wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:21 AM EST

PDB ID	:	7N65
EMDB ID	:	EMD-24195
Title	:	Complex structure of HIV superinfection Fab QA013.2 and BG505.SOSIP.664
Authors	:	Mangala Prasad, V.; Shipley, M.M.; Overbaugh, J.M.; Lee, K.K.
Deposited on	:	2021-06-07
Resolution	:	4.15 Å(reported)
Based on initial model	:	5ACO

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

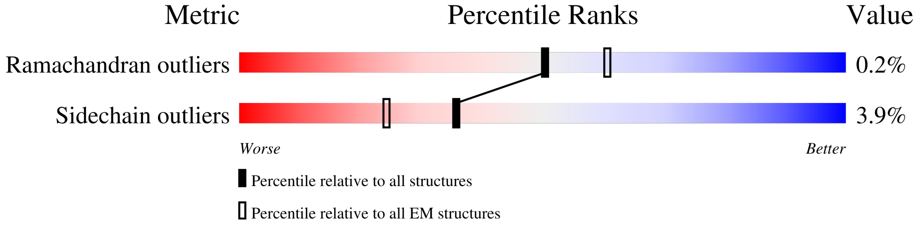
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

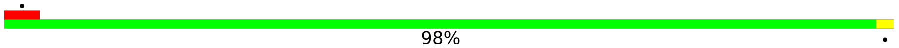
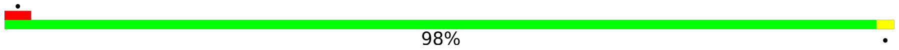
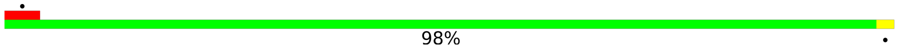
The reported resolution of this entry is 4.15 Å.

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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	508	
1	E	508	
1	I	508	
2	B	161	
2	F	161	
2	J	161	
3	C	128	
3	G	128	
3	K	128	

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Mol	Chain	Length	Quality of chain
4	D	108	• 95% • •
4	H	108	95% • •
4	L	108	• 95% • •
5	1	3	33% 100%
5	6	3	33% 67%
5	7	3	33% 67%
5	M	3	67% 33% 67%
5	O	3	100%
5	P	3	33% 33% 67%
5	T	3	33% 100%
5	Y	3	33% 33% 67%
5	Z	3	33% 67%
5	d	3	67% 33% 67%
5	f	3	100%
5	g	3	33% 33% 67%
5	k	3	100%
5	p	3	33% 33% 67%
5	q	3	33% 67%
5	u	3	67% 67% 33%
5	w	3	100%
5	x	3	33% 33% 67%
6	5	2	50% 50% 50%
6	8	2	100%
6	9	2	100%
6	AA	2	50% 100%

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Mol	Chain	Length	Quality of chain
6	N	2	🟩 100%
6	Q	2	🟩 50% 🟨 50%
6	R	2	🟨 100%
6	X	2	🟥 100% 🟩 50% 🟨 50%
6	a	2	🟩 100%
6	b	2	🟨 100%
6	c	2	🟥 50% 🟩 100%
6	e	2	🟩 100%
6	h	2	🟩 50% 🟨 50%
6	i	2	🟩 50% 🟨 50%
6	o	2	🟥 100% 🟩 50% 🟨 50%
6	r	2	🟩 100%
6	s	2	🟨 100%
6	t	2	🟥 50% 🟩 100%
6	v	2	🟩 100%
6	y	2	🟩 50% 🟨 50%
6	z	2	🟥 50% 🟩 50% 🟨 50%
7	0	7	🟥 14% 🟨 100%
7	S	7	🟥 14% 🟨 100%
7	j	7	🟥 14% 🟨 100%
8	2	5	🟩 60% 🟨 40%
8	U	5	🟩 60% 🟨 40%
8	l	5	🟩 60% 🟨 40%
9	3	7	🟨 100%
9	V	7	🟨 100%

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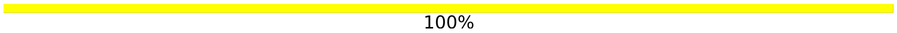
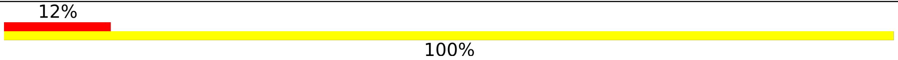
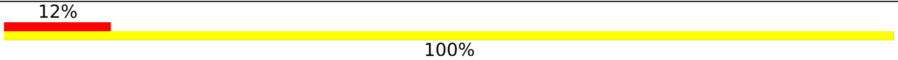
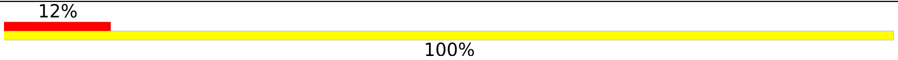
Mol	Chain	Length	Quality of chain
9	m	7	
10	4	8	
10	W	8	
10	n	8	

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 21525 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	450	3522	2213	623	658	28	0	0
1	E	450	3522	2213	623	658	28	0	0
1	I	450	3522	2213	623	658	28	0	0

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP A0A6H1VCM1
A	-3	ASP	-	expression tag	UNP A0A6H1VCM1
A	-2	ALA	-	expression tag	UNP A0A6H1VCM1
A	-1	MET	-	expression tag	UNP A0A6H1VCM1
A	0	LYS	-	expression tag	UNP A0A6H1VCM1
A	1	ARG	-	expression tag	UNP A0A6H1VCM1
A	2	GLY	-	expression tag	UNP A0A6H1VCM1
A	3	LEU	-	expression tag	UNP A0A6H1VCM1
A	4	CYS	-	expression tag	UNP A0A6H1VCM1
A	5	CYS	-	expression tag	UNP A0A6H1VCM1
A	6	VAL	-	expression tag	UNP A0A6H1VCM1
A	7	LEU	-	expression tag	UNP A0A6H1VCM1
A	8	LEU	-	expression tag	UNP A0A6H1VCM1
A	9	LEU	-	expression tag	UNP A0A6H1VCM1
A	10	CYS	-	expression tag	UNP A0A6H1VCM1
A	11	GLY	-	expression tag	UNP A0A6H1VCM1
A	12	ALA	-	expression tag	UNP A0A6H1VCM1
A	13	VAL	-	expression tag	UNP A0A6H1VCM1
A	14	PHE	-	expression tag	UNP A0A6H1VCM1
A	15	VAL	-	expression tag	UNP A0A6H1VCM1
A	16	SER	-	expression tag	UNP A0A6H1VCM1
A	17	PRO	-	expression tag	UNP A0A6H1VCM1
A	18	SER	-	expression tag	UNP A0A6H1VCM1
A	19	GLN	-	expression tag	UNP A0A6H1VCM1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	expression tag	UNP A0A6H1VCM1
A	21	ILE	-	expression tag	UNP A0A6H1VCM1
A	22	HIS	-	expression tag	UNP A0A6H1VCM1
A	23	ALA	-	expression tag	UNP A0A6H1VCM1
A	24	ARG	-	expression tag	UNP A0A6H1VCM1
A	25	PHE	-	expression tag	UNP A0A6H1VCM1
A	26	ARG	-	expression tag	UNP A0A6H1VCM1
A	27	ARG	-	expression tag	UNP A0A6H1VCM1
A	28	GLY	-	expression tag	UNP A0A6H1VCM1
A	29	ALA	-	expression tag	UNP A0A6H1VCM1
A	30	ARG	-	expression tag	UNP A0A6H1VCM1
A	375	SER	TYR	conflict	UNP A0A6H1VCM1
A	501	CYS	ALA	conflict	UNP A0A6H1VCM1
E	-4	MET	-	initiating methionine	UNP A0A6H1VCM1
E	-3	ASP	-	expression tag	UNP A0A6H1VCM1
E	-2	ALA	-	expression tag	UNP A0A6H1VCM1
E	-1	MET	-	expression tag	UNP A0A6H1VCM1
E	0	LYS	-	expression tag	UNP A0A6H1VCM1
E	1	ARG	-	expression tag	UNP A0A6H1VCM1
E	2	GLY	-	expression tag	UNP A0A6H1VCM1
E	3	LEU	-	expression tag	UNP A0A6H1VCM1
E	4	CYS	-	expression tag	UNP A0A6H1VCM1
E	5	CYS	-	expression tag	UNP A0A6H1VCM1
E	6	VAL	-	expression tag	UNP A0A6H1VCM1
E	7	LEU	-	expression tag	UNP A0A6H1VCM1
E	8	LEU	-	expression tag	UNP A0A6H1VCM1
E	9	LEU	-	expression tag	UNP A0A6H1VCM1
E	10	CYS	-	expression tag	UNP A0A6H1VCM1
E	11	GLY	-	expression tag	UNP A0A6H1VCM1
E	12	ALA	-	expression tag	UNP A0A6H1VCM1
E	13	VAL	-	expression tag	UNP A0A6H1VCM1
E	14	PHE	-	expression tag	UNP A0A6H1VCM1
E	15	VAL	-	expression tag	UNP A0A6H1VCM1
E	16	SER	-	expression tag	UNP A0A6H1VCM1
E	17	PRO	-	expression tag	UNP A0A6H1VCM1
E	18	SER	-	expression tag	UNP A0A6H1VCM1
E	19	GLN	-	expression tag	UNP A0A6H1VCM1
E	20	GLU	-	expression tag	UNP A0A6H1VCM1
E	21	ILE	-	expression tag	UNP A0A6H1VCM1
E	22	HIS	-	expression tag	UNP A0A6H1VCM1
E	23	ALA	-	expression tag	UNP A0A6H1VCM1
E	24	ARG	-	expression tag	UNP A0A6H1VCM1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	25	PHE	-	expression tag	UNP A0A6H1VCM1
E	26	ARG	-	expression tag	UNP A0A6H1VCM1
E	27	ARG	-	expression tag	UNP A0A6H1VCM1
E	28	GLY	-	expression tag	UNP A0A6H1VCM1
E	29	ALA	-	expression tag	UNP A0A6H1VCM1
E	30	ARG	-	expression tag	UNP A0A6H1VCM1
E	375	SER	TYR	conflict	UNP A0A6H1VCM1
E	501	CYS	ALA	conflict	UNP A0A6H1VCM1
I	-4	MET	-	initiating methionine	UNP A0A6H1VCM1
I	-3	ASP	-	expression tag	UNP A0A6H1VCM1
I	-2	ALA	-	expression tag	UNP A0A6H1VCM1
I	-1	MET	-	expression tag	UNP A0A6H1VCM1
I	0	LYS	-	expression tag	UNP A0A6H1VCM1
I	1	ARG	-	expression tag	UNP A0A6H1VCM1
I	2	GLY	-	expression tag	UNP A0A6H1VCM1
I	3	LEU	-	expression tag	UNP A0A6H1VCM1
I	4	CYS	-	expression tag	UNP A0A6H1VCM1
I	5	CYS	-	expression tag	UNP A0A6H1VCM1
I	6	VAL	-	expression tag	UNP A0A6H1VCM1
I	7	LEU	-	expression tag	UNP A0A6H1VCM1
I	8	LEU	-	expression tag	UNP A0A6H1VCM1
I	9	LEU	-	expression tag	UNP A0A6H1VCM1
I	10	CYS	-	expression tag	UNP A0A6H1VCM1
I	11	GLY	-	expression tag	UNP A0A6H1VCM1
I	12	ALA	-	expression tag	UNP A0A6H1VCM1
I	13	VAL	-	expression tag	UNP A0A6H1VCM1
I	14	PHE	-	expression tag	UNP A0A6H1VCM1
I	15	VAL	-	expression tag	UNP A0A6H1VCM1
I	16	SER	-	expression tag	UNP A0A6H1VCM1
I	17	PRO	-	expression tag	UNP A0A6H1VCM1
I	18	SER	-	expression tag	UNP A0A6H1VCM1
I	19	GLN	-	expression tag	UNP A0A6H1VCM1
I	20	GLU	-	expression tag	UNP A0A6H1VCM1
I	21	ILE	-	expression tag	UNP A0A6H1VCM1
I	22	HIS	-	expression tag	UNP A0A6H1VCM1
I	23	ALA	-	expression tag	UNP A0A6H1VCM1
I	24	ARG	-	expression tag	UNP A0A6H1VCM1
I	25	PHE	-	expression tag	UNP A0A6H1VCM1
I	26	ARG	-	expression tag	UNP A0A6H1VCM1
I	27	ARG	-	expression tag	UNP A0A6H1VCM1
I	28	GLY	-	expression tag	UNP A0A6H1VCM1
I	29	ALA	-	expression tag	UNP A0A6H1VCM1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	30	ARG	-	expression tag	UNP A0A6H1VCM1
I	375	SER	TYR	conflict	UNP A0A6H1VCM1
I	501	CYS	ALA	conflict	UNP A0A6H1VCM1

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	133	Total 1056	C 670	N 181	O 199	S 6	0	0
2	F	133	Total 1056	C 670	N 181	O 199	S 6	0	0
2	J	133	Total 1056	C 670	N 181	O 199	S 6	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	504	VAL	-	expression tag	UNP Q2N0S7
B	505	GLY	-	expression tag	UNP Q2N0S7
B	506	ARG	-	expression tag	UNP Q2N0S7
B	507	ARG	-	expression tag	UNP Q2N0S7
B	508	ARG	-	expression tag	UNP Q2N0S7
B	509	ARG	-	expression tag	UNP Q2N0S7
B	510	ARG	-	expression tag	UNP Q2N0S7
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
F	504	VAL	-	expression tag	UNP Q2N0S7
F	505	GLY	-	expression tag	UNP Q2N0S7
F	506	ARG	-	expression tag	UNP Q2N0S7
F	507	ARG	-	expression tag	UNP Q2N0S7
F	508	ARG	-	expression tag	UNP Q2N0S7
F	509	ARG	-	expression tag	UNP Q2N0S7
F	510	ARG	-	expression tag	UNP Q2N0S7
F	559	PRO	ILE	conflict	UNP Q2N0S7
F	605	CYS	THR	conflict	UNP Q2N0S7
J	504	VAL	-	expression tag	UNP Q2N0S7
J	505	GLY	-	expression tag	UNP Q2N0S7
J	506	ARG	-	expression tag	UNP Q2N0S7
J	507	ARG	-	expression tag	UNP Q2N0S7
J	508	ARG	-	expression tag	UNP Q2N0S7
J	509	ARG	-	expression tag	UNP Q2N0S7
J	510	ARG	-	expression tag	UNP Q2N0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	559	PRO	ILE	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

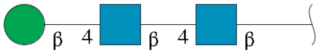
- Molecule 3 is a protein called Fab QA013.2 Heavy Chain, variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	128	Total 1015	C 640	N 180	O 192	S 3	0	0
3	G	128	Total 1015	C 640	N 180	O 192	S 3	0	0
3	K	128	Total 1015	C 640	N 180	O 192	S 3	0	0

- Molecule 4 is a protein called Fab QA013.2 Light Chain, , variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total 778	C 480	N 136	O 160	S 2	0	0
4	H	107	Total 778	C 480	N 136	O 160	S 2	0	0
4	L	107	Total 778	C 480	N 136	O 160	S 2	0	0

- Molecule 5 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
5	M	3	Total 39	C 22	N 2	O 15	0	0
5	O	3	Total 39	C 22	N 2	O 15	0	0
5	P	3	Total 39	C 22	N 2	O 15	0	0
5	T	3	Total 39	C 22	N 2	O 15	0	0
5	Y	3	Total 39	C 22	N 2	O 15	0	0

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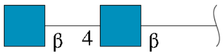
Mol	Chain	Residues	Atoms	AltConf	Trace
5	Z	3	Total C N O 39 22 2 15	0	0
5	d	3	Total C N O 39 22 2 15	0	0
5	f	3	Total C N O 39 22 2 15	0	0
5	g	3	Total C N O 39 22 2 15	0	0
5	k	3	Total C N O 39 22 2 15	0	0
5	p	3	Total C N O 39 22 2 15	0	0
5	q	3	Total C N O 39 22 2 15	0	0
5	u	3	Total C N O 39 22 2 15	0	0
5	w	3	Total C N O 39 22 2 15	0	0
5	x	3	Total C N O 39 22 2 15	0	0
5	1	3	Total C N O 39 22 2 15	0	0
5	6	3	Total C N O 39 22 2 15	0	0
5	7	3	Total C N O 39 22 2 15	0	0

- Molecule 6 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
6	N	2	Total C N O 28 16 2 10	0	0
6	Q	2	Total C N O 28 16 2 10	0	0
6	R	2	Total C N O 28 16 2 10	0	0
6	X	2	Total C N O 28 16 2 10	0	0

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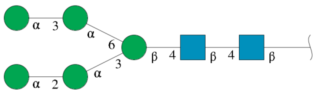
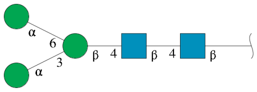
Mol	Chain	Residues	Atoms	AltConf	Trace
6	a	2	Total C N O 28 16 2 10	0	0
6	b	2	Total C N O 28 16 2 10	0	0
6	c	2	Total C N O 28 16 2 10	0	0
6	e	2	Total C N O 28 16 2 10	0	0
6	h	2	Total C N O 28 16 2 10	0	0
6	i	2	Total C N O 28 16 2 10	0	0
6	o	2	Total C N O 28 16 2 10	0	0
6	r	2	Total C N O 28 16 2 10	0	0
6	s	2	Total C N O 28 16 2 10	0	0
6	t	2	Total C N O 28 16 2 10	0	0
6	v	2	Total C N O 28 16 2 10	0	0
6	y	2	Total C N O 28 16 2 10	0	0
6	z	2	Total C N O 28 16 2 10	0	0
6	5	2	Total C N O 28 16 2 10	0	0
6	8	2	Total C N O 28 16 2 10	0	0
6	9	2	Total C N O 28 16 2 10	0	0
6	AA	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



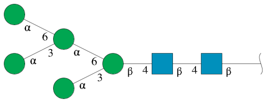
Mol	Chain	Residues	Atoms	AltConf	Trace
7	S	7	Total C N O 83 46 2 35	0	0
7	j	7	Total C N O 83 46 2 35	0	0
7	0	7	Total C N O 83 46 2 35	0	0

- Molecule 8 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
8	U	5	Total C N O 61 34 2 25	0	0
8	l	5	Total C N O 61 34 2 25	0	0
8	2	5	Total C N O 61 34 2 25	0	0

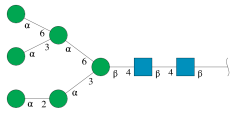
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
9	V	7	Total C N O 83 46 2 35	0	0
9	m	7	Total C N O 83 46 2 35	0	0
9	3	7	Total C N O 83 46 2 35	0	0

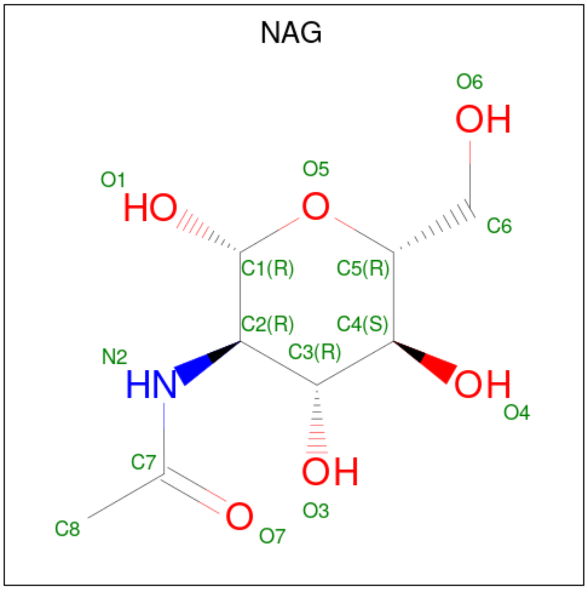
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-

2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
10	W	8	Total C N O 94 52 2 40	0	0
10	n	8	Total C N O 94 52 2 40	0	0
10	4	8	Total C N O 94 52 2 40	0	0

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



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O 14 8 1 5	0
11	B	1	Total C N O 28 16 2 10	0
11	B	1	Total C N O 28 16 2 10	0
11	E	1	Total C N O 14 8 1 5	0
11	F	1	Total C N O 28 16 2 10	0

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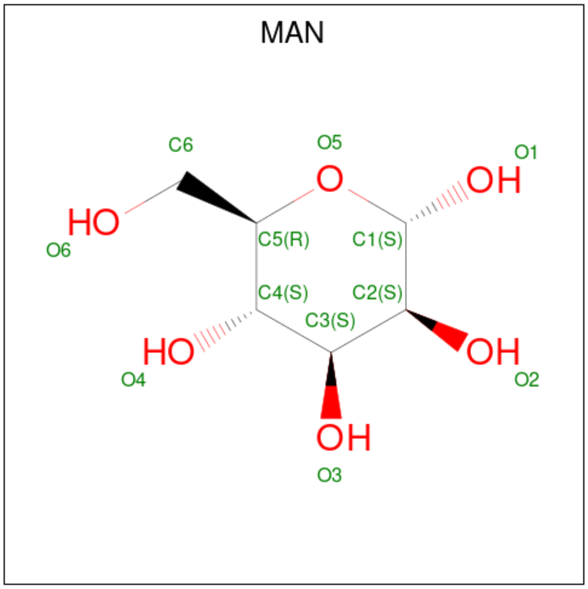
Mol	Chain	Residues	Atoms	AltConf
11	F	1	Total C N O 28 16 2 10	0
11	I	1	Total C N O 14 8 1 5	0
11	J	1	Total C N O 28 16 2 10	0
11	J	1	Total C N O 28 16 2 10	0

- Molecule 12 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



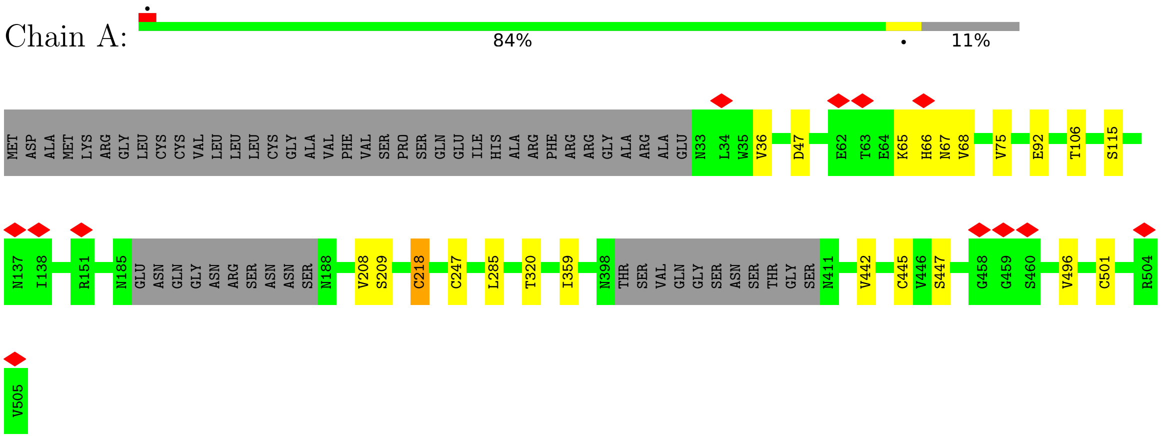
Mol	Chain	Residues	Atoms	AltConf
12	C	1	Total C O 11 6 5	0
12	G	1	Total C O 11 6 5	0
12	K	1	Total C O 11 6 5	0

3 Residue-property plots ⓘ

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

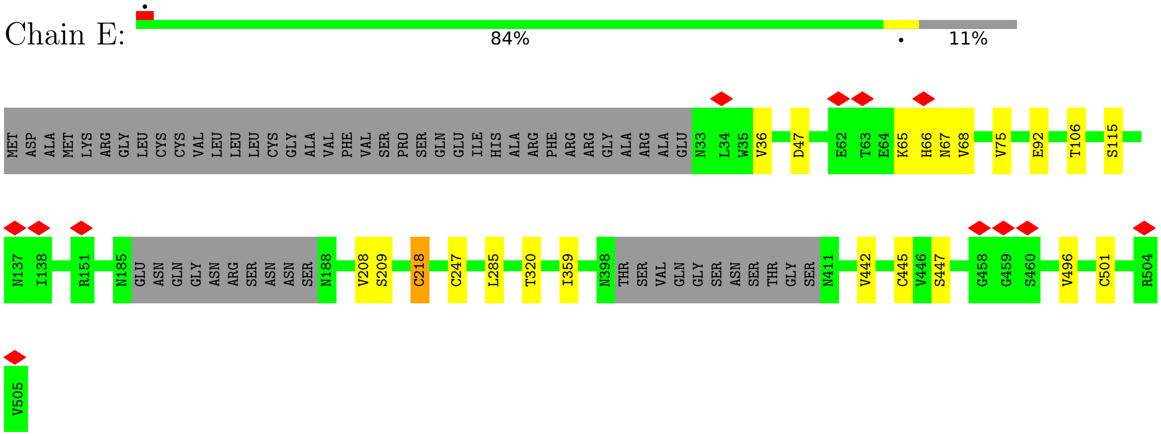
- Molecule 1: Envelope glycoprotein gp41

Chain A:



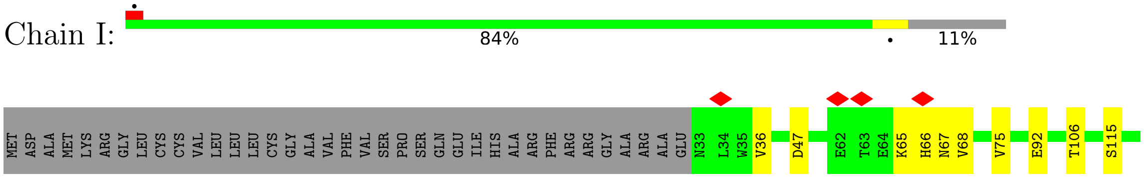
- Molecule 1: Envelope glycoprotein gp41

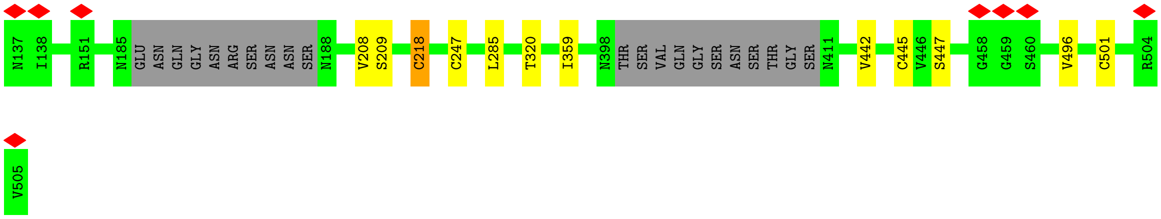
Chain E:



- Molecule 1: Envelope glycoprotein gp41

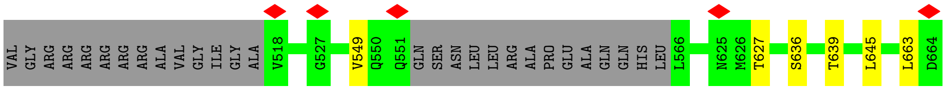
Chain I:





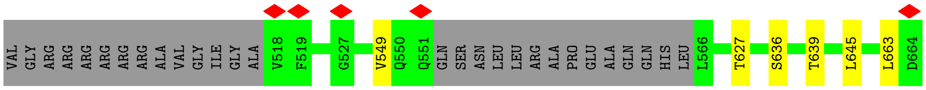
- Molecule 2: Envelope glycoprotein gp41

Chain B:



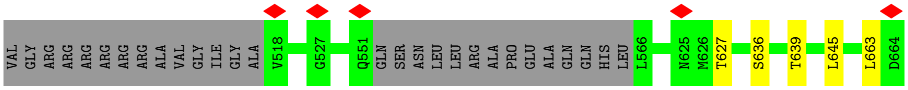
- Molecule 2: Envelope glycoprotein gp41

Chain F:



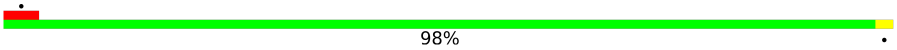
- Molecule 2: Envelope glycoprotein gp41

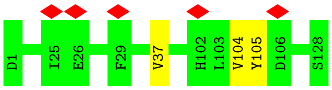
Chain J:



- Molecule 3: Fab QA013.2 Heavy Chain, variable region

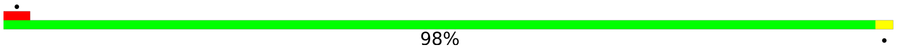
Chain C:

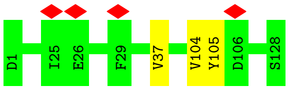




- Molecule 3: Fab QA013.2 Heavy Chain, variable region

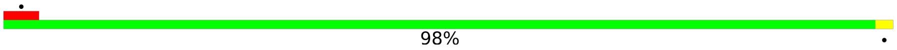
Chain G:

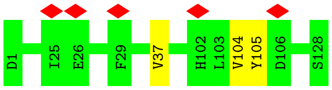




- Molecule 3: Fab QA013.2 Heavy Chain, variable region

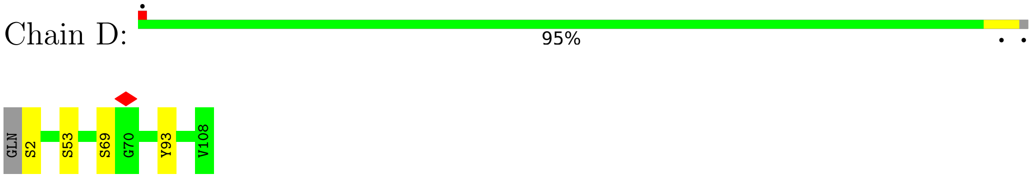
Chain K:





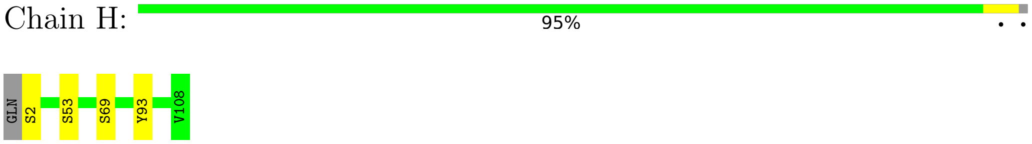
- Molecule 4: Fab QA013.2 Light Chain, , variable region

Chain D:



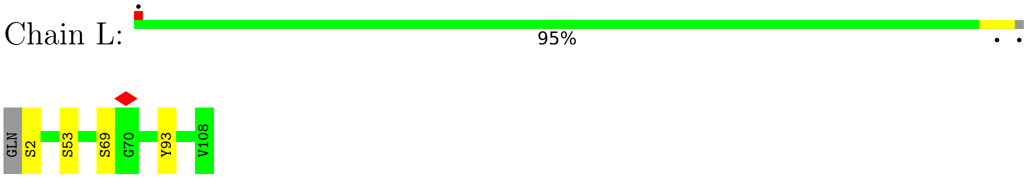
- Molecule 4: Fab QA013.2 Light Chain, , variable region

Chain H:



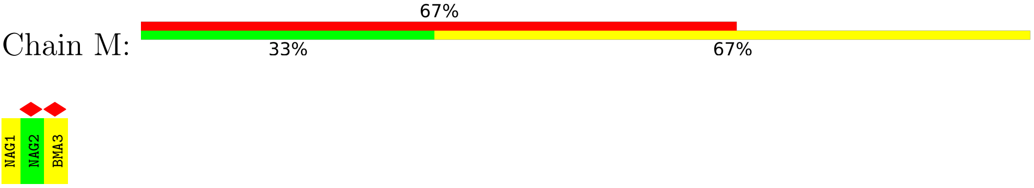
- Molecule 4: Fab QA013.2 Light Chain, , variable region

Chain L:



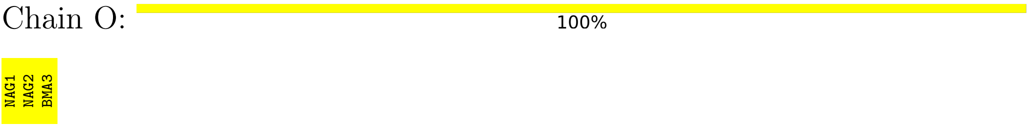
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



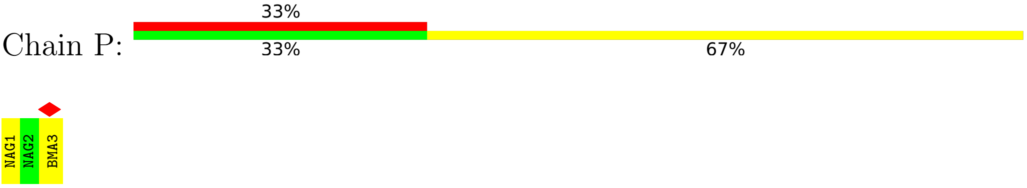
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



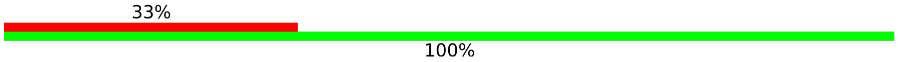
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



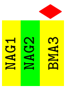
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain Y:



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

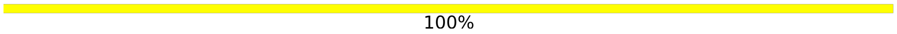
Chain Z:

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

Chain d:

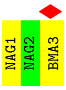
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



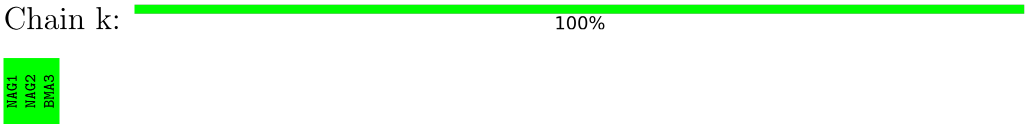
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



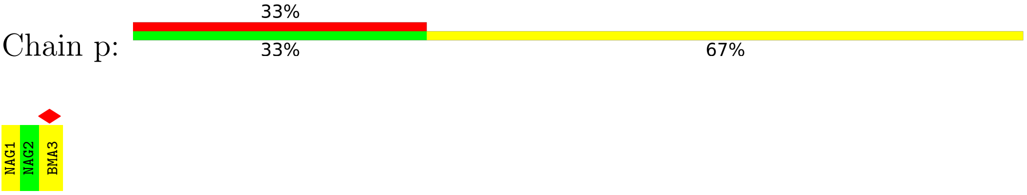
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



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

Chain p:

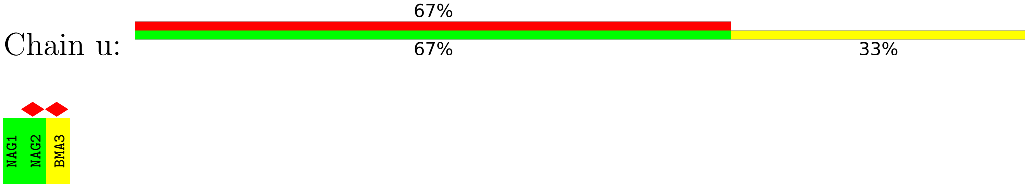


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

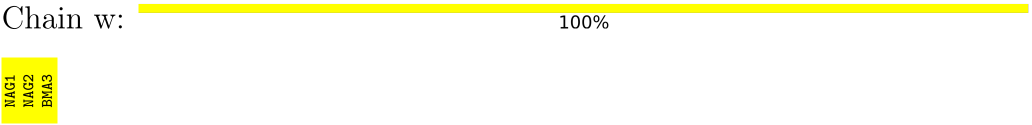
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



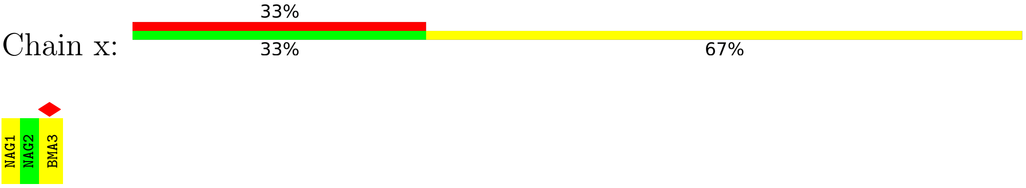
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



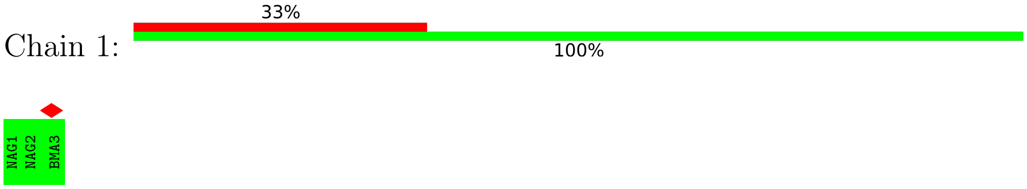
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



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

Chain 1:



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

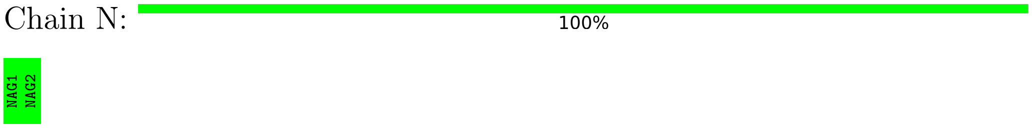
Chain 6:

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

Chain 7:

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

Chain N:

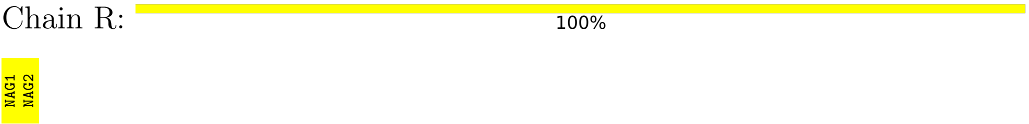


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

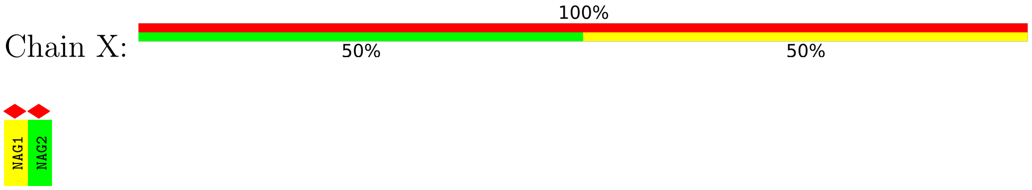
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



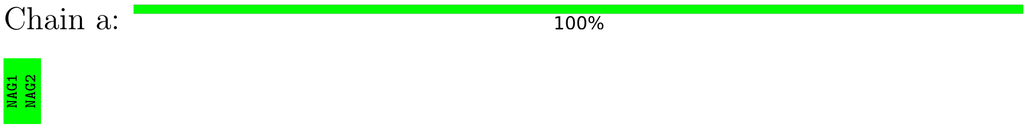
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



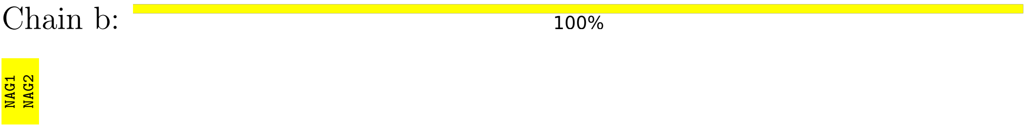
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



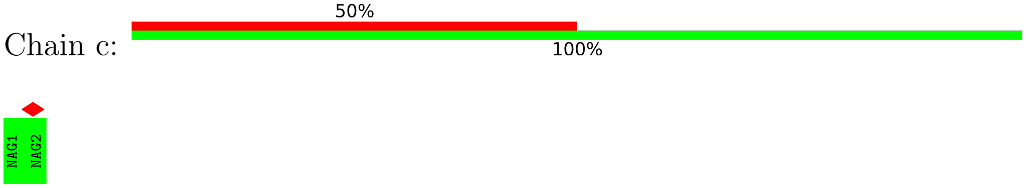
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



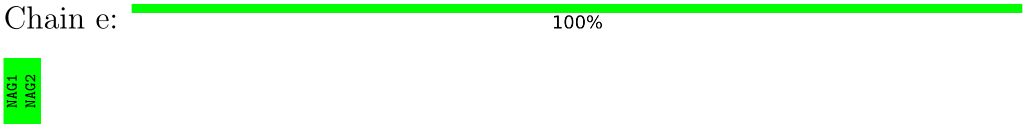
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain e:



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

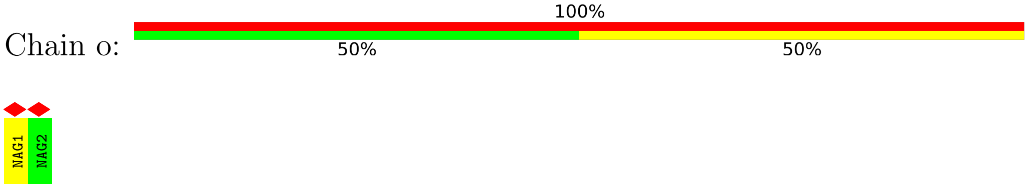
Chain h:

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

Chain i:

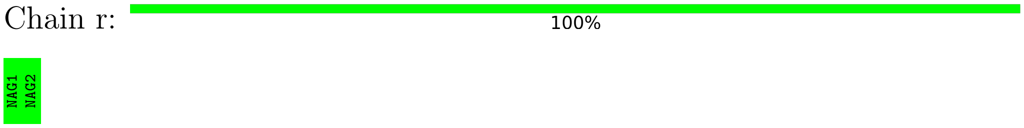
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



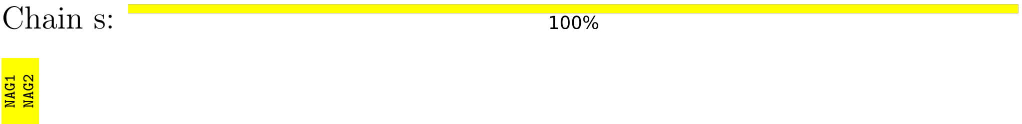
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



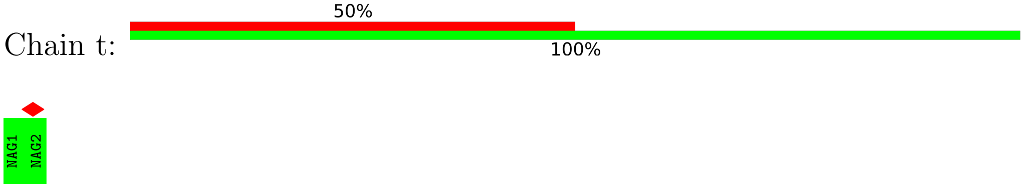
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



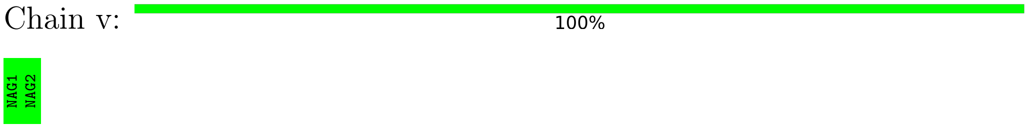
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



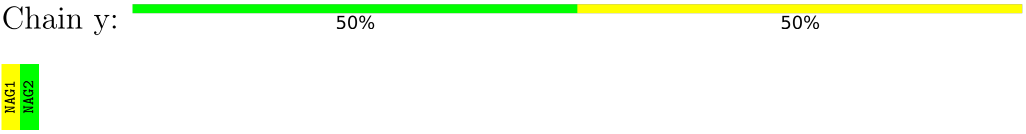
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



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

Chain y:



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

Chain z:

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

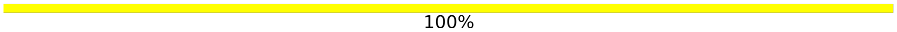
Chain 5:

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

Chain 8:

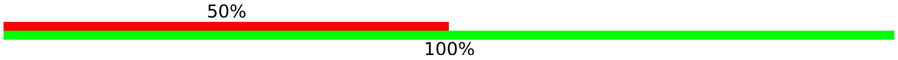
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:



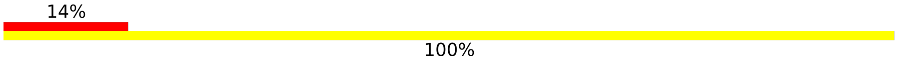
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



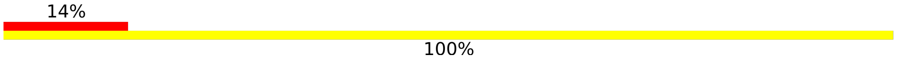
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



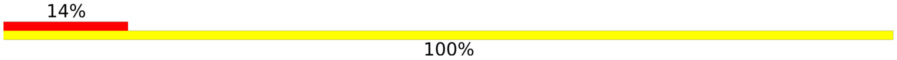
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



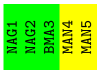
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



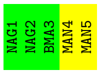
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



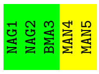
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



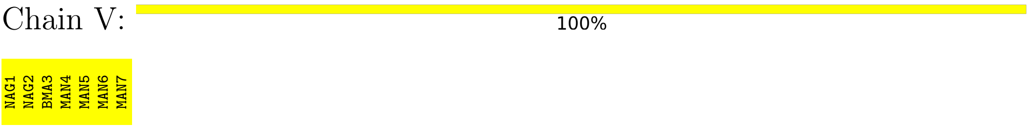
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



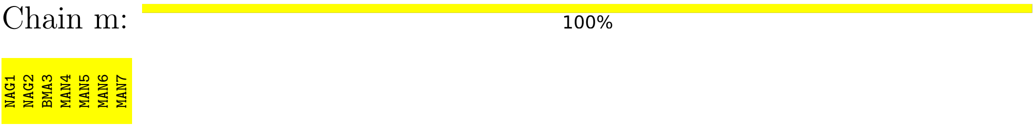
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



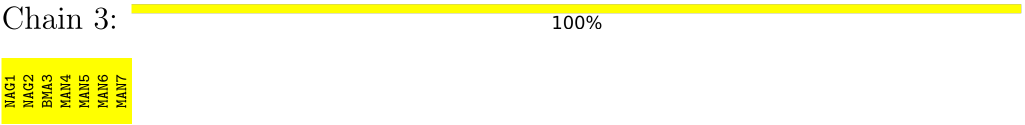
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



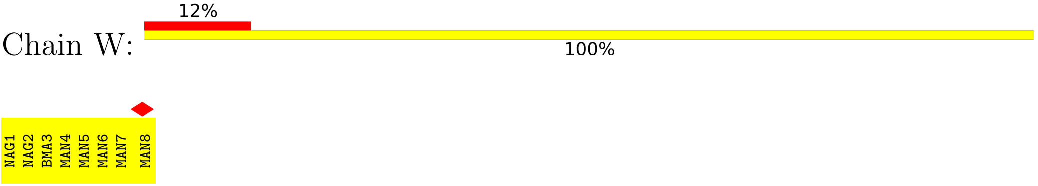
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



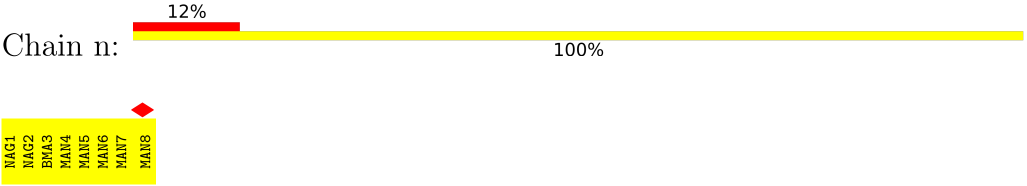
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



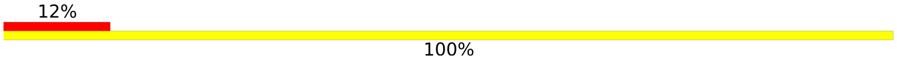
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

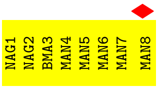
Chain n:



- Molecule 10: 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 4:




NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	113470	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 $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	110000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	56.840	Depositor
Minimum map value	-26.521	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7.8	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.60	1/3595 (0.0%)	0.68	3/4884 (0.1%)
1	E	0.60	1/3595 (0.0%)	0.68	3/4884 (0.1%)
1	I	0.60	1/3595 (0.0%)	0.68	3/4884 (0.1%)
2	B	0.46	0/1074	0.59	0/1455
2	F	0.46	0/1074	0.59	0/1455
2	J	0.46	0/1074	0.59	0/1455
3	C	0.44	0/1040	0.59	0/1411
3	G	0.44	0/1040	0.59	0/1411
3	K	0.44	0/1040	0.59	0/1411
4	D	0.44	0/794	0.63	2/1078 (0.2%)
4	H	0.44	0/794	0.63	2/1078 (0.2%)
4	L	0.44	0/794	0.63	2/1078 (0.2%)
All	All	0.54	3/19509 (0.0%)	0.65	15/26484 (0.1%)

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	2
1	E	0	2
1	I	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CYS	C-N	-6.35	1.19	1.34
1	I	218	CYS	C-N	-6.35	1.19	1.34
1	E	218	CYS	C-N	-6.31	1.19	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	CYS	CA-CB-SG	6.75	126.16	114.00
1	I	445	CYS	CA-CB-SG	6.75	126.14	114.00
1	E	445	CYS	CA-CB-SG	6.74	126.13	114.00
1	A	247	CYS	CA-CB-SG	6.59	125.86	114.00
1	E	247	CYS	CA-CB-SG	6.59	125.85	114.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	501	CYS	Peptide
1	A	66	HIS	Peptide
1	E	501	CYS	Peptide
1	E	66	HIS	Peptide
1	I	66	HIS	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/508 (87%)	377 (85%)	66 (15%)	1 (0%)	47	80
1	E	444/508 (87%)	377 (85%)	66 (15%)	1 (0%)	47	80
1	I	444/508 (87%)	377 (85%)	66 (15%)	1 (0%)	47	80
2	B	129/161 (80%)	103 (80%)	25 (19%)	1 (1%)	19	59
2	F	129/161 (80%)	103 (80%)	25 (19%)	1 (1%)	19	59
2	J	129/161 (80%)	103 (80%)	26 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	126/128 (98%)	107 (85%)	19 (15%)	0	100	100
3	G	126/128 (98%)	107 (85%)	19 (15%)	0	100	100
3	K	126/128 (98%)	107 (85%)	19 (15%)	0	100	100
4	D	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
4	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
4	L	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	2412/2715 (89%)	2040 (85%)	367 (15%)	5 (0%)	50	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	E	67	ASN
1	I	67	ASN
2	B	549	VAL
2	F	549	VAL

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	395/449 (88%)	379 (96%)	16 (4%)	30	56
1	E	395/449 (88%)	379 (96%)	16 (4%)	30	56
1	I	395/449 (88%)	379 (96%)	16 (4%)	30	56
2	B	114/136 (84%)	109 (96%)	5 (4%)	28	54
2	F	114/136 (84%)	109 (96%)	5 (4%)	28	54
2	J	114/136 (84%)	109 (96%)	5 (4%)	28	54
3	C	106/106 (100%)	103 (97%)	3 (3%)	43	65
3	G	106/106 (100%)	103 (97%)	3 (3%)	43	65
3	K	106/106 (100%)	103 (97%)	3 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	85/86 (99%)	82 (96%)	3 (4%)	36	60
4	H	85/86 (99%)	82 (96%)	3 (4%)	36	60
4	L	85/86 (99%)	82 (96%)	3 (4%)	36	60
All	All	2100/2331 (90%)	2019 (96%)	81 (4%)	36	57

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	75	VAL
2	J	636	SER
1	I	106	THR
1	I	320	THR
3	K	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	374	HIS
4	L	91	GLN
1	I	422	GLN
3	K	52	ASN
1	E	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

177 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	$\#\|Z\| > 2$
7	NAG	0	1	7,1	14,14,15	1.00	1 (7%)	17,19,21	0.48	0
7	NAG	0	2	7	14,14,15	0.77	1 (7%)	17,19,21	0.68	0
7	BMA	0	3	7	11,11,12	0.91	1 (9%)	15,15,17	0.86	0
7	MAN	0	4	7	11,11,12	0.76	0	15,15,17	1.35	2 (13%)
7	MAN	0	5	7	11,11,12	0.65	0	15,15,17	1.53	2 (13%)
7	MAN	0	6	7	11,11,12	0.61	0	15,15,17	0.95	1 (6%)
7	MAN	0	7	7	11,11,12	0.49	0	15,15,17	1.13	2 (13%)
5	NAG	1	1	5,1	14,14,15	0.50	0	17,19,21	0.33	0
5	NAG	1	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	BMA	1	3	5	11,11,12	0.49	0	15,15,17	0.82	0
8	NAG	2	1	8,1	14,14,15	0.47	0	17,19,21	0.52	0
8	NAG	2	2	8	14,14,15	0.31	0	17,19,21	0.47	0
8	BMA	2	3	8	11,11,12	0.62	0	15,15,17	0.70	0
8	MAN	2	4	8	11,11,12	0.49	0	15,15,17	1.07	2 (13%)
8	MAN	2	5	8	11,11,12	0.68	0	15,15,17	1.06	1 (6%)
9	NAG	3	1	9,1	14,14,15	0.29	0	17,19,21	1.11	1 (5%)
9	NAG	3	2	9	14,14,15	1.50	1 (7%)	17,19,21	1.12	1 (5%)
9	BMA	3	3	9	11,11,12	1.44	1 (9%)	15,15,17	1.38	2 (13%)
9	MAN	3	4	9	11,11,12	0.99	1 (9%)	15,15,17	1.17	1 (6%)
9	MAN	3	5	9	11,11,12	1.42	1 (9%)	15,15,17	1.91	4 (26%)
9	MAN	3	6	9	11,11,12	0.85	1 (9%)	15,15,17	0.92	1 (6%)
9	MAN	3	7	9	11,11,12	1.05	1 (9%)	15,15,17	1.12	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.61	1 (7%)	17,19,21	0.52	0
10	NAG	4	2	10	14,14,15	0.86	1 (7%)	17,19,21	0.57	0
10	BMA	4	3	10	11,11,12	1.24	2 (18%)	15,15,17	1.35	3 (20%)
10	MAN	4	4	10	11,11,12	1.66	1 (9%)	15,15,17	1.42	3 (20%)
10	MAN	4	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.57	3 (20%)
10	MAN	4	6	10	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
10	MAN	4	7	10	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
10	MAN	4	8	10	11,11,12	1.03	1 (9%)	15,15,17	1.72	3 (20%)
6	NAG	5	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	0.56	0
6	NAG	5	2	6	14,14,15	0.37	0	17,19,21	0.45	0
5	NAG	6	1	5,1	14,14,15	1.02	1 (7%)	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	6	2	5	14,14,15	0.36	0	17,19,21	0.47	0
5	BMA	6	3	5	11,11,12	0.84	1 (9%)	15,15,17	0.91	0
5	NAG	7	1	5,1	14,14,15	0.58	1 (7%)	17,19,21	0.51	0
5	NAG	7	2	5	14,14,15	0.21	0	17,19,21	0.52	0
5	BMA	7	3	5	11,11,12	0.63	0	15,15,17	0.97	1 (6%)
6	NAG	8	1	6,1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	8	2	6	14,14,15	0.35	0	17,19,21	0.49	0
6	NAG	9	1	6,1	14,14,15	0.80	1 (7%)	17,19,21	0.67	0
6	NAG	9	2	6	14,14,15	0.25	0	17,19,21	0.71	1 (5%)
6	NAG	AA	1	2,6	14,14,15	0.41	0	17,19,21	0.40	0
6	NAG	AA	2	6	14,14,15	0.31	0	17,19,21	0.35	0
5	NAG	M	1	5,1	14,14,15	0.34	0	17,19,21	0.65	1 (5%)
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.40	0
5	BMA	M	3	5	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
6	NAG	N	1	6,1	14,14,15	0.45	0	17,19,21	0.73	0
6	NAG	N	2	6	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	O	1	5,1	14,14,15	0.85	1 (7%)	17,19,21	0.55	0
5	NAG	O	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.67	0
5	BMA	O	3	5	11,11,12	0.49	0	15,15,17	0.96	1 (6%)
5	NAG	P	1	5,1	14,14,15	1.39	2 (14%)	17,19,21	0.67	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.37	0
5	BMA	P	3	5	11,11,12	0.55	0	15,15,17	0.85	1 (6%)
6	NAG	Q	1	6,1	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
6	NAG	Q	2	6	14,14,15	0.23	0	17,19,21	0.62	0
6	NAG	R	1	6,1	14,14,15	0.80	1 (7%)	17,19,21	0.67	0
6	NAG	R	2	6	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
7	NAG	S	1	7,1	14,14,15	1.00	1 (7%)	17,19,21	0.47	0
7	NAG	S	2	7	14,14,15	0.76	1 (7%)	17,19,21	0.68	0
7	BMA	S	3	7	11,11,12	0.92	1 (9%)	15,15,17	0.85	0
7	MAN	S	4	7	11,11,12	0.78	0	15,15,17	1.34	2 (13%)
7	MAN	S	5	7	11,11,12	0.65	0	15,15,17	1.53	2 (13%)
7	MAN	S	6	7	11,11,12	0.61	0	15,15,17	0.95	1 (6%)
7	MAN	S	7	7	11,11,12	0.49	0	15,15,17	1.14	2 (13%)
5	NAG	T	1	5,1	14,14,15	0.49	0	17,19,21	0.34	0
5	NAG	T	2	5	14,14,15	0.22	0	17,19,21	0.45	0
5	BMA	T	3	5	11,11,12	0.49	0	15,15,17	0.83	0
8	NAG	U	1	8,1	14,14,15	0.46	0	17,19,21	0.52	0
8	NAG	U	2	8	14,14,15	0.32	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BMA	U	3	8	11,11,12	0.63	0	15,15,17	0.70	0
8	MAN	U	4	8	11,11,12	0.50	0	15,15,17	1.06	2 (13%)
8	MAN	U	5	8	11,11,12	0.67	0	15,15,17	1.05	1 (6%)
9	NAG	V	1	9,1	14,14,15	0.29	0	17,19,21	1.11	1 (5%)
9	NAG	V	2	9	14,14,15	1.51	1 (7%)	17,19,21	1.12	1 (5%)
9	BMA	V	3	9	11,11,12	1.44	1 (9%)	15,15,17	1.37	2 (13%)
9	MAN	V	4	9	11,11,12	0.98	1 (9%)	15,15,17	1.17	1 (6%)
9	MAN	V	5	9	11,11,12	1.43	1 (9%)	15,15,17	1.91	4 (26%)
9	MAN	V	6	9	11,11,12	0.84	1 (9%)	15,15,17	0.91	1 (6%)
9	MAN	V	7	9	11,11,12	1.04	1 (9%)	15,15,17	1.13	1 (6%)
10	NAG	W	1	10,1	14,14,15	0.61	1 (7%)	17,19,21	0.53	0
10	NAG	W	2	10	14,14,15	0.87	1 (7%)	17,19,21	0.57	0
10	BMA	W	3	10	11,11,12	1.24	2 (18%)	15,15,17	1.35	3 (20%)
10	MAN	W	4	10	11,11,12	1.67	1 (9%)	15,15,17	1.42	3 (20%)
10	MAN	W	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.56	3 (20%)
10	MAN	W	6	10	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
10	MAN	W	7	10	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
10	MAN	W	8	10	11,11,12	1.04	1 (9%)	15,15,17	1.71	3 (20%)
6	NAG	X	1	6,1	14,14,15	0.72	1 (7%)	17,19,21	0.56	0
6	NAG	X	2	6	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	Y	1	5,1	14,14,15	1.03	1 (7%)	17,19,21	0.72	0
5	NAG	Y	2	5	14,14,15	0.38	0	17,19,21	0.47	0
5	BMA	Y	3	5	11,11,12	0.83	1 (9%)	15,15,17	0.92	0
5	NAG	Z	1	5,1	14,14,15	0.58	1 (7%)	17,19,21	0.51	0
5	NAG	Z	2	5	14,14,15	0.21	0	17,19,21	0.53	0
5	BMA	Z	3	5	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
6	NAG	a	1	6,1	14,14,15	0.32	0	17,19,21	0.46	0
6	NAG	a	2	6	14,14,15	0.35	0	17,19,21	0.49	0
6	NAG	b	1	6,1	14,14,15	0.80	1 (7%)	17,19,21	0.68	0
6	NAG	b	2	6	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
6	NAG	c	1	2,6	14,14,15	0.41	0	17,19,21	0.39	0
6	NAG	c	2	6	14,14,15	0.29	0	17,19,21	0.36	0
5	NAG	d	1	5,1	14,14,15	0.35	0	17,19,21	0.65	1 (5%)
5	NAG	d	2	5	14,14,15	0.23	0	17,19,21	0.40	0
5	BMA	d	3	5	11,11,12	0.58	0	15,15,17	1.00	1 (6%)
6	NAG	e	1	6,1	14,14,15	0.45	0	17,19,21	0.74	0
6	NAG	e	2	6	14,14,15	0.30	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	f	1	5,1	14,14,15	0.87	1 (7%)	17,19,21	0.54	0
5	NAG	f	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
5	BMA	f	3	5	11,11,12	0.49	0	15,15,17	0.96	1 (6%)
5	NAG	g	1	5,1	14,14,15	1.41	2 (14%)	17,19,21	0.67	0
5	NAG	g	2	5	14,14,15	0.23	0	17,19,21	0.37	0
5	BMA	g	3	5	11,11,12	0.55	0	15,15,17	0.84	1 (6%)
6	NAG	h	1	6,1	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
6	NAG	h	2	6	14,14,15	0.23	0	17,19,21	0.61	0
6	NAG	i	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	0.66	0
6	NAG	i	2	6	14,14,15	0.55	0	17,19,21	0.56	0
7	NAG	j	1	7,1	14,14,15	0.99	1 (7%)	17,19,21	0.47	0
7	NAG	j	2	7	14,14,15	0.78	1 (7%)	17,19,21	0.67	0
7	BMA	j	3	7	11,11,12	0.91	1 (9%)	15,15,17	0.85	0
7	MAN	j	4	7	11,11,12	0.75	0	15,15,17	1.35	2 (13%)
7	MAN	j	5	7	11,11,12	0.65	0	15,15,17	1.54	2 (13%)
7	MAN	j	6	7	11,11,12	0.63	0	15,15,17	0.95	1 (6%)
7	MAN	j	7	7	11,11,12	0.50	0	15,15,17	1.14	2 (13%)
5	NAG	k	1	5,1	14,14,15	0.50	0	17,19,21	0.34	0
5	NAG	k	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	BMA	k	3	5	11,11,12	0.50	0	15,15,17	0.83	0
8	NAG	l	1	8,1	14,14,15	0.47	0	17,19,21	0.51	0
8	NAG	l	2	8	14,14,15	0.31	0	17,19,21	0.47	0
8	BMA	l	3	8	11,11,12	0.61	0	15,15,17	0.70	0
8	MAN	l	4	8	11,11,12	0.48	0	15,15,17	1.06	2 (13%)
8	MAN	l	5	8	11,11,12	0.68	0	15,15,17	1.05	1 (6%)
9	NAG	m	1	9,1	14,14,15	0.29	0	17,19,21	1.11	1 (5%)
9	NAG	m	2	9	14,14,15	1.52	1 (7%)	17,19,21	1.12	1 (5%)
9	BMA	m	3	9	11,11,12	1.45	1 (9%)	15,15,17	1.36	2 (13%)
9	MAN	m	4	9	11,11,12	0.99	1 (9%)	15,15,17	1.17	1 (6%)
9	MAN	m	5	9	11,11,12	1.42	1 (9%)	15,15,17	1.91	4 (26%)
9	MAN	m	6	9	11,11,12	0.84	1 (9%)	15,15,17	0.92	1 (6%)
9	MAN	m	7	9	11,11,12	1.05	1 (9%)	15,15,17	1.12	1 (6%)
10	NAG	n	1	10,1	14,14,15	0.60	1 (7%)	17,19,21	0.52	0
10	NAG	n	2	10	14,14,15	0.87	1 (7%)	17,19,21	0.57	0
10	BMA	n	3	10	11,11,12	1.24	2 (18%)	15,15,17	1.35	3 (20%)
10	MAN	n	4	10	11,11,12	1.67	1 (9%)	15,15,17	1.42	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
10	MAN	n	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.56	3 (20%)
10	MAN	n	6	10	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
10	MAN	n	7	10	11,11,12	0.72	0	15,15,17	0.93	1 (6%)
10	MAN	n	8	10	11,11,12	1.04	1 (9%)	15,15,17	1.71	3 (20%)
6	NAG	o	1	6,1	14,14,15	0.72	1 (7%)	17,19,21	0.56	0
6	NAG	o	2	6	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	p	1	5,1	14,14,15	1.02	1 (7%)	17,19,21	0.72	0
5	NAG	p	2	5	14,14,15	0.36	0	17,19,21	0.47	0
5	BMA	p	3	5	11,11,12	0.85	1 (9%)	15,15,17	0.91	0
5	NAG	q	1	5,1	14,14,15	0.58	1 (7%)	17,19,21	0.51	0
5	NAG	q	2	5	14,14,15	0.22	0	17,19,21	0.53	0
5	BMA	q	3	5	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
6	NAG	r	1	6,1	14,14,15	0.33	0	17,19,21	0.46	0
6	NAG	r	2	6	14,14,15	0.34	0	17,19,21	0.49	0
6	NAG	s	1	6,1	14,14,15	0.79	1 (7%)	17,19,21	0.68	0
6	NAG	s	2	6	14,14,15	0.25	0	17,19,21	0.72	1 (5%)
6	NAG	t	1	2,6	14,14,15	0.40	0	17,19,21	0.40	0
6	NAG	t	2	6	14,14,15	0.30	0	17,19,21	0.36	0
5	NAG	u	1	5,1	14,14,15	0.35	0	17,19,21	0.64	0
5	NAG	u	2	5	14,14,15	0.22	0	17,19,21	0.40	0
5	BMA	u	3	5	11,11,12	0.59	0	15,15,17	1.01	1 (6%)
6	NAG	v	1	6,1	14,14,15	0.45	0	17,19,21	0.73	0
6	NAG	v	2	6	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	w	1	5,1	14,14,15	0.86	1 (7%)	17,19,21	0.54	0
5	NAG	w	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.67	0
5	BMA	w	3	5	11,11,12	0.48	0	15,15,17	0.96	1 (6%)
5	NAG	x	1	5,1	14,14,15	1.41	2 (14%)	17,19,21	0.66	0
5	NAG	x	2	5	14,14,15	0.24	0	17,19,21	0.37	0
5	BMA	x	3	5	11,11,12	0.56	0	15,15,17	0.85	1 (6%)
6	NAG	y	1	6,1	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
6	NAG	y	2	6	14,14,15	0.21	0	17,19,21	0.62	0
6	NAG	z	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	0.67	0
6	NAG	z	2	6	14,14,15	0.56	0	17,19,21	0.57	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
7	NAG	0	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	0	2	7	-	3/6/23/26	0/1/1/1
7	BMA	0	3	7	-	2/2/19/22	0/1/1/1
7	MAN	0	4	7	-	2/2/19/22	0/1/1/1
7	MAN	0	5	7	-	1/2/19/22	0/1/1/1
7	MAN	0	6	7	-	0/2/19/22	0/1/1/1
7	MAN	0	7	7	-	2/2/19/22	0/1/1/1
5	NAG	1	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	1	2	5	-	2/6/23/26	0/1/1/1
5	BMA	1	3	5	-	2/2/19/22	0/1/1/1
8	NAG	2	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	2	2	8	-	4/6/23/26	0/1/1/1
8	BMA	2	3	8	-	0/2/19/22	0/1/1/1
8	MAN	2	4	8	-	2/2/19/22	0/1/1/1
8	MAN	2	5	8	-	1/2/19/22	0/1/1/1
9	NAG	3	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	3	2	9	-	3/6/23/26	0/1/1/1
9	BMA	3	3	9	-	2/2/19/22	0/1/1/1
9	MAN	3	4	9	-	1/2/19/22	0/1/1/1
9	MAN	3	5	9	-	0/2/19/22	0/1/1/1
9	MAN	3	6	9	-	1/2/19/22	0/1/1/1
9	MAN	3	7	9	-	1/2/19/22	0/1/1/1
10	NAG	4	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	4	2	10	-	2/6/23/26	0/1/1/1
10	BMA	4	3	10	-	0/2/19/22	0/1/1/1
10	MAN	4	4	10	-	1/2/19/22	0/1/1/1
10	MAN	4	5	10	-	0/2/19/22	0/1/1/1
10	MAN	4	6	10	-	0/2/19/22	0/1/1/1
10	MAN	4	7	10	-	1/2/19/22	0/1/1/1
10	MAN	4	8	10	-	0/2/19/22	0/1/1/1
6	NAG	5	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	5	2	6	-	2/6/23/26	0/1/1/1
5	NAG	6	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	1/6/23/26	0/1/1/1
5	BMA	6	3	5	-	0/2/19/22	0/1/1/1
5	NAG	7	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	7	2	5	-	0/6/23/26	0/1/1/1
5	BMA	7	3	5	-	0/2/19/22	0/1/1/1
6	NAG	8	1	6,1	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	V	2	9	-	3/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	1/2/19/22	0/1/1/1
9	MAN	V	5	9	-	0/2/19/22	0/1/1/1
9	MAN	V	6	9	-	1/2/19/22	0/1/1/1
9	MAN	V	7	9	-	1/2/19/22	0/1/1/1
10	NAG	W	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
10	MAN	W	4	10	-	1/2/19/22	0/1/1/1
10	MAN	W	5	10	-	0/2/19/22	0/1/1/1
10	MAN	W	6	10	-	0/2/19/22	0/1/1/1
10	MAN	W	7	10	-	1/2/19/22	0/1/1/1
10	MAN	W	8	10	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	3/6/23/26	0/1/1/1
6	NAG	b	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1
6	NAG	c	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	c	2	6	-	0/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
6	NAG	e	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
5	NAG	f	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	BMA	f	3	5	-	2/2/19/22	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
6	NAG	h	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
6	NAG	i	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
7	NAG	j	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	j	2	7	-	3/6/23/26	0/1/1/1
7	BMA	j	3	7	-	2/2/19/22	0/1/1/1
7	MAN	j	4	7	-	2/2/19/22	0/1/1/1
7	MAN	j	5	7	-	1/2/19/22	0/1/1/1
7	MAN	j	6	7	-	0/2/19/22	0/1/1/1
7	MAN	j	7	7	-	2/2/19/22	0/1/1/1
5	NAG	k	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
5	BMA	k	3	5	-	2/2/19/22	0/1/1/1
8	NAG	l	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	l	2	8	-	4/6/23/26	0/1/1/1
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
8	MAN	l	4	8	-	2/2/19/22	0/1/1/1
8	MAN	l	5	8	-	1/2/19/22	0/1/1/1
9	NAG	m	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	m	2	9	-	3/6/23/26	0/1/1/1
9	BMA	m	3	9	-	2/2/19/22	0/1/1/1
9	MAN	m	4	9	-	1/2/19/22	0/1/1/1
9	MAN	m	5	9	-	0/2/19/22	0/1/1/1
9	MAN	m	6	9	-	1/2/19/22	0/1/1/1
9	MAN	m	7	9	-	1/2/19/22	0/1/1/1
10	NAG	n	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	n	2	10	-	2/6/23/26	0/1/1/1
10	BMA	n	3	10	-	0/2/19/22	0/1/1/1
10	MAN	n	4	10	-	1/2/19/22	0/1/1/1
10	MAN	n	5	10	-	0/2/19/22	0/1/1/1
10	MAN	n	6	10	-	0/2/19/22	0/1/1/1
10	MAN	n	7	10	-	1/2/19/22	0/1/1/1
10	MAN	n	8	10	-	0/2/19/22	0/1/1/1
6	NAG	o	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	o	2	6	-	2/6/23/26	0/1/1/1
5	NAG	p	1	5,1	-	0/6/23/26	0/1/1/1

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

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	m	2	NAG	C1-C2	5.24	1.60	1.52
9	V	2	NAG	C1-C2	5.23	1.60	1.52
9	3	2	NAG	C1-C2	5.19	1.60	1.52
5	g	1	NAG	O5-C1	-4.77	1.36	1.43
5	x	1	NAG	O5-C1	-4.77	1.36	1.43

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	j	5	MAN	C1-O5-C5	4.80	118.70	112.19
7	S	5	MAN	C1-O5-C5	4.78	118.67	112.19
7	0	5	MAN	C1-O5-C5	4.77	118.66	112.19
10	4	8	MAN	C1-O5-C5	4.22	117.90	112.19
10	W	8	MAN	C1-O5-C5	4.21	117.90	112.19

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

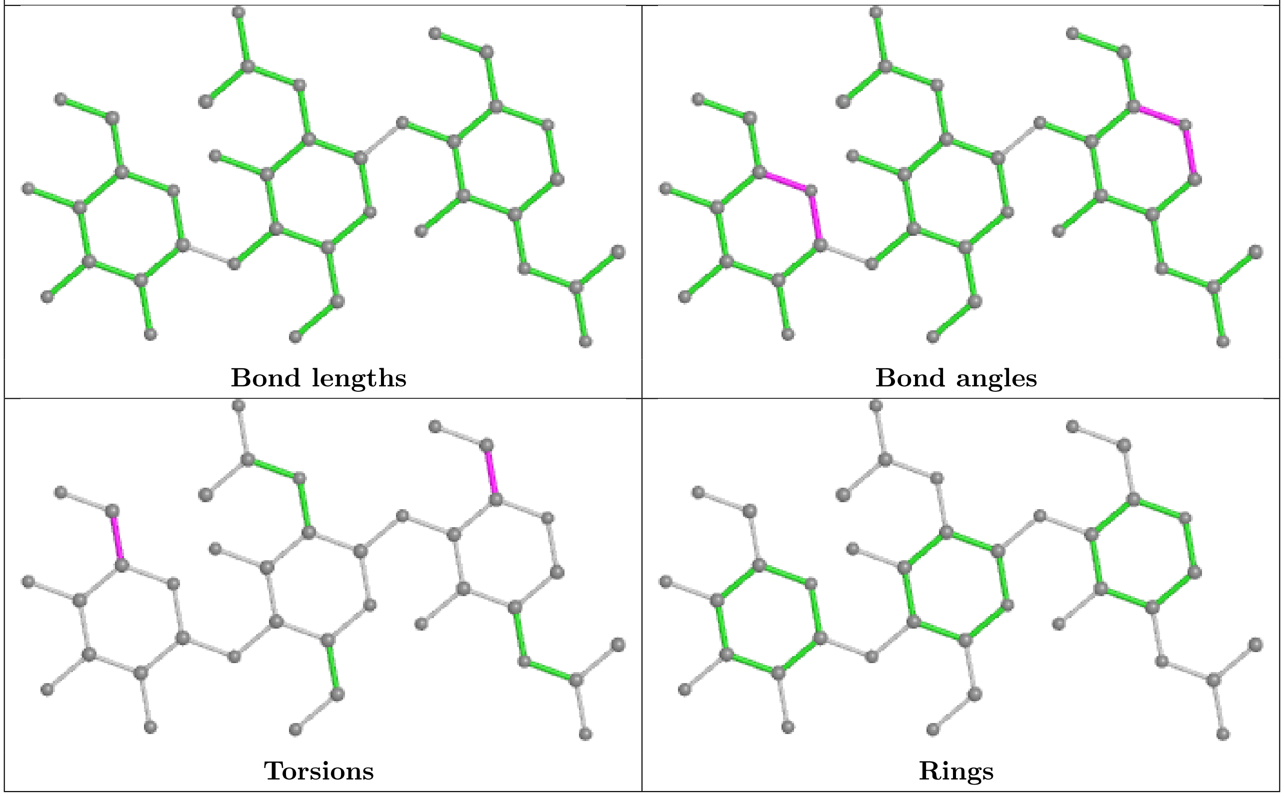
Mol	Chain	Res	Type	Atoms
6	X	1	NAG	O5-C5-C6-O6
6	o	1	NAG	O5-C5-C6-O6
6	5	1	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	o	2	NAG	O5-C5-C6-O6

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 M



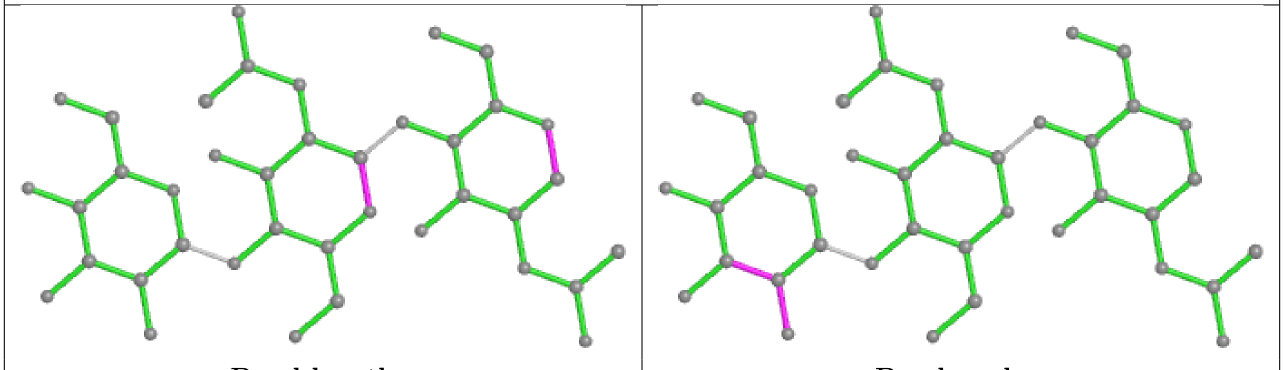
Bond lengths

Bond angles

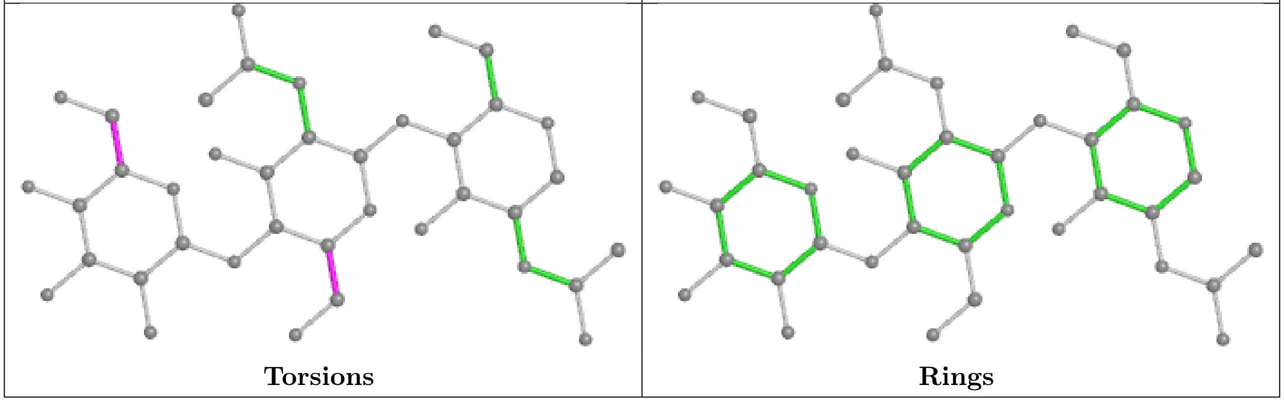
Torsions

Rings

Oligosaccharide Chain O

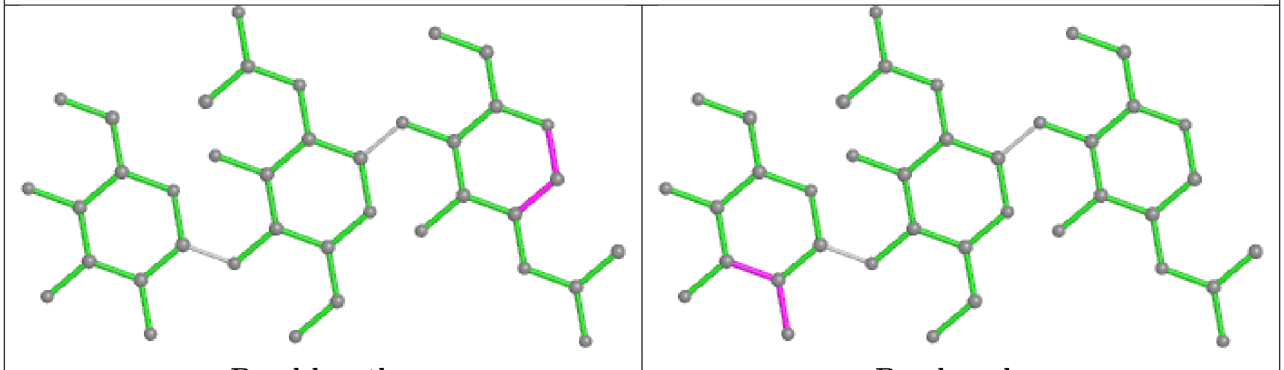


Bond lengths Bond angles

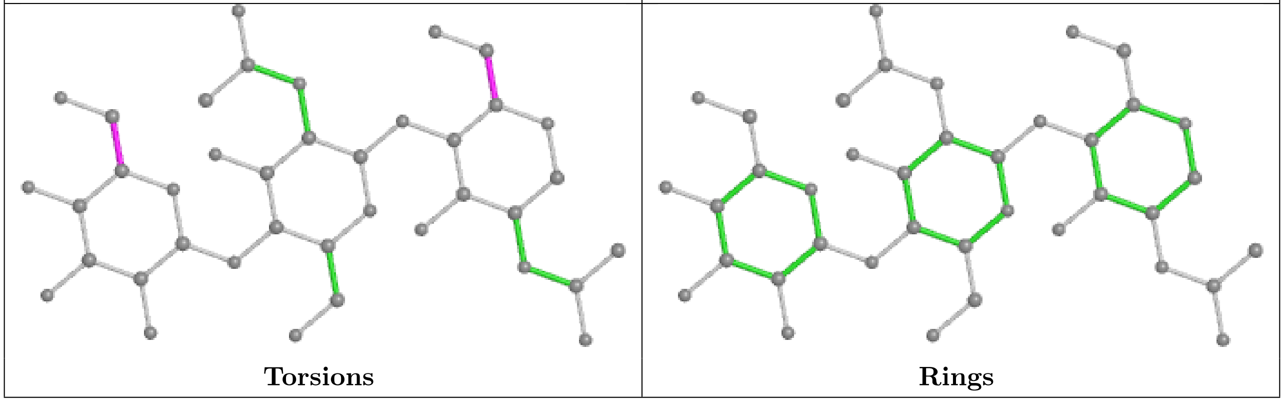


Torsions Rings

Oligosaccharide Chain P

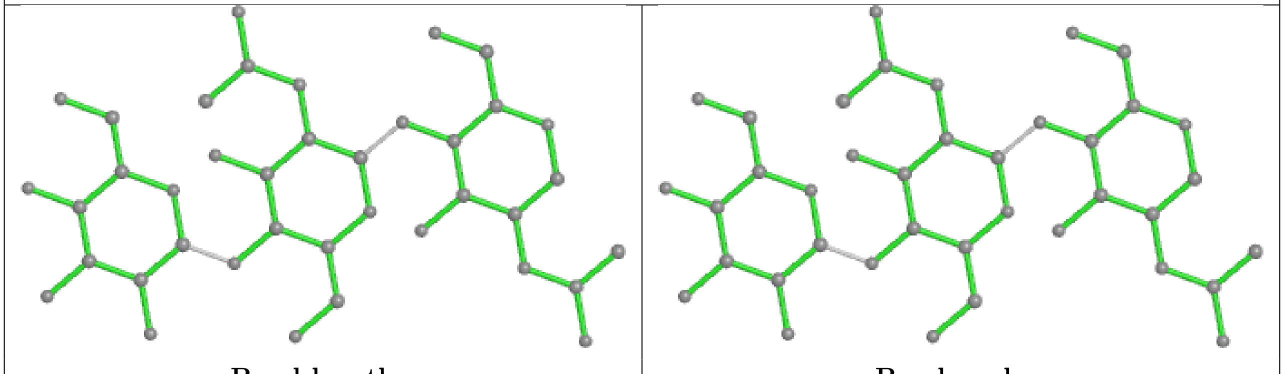


Bond lengths Bond angles

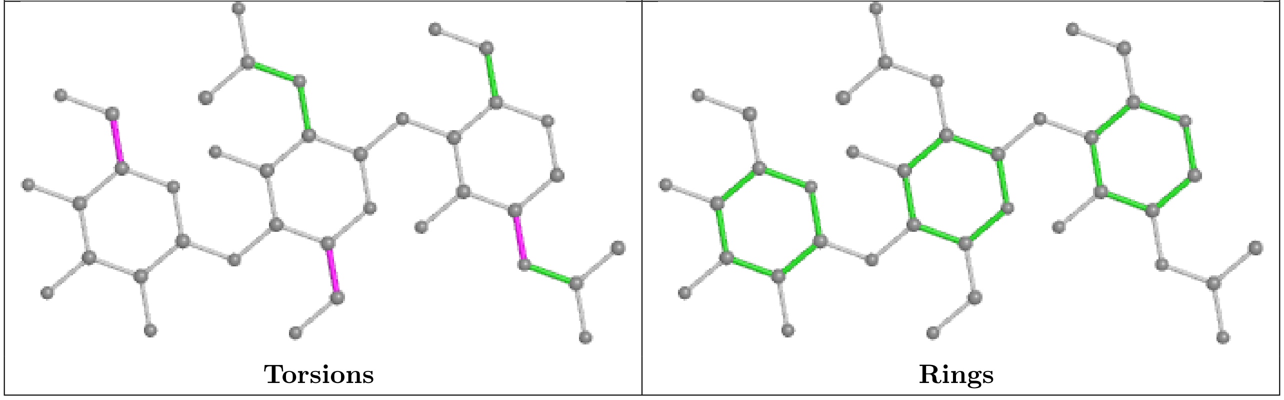


Torsions Rings

Oligosaccharide Chain T

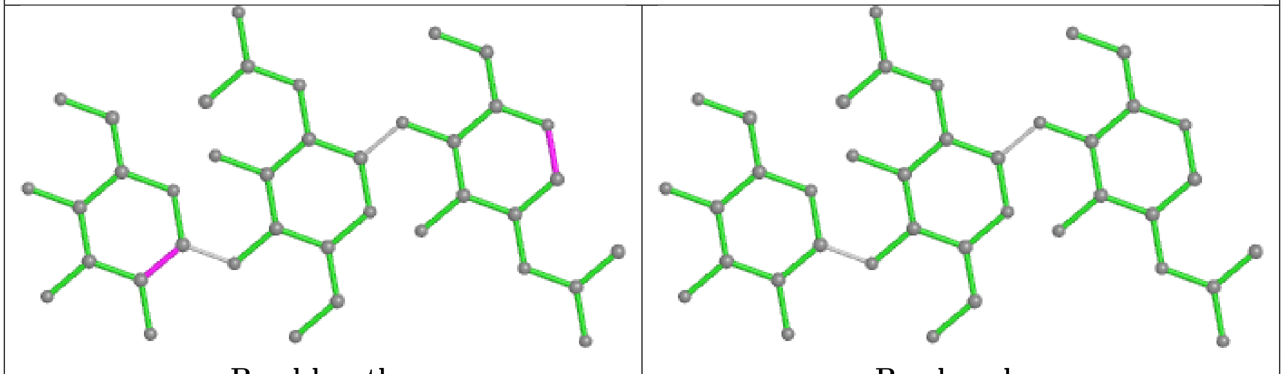


Bond lengths **Bond angles**

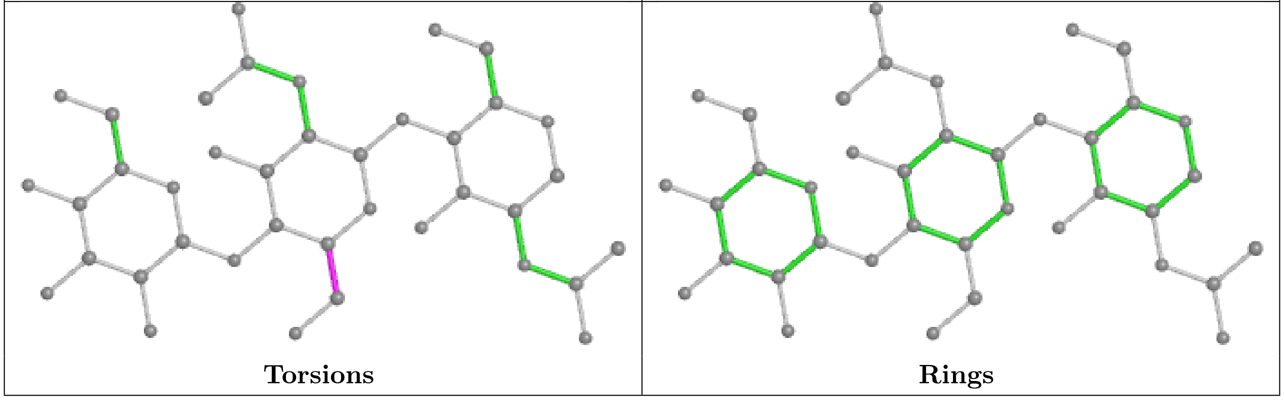


Torsions **Rings**

Oligosaccharide Chain Y

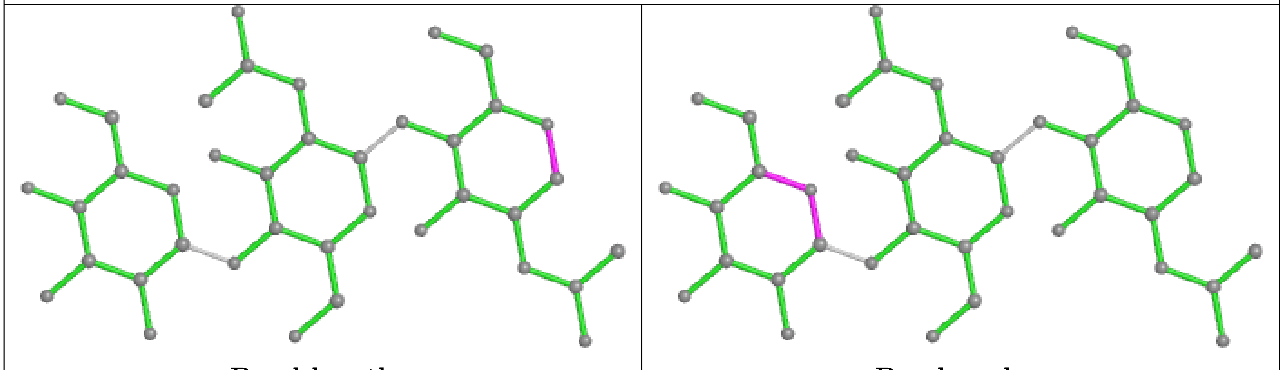


Bond lengths **Bond angles**

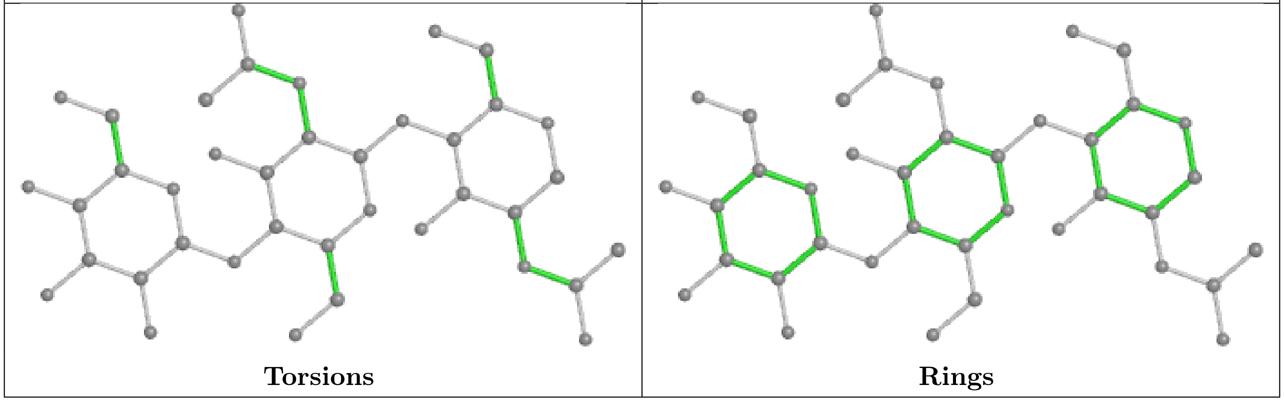


Torsions **Rings**

Oligosaccharide Chain Z

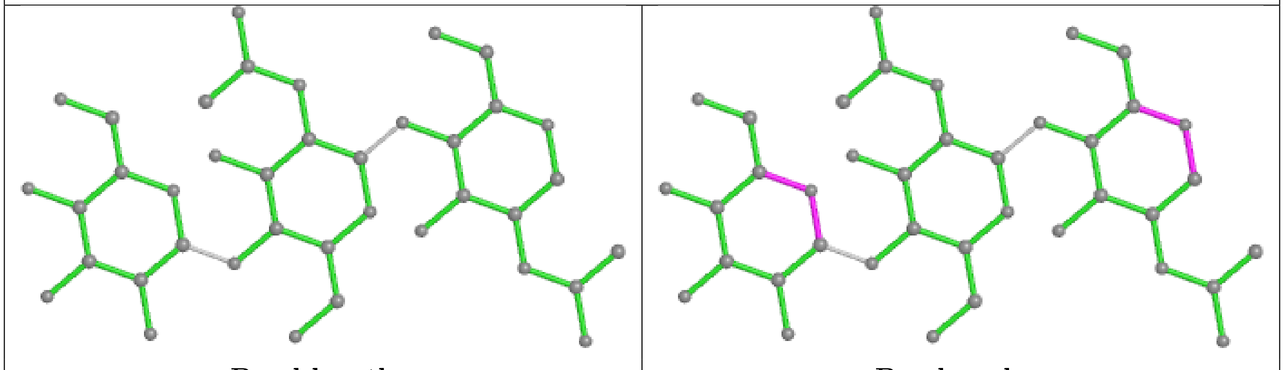


Bond lengths Bond angles

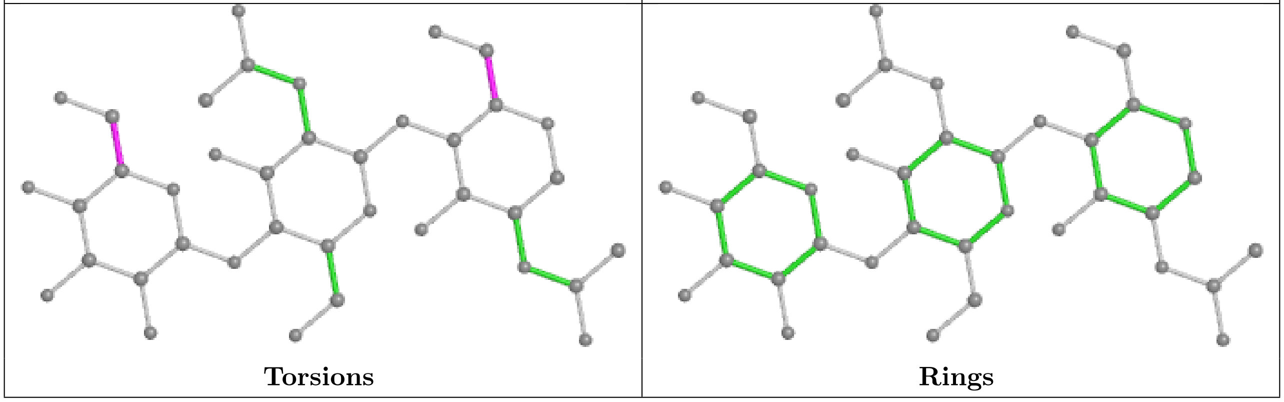


Torsions Rings

Oligosaccharide Chain d

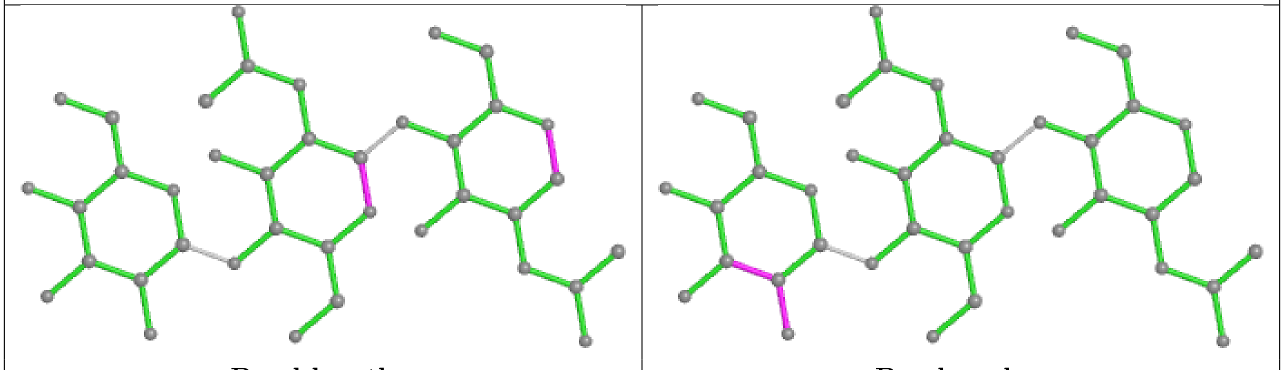


Bond lengths Bond angles

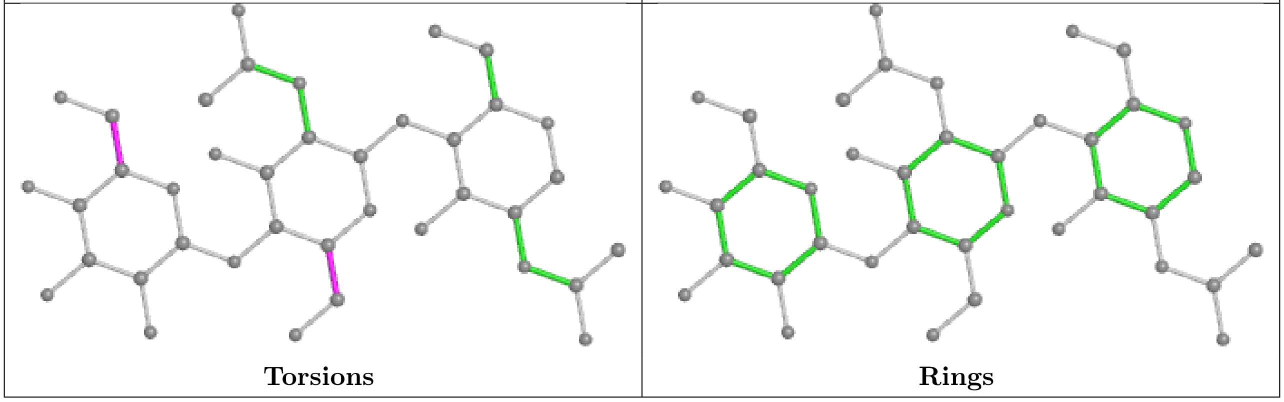


Torsions Rings

Oligosaccharide Chain f

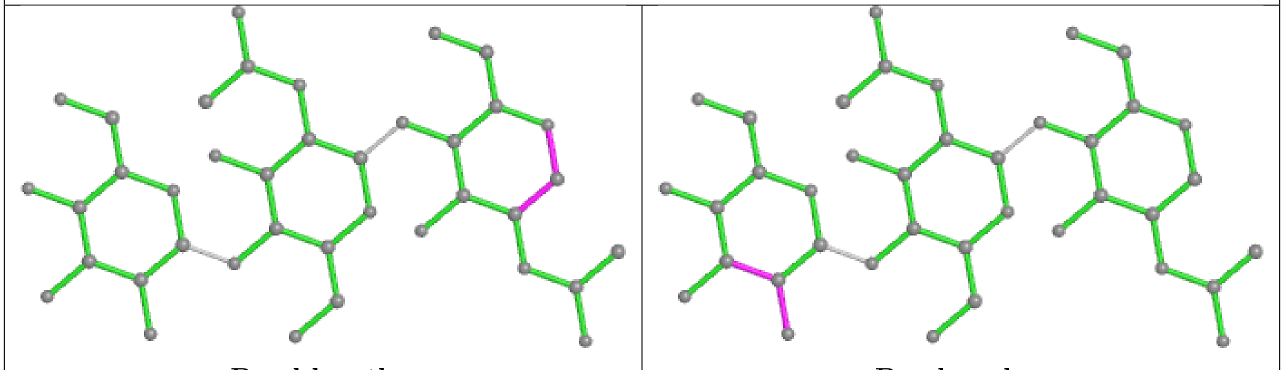


Bond lengths Bond angles

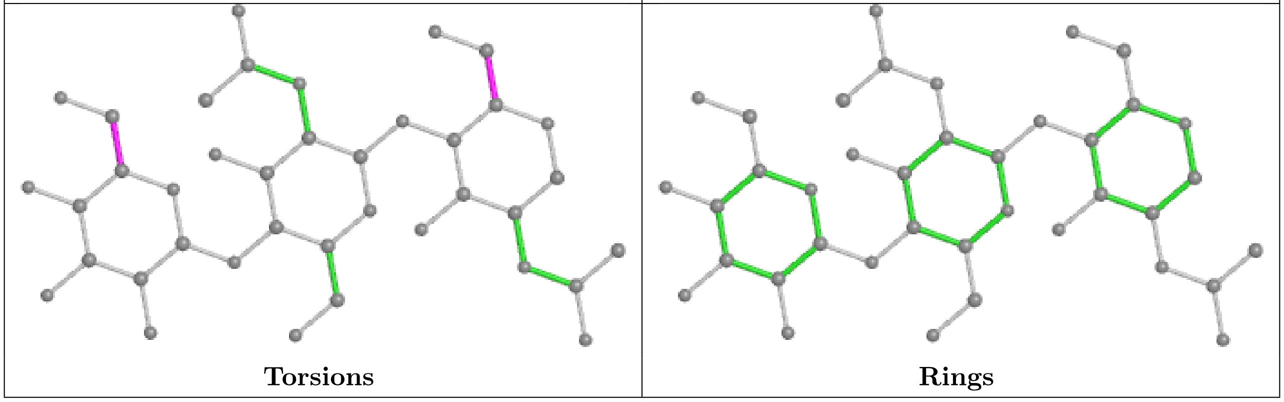


Torsions Rings

Oligosaccharide Chain g

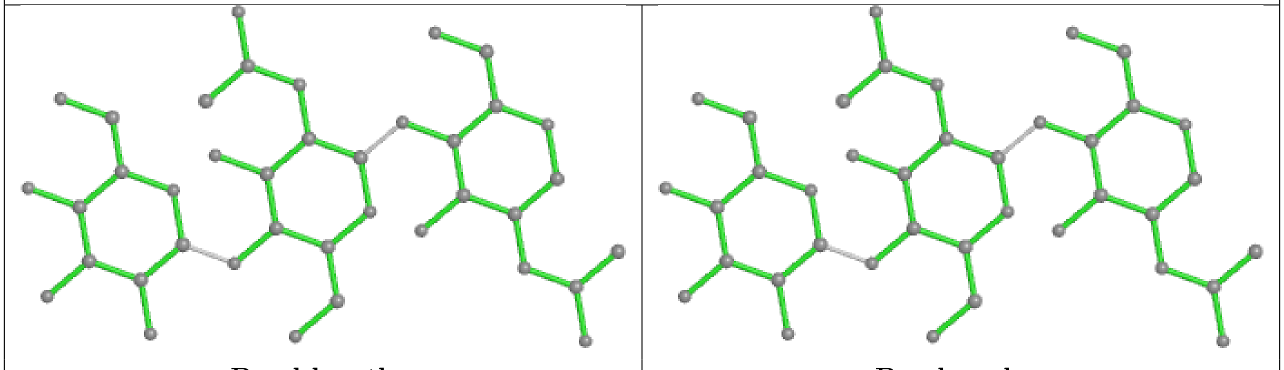


Bond lengths Bond angles

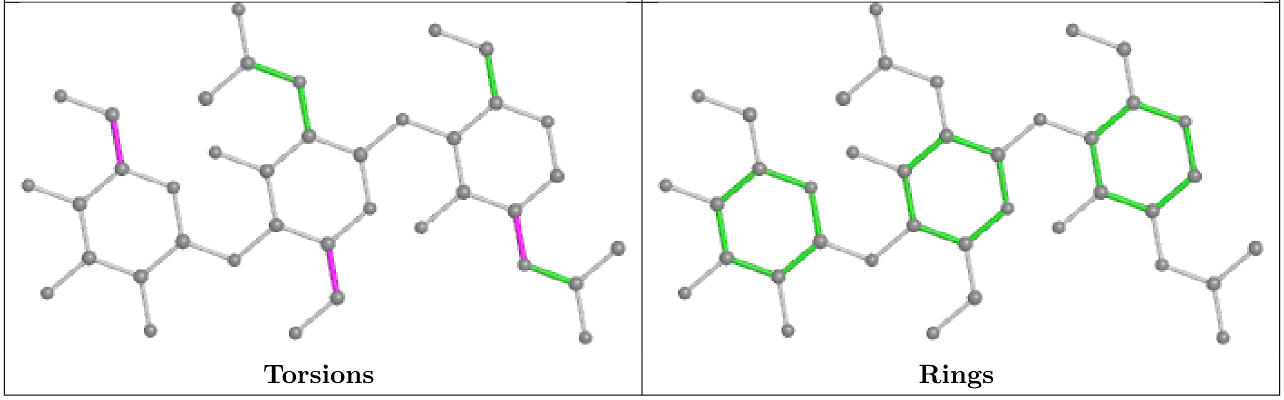


Torsions Rings

Oligosaccharide Chain k

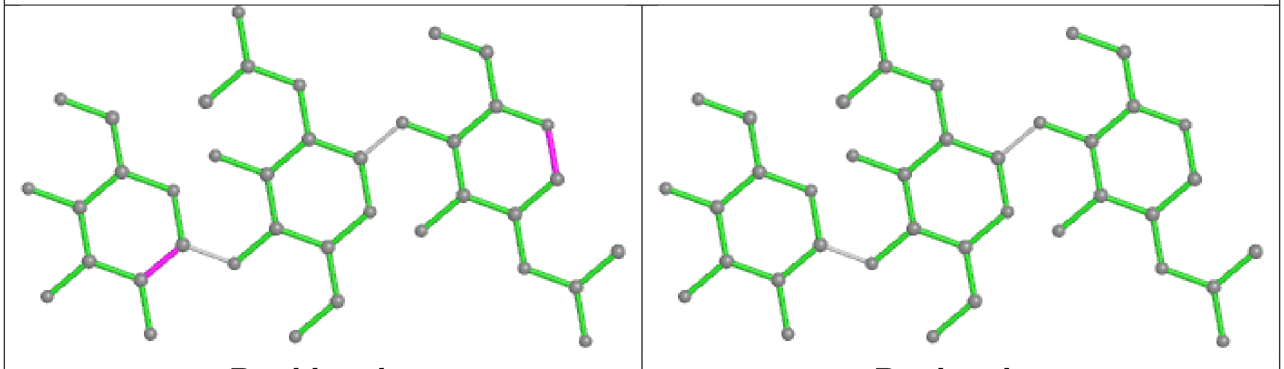


Bond lengths **Bond angles**

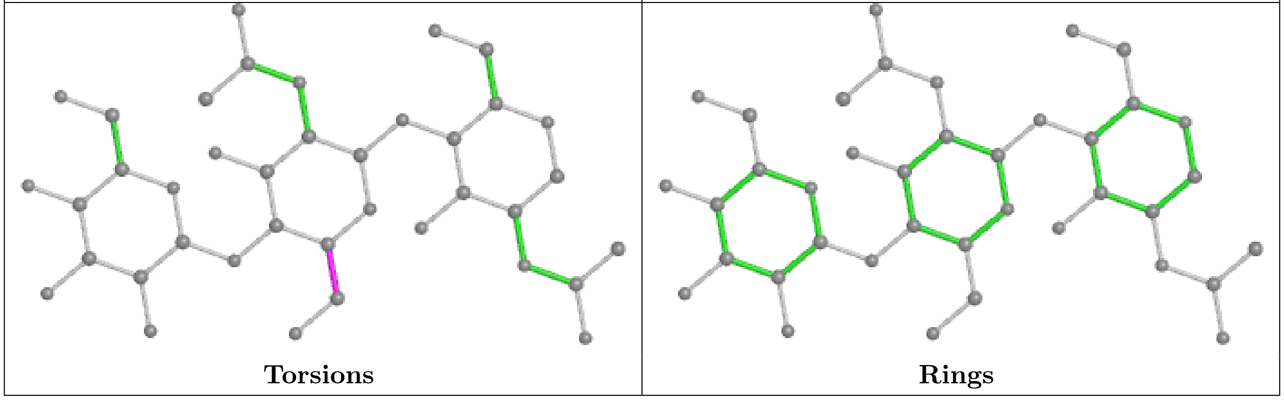


Torsions **Rings**

Oligosaccharide Chain p

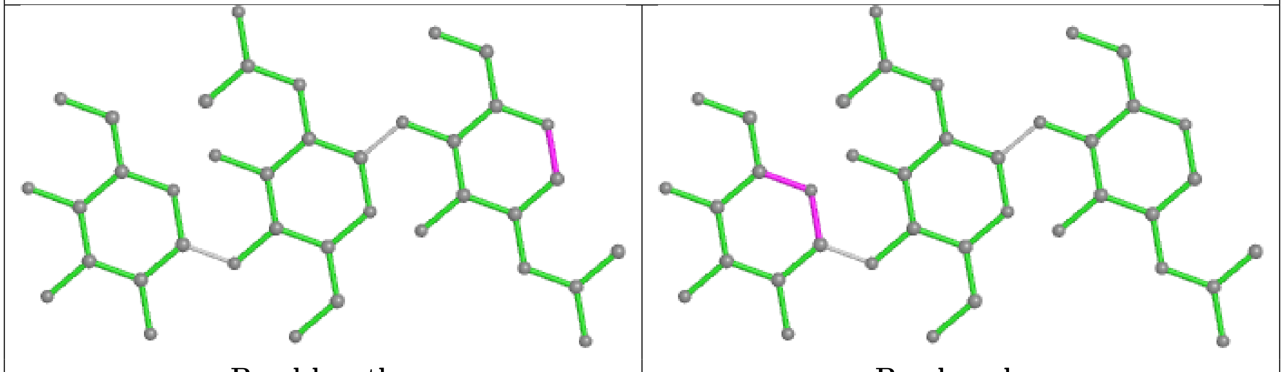


Bond lengths **Bond angles**



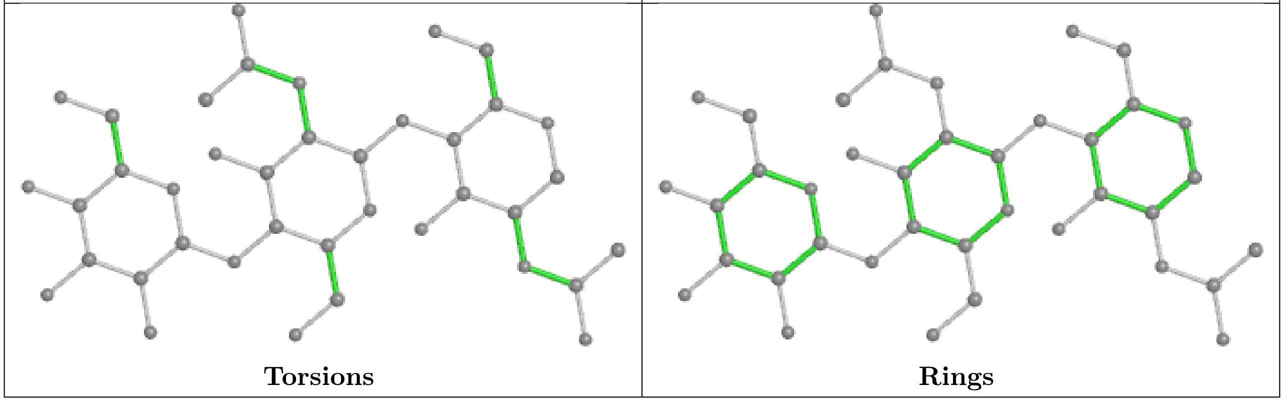
Torsions **Rings**

Oligosaccharide Chain q



Bond lengths

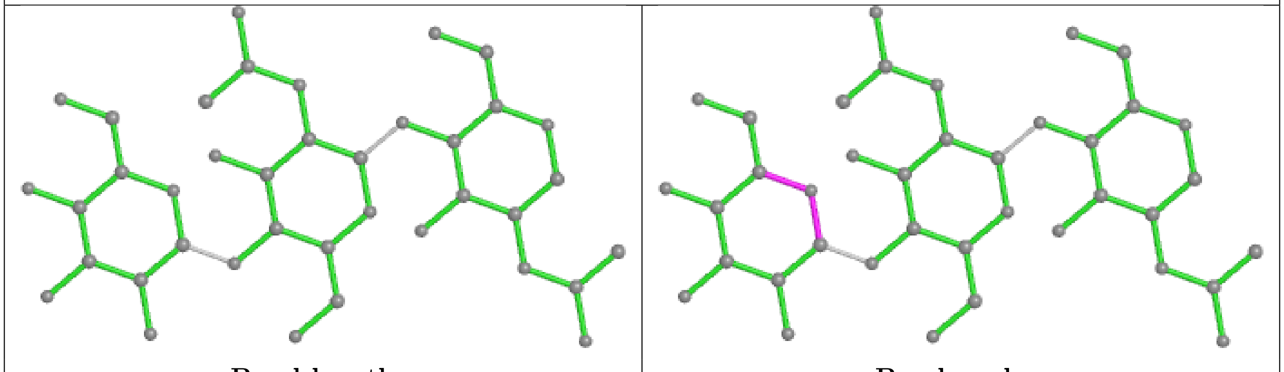
Bond angles



Torsions

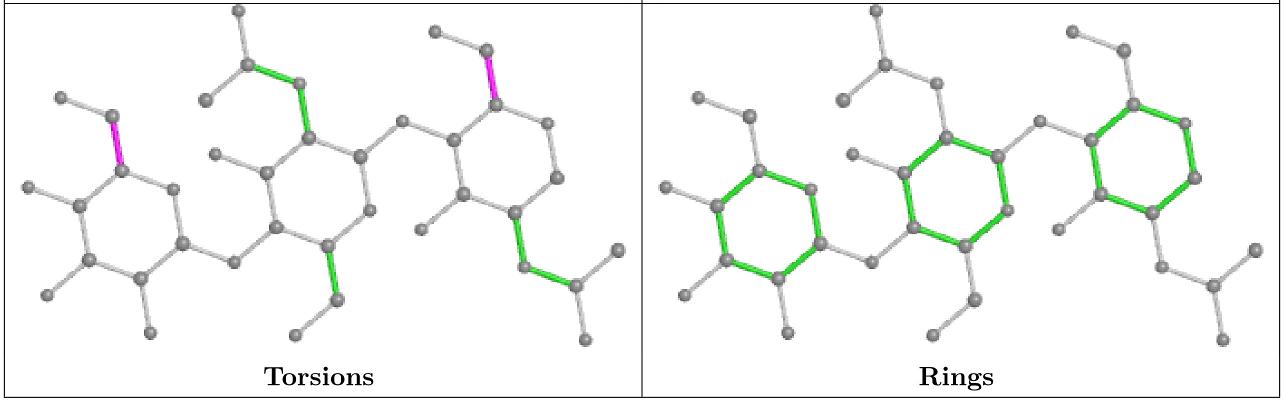
Rings

Oligosaccharide Chain u



Bond lengths

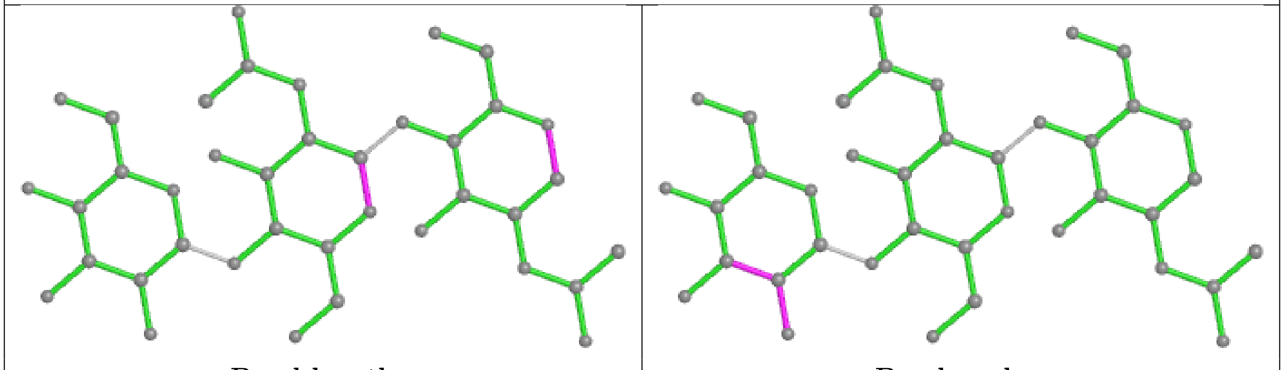
Bond angles



Torsions

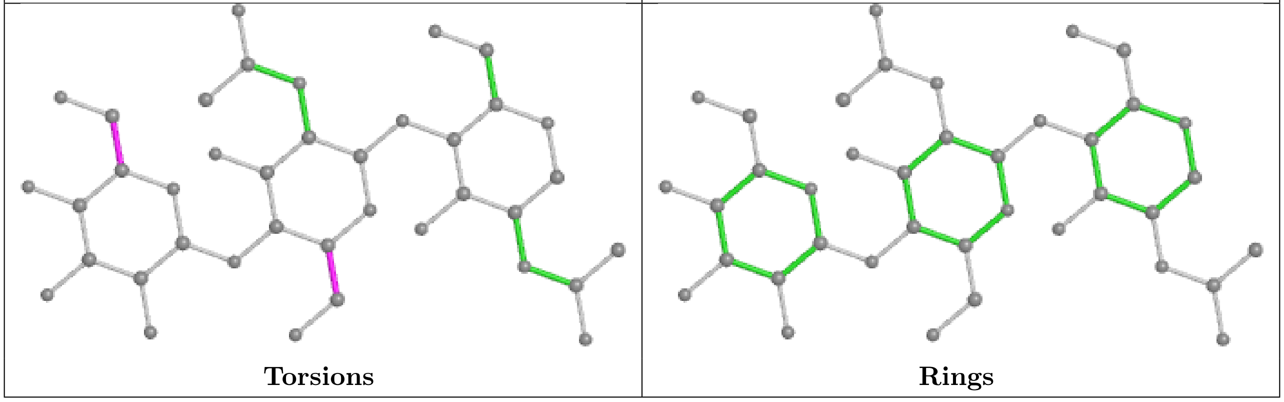
Rings

Oligosaccharide Chain w



Bond lengths

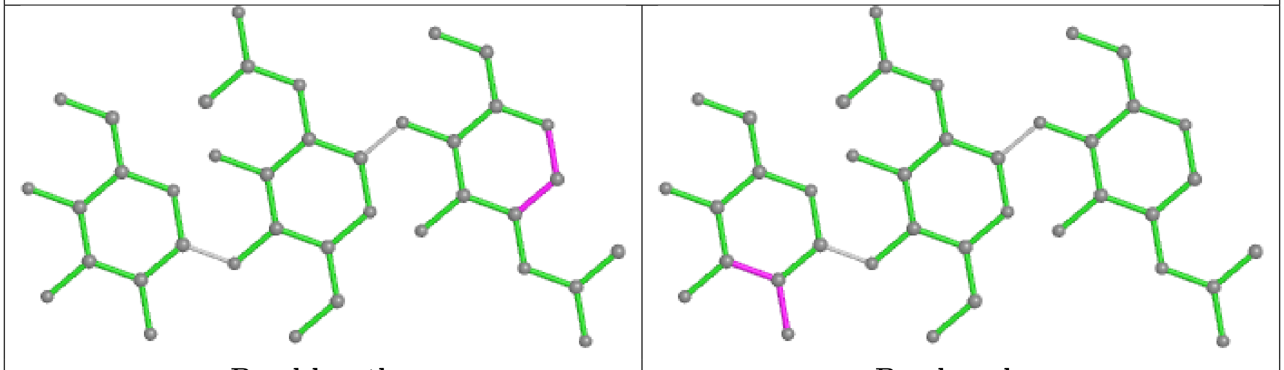
Bond angles



Torsions

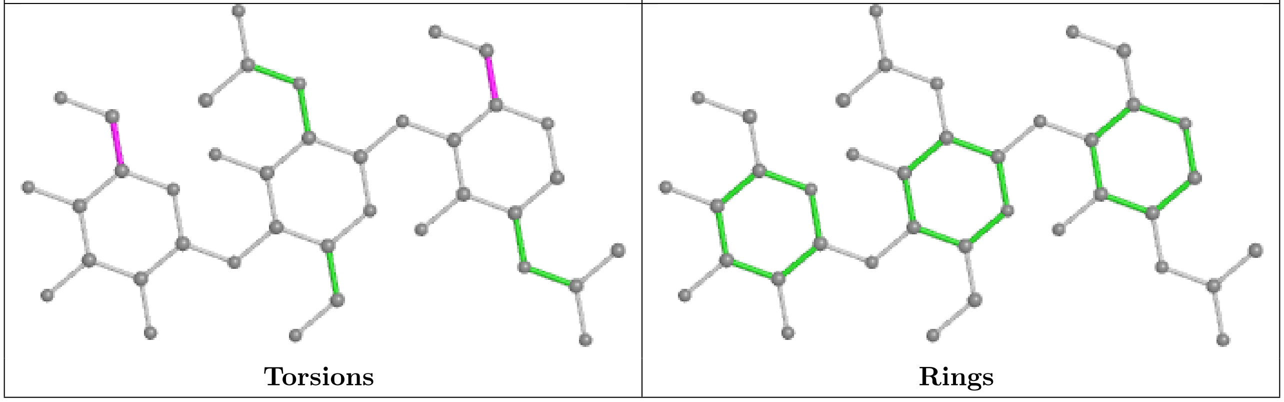
Rings

Oligosaccharide Chain x



Bond lengths

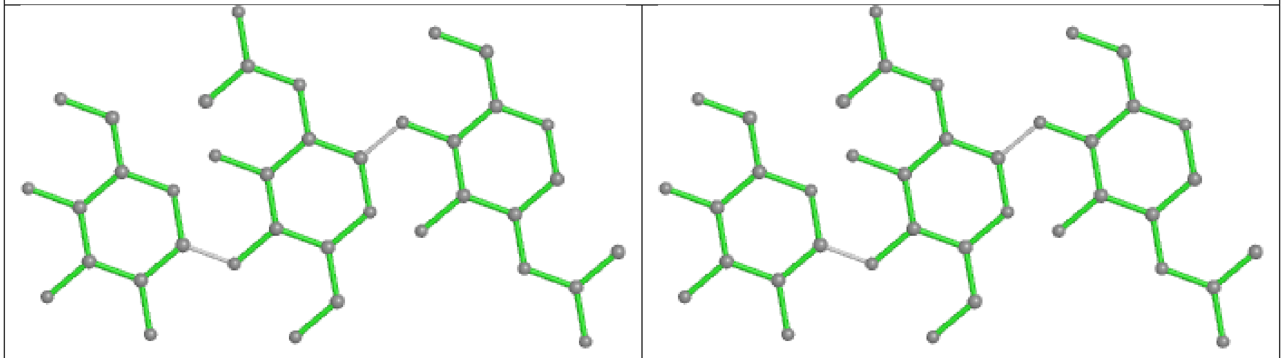
Bond angles



Torsions

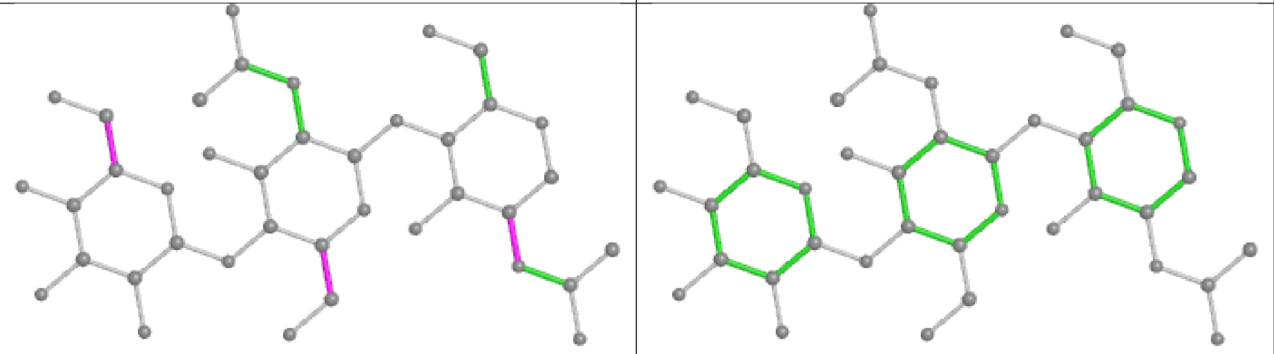
Rings

Oligosaccharide Chain 1



Bond lengths

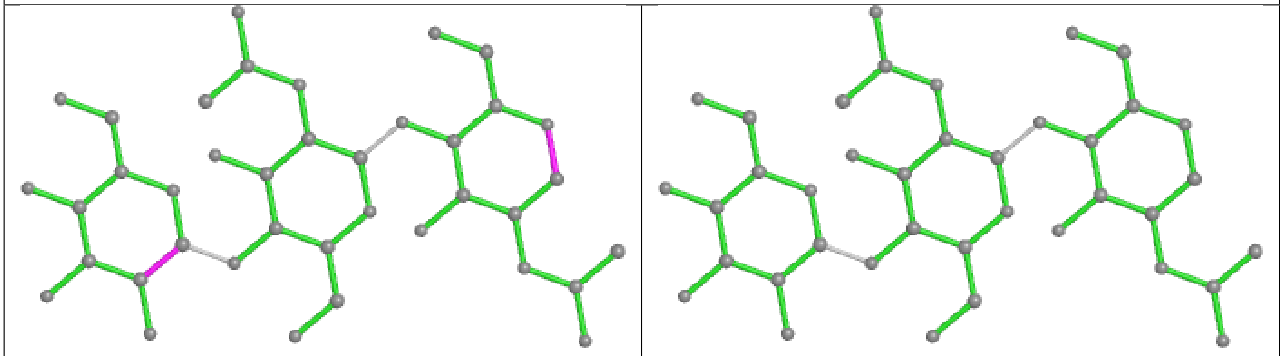
Bond angles



Torsions

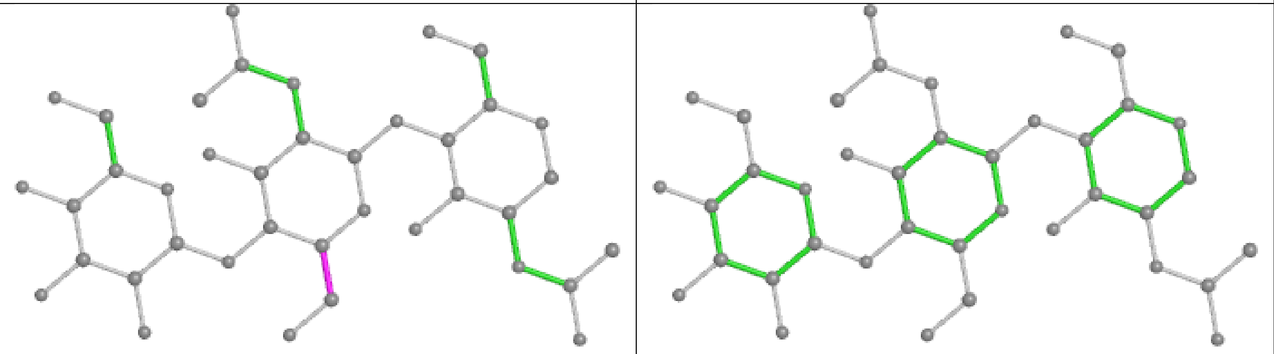
Rings

Oligosaccharide Chain 6



Bond lengths

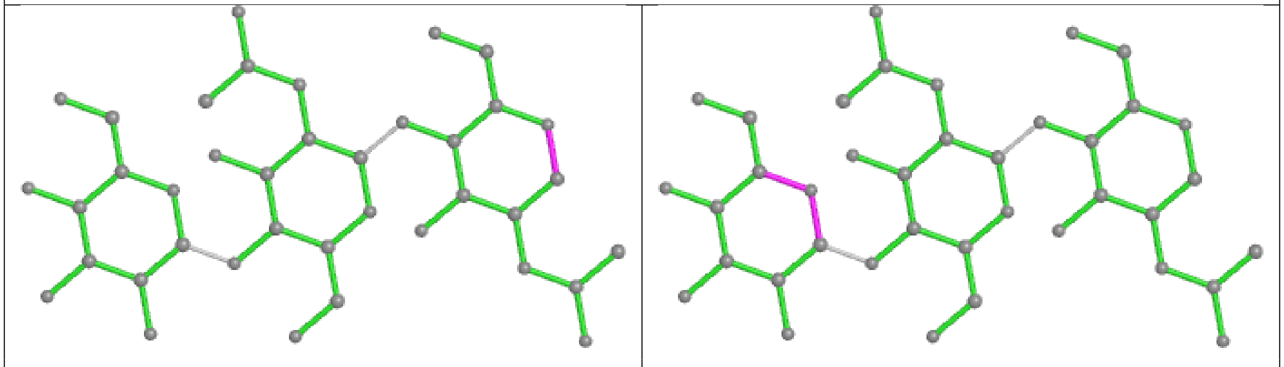
Bond angles



Torsions

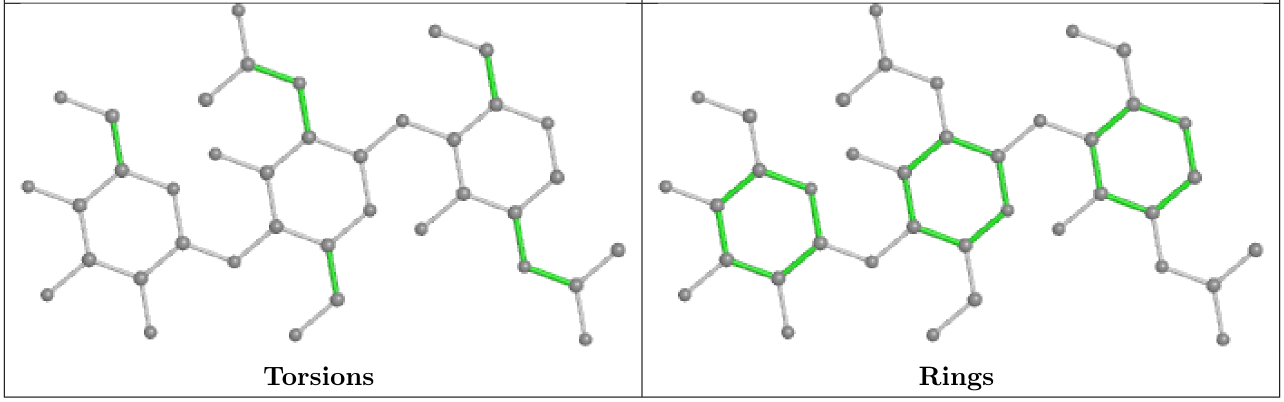
Rings

Oligosaccharide Chain 7



Bond lengths

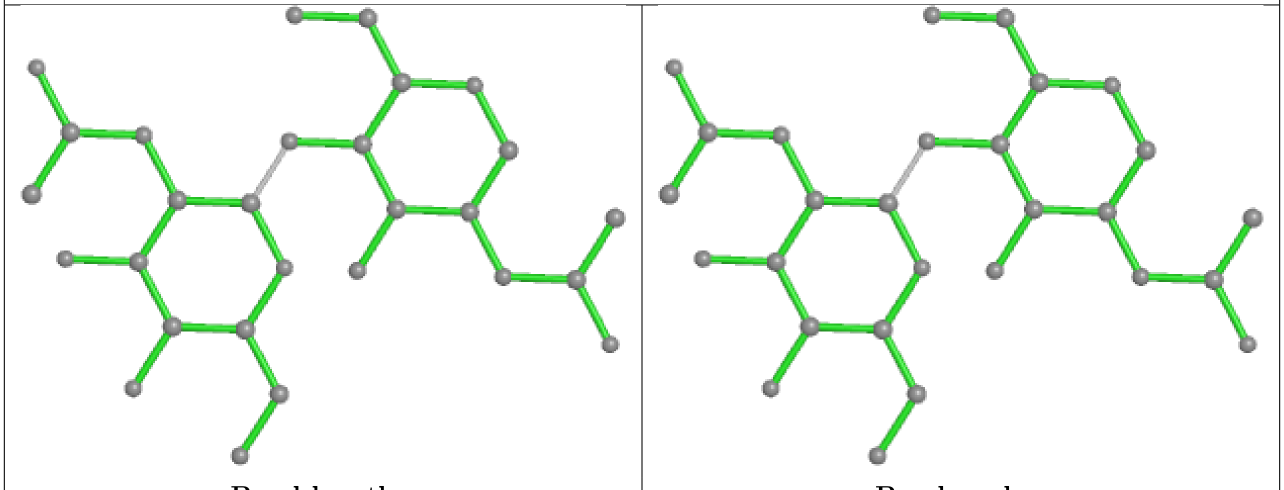
Bond angles



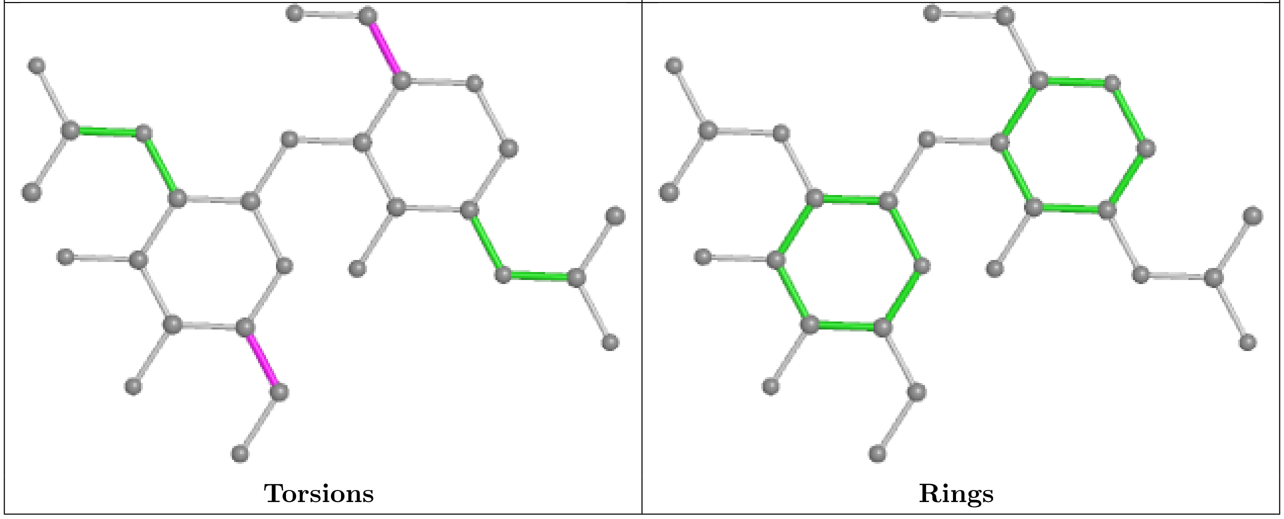
Torsions

Rings

Oligosaccharide Chain N

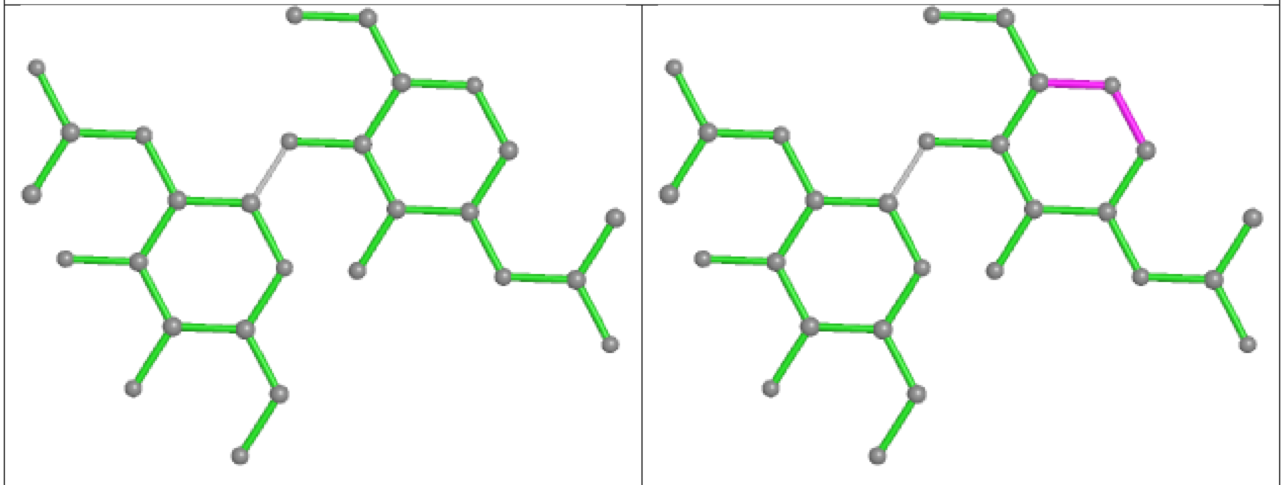


Bond lengths **Bond angles**



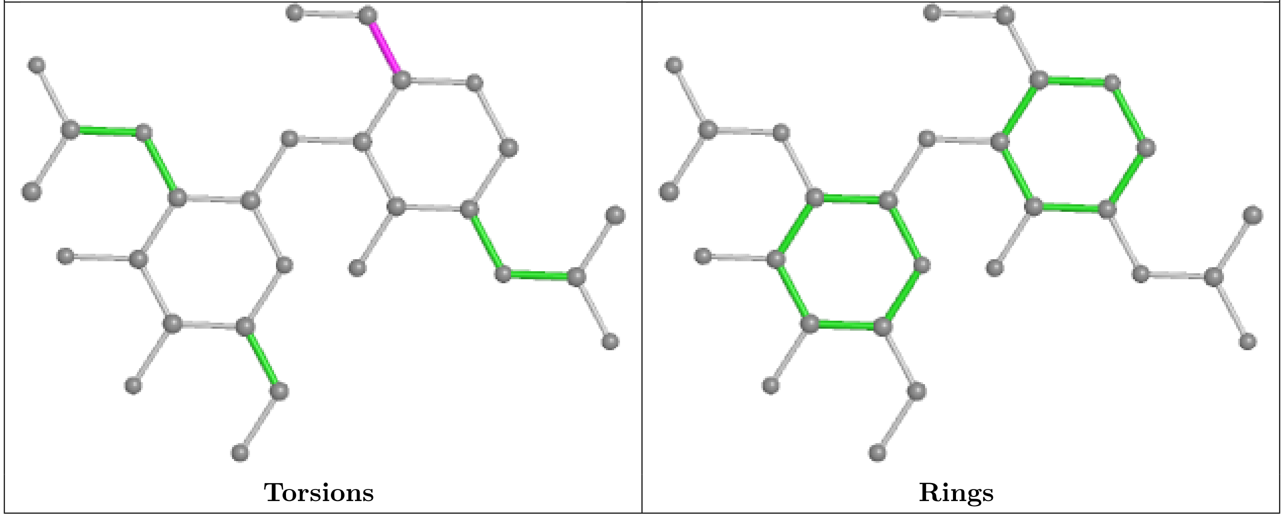
Torsions **Rings**

Oligosaccharide Chain Q



Bond lengths

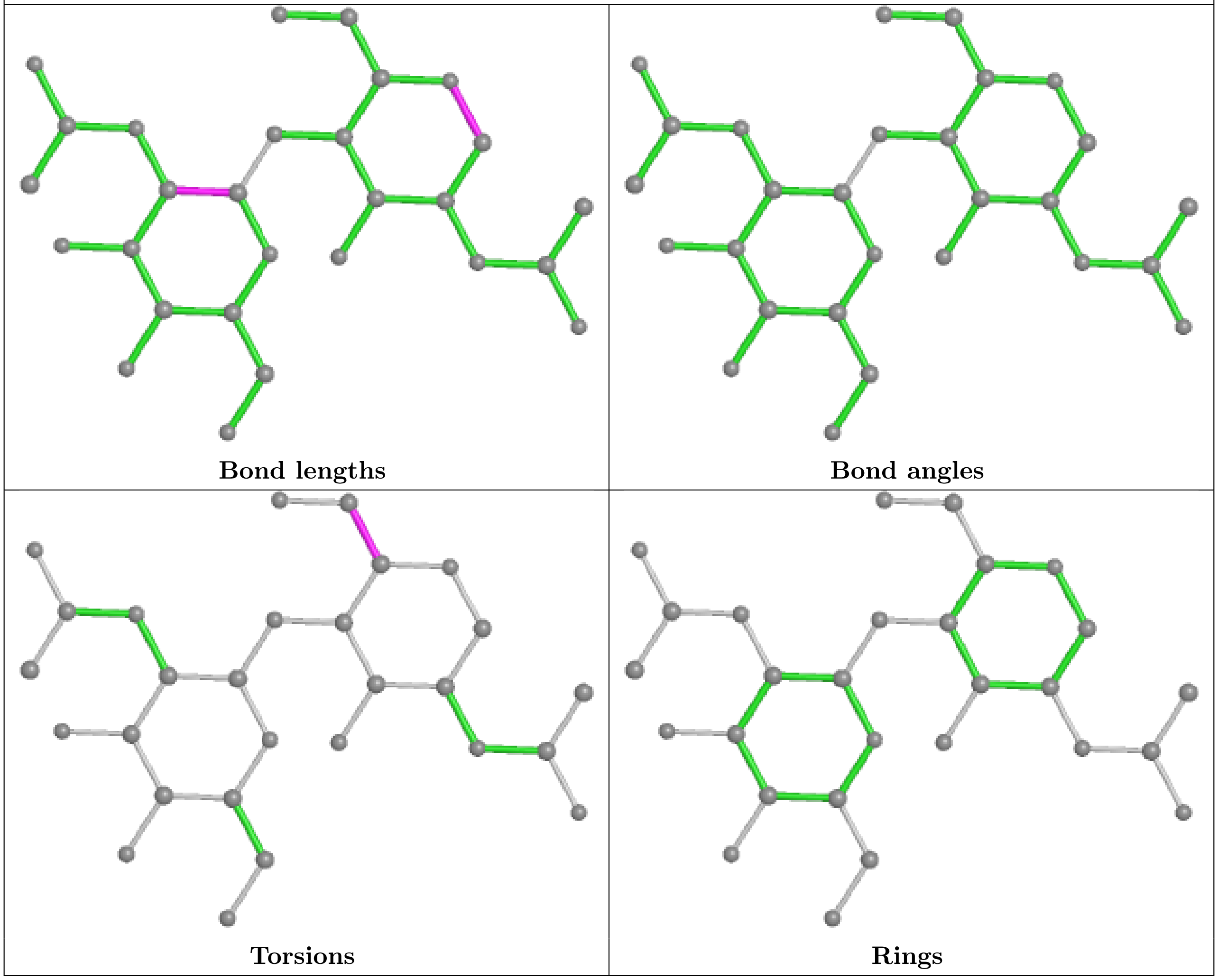
Bond angles



Torsions

Rings

Oligosaccharide Chain R



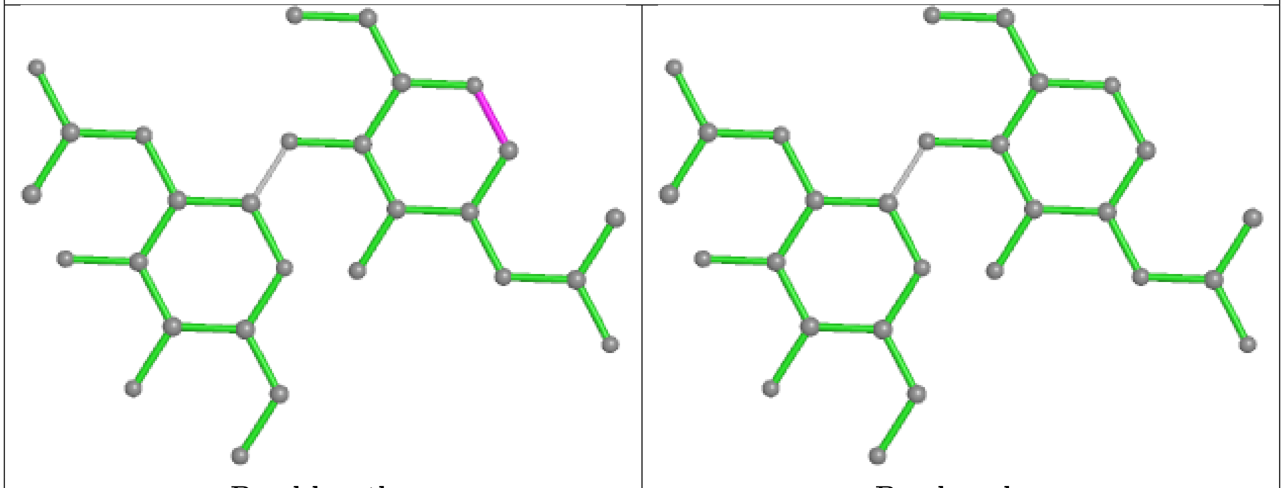
Bond lengths

Bond angles

Torsions

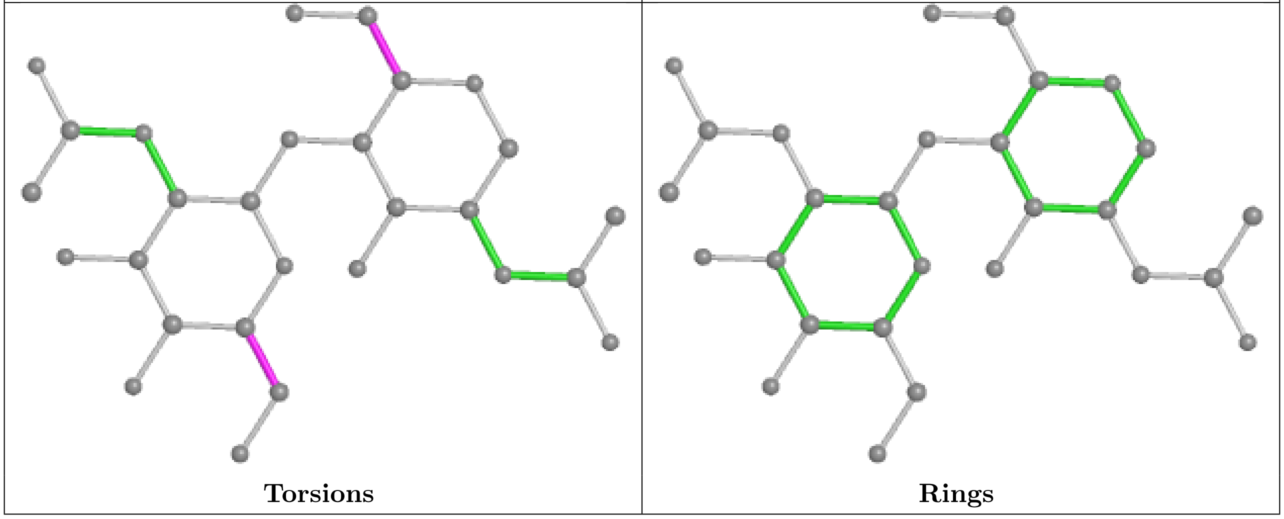
Rings

Oligosaccharide Chain X



Bond lengths

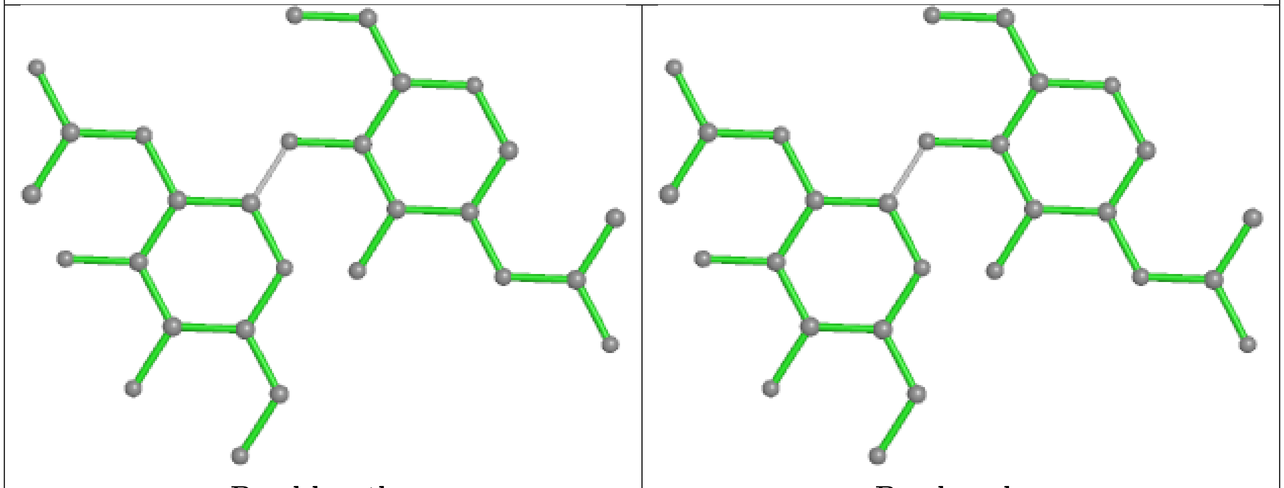
Bond angles



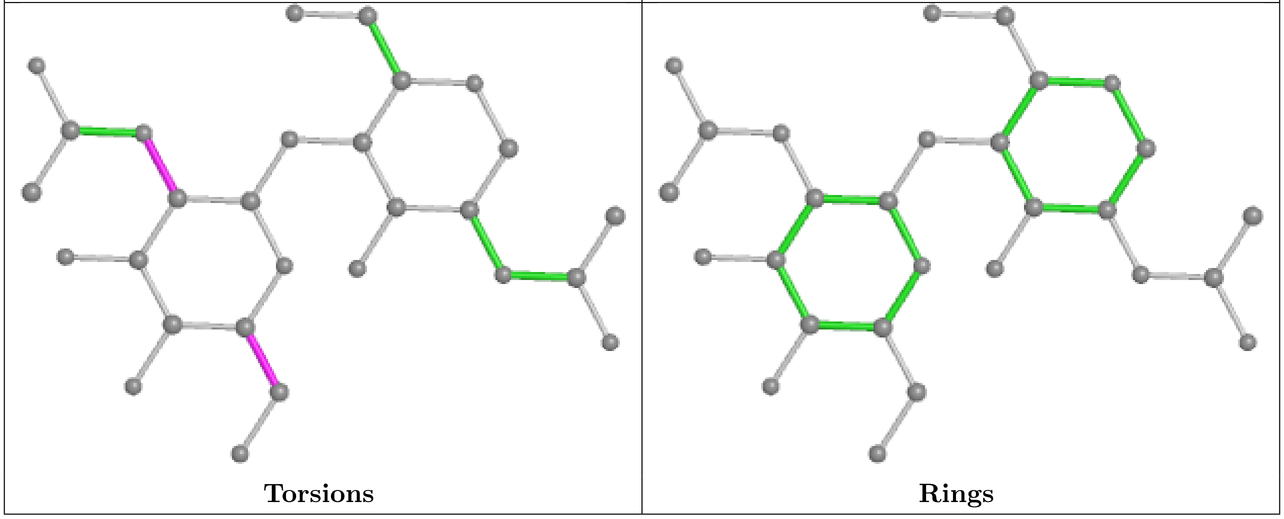
Torsions

Rings

Oligosaccharide Chain a

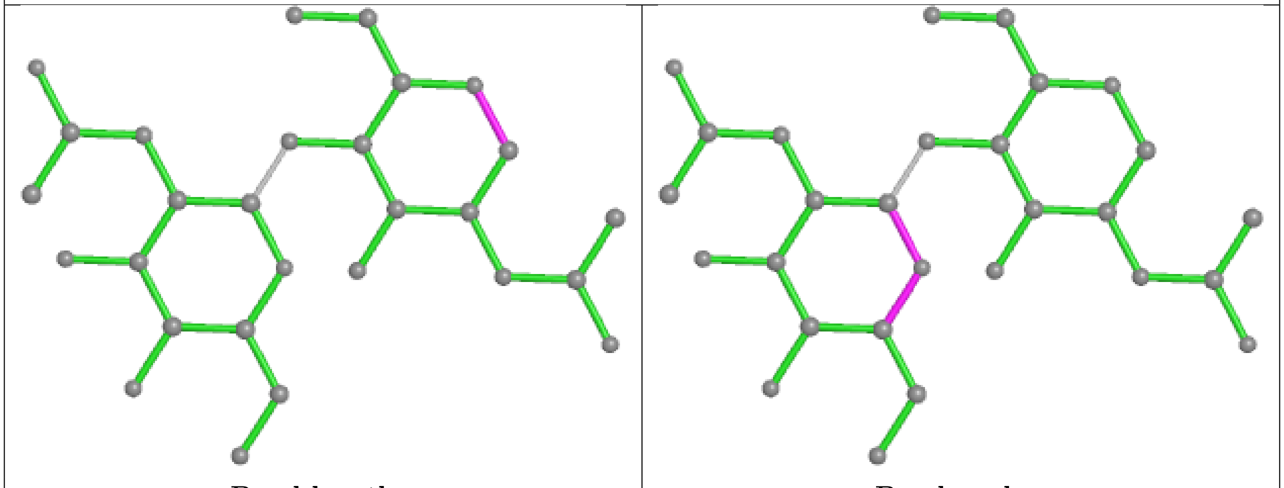


Bond lengths Bond angles



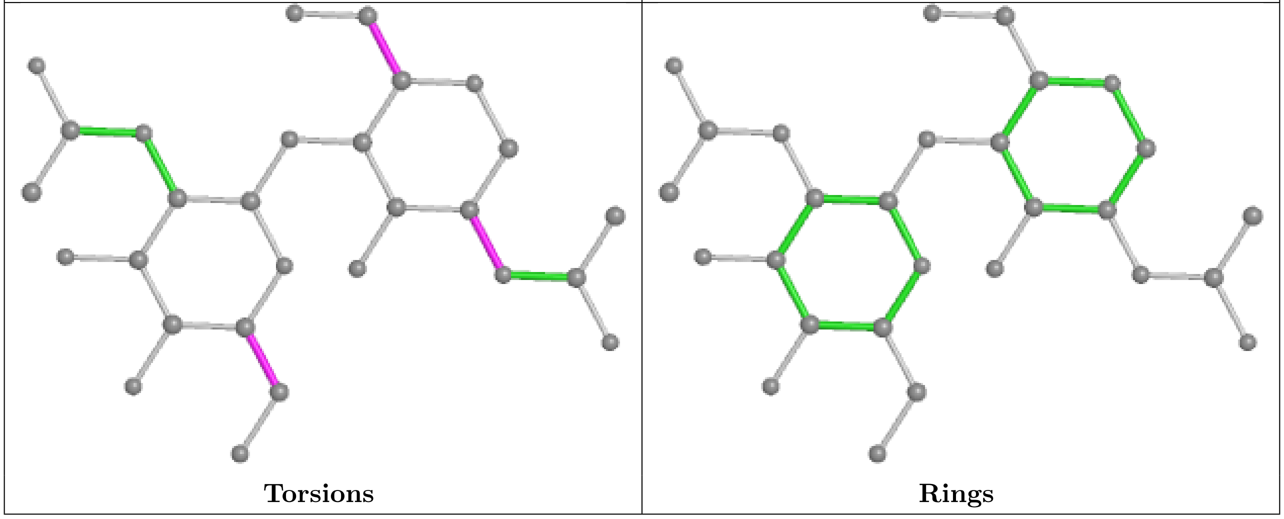
Torsions Rings

Oligosaccharide Chain b



Bond lengths

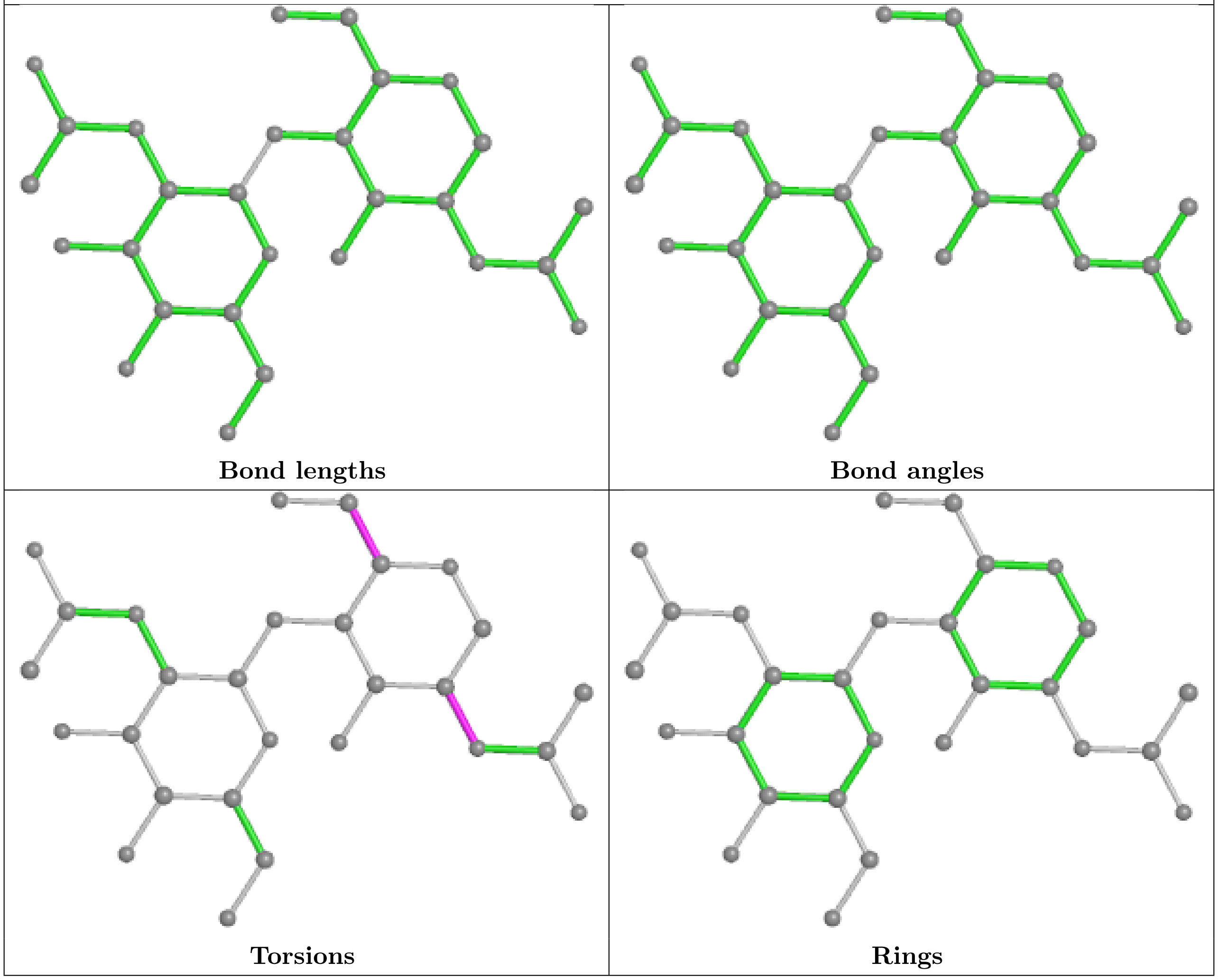
Bond angles



Torsions

Rings

Oligosaccharide Chain c



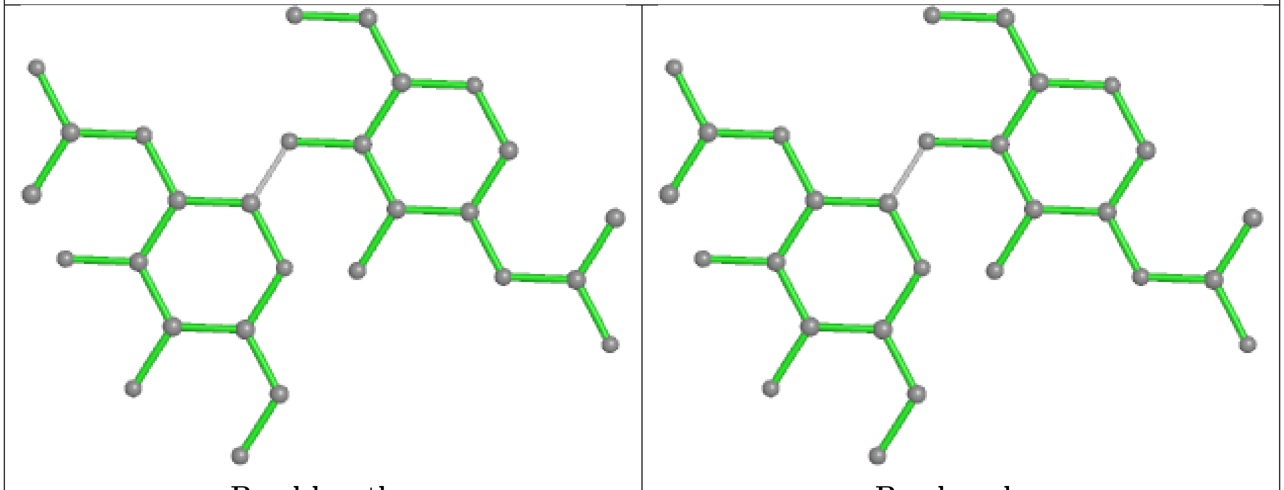
Bond lengths

Bond angles

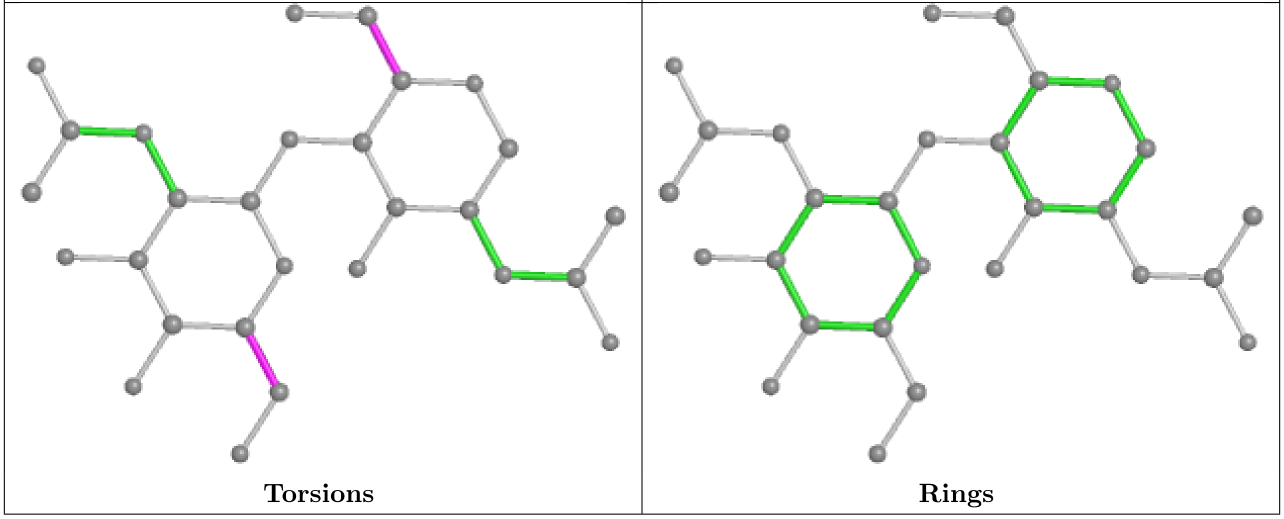
Torsions

Rings

Oligosaccharide Chain e

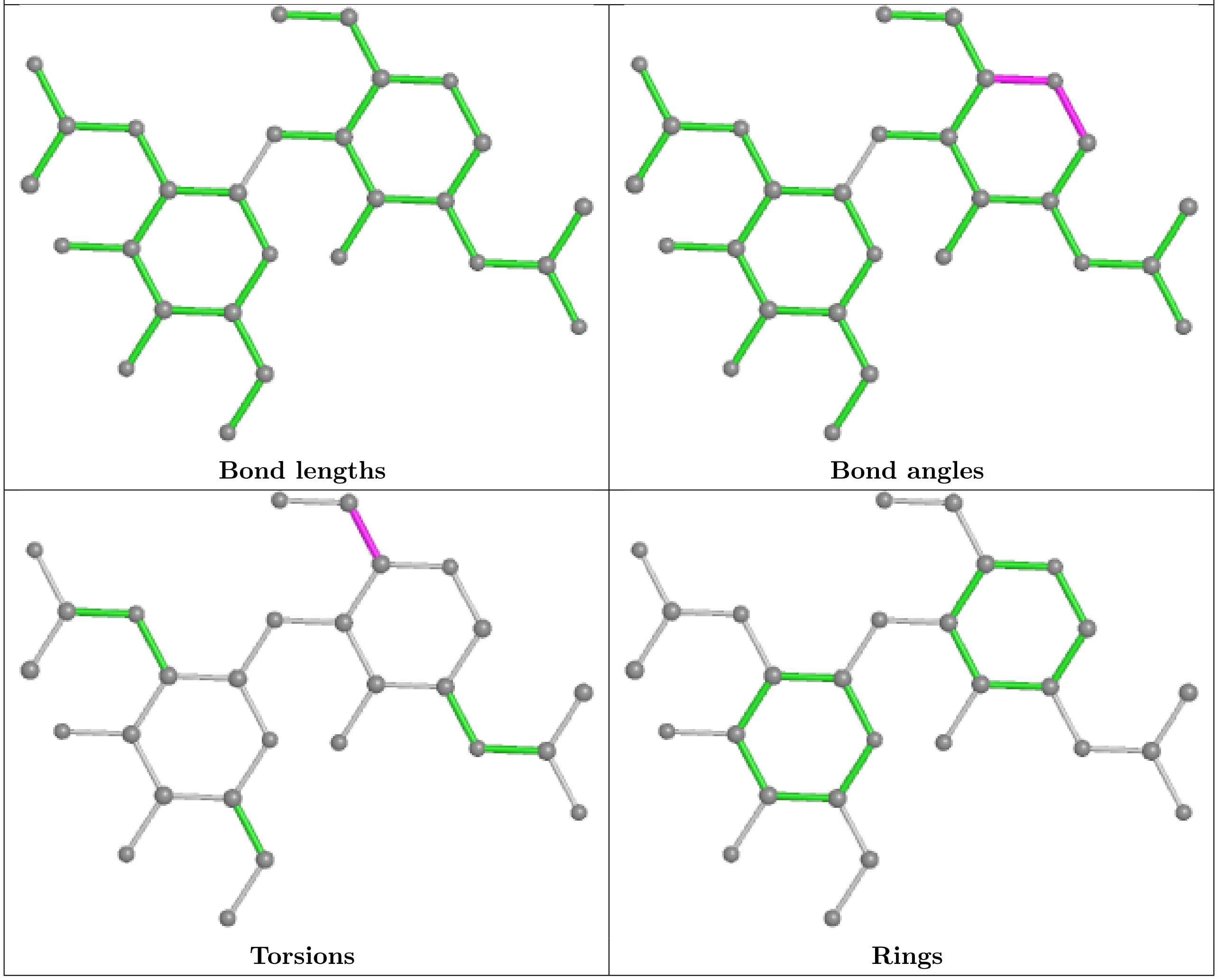


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain h



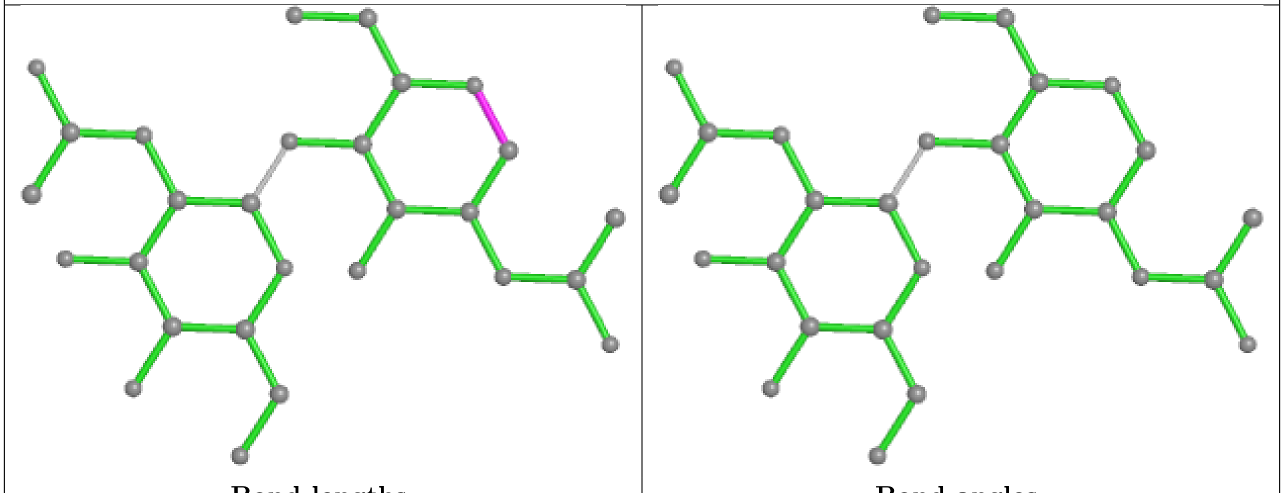
Bond lengths

Bond angles

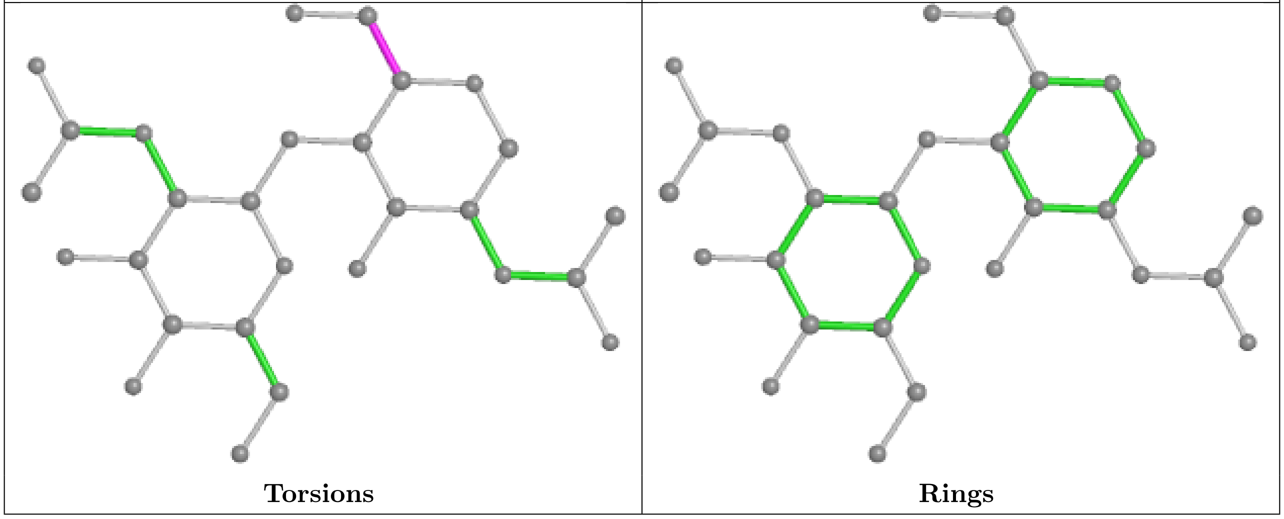
Torsions

Rings

Oligosaccharide Chain i

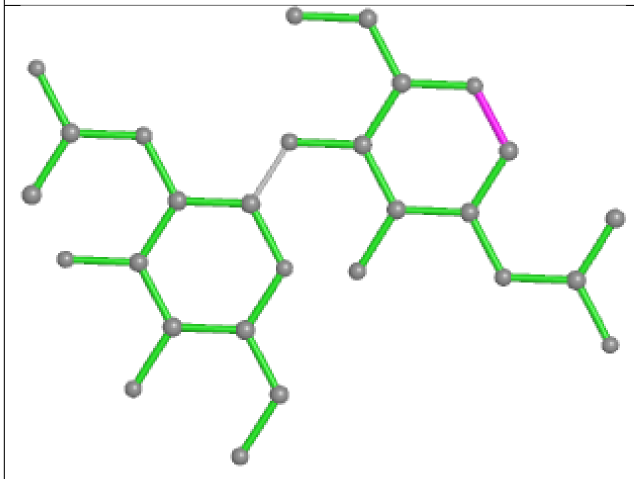


Bond lengths **Bond angles**

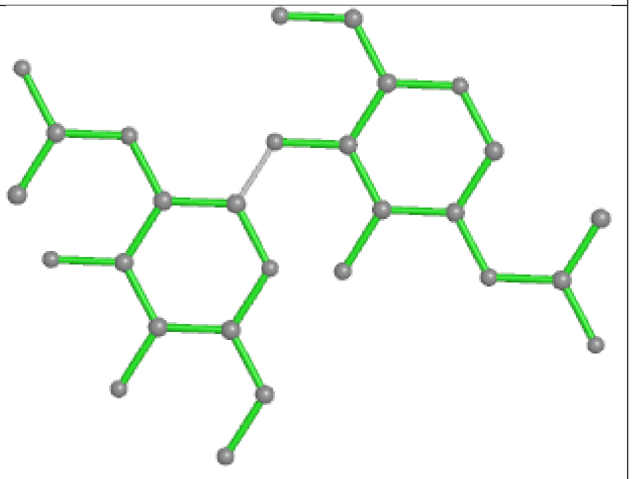


Torsions **Rings**

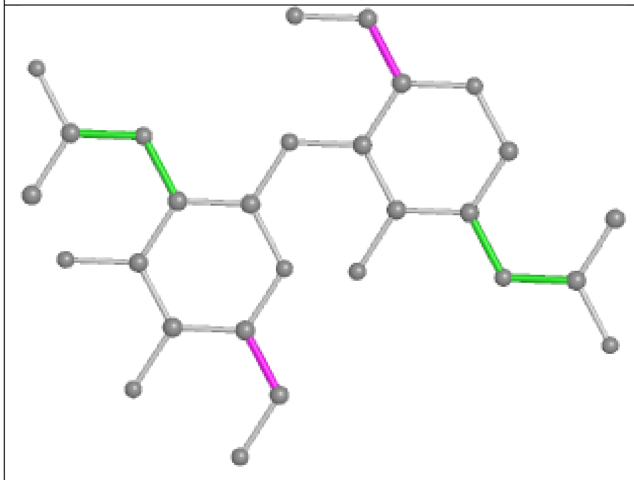
Oligosaccharide Chain o



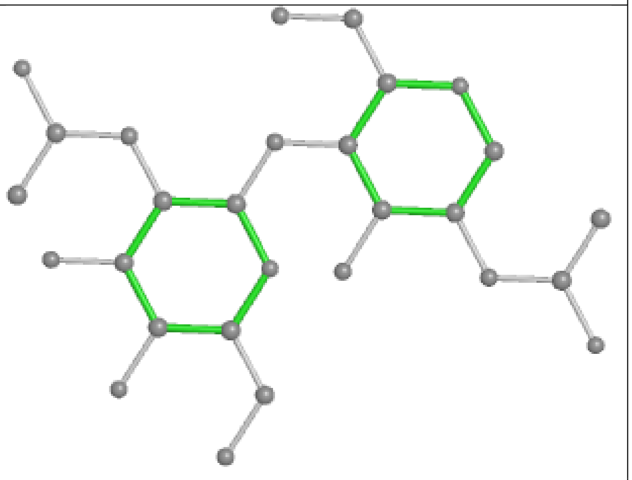
Bond lengths



Bond angles

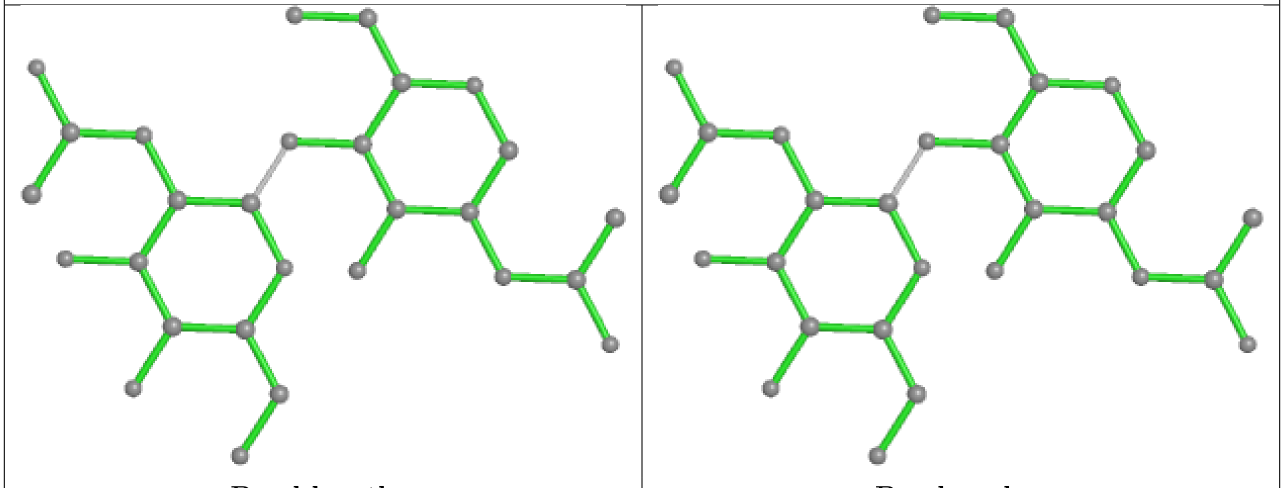


Torsions

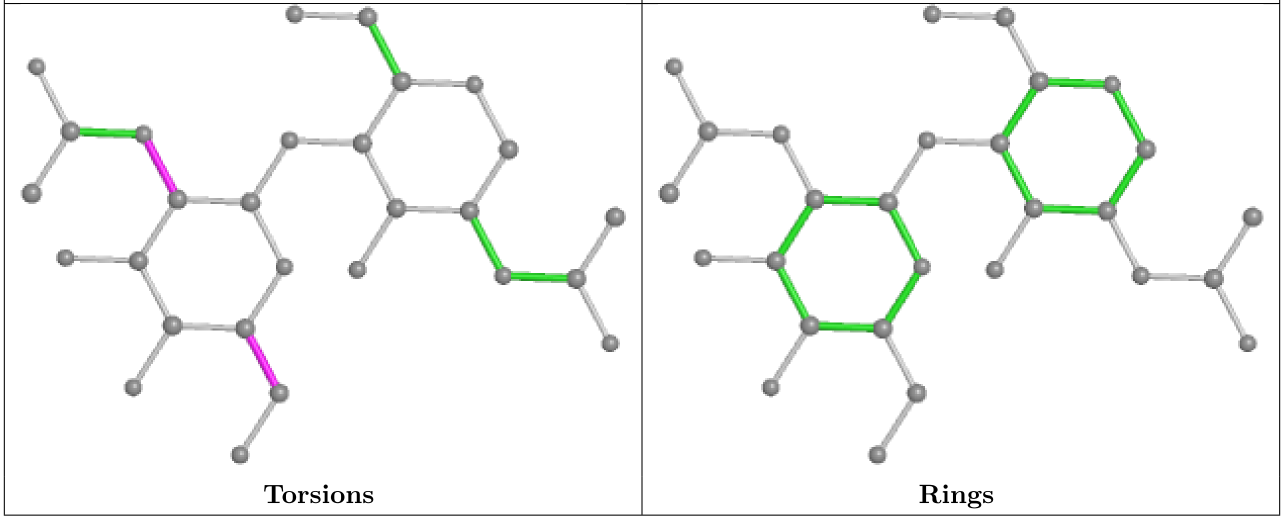


Rings

Oligosaccharide Chain r

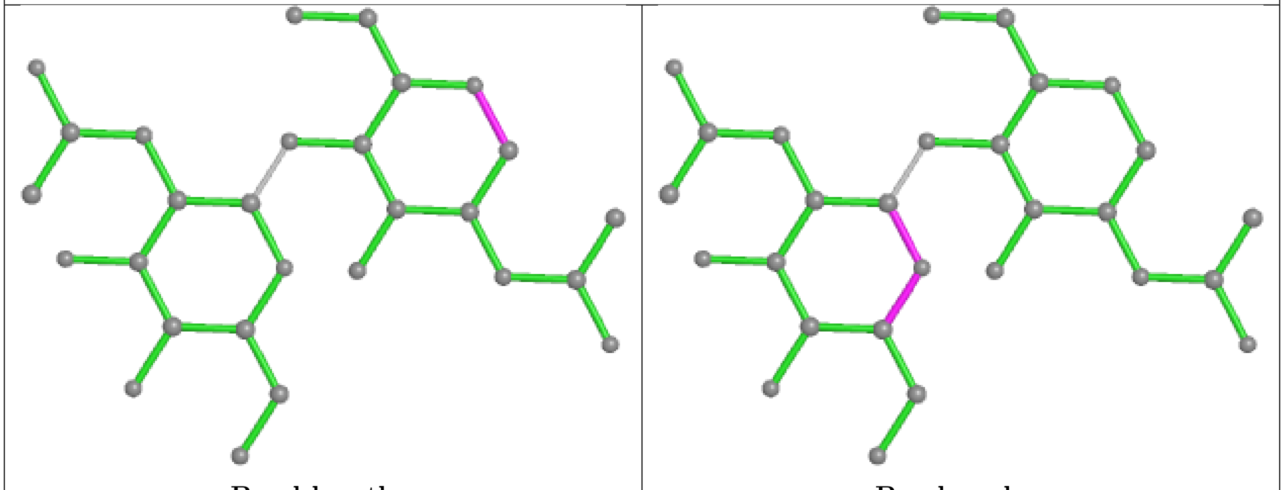


Bond lengths **Bond angles**

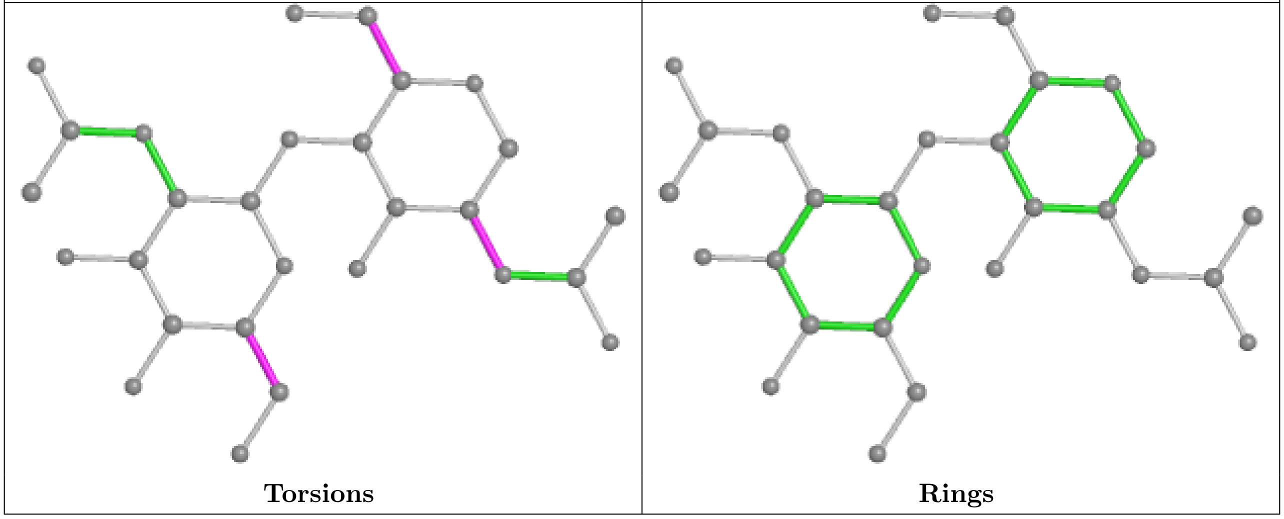


Torsions **Rings**

Oligosaccharide Chain s

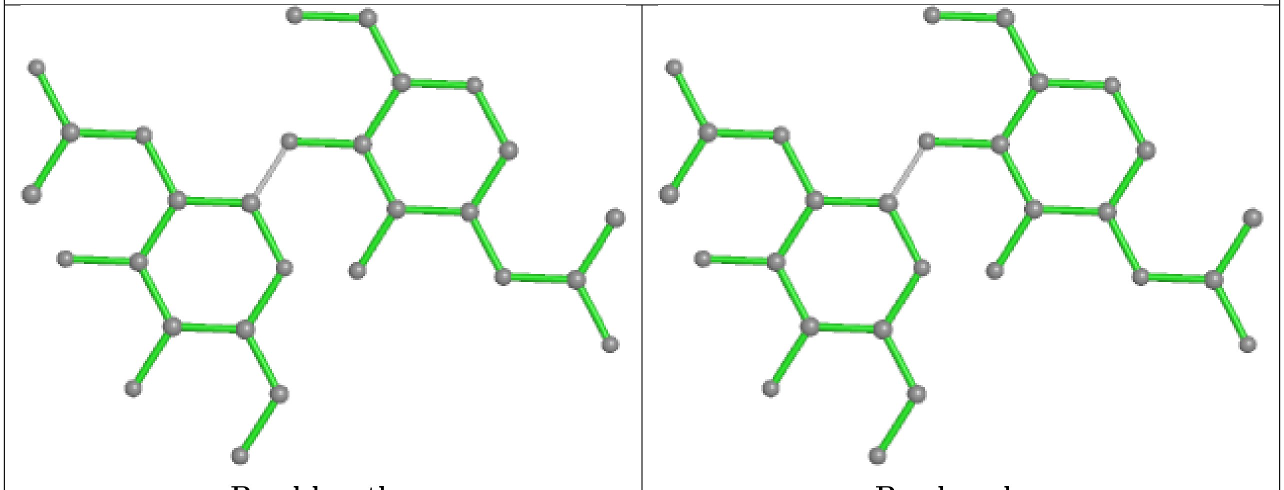


Bond lengths **Bond angles**

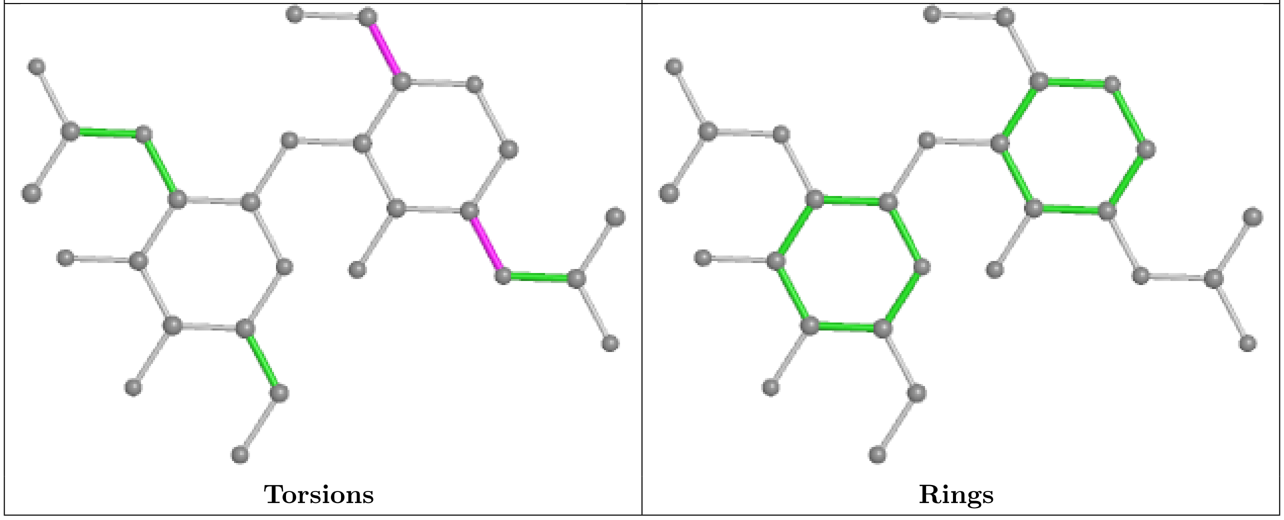


Torsions **Rings**

Oligosaccharide Chain t

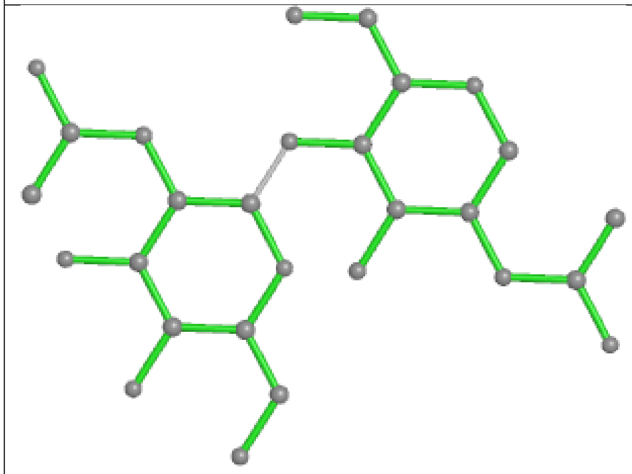


Bond lengths **Bond angles**

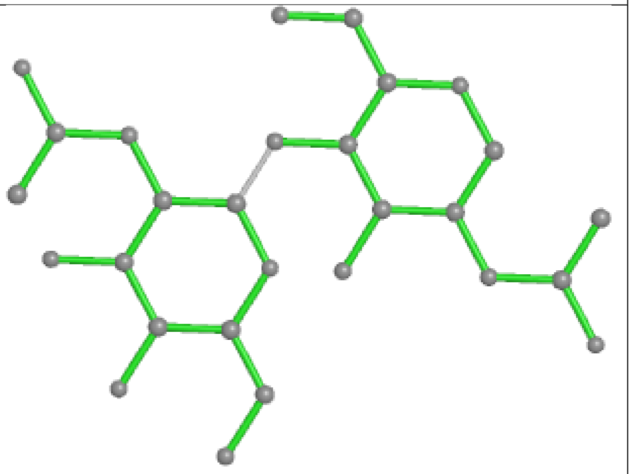


Torsions **Rings**

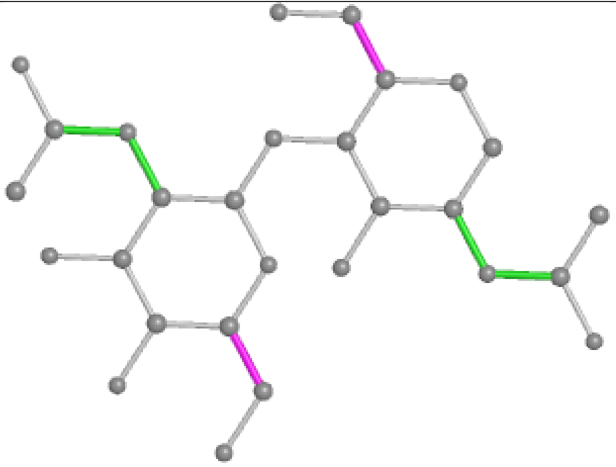
Oligosaccharide Chain v



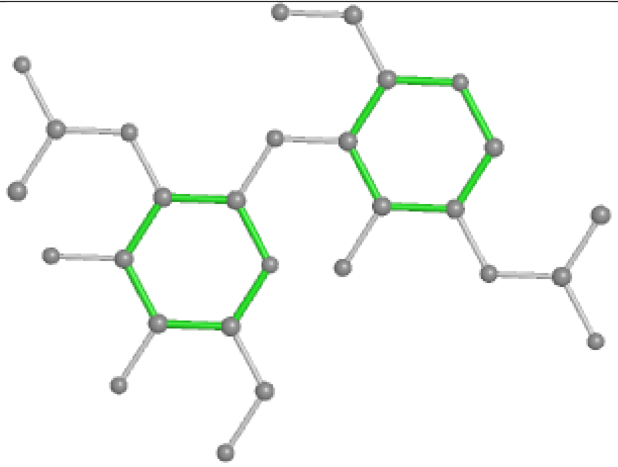
Bond lengths



Bond angles

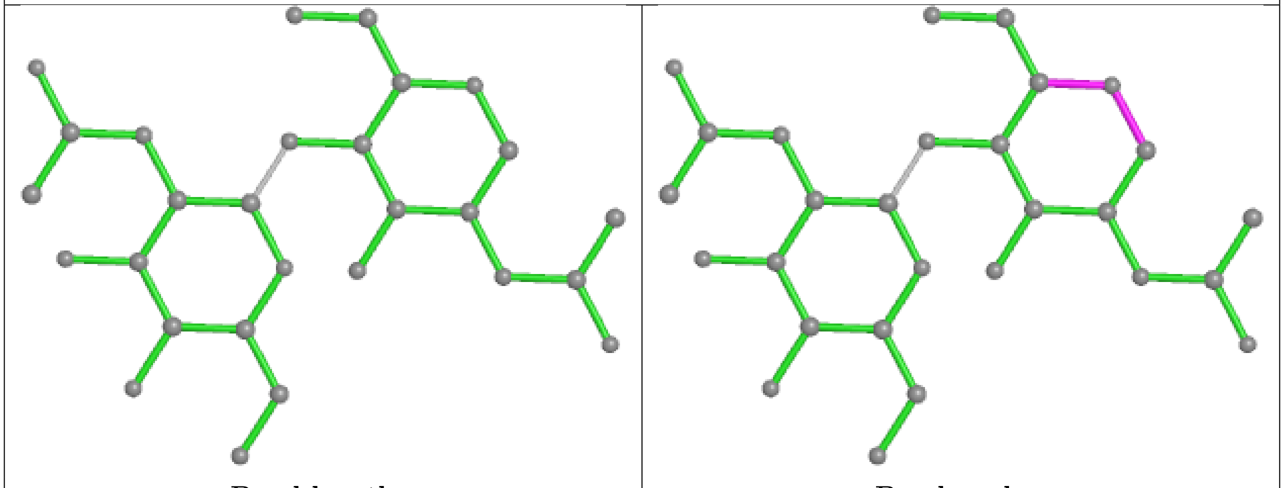


Torsions



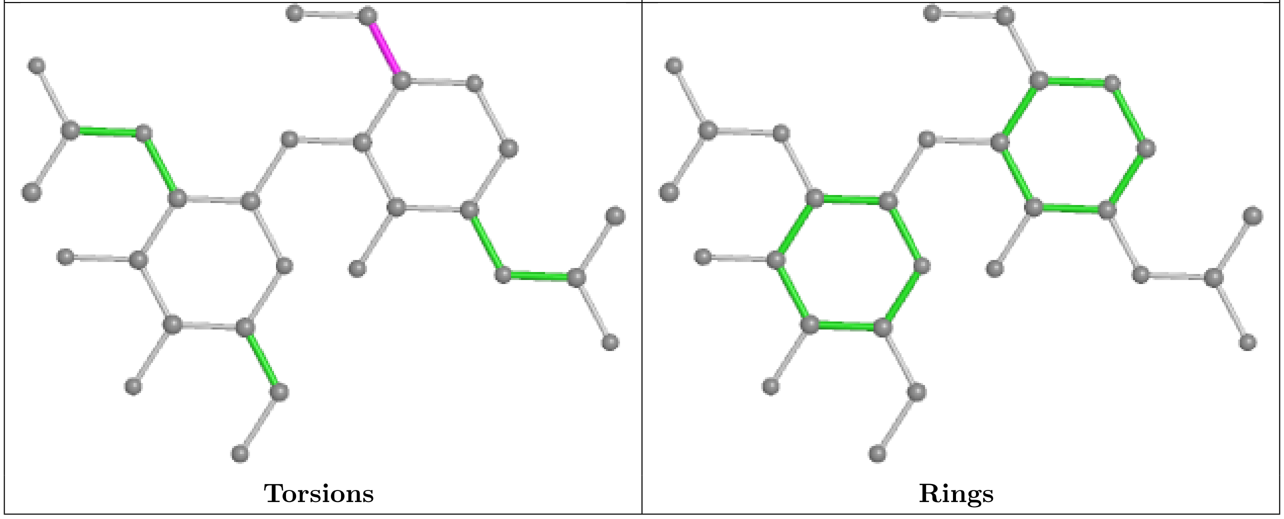
Rings

Oligosaccharide Chain y



Bond lengths

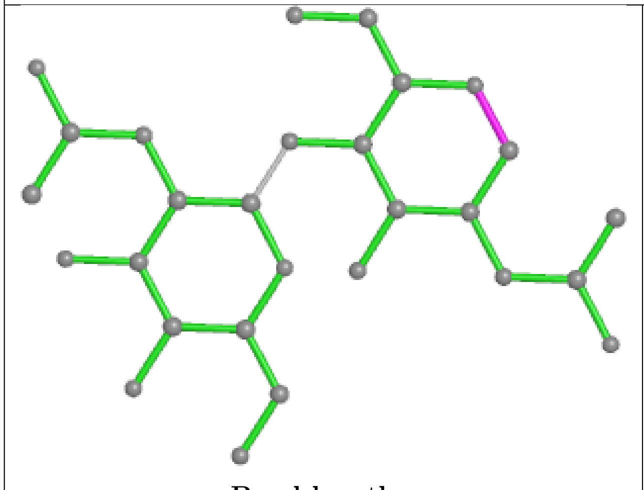
Bond angles



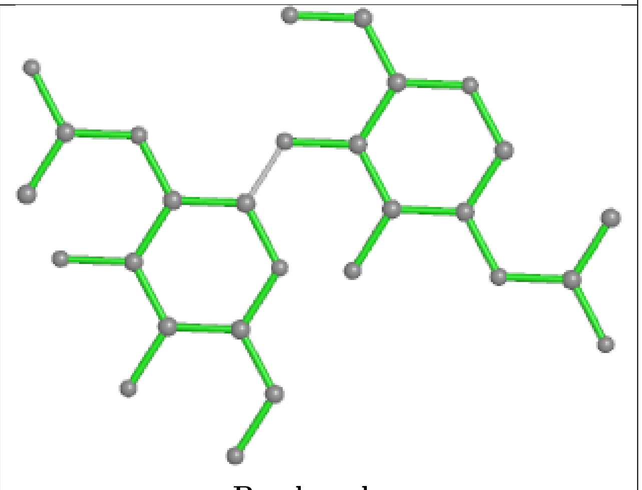
Torsions

Rings

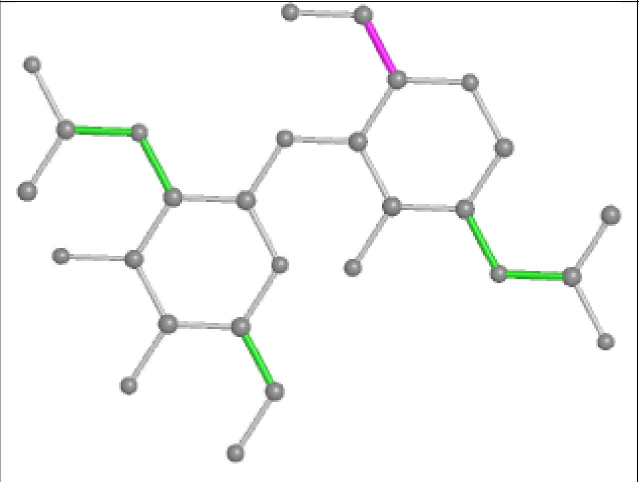
Oligosaccharide Chain z



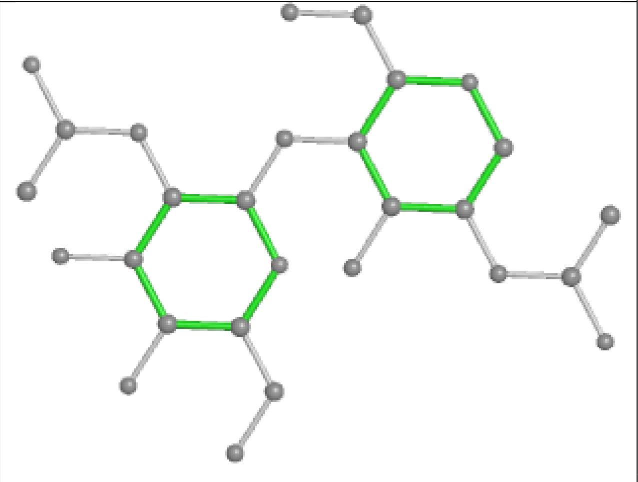
Bond lengths



Bond angles

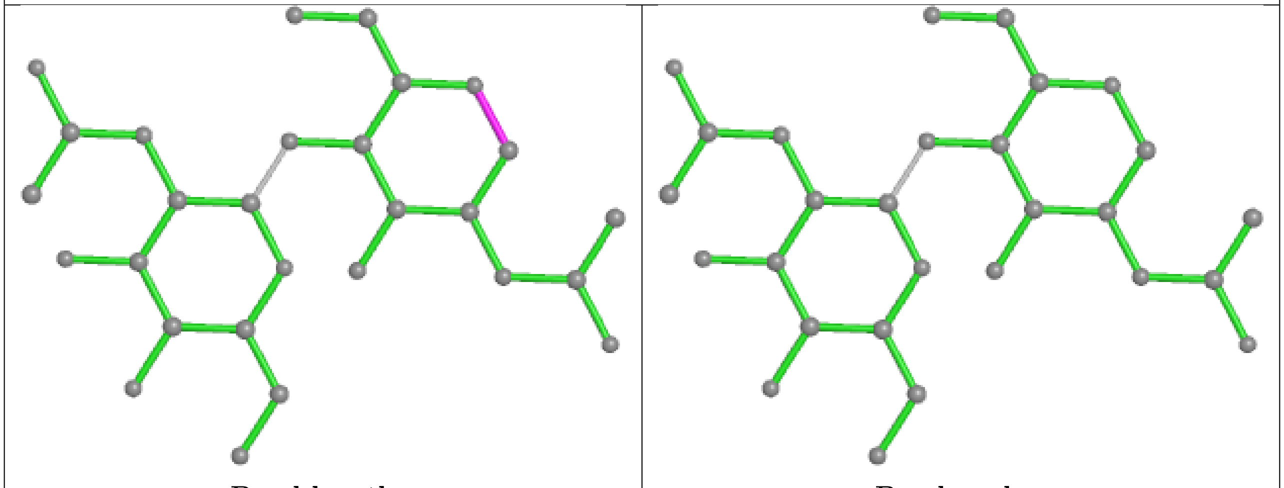


Torsions

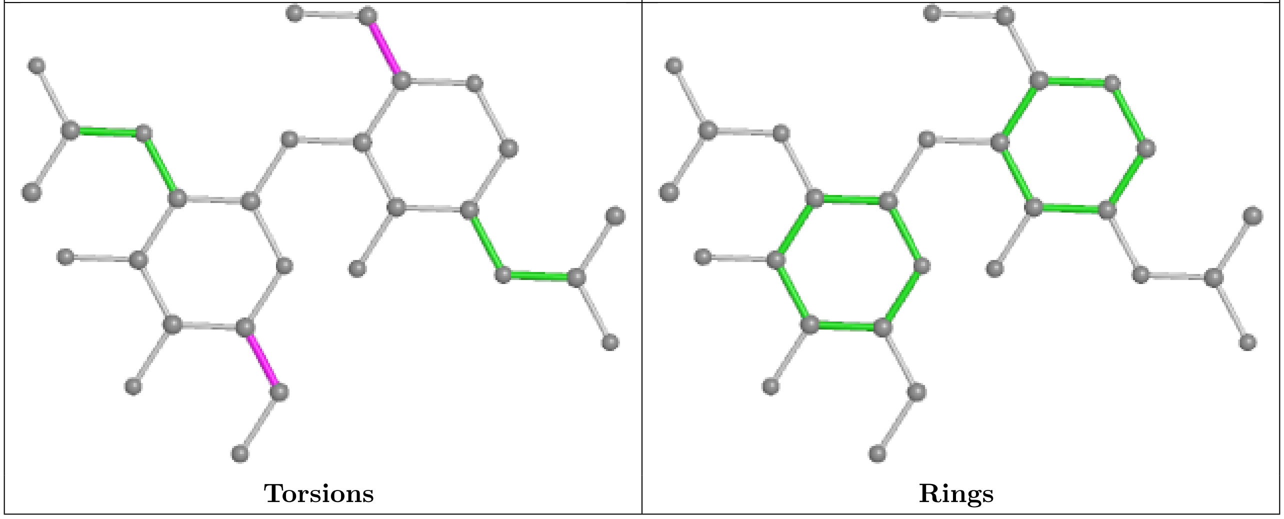


Rings

Oligosaccharide Chain 5

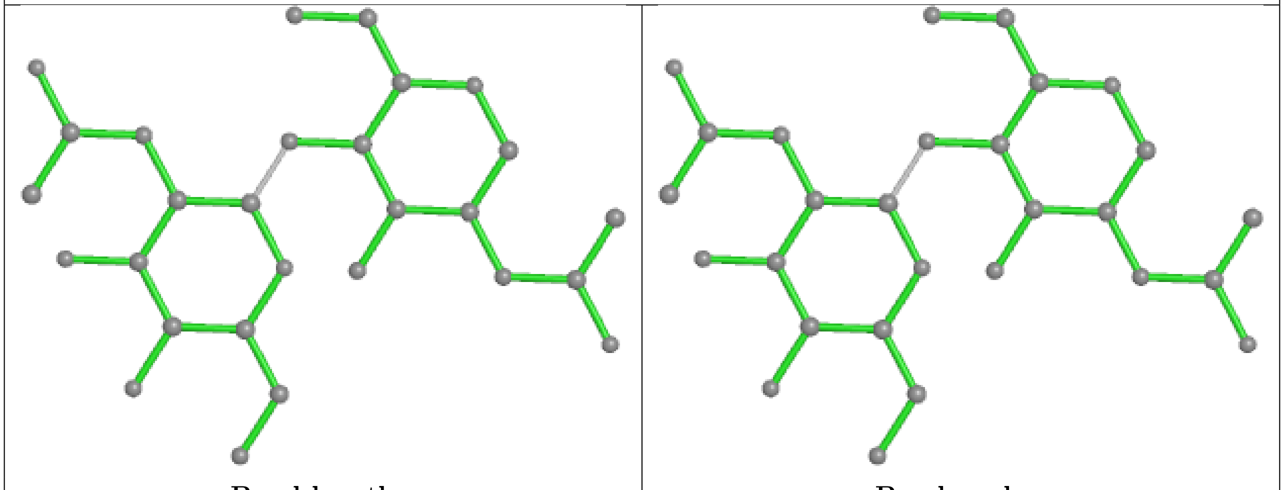


Bond lengths **Bond angles**

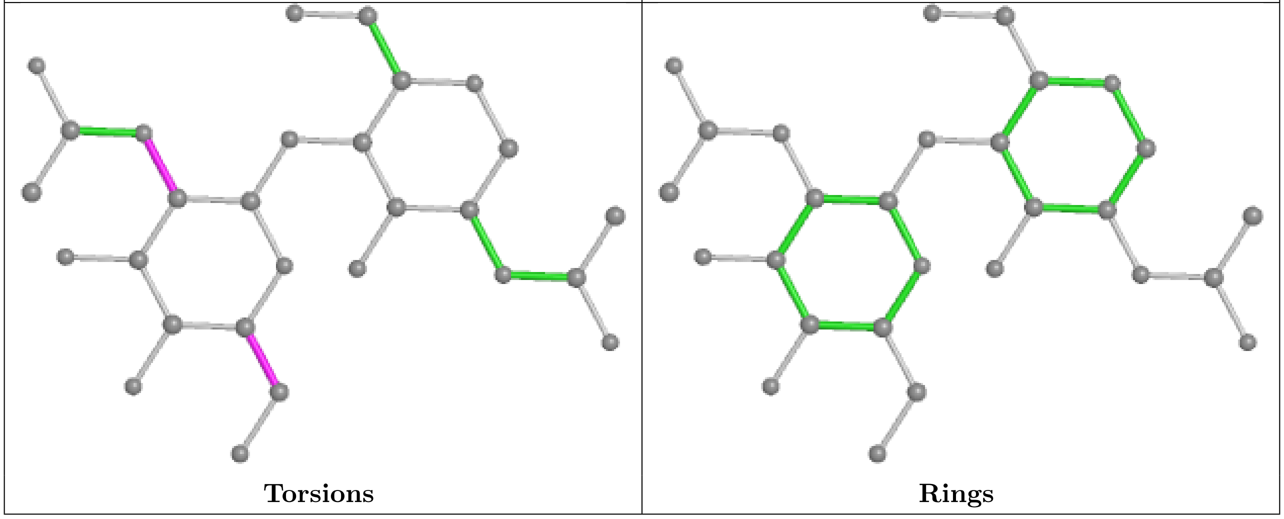


Torsions **Rings**

Oligosaccharide Chain 8

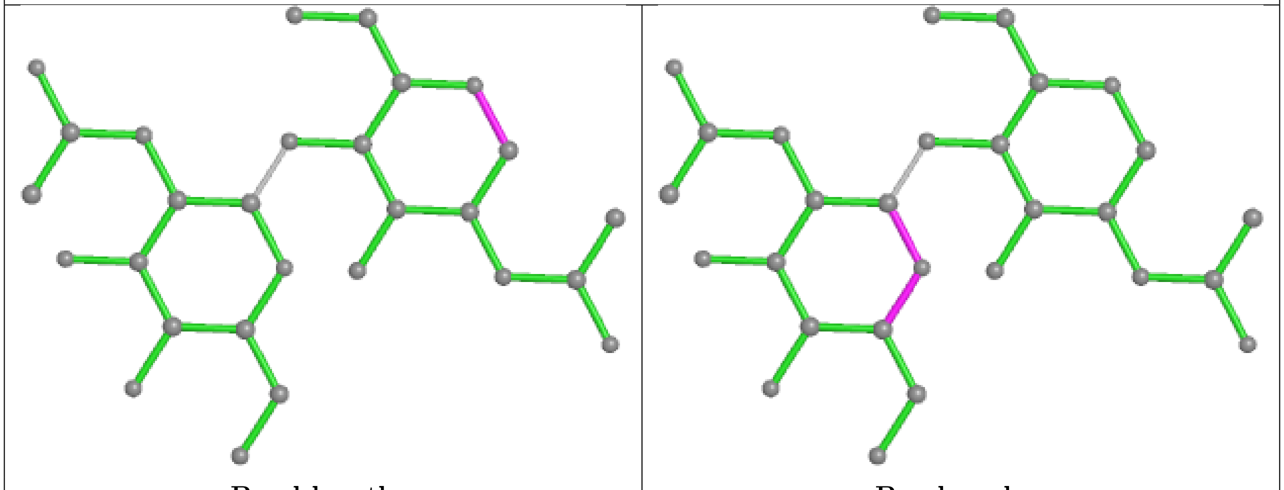


Bond lengths **Bond angles**



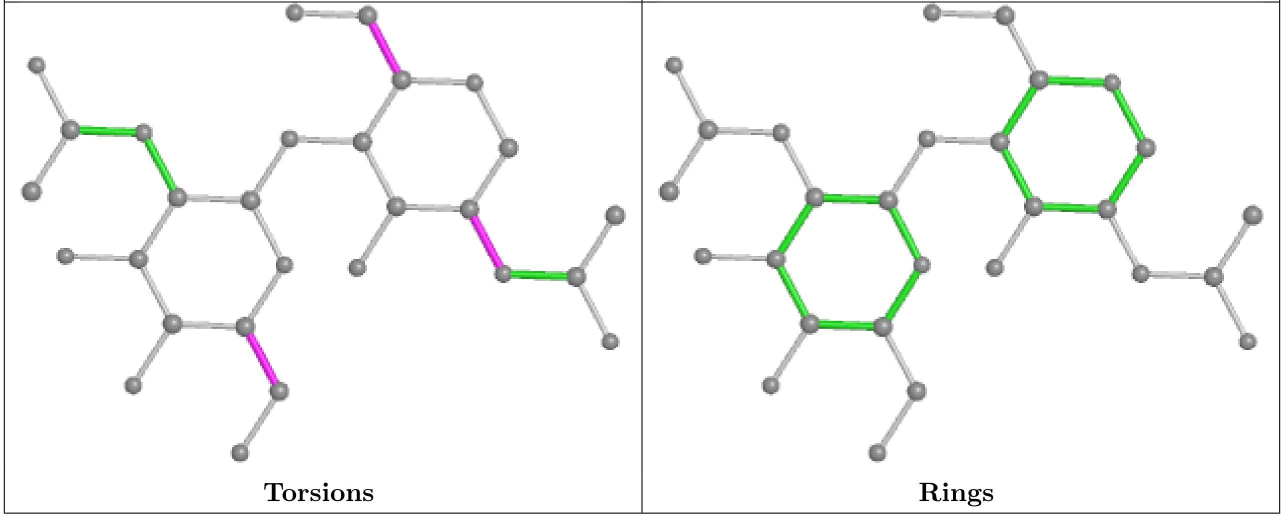
Torsions **Rings**

Oligosaccharide Chain 9



Bond lengths

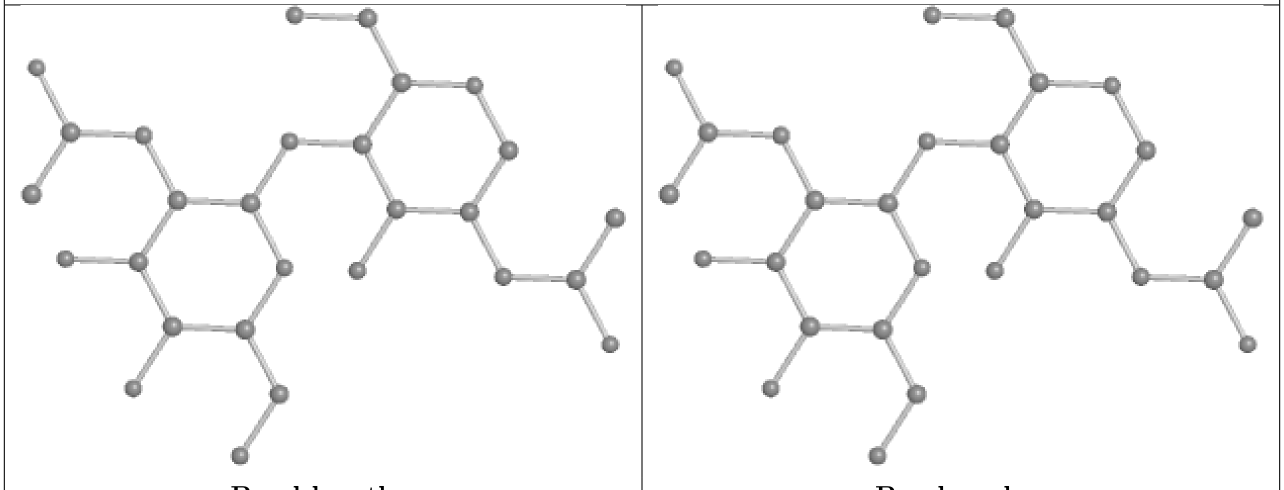
Bond angles



Torsions

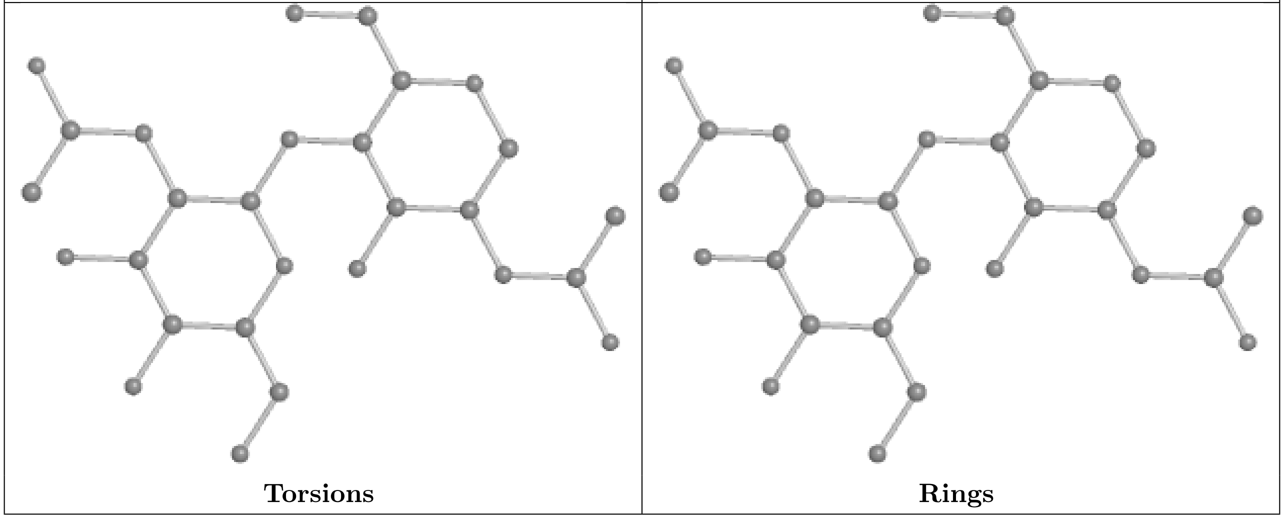
Rings

Oligosaccharide Chain AA



Bond lengths

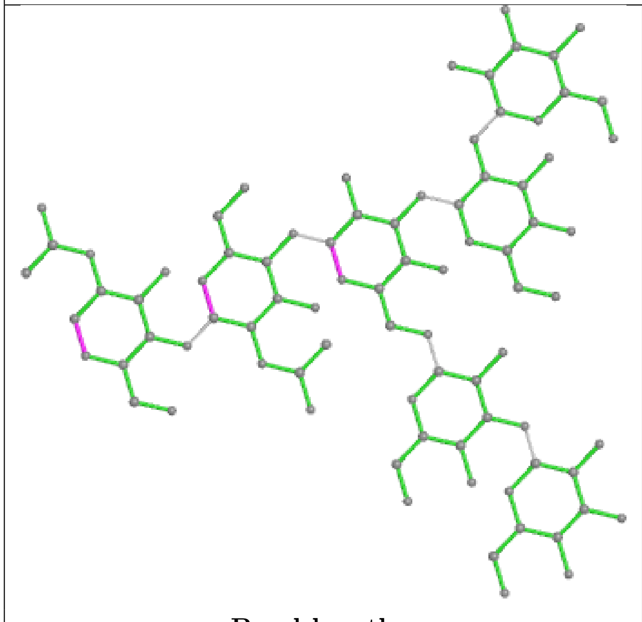
Bond angles



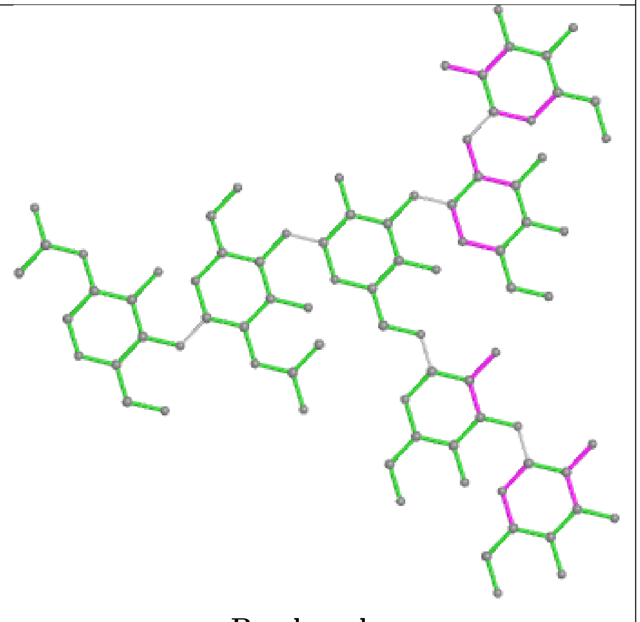
Torsions

Rings

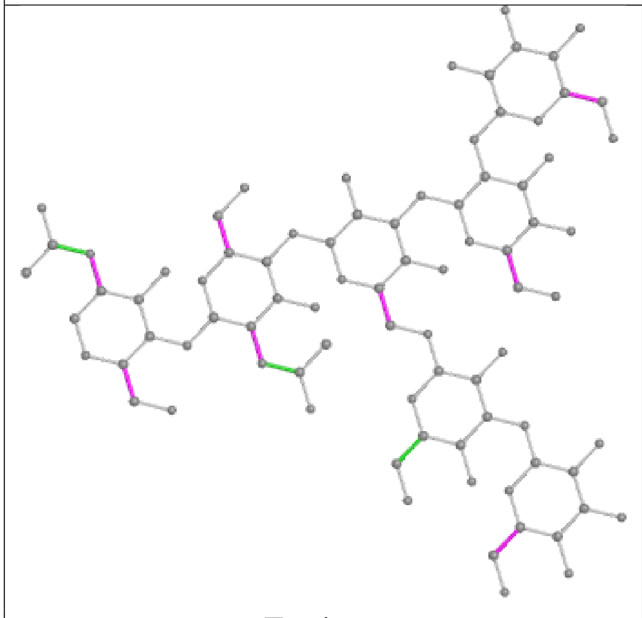
Oligosaccharide Chain S



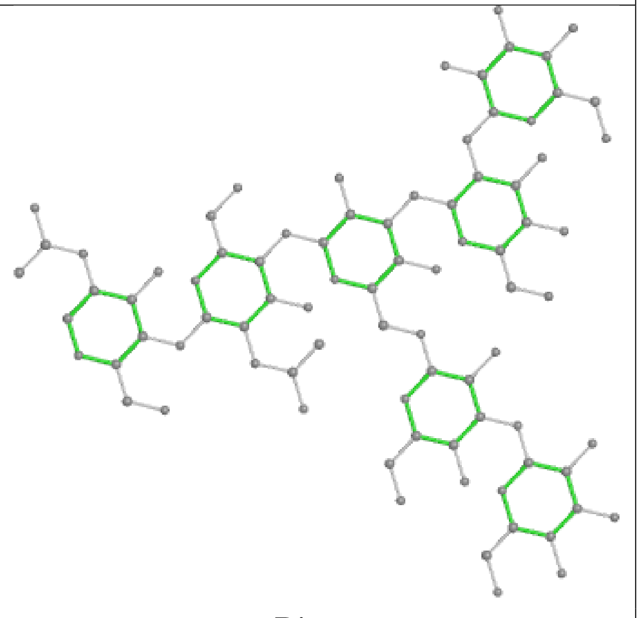
Bond lengths



Bond angles

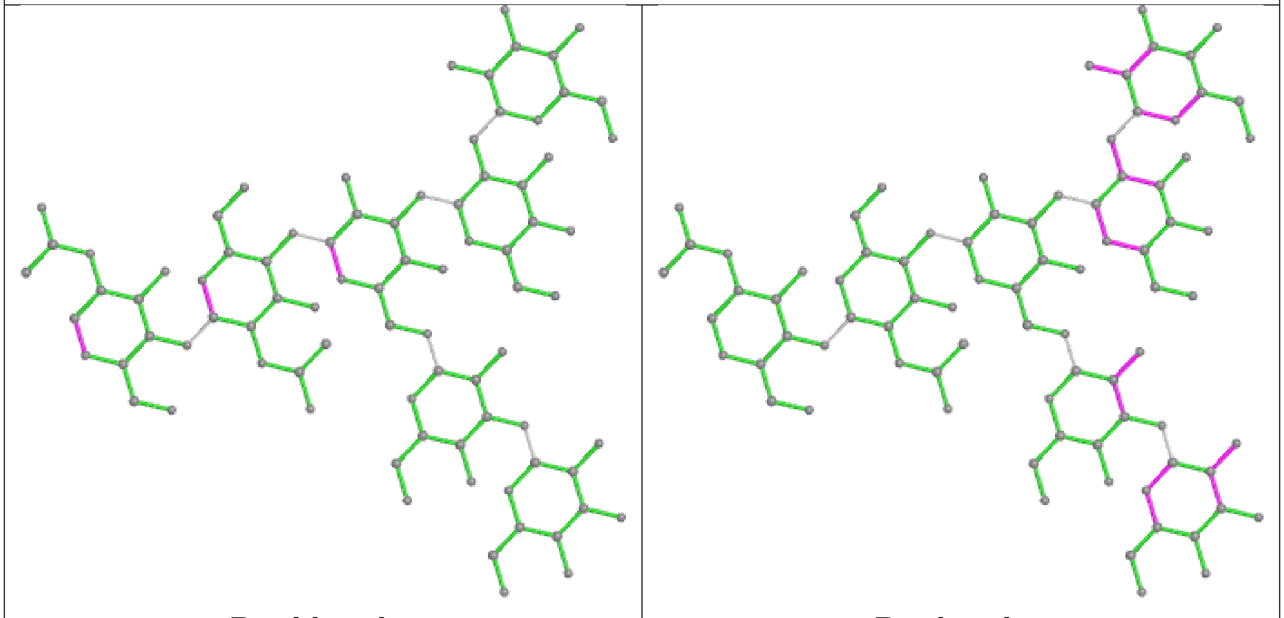


Torsions

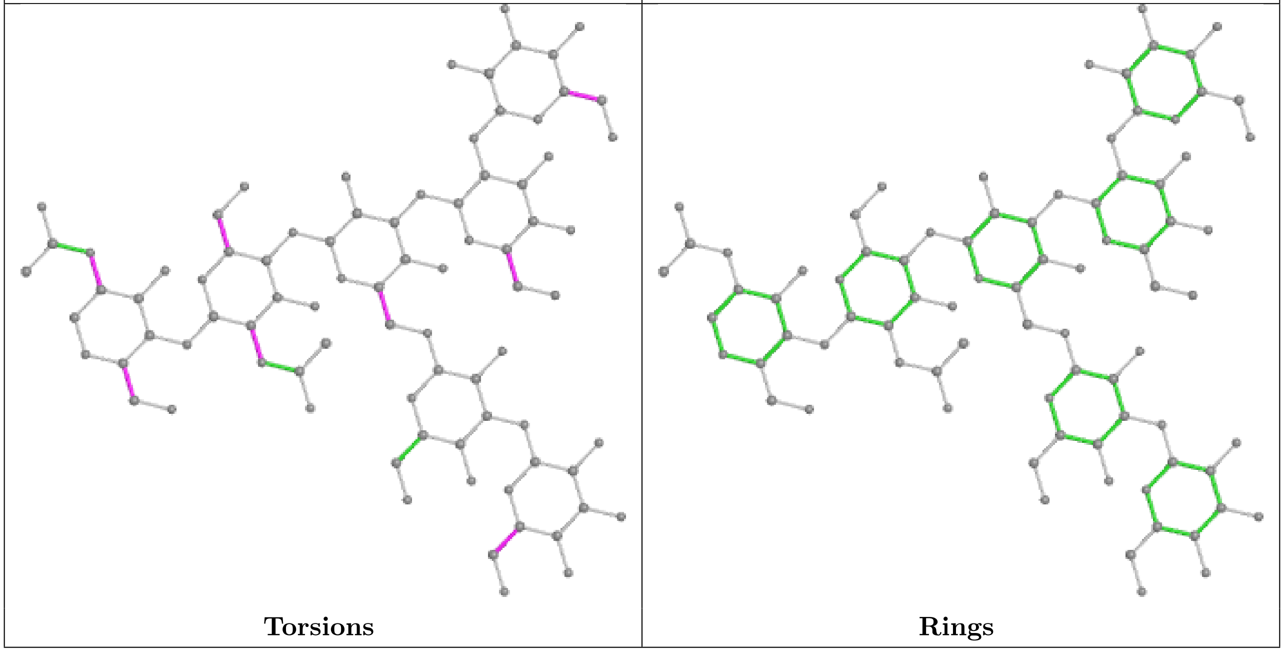


Rings

Oligosaccharide Chain j

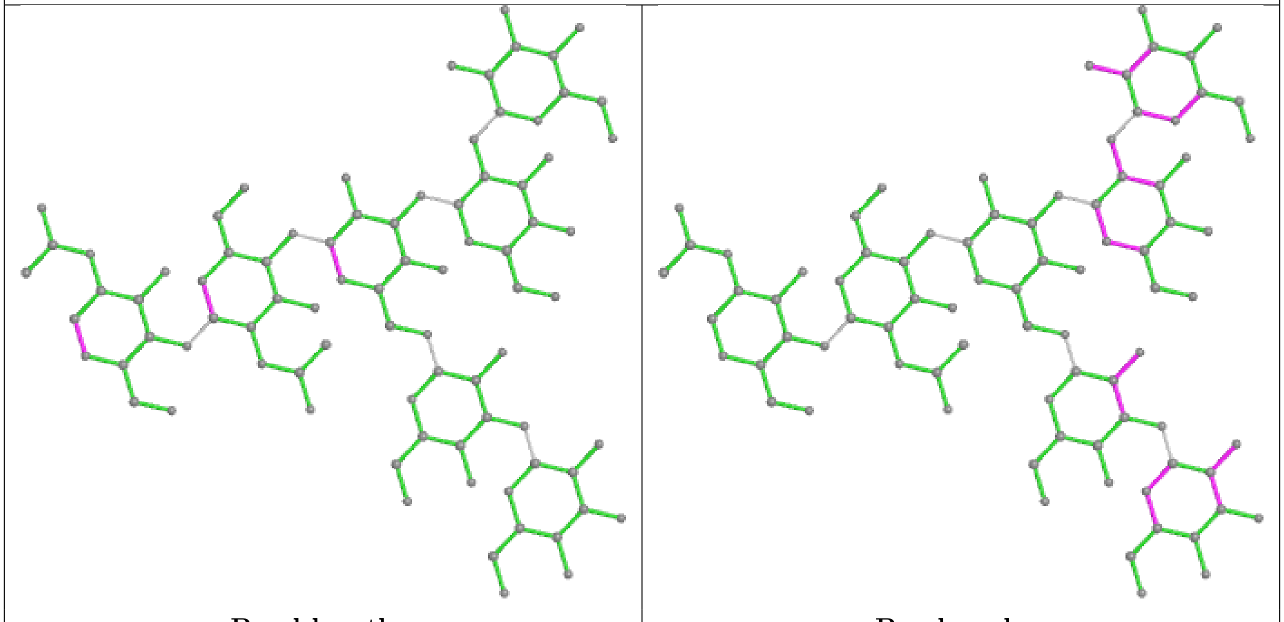


Bond lengths **Bond angles**



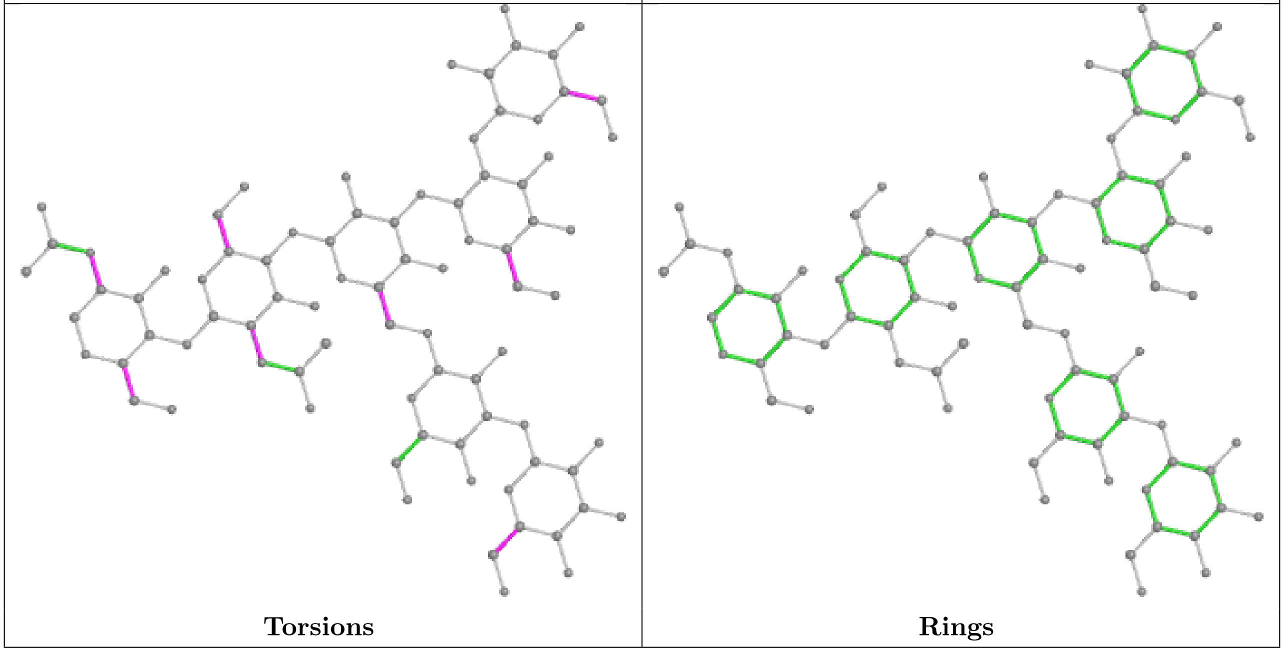
Torsions **Rings**

Oligosaccharide Chain 0



Bond lengths

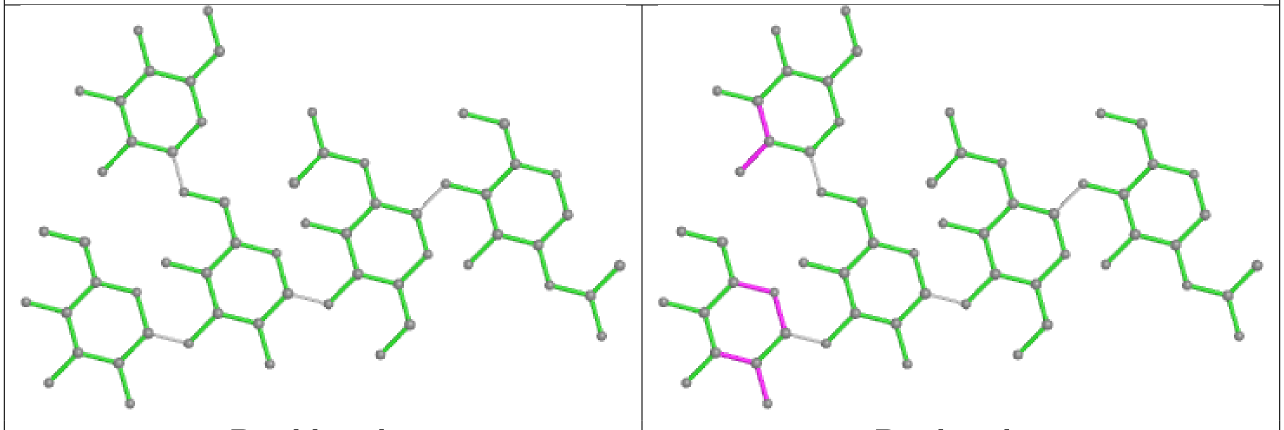
Bond angles



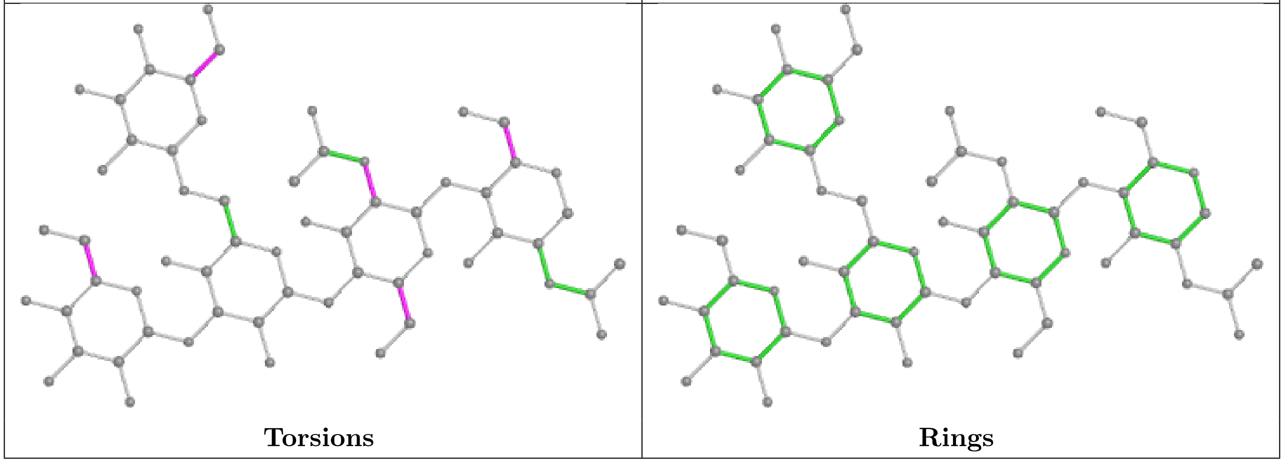
Torsions

Rings

Oligosaccharide Chain U

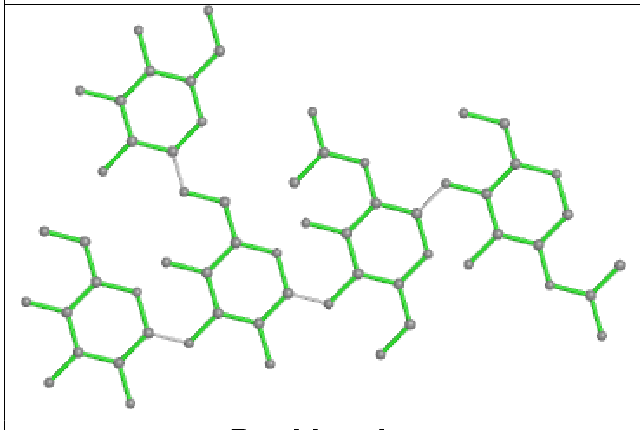


Bond lengths Bond angles

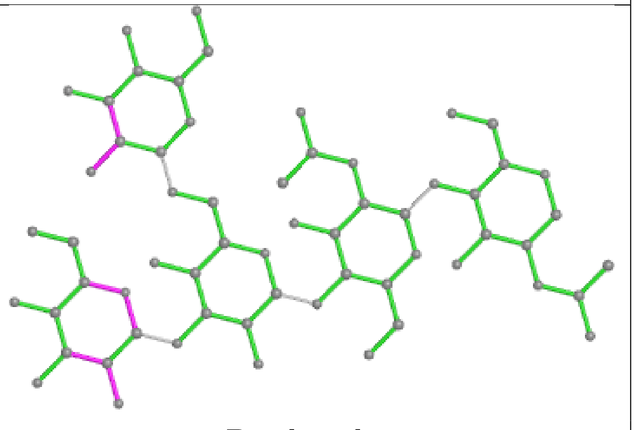


Torsions Rings

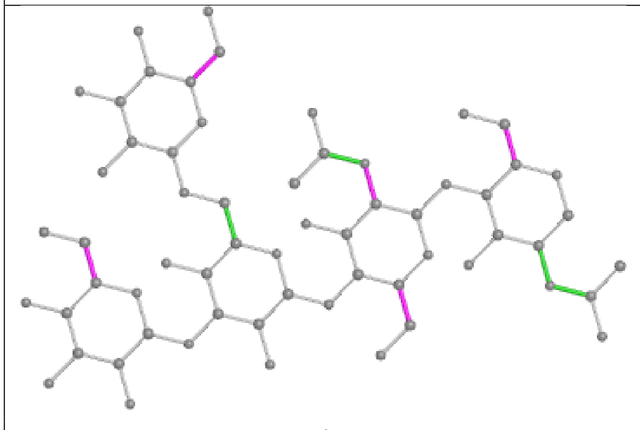
Oligosaccharide Chain l



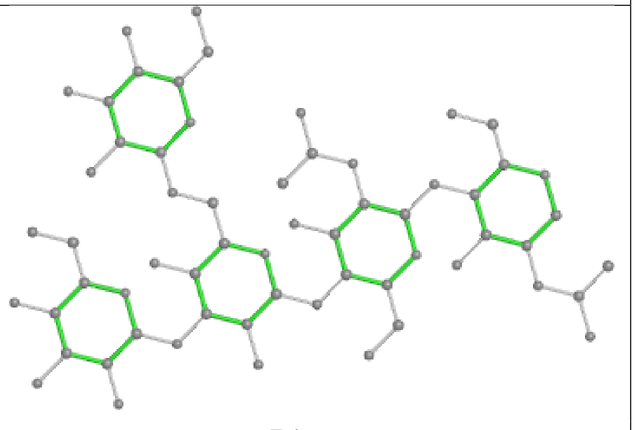
Bond lengths



Bond angles

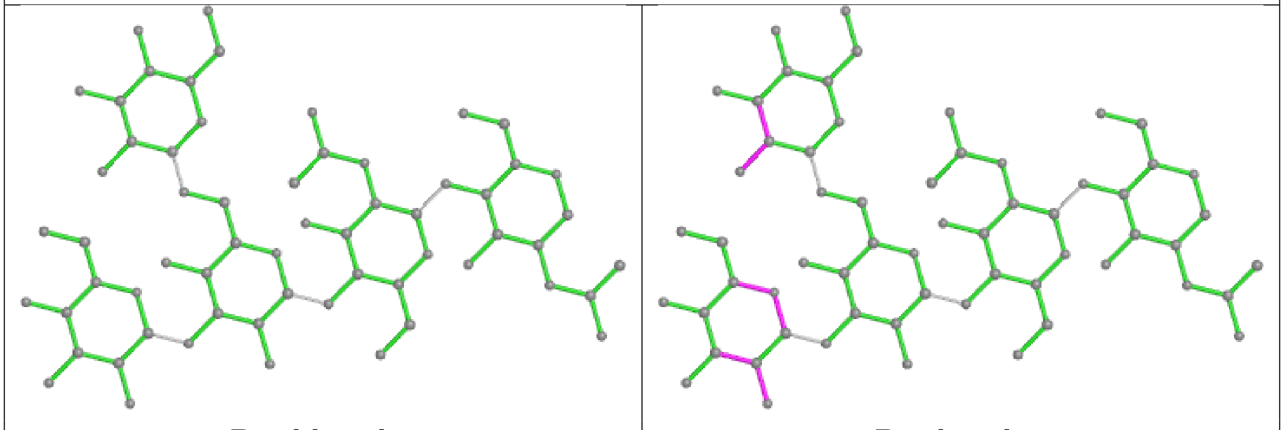


Torsions

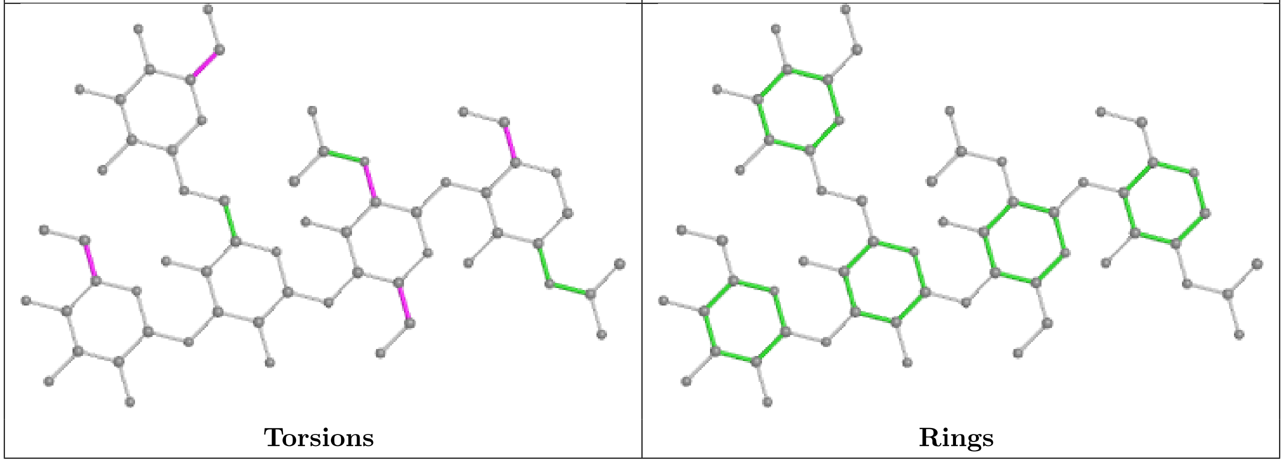


Rings

Oligosaccharide Chain 2

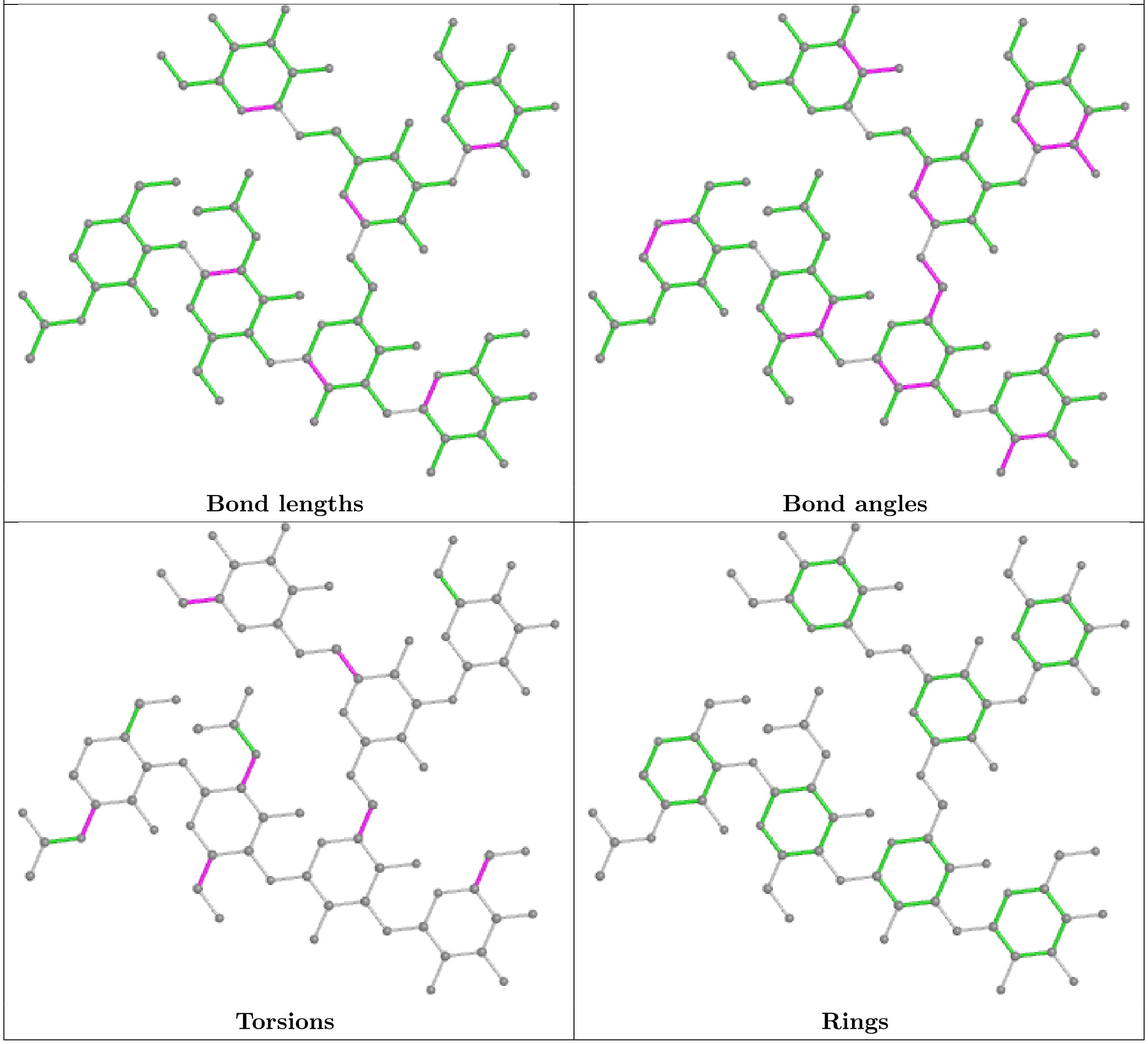


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain V



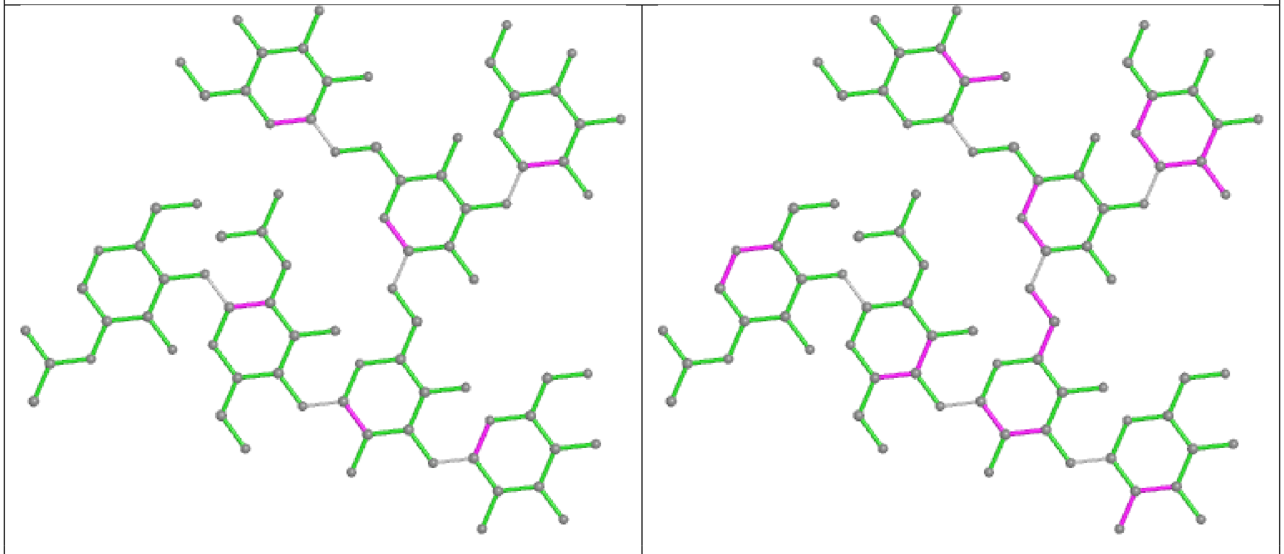
Bond lengths

Bond angles

Torsions

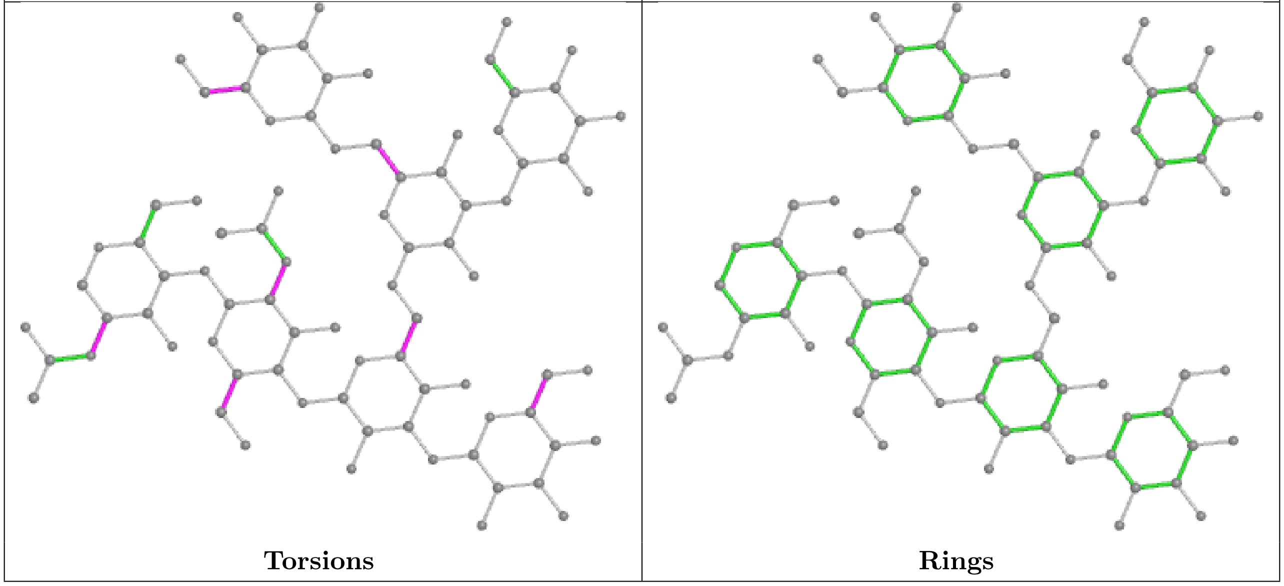
Rings

Oligosaccharide Chain m



Bond lengths

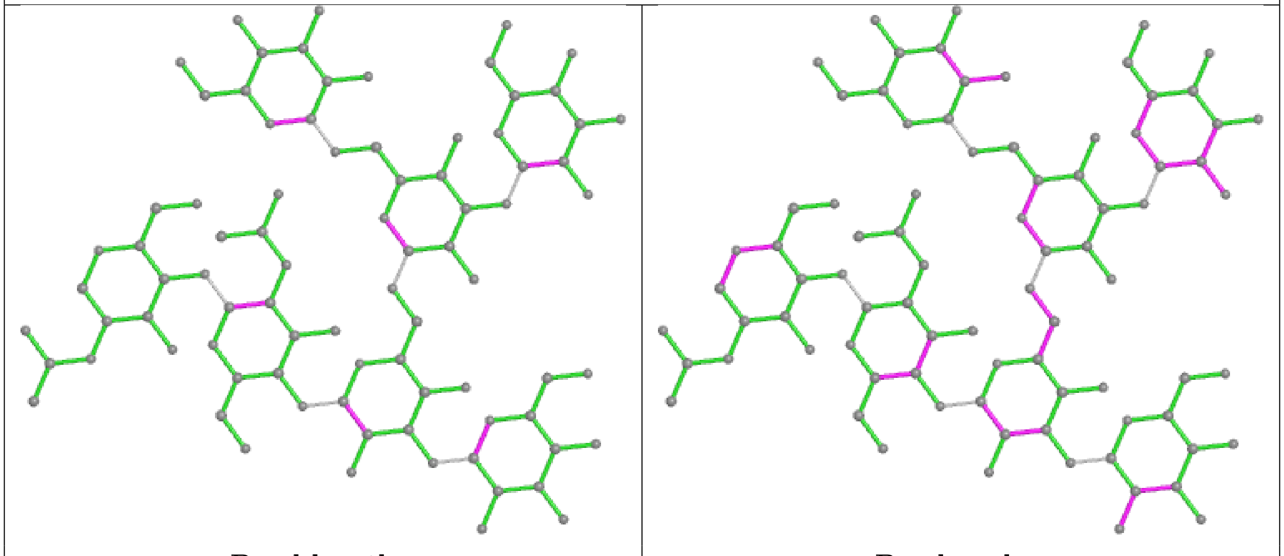
Bond angles



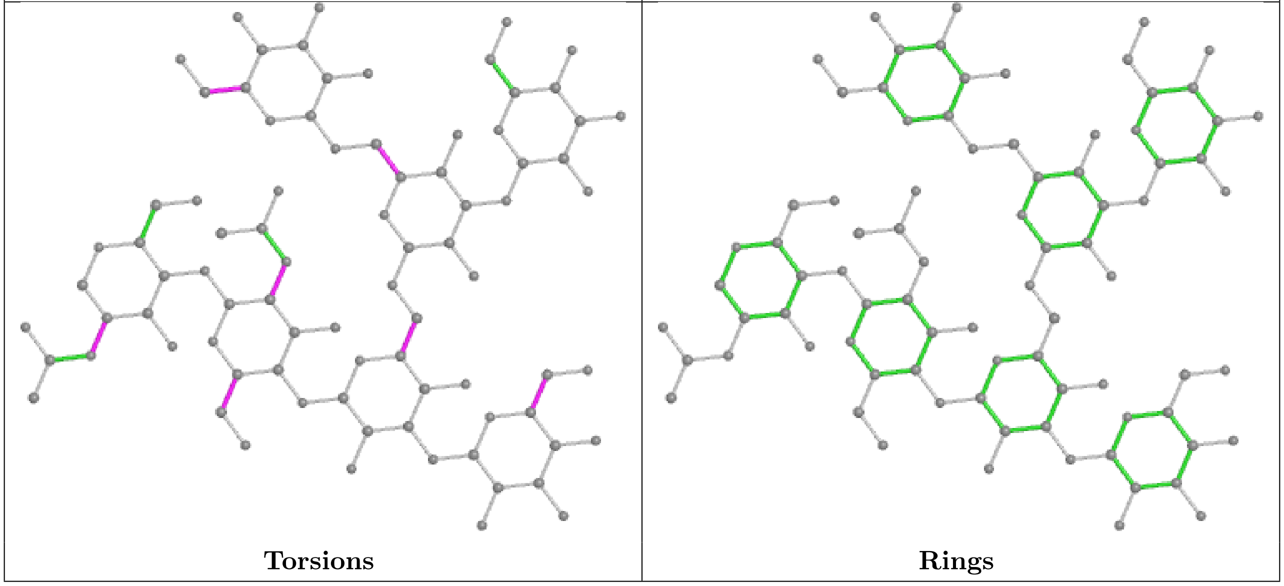
Torsions

Rings

Oligosaccharide Chain 3

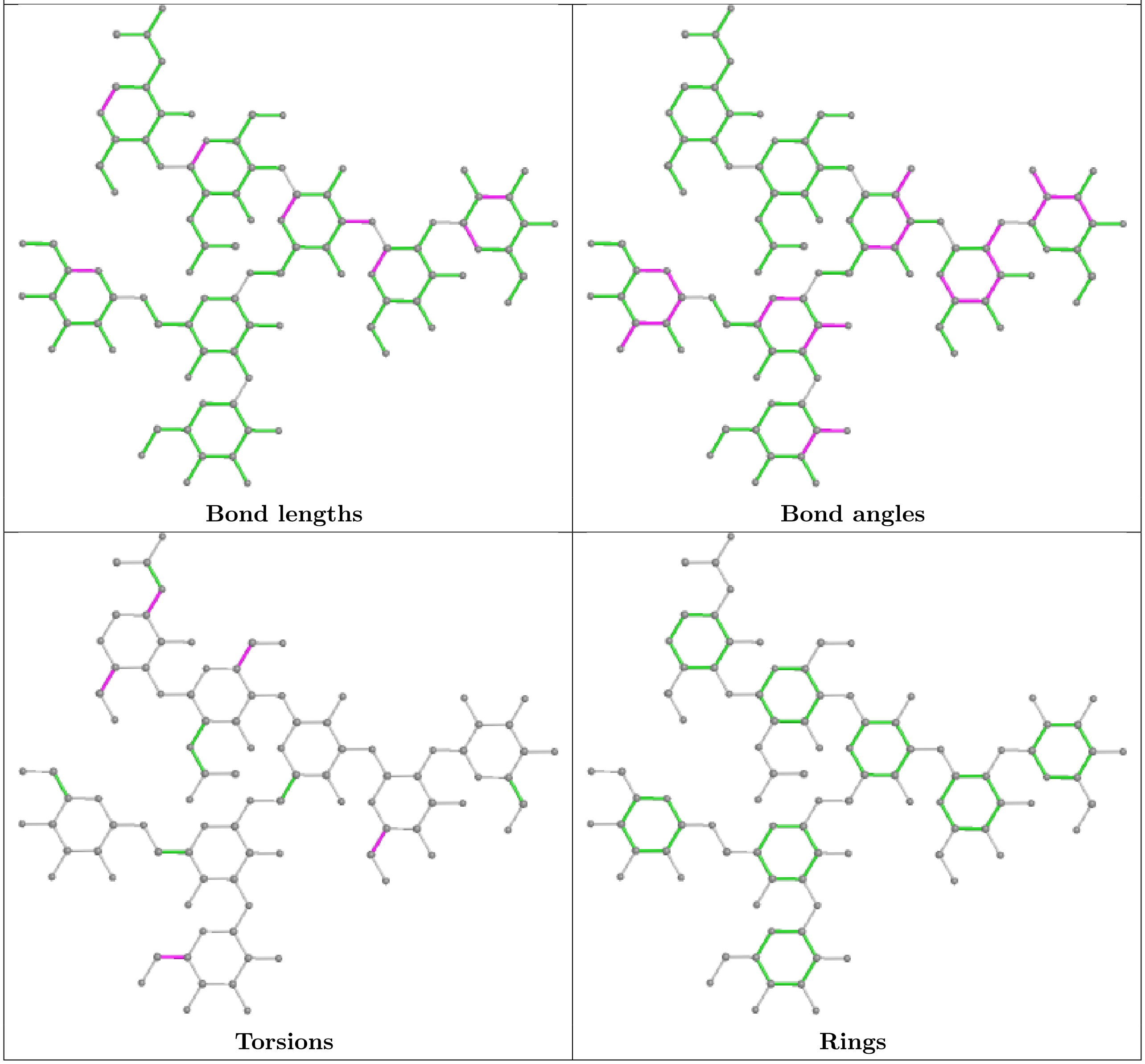


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain W



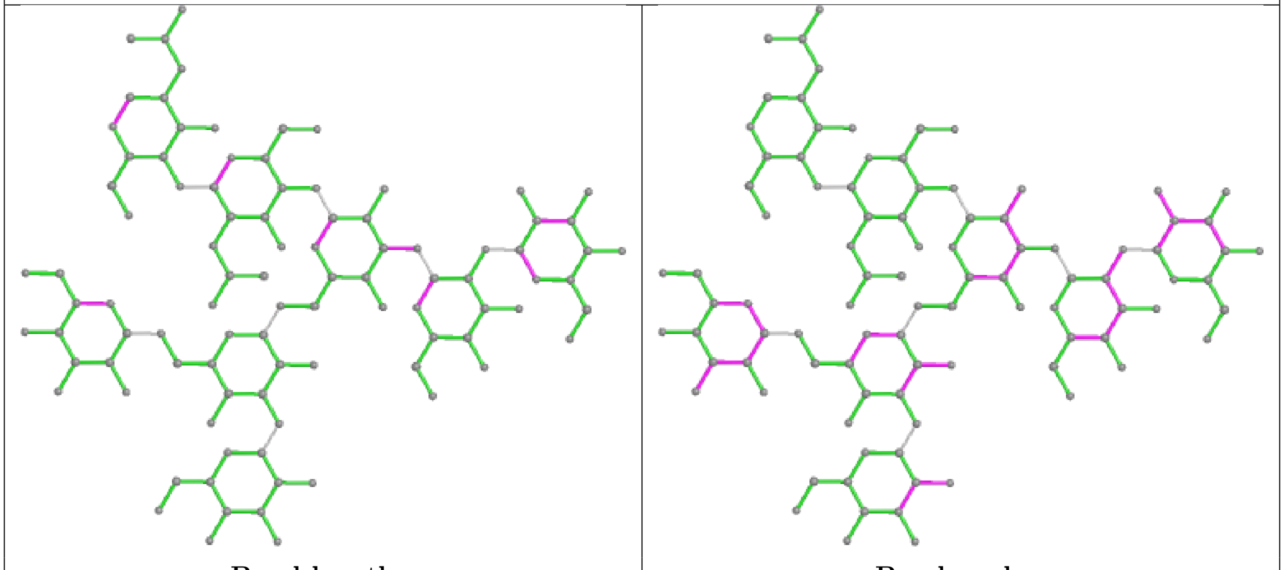
Bond lengths

Bond angles

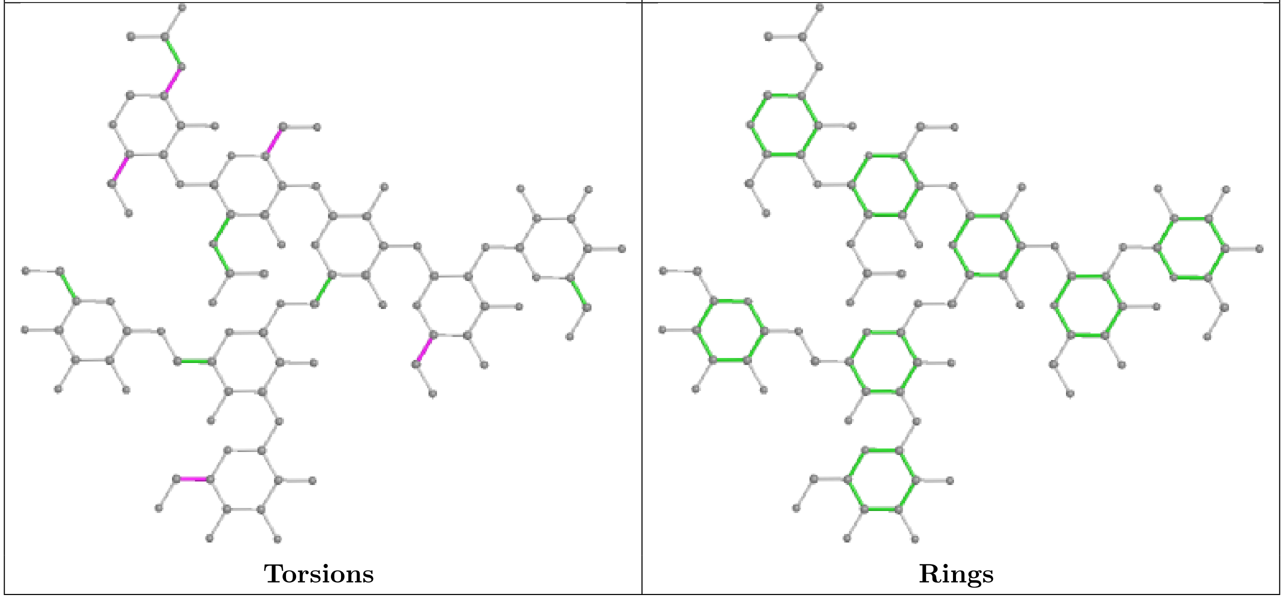
Torsions

Rings

Oligosaccharide Chain n

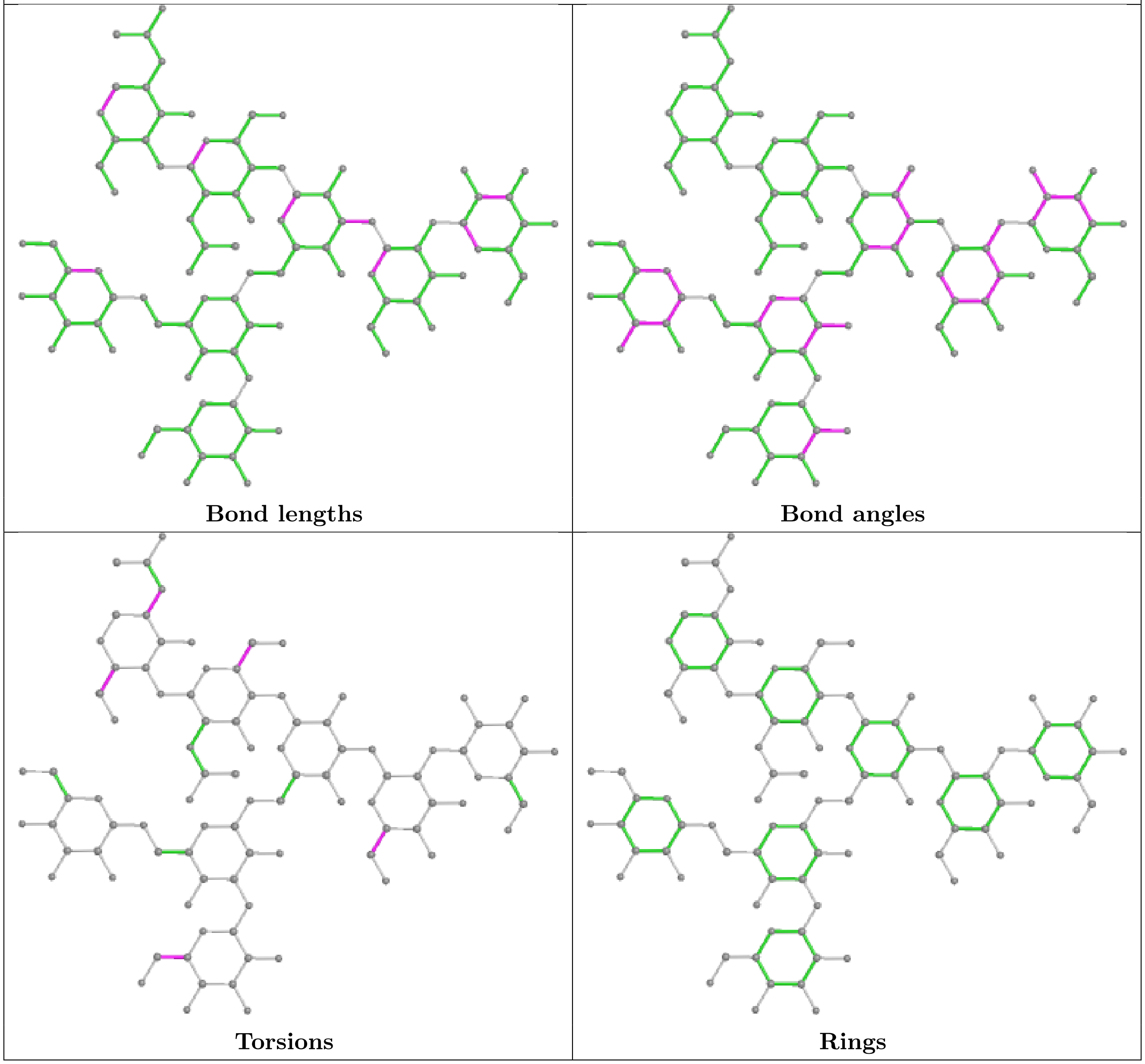


Bond lengths Bond angles



Torsions Rings

Oligosaccharide Chain 4



5.6 Ligand geometry ⓘ

12 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	$\#\|Z\|>2$
12	MAN	C	201	-	11,11,12	1.21	1 (9%)	15,15,17	1.19	1 (6%)
11	NAG	J	701	2	14,14,15	0.27	0	17,19,21	0.40	0
11	NAG	F	702	2	14,14,15	0.14	0	17,19,21	0.51	0
11	NAG	E	601	1	14,14,15	0.30	0	17,19,21	0.38	0
11	NAG	B	702	2	14,14,15	0.14	0	17,19,21	0.51	0
11	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.38	0
11	NAG	I	601	1	14,14,15	0.30	0	17,19,21	0.38	0
11	NAG	B	701	2	14,14,15	0.28	0	17,19,21	0.40	0
11	NAG	J	702	2	14,14,15	0.14	0	17,19,21	0.51	0
12	MAN	G	201	-	11,11,12	1.22	1 (9%)	15,15,17	1.19	1 (6%)
12	MAN	K	201	-	11,11,12	1.22	1 (9%)	15,15,17	1.19	1 (6%)
11	NAG	F	701	2	14,14,15	0.26	0	17,19,21	0.41	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
12	MAN	C	201	-	-	1/2/19/22	0/1/1/1
11	NAG	J	701	2	-	1/6/23/26	0/1/1/1
11	NAG	F	702	2	-	2/6/23/26	0/1/1/1
11	NAG	E	601	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	NAG	I	601	1	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	1/6/23/26	0/1/1/1
11	NAG	J	702	2	-	2/6/23/26	0/1/1/1
12	MAN	G	201	-	-	1/2/19/22	0/1/1/1
12	MAN	K	201	-	-	1/2/19/22	0/1/1/1
11	NAG	F	701	2	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	201	MAN	C4-C5	2.60	1.58	1.53
12	K	201	MAN	C4-C5	2.59	1.58	1.53
12	G	201	MAN	C4-C5	2.58	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	201	MAN	O2-C2-C3	-2.80	104.53	110.14
12	K	201	MAN	O2-C2-C3	-2.79	104.55	110.14
12	C	201	MAN	O2-C2-C3	-2.79	104.56	110.14

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	702	NAG	C4-C5-C6-O6
11	F	702	NAG	C4-C5-C6-O6
11	J	702	NAG	C4-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	F	702	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	E	1
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	218:CYS	C	219:ALA	N	1.19
1	E	218:CYS	C	219:ALA	N	1.19
1	I	218:CYS	C	219:ALA	N	1.19

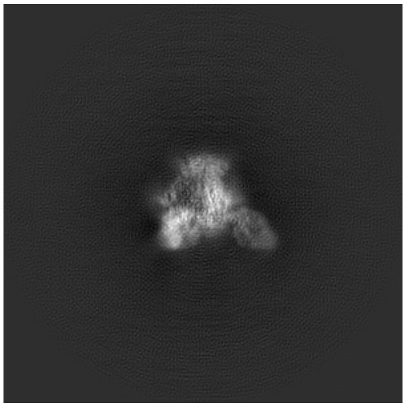
6 Map visualisation ⓘ

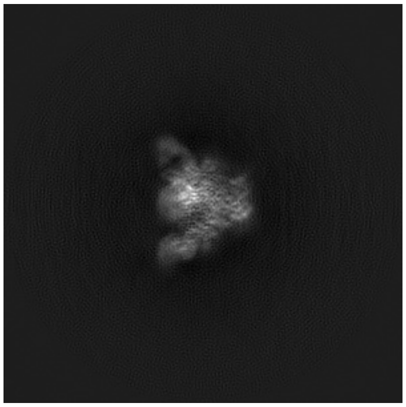
This section contains visualisations of the EMDB entry EMD-24195. These allow visual inspection of the internal detail of the map and identification of artifacts.

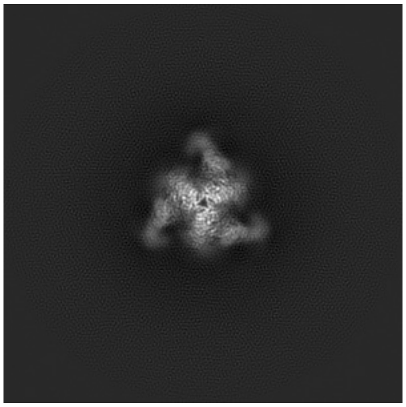
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map


X

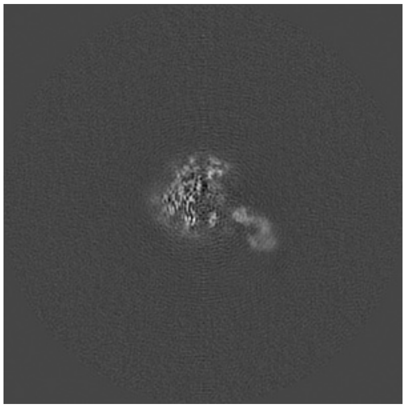

Y

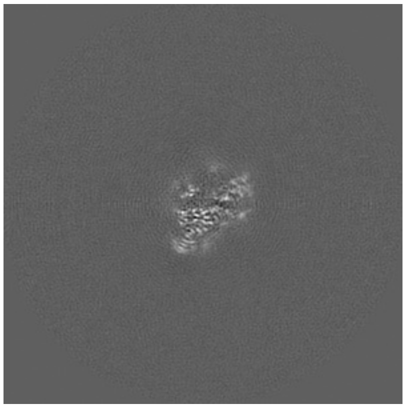

Z

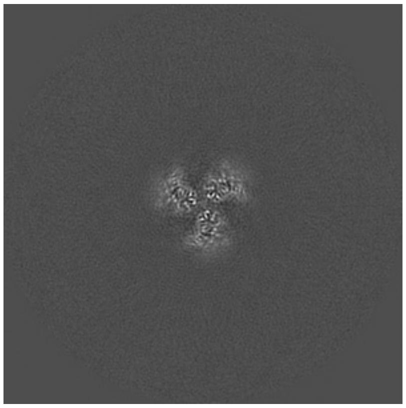
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map


X Index: 200

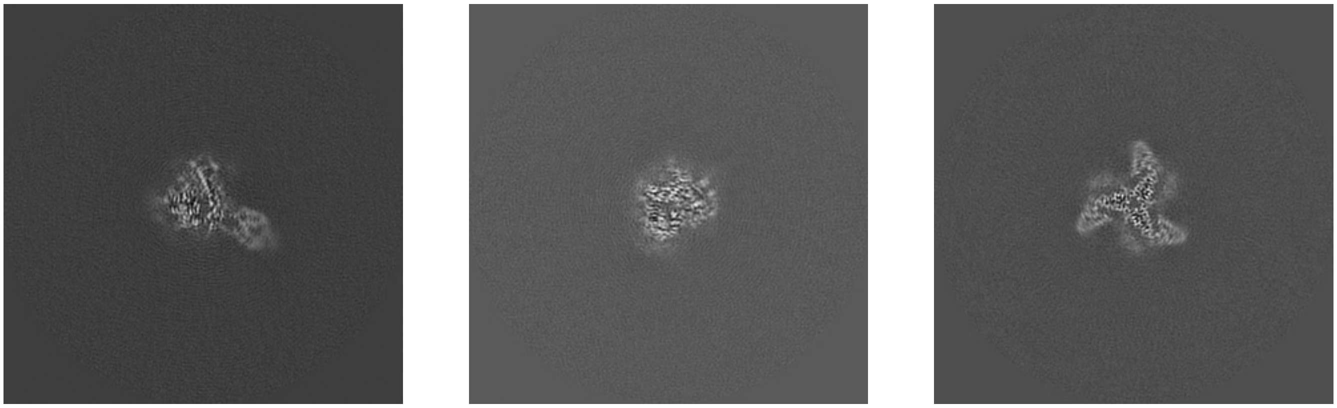

Y Index: 200


Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 205 Y Index: 206 Z Index: 186

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

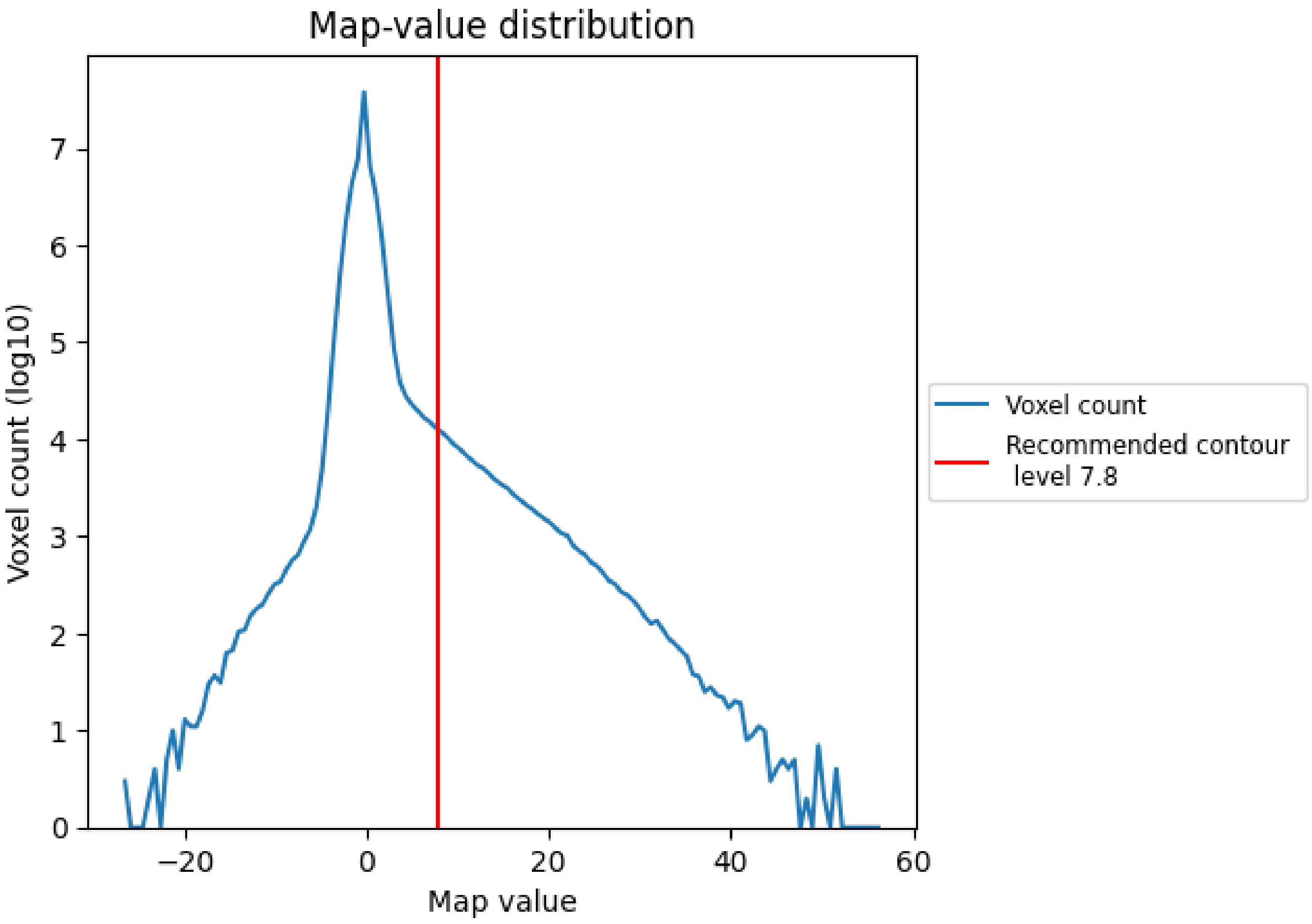
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

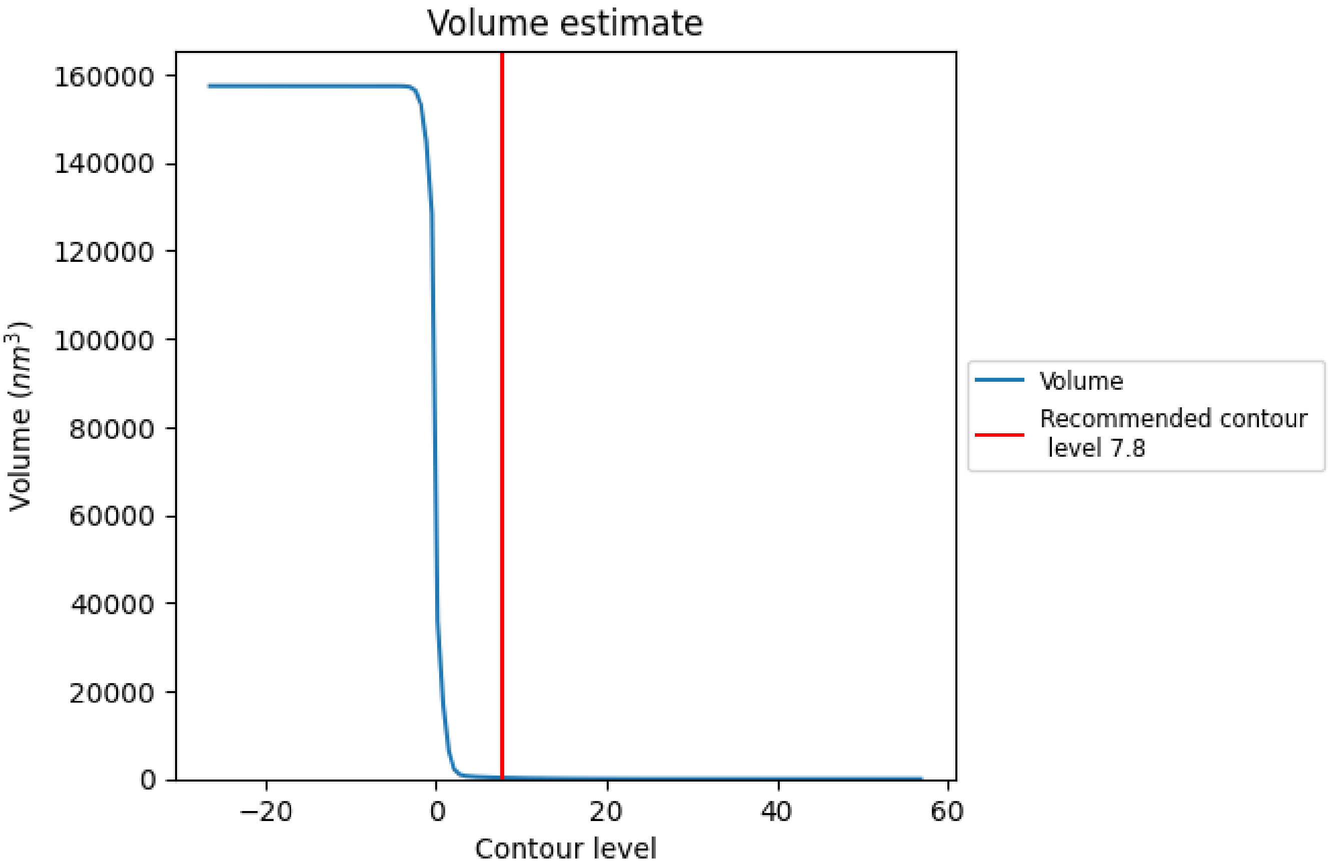
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

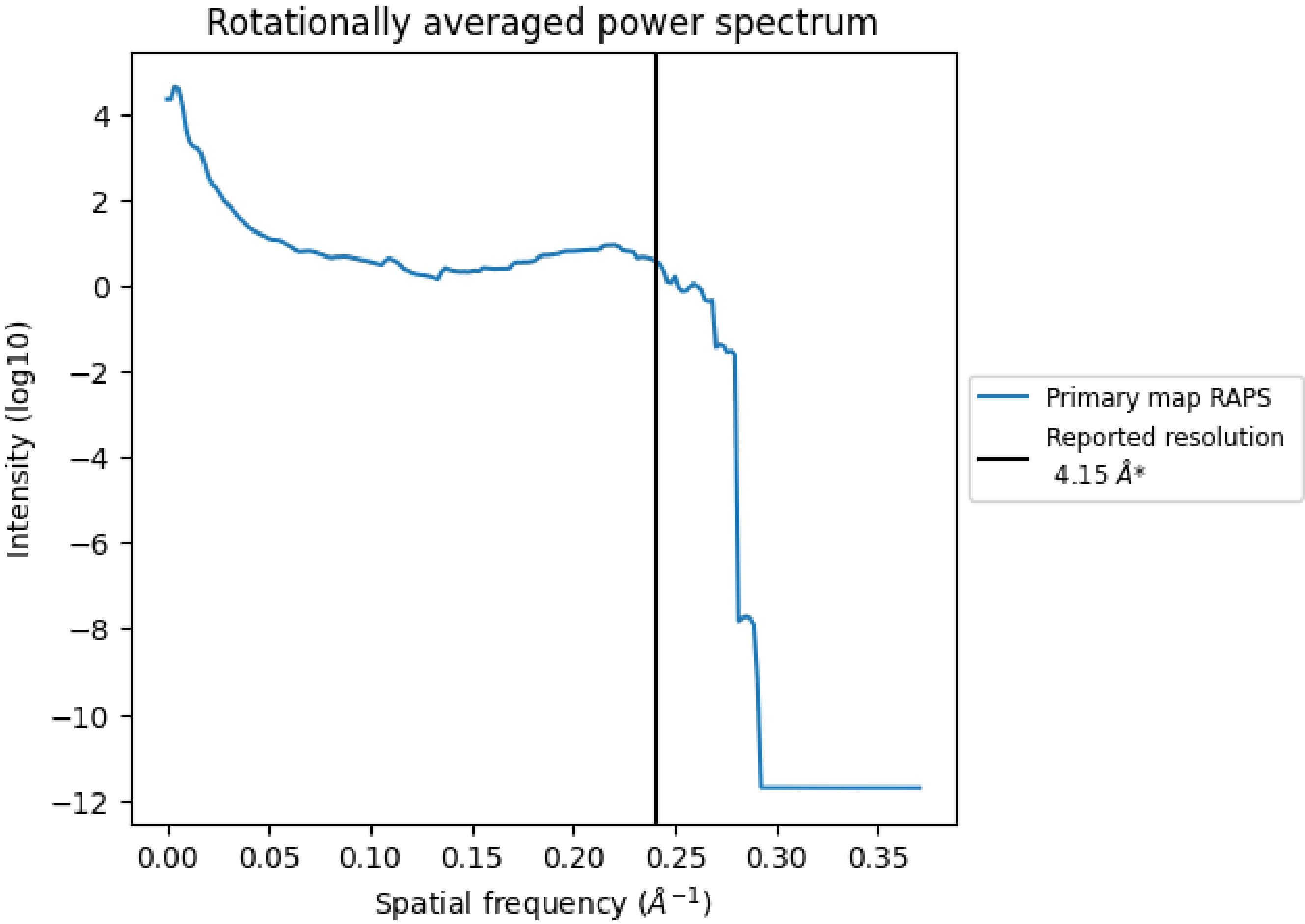
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 270 nm^3; this corresponds to an approximate mass of 244 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 ⓘ

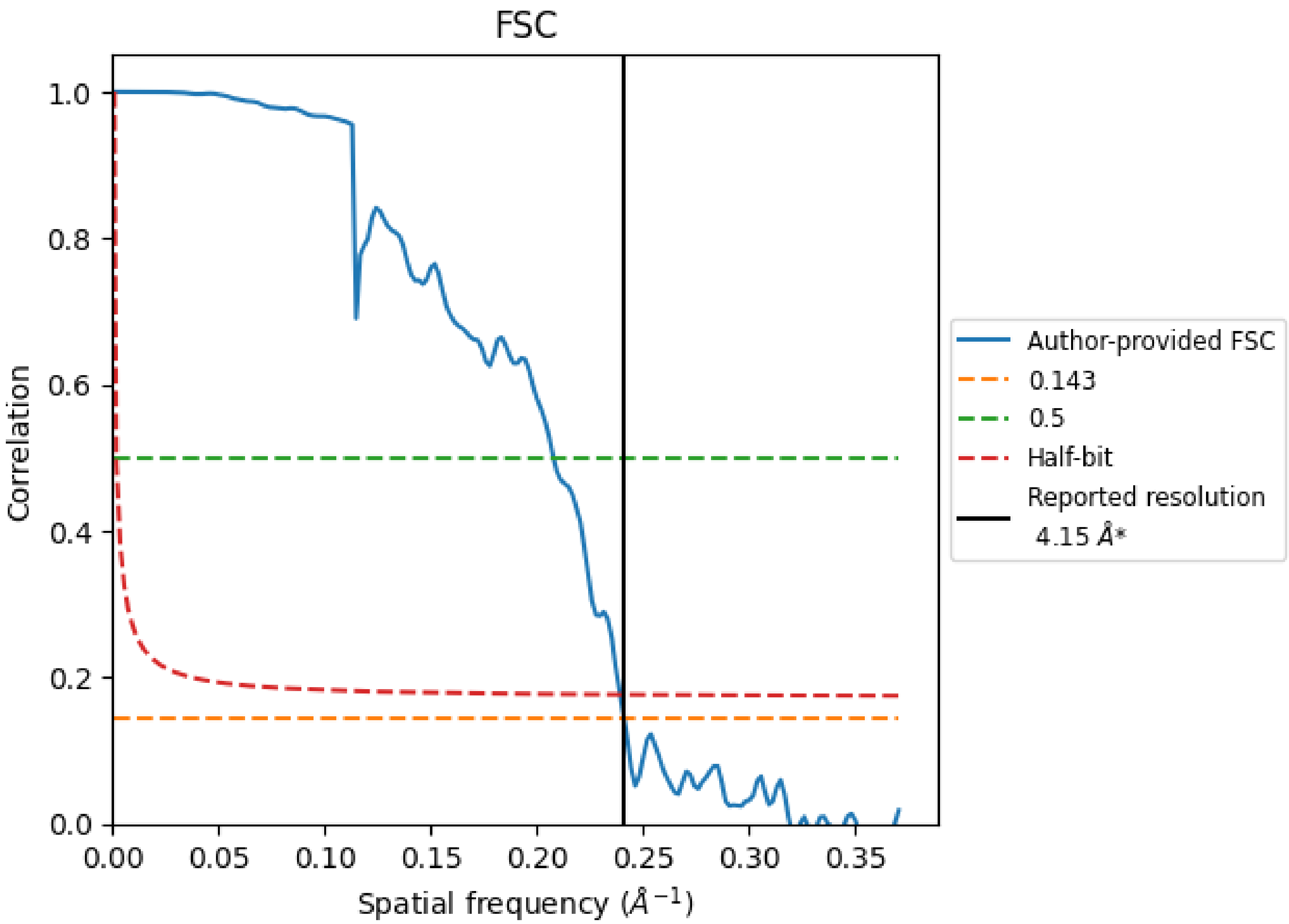


*Reported resolution corresponds to spatial frequency of 0.241 $Å^{-1}$

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 0.241 $Å^{-1}$

8.2 Resolution estimates ⓘ

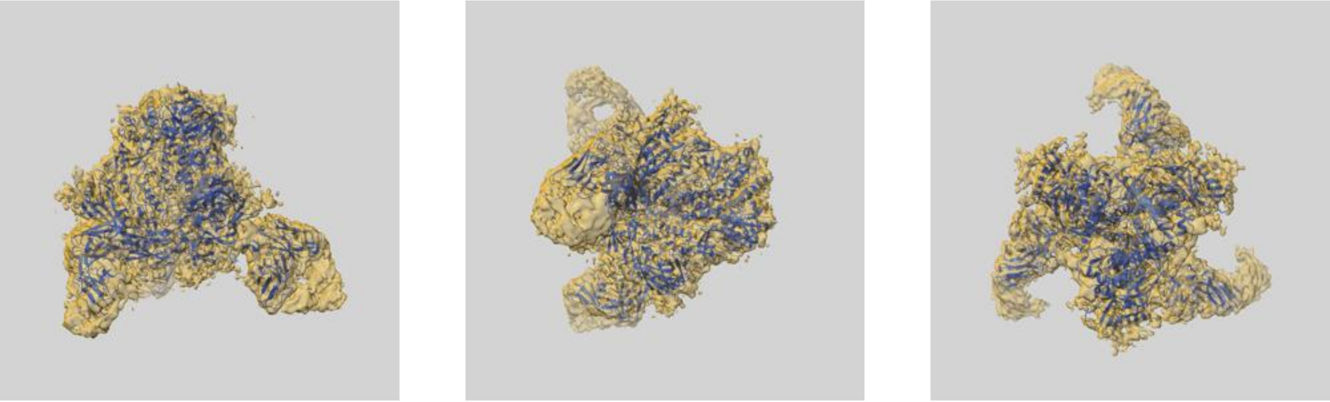
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	4.15	4.81	4.18
Unmasked-calculated*	-	-	-

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-24195 and PDB model 7N65. Per-residue inclusion information can be found in section 3 on page 16.

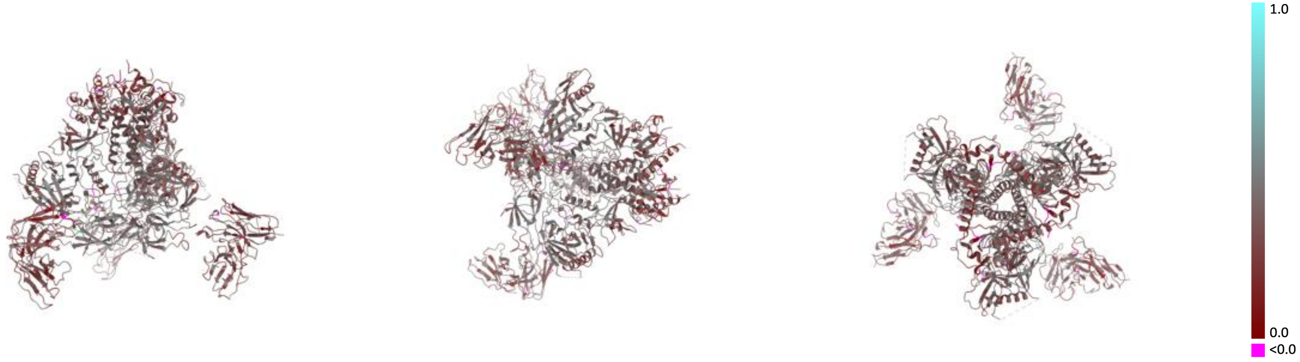
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

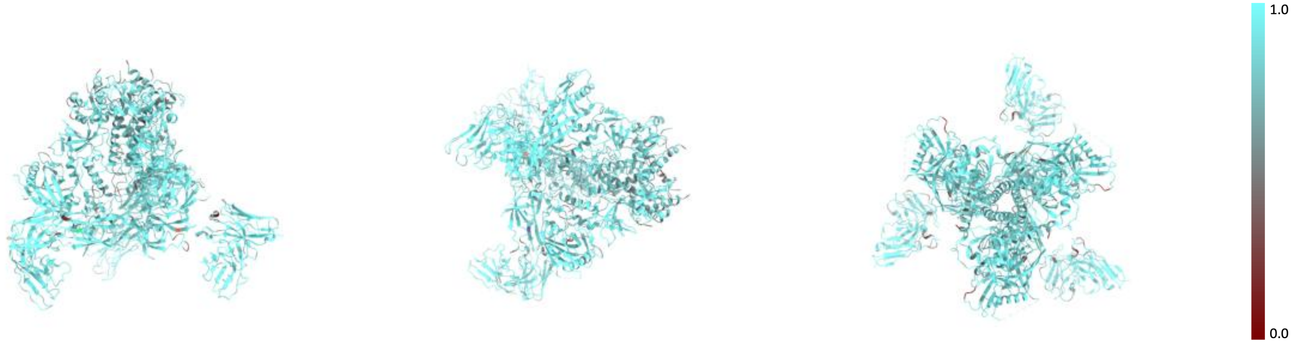
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

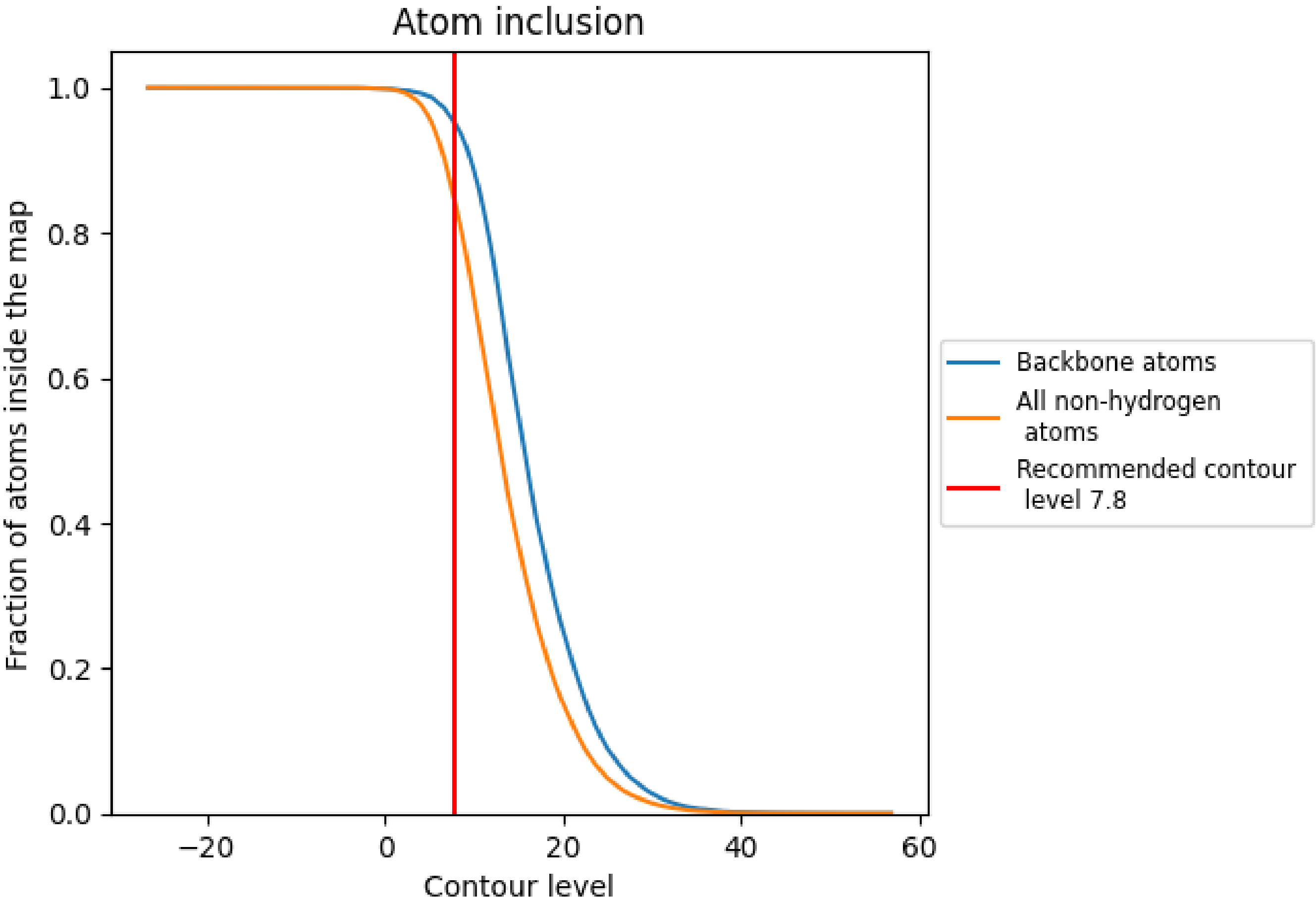
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 85% 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 (7.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8481	0.3480
0	0.7229	0.3980
1	0.5385	0.3760
2	0.7049	0.3580
3	0.8072	0.2530
4	0.8404	0.4010
5	0.2500	0.2770
6	0.7179	0.3350
7	0.8205	0.3400
8	0.5714	0.3810
9	0.7857	0.4260
A	0.8779	0.3860
AA	0.3571	0.3100
B	0.8036	0.2970
C	0.8853	0.2920
D	0.8949	0.2960
E	0.8771	0.3880
F	0.8111	0.3100
G	0.8883	0.2890
H	0.9014	0.3040
I	0.8776	0.3860
J	0.7932	0.2820
K	0.8843	0.2920
L	0.8857	0.2800
M	0.2051	0.3230
N	0.6429	0.3860
O	0.8462	0.5020
P	0.6923	0.4190
Q	0.7857	0.4320
R	0.6786	0.3680
S	0.7229	0.4150
T	0.5128	0.3700
U	0.6721	0.3510
V	0.7952	0.2410
W	0.8298	0.3830

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Chain	Atom inclusion	Q-score
X	0.2143	0.2760
Y	0.7436	0.3270
Z	0.8205	0.3650
a	0.6071	0.4040
b	0.7500	0.4400
c	0.3214	0.3960
d	0.2051	0.3310
e	0.6429	0.4080
f	0.8718	0.4960
g	0.6923	0.4420
h	0.7143	0.4190
i	0.6786	0.3680
j	0.7590	0.4130
k	0.5897	0.3860
l	0.7049	0.3680
m	0.8072	0.2580
n	0.8511	0.3960
o	0.2143	0.2550
p	0.7436	0.3370
q	0.7949	0.3450
r	0.5714	0.3980
s	0.8214	0.4500
t	0.3929	0.4000
u	0.2051	0.3240
v	0.6429	0.3770
w	0.8462	0.4840
x	0.6667	0.4240
y	0.6786	0.4150
z	0.6429	0.3760