Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 08:22 am GMT

PDB ID	:	5ACO
EMDB ID	:	EMD-3121
Title	:	Cryo-EM structure of PGT128 Fab in complex with BG505 SOSIP.664 Env trimer
Authors	:	Lee, J.H.; Ward, A.B.
Deposited on	:	2015-08-17
Resolution	:	4.36 Å(reported)

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

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

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

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

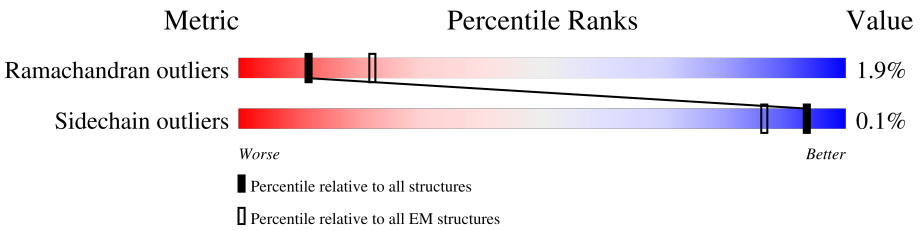
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.36 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	476	7% 89% • • 8%
1	C	476	7% 89% • • 8%
1	D	476	7% 89% • • 8%
2	B	153	14% 82% 5% 14%
2	E	153	14% 82% 5% 14%
2	F	153	14% 82% 5% 14%
3	G	239	8% 55% 45%
3	H	239	8% 55% 45%
3	I	239	8% 55% 45%

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Mol	Chain	Length	Quality of chain
4	J	211	11% 47% • 51%
4	K	211	11% 47% • 51%
4	L	211	10% 47% • 51%
5	0	3	100% 100%
5	5	3	67% 100%
5	6	3	33% 100%
5	M	3	100% 100%
5	O	3	67% 100%
5	P	3	67% 100%
5	T	3	100% 100%
5	Y	3	67% 100%
5	Z	3	33% 100%
5	d	3	100% 100%
5	f	3	67% 100%
5	g	3	67% 100%
5	k	3	100% 100%
5	p	3	67% 100%
5	q	3	33% 100%
5	t	3	100% 100%
5	v	3	67% 100%
5	w	3	67% 100%
6	4	2	100% 100%
6	7	2	100% 100%
6	8	2	50% 100%
6	9	2	100% 100%

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Mol	Chain	Length	Quality of chain
6	AA	2	100% 100%
6	N	2	50% 100%
6	Q	2	50% 100%
6	R	2	50% 100%
6	X	2	100% 100%
6	a	2	100% 100%
6	b	2	50% 100%
6	c	2	100% 100%
6	e	2	50% 100%
6	h	2	50% 100%
6	i	2	50% 100%
6	o	2	100% 100%
6	r	2	100% 100%
6	s	2	50% 100%
6	u	2	50% 100%
6	x	2	50% 100%
6	y	2	50% 100%
7	2	7	29% 100%
7	S	7	57% 86% 14%
7	V	7	29% 100%
7	j	7	57% 86% 14%
7	m	7	29% 100%
7	z	7	57% 86% 14%
8	1	5	60% 100%
8	U	5	60% 100%

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Mol	Chain	Length	Quality of chain
8	l	5	60% 100%
9	3	10	10% 20% 80%
9	W	10	10% 20% 80%
9	n	10	20% 20% 80%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21297 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 HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	438	3453	2170	610	645	28	0	0
1	C	438	3453	2170	610	645	28	0	0
1	D	438	3453	2170	610	645	28	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1051	667	180	198	6	0	0
2	E	132	1051	667	180	198	6	0	0
2	F	132	1051	667	180	198	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
E	559	PRO	ILE	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

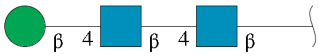
- Molecule 3 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	132	1028	659	175	190	4	0	0
3	H	132	1028	659	175	190	4	0	0
3	I	132	1028	659	175	190	4	0	0

- Molecule 4 is a protein called PGT128 FAB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	103	752	469	128	153	2	0	0
4	K	103	752	469	128	153	2	0	0
4	L	103	752	469	128	153	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
			Total	C	N	O		
5	M	3	39	22	2	15	0	0
5	O	3	39	22	2	15	0	0
5	P	3	39	22	2	15	0	0
5	T	3	39	22	2	15	0	0
5	Y	3	39	22	2	15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Z	3	39	22	2	15	0	0
5	d	3	39	22	2	15	0	0
5	f	3	39	22	2	15	0	0
5	g	3	39	22	2	15	0	0
5	k	3	39	22	2	15	0	0
5	p	3	39	22	2	15	0	0
5	q	3	39	22	2	15	0	0
5	t	3	39	22	2	15	0	0
5	v	3	39	22	2	15	0	0
5	w	3	39	22	2	15	0	0
5	0	3	39	22	2	15	0	0
5	5	3	39	22	2	15	0	0
5	6	3	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
			Total	C	N	O		
6	N	2	28	16	2	10	0	0
6	Q	2	28	16	2	10	0	0
6	R	2	28	16	2	10	0	0
6	X	2	28	16	2	10	0	0

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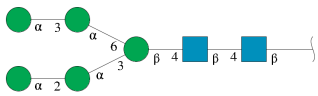
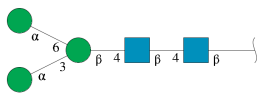
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	a	2	28	16	2	10	0	0
6	b	2	28	16	2	10	0	0
6	c	2	28	16	2	10	0	0
6	e	2	28	16	2	10	0	0
6	h	2	28	16	2	10	0	0
6	i	2	28	16	2	10	0	0
6	o	2	28	16	2	10	0	0
6	r	2	28	16	2	10	0	0
6	s	2	28	16	2	10	0	0
6	u	2	28	16	2	10	0	0
6	x	2	28	16	2	10	0	0
6	y	2	28	16	2	10	0	0
6	4	2	28	16	2	10	0	0
6	7	2	28	16	2	10	0	0
6	8	2	28	16	2	10	0	0
6	9	2	28	16	2	10	0	0
6	AA	2	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.



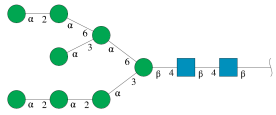
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S	7	83	46	2	35	0	0
7	V	7	83	46	2	35	0	0
7	j	7	83	46	2	35	0	0
7	m	7	83	46	2	35	0	0
7	z	7	83	46	2	35	0	0
7	2	7	83	46	2	35	0	0

- 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
			Total	C	N	O		
8	U	5	61	34	2	25	0	0
8	l	5	61	34	2	25	0	0
8	1	5	61	34	2	25	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
			Total	C	N	O		
9	W	10	116	64	2	50	0	0

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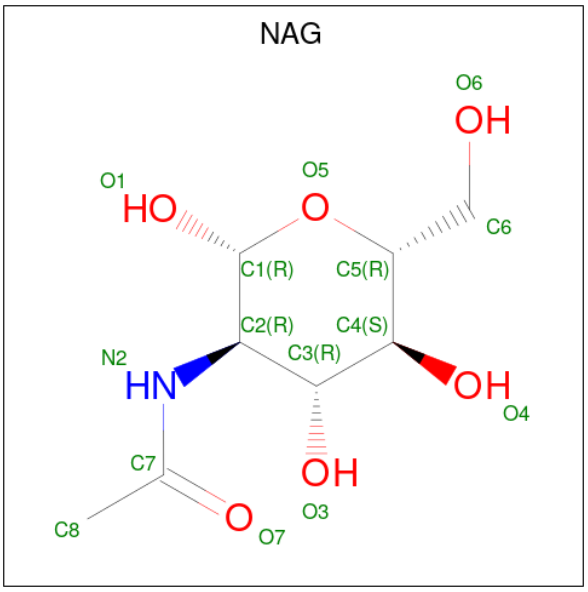
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	n	10	116	64	2	50	0	0
			Total	C	N	O		
9	3	10	116	64	2	50	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



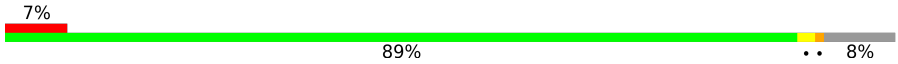
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	A	1	14	8	1	5	0
			Total	C	N	O	
10	B	1	28	16	2	10	0
			Total	C	N	O	
10	B	1	28	16	2	10	0
			Total	C	N	O	
10	C	1	14	8	1	5	0
			Total	C	N	O	
10	D	1	14	8	1	5	0
			Total	C	N	O	
10	E	1	28	16	2	10	0
			Total	C	N	O	
10	E	1	28	16	2	10	0
			Total	C	N	O	
10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

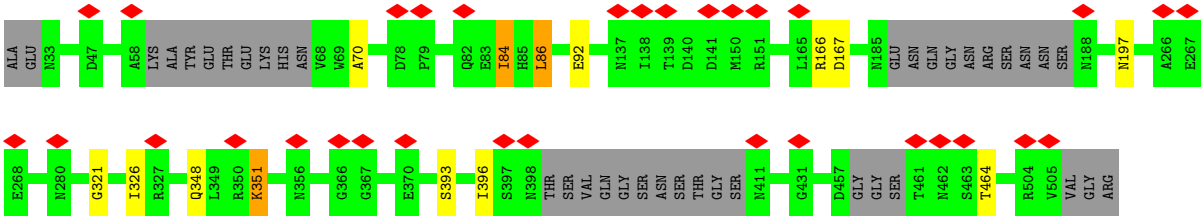
3 Residue-property plots (i)

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

• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

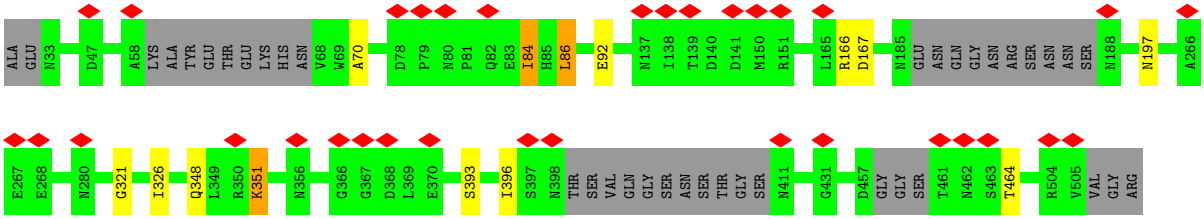
Chain A:





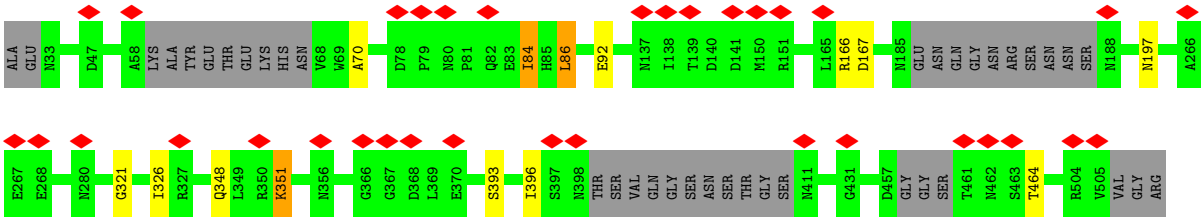
• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

Chain C:



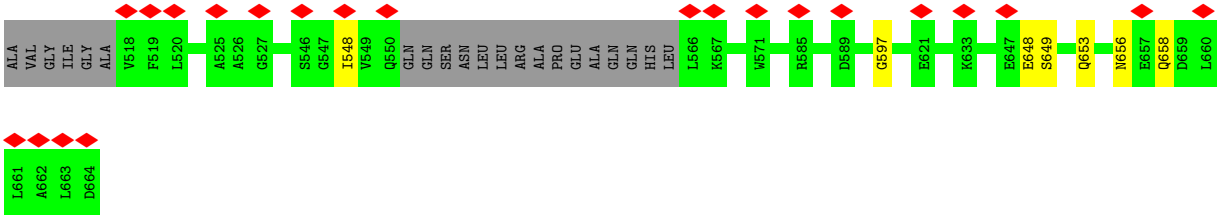
• Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN

Chain D:



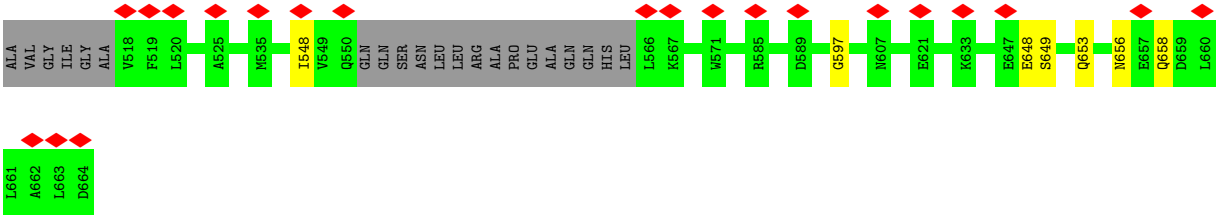
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain B:



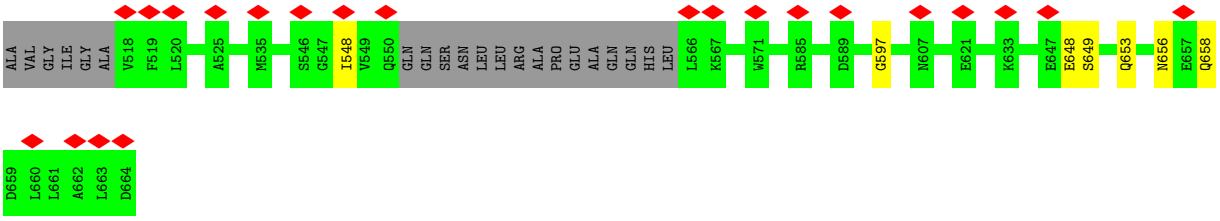
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain E:



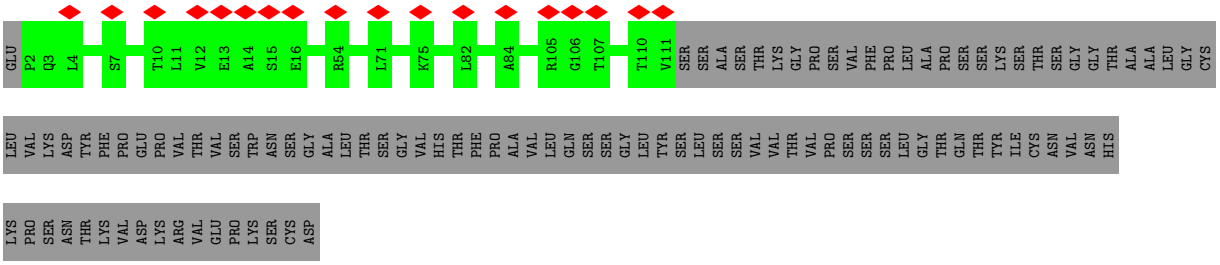
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN

Chain F:



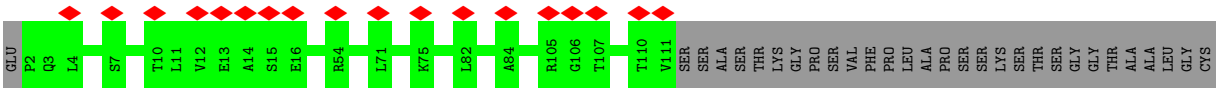
• Molecule 3: PGT128 FAB

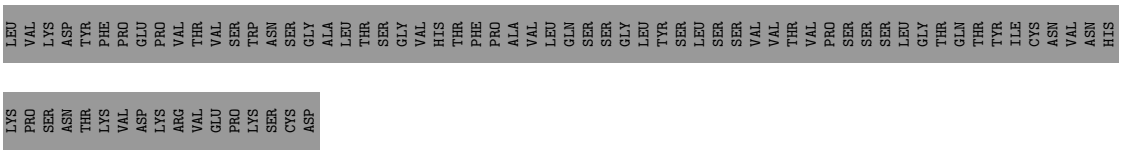
Chain G:



• Molecule 3: PGT128 FAB

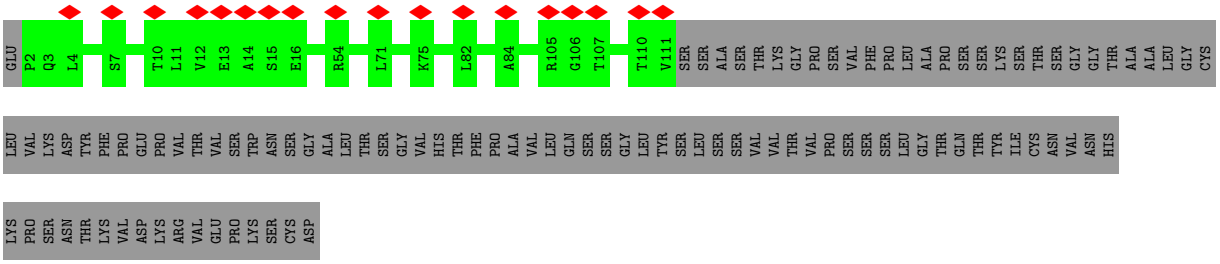
Chain H:





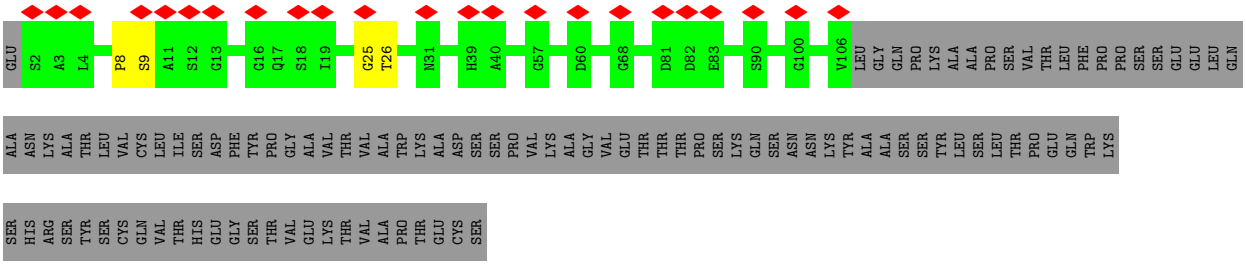
• Molecule 3: PGT128 FAB

Chain I:



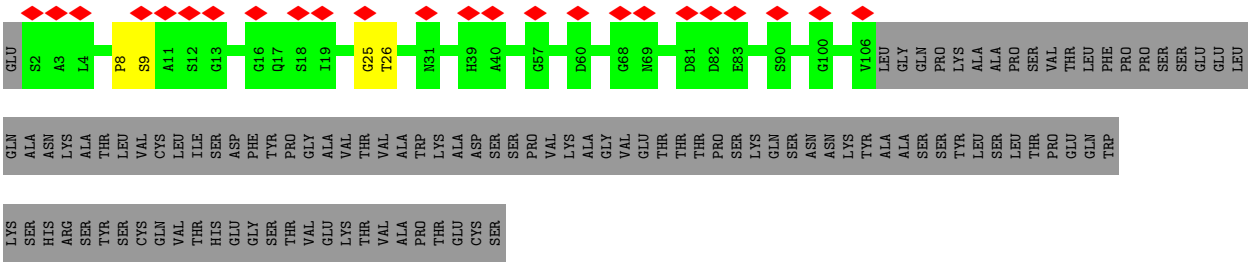
• Molecule 4: PGT128 FAB

Chain J:



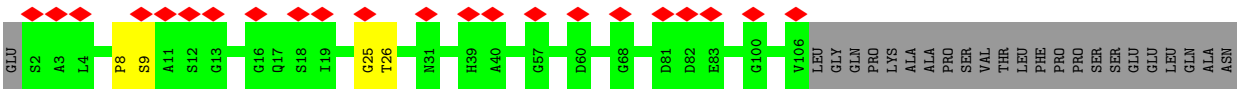
• Molecule 4: PGT128 FAB

Chain K:



• Molecule 4: PGT128 FAB

Chain L:



LYS ALA THR LEU VAL CYS LEU ILE SER ASP PHE TYR PRO GLY ALA VAL THR VAL ALA TRP LYS ALA ASP SER SER PRO VAL LYS ALA GLY VAL GLU THR THR THR PRO SER LYS GLN SER ASN ASN LYS TYR ALA ALA SER SER TYR LEU SER LEU THR PRO GLU GLN TRP LYS SER HIS

ARG SER TYR SER CYS GLN VAL THR HIS GLU GLY SER THR VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

• 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: 100% 100%

NAG1 NAG2 BMA3

• 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: 67% 100%

NAG1 NAG2 BMA3

• 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: 67% 100%

NAG1 NAG2 BMA3

• 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: 100% 100%

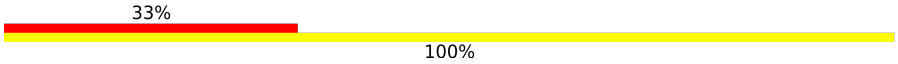
NAG1 NAG2 BMA3

• 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: 67% 100%

NAG1 NAG2 BMA3

• 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: 

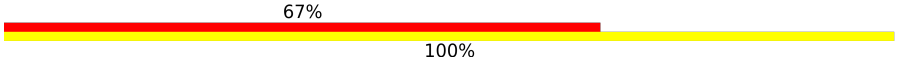
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

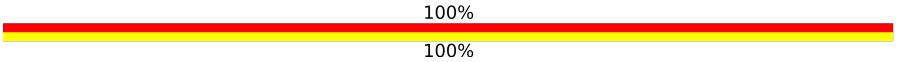
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

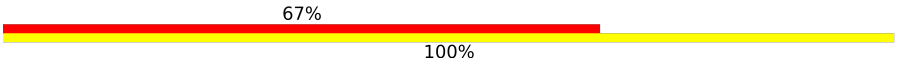
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 33% 100%

• 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: 100% 100%

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

Chain v: 67% 100%

• 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: 67% 100%

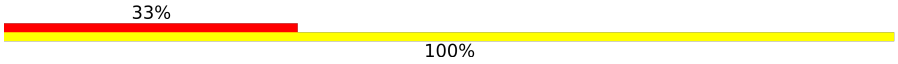
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0: 100% 100%

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

Chain 5: 67% 100%

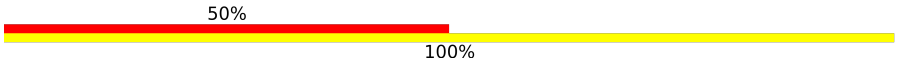
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6: 

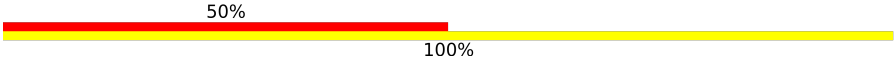
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 

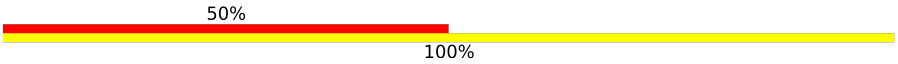
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

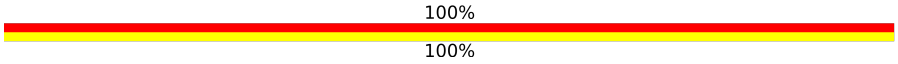
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

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

Chain b: 

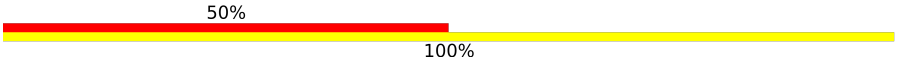
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

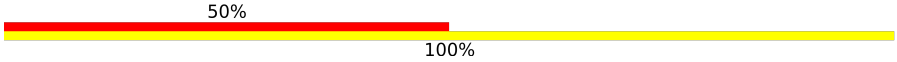
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 100% 100%

NAG1 NAG2

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

Chain r: 100% 100%

NAG1 NAG2

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

Chain s: 50% 100%

NAG1 NAG2

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

Chain u: 50% 100%

NAG1 NAG2

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

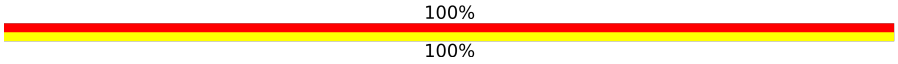
Chain x: 50% 100%

NAG1 NAG2

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

Chain y: 50% 100%

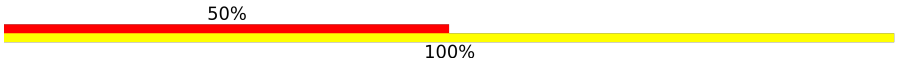
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 

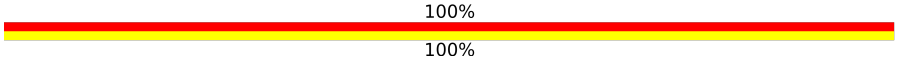
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:

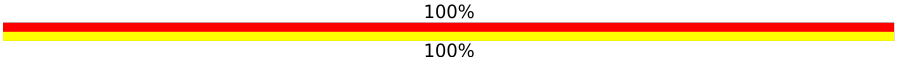
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8: 

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

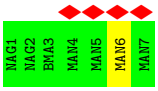
Chain 9: 

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

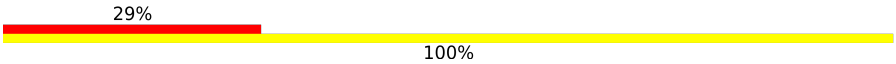
Chain AA: 

• 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:

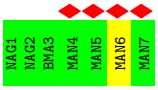


• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

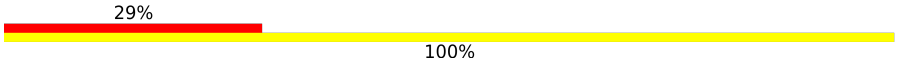
Chain V: 

• 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:

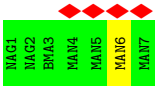


• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

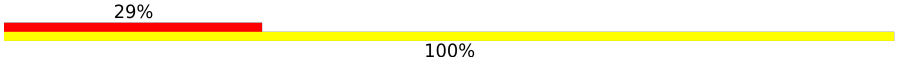
Chain m: 

• 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

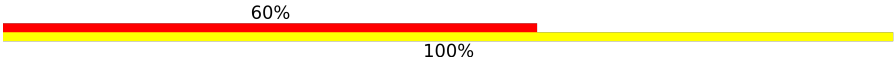
Chain z:



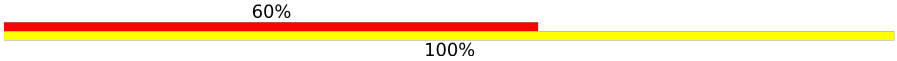
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2: 

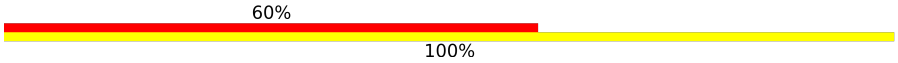
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

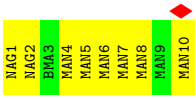
Chain l: 

• 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 1: 

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

Chain W:



• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 n:

• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 3:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	92095	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.041	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	C	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	D	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
2	B	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	E	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	F	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
3	G	0.66	0/1061	0.72	0/1455
3	H	0.65	0/1061	0.72	0/1455
3	I	0.65	0/1061	0.72	0/1455
4	J	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	K	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
4	L	0.75	2/769 (0.3%)	0.92	3/1048 (0.3%)
All	All	0.67	15/19266 (0.1%)	0.77	69/26202 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	658	GLN	C-N	12.04	1.61	1.34
2	F	658	GLN	C-N	12.04	1.61	1.34
2	E	658	GLN	C-N	12.00	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	8	PRO	C-N	10.79	1.58	1.34
4	J	8	PRO	C-N	10.77	1.58	1.34
4	K	8	PRO	C-N	10.77	1.58	1.34
1	C	92	GLU	C-N	-6.48	1.19	1.34
1	D	92	GLU	C-N	-6.47	1.19	1.34
1	A	92	GLU	C-N	-6.45	1.19	1.34
1	A	84	ILE	C-N	6.02	1.48	1.34
1	C	84	ILE	C-N	6.01	1.47	1.34
1	D	84	ILE	C-N	6.01	1.47	1.34
4	J	9	SER	C-N	5.30	1.46	1.34
4	K	9	SER	C-N	5.29	1.46	1.34
4	L	9	SER	C-N	5.26	1.46	1.34

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	648	GLU	N-CA-C	14.16	149.23	111.00
2	B	648	GLU	N-CA-C	14.16	149.22	111.00
2	F	648	GLU	N-CA-C	14.14	149.18	111.00
1	C	84	ILE	O-C-N	12.71	143.04	122.70
1	D	84	ILE	O-C-N	12.70	143.01	122.70
1	A	84	ILE	O-C-N	12.69	143.01	122.70
1	D	86	LEU	O-C-N	-12.63	102.49	122.70
1	A	86	LEU	O-C-N	-12.63	102.49	122.70
1	C	86	LEU	O-C-N	-12.62	102.52	122.70
1	D	393	SER	O-C-N	11.17	140.57	122.70
1	C	393	SER	O-C-N	11.17	140.57	122.70
1	A	393	SER	O-C-N	11.15	140.54	122.70
1	C	84	ILE	CA-C-N	-10.75	93.55	117.20
1	A	84	ILE	CA-C-N	-10.74	93.57	117.20
1	D	84	ILE	CA-C-N	-10.72	93.61	117.20
1	D	348	GLN	O-C-N	10.57	139.61	122.70
1	A	348	GLN	O-C-N	10.56	139.60	122.70
1	C	348	GLN	O-C-N	10.56	139.60	122.70
2	E	658	GLN	O-C-N	10.31	139.20	122.70
2	B	658	GLN	O-C-N	10.31	139.19	122.70
2	F	658	GLN	O-C-N	10.31	139.19	122.70
1	D	351	LYS	O-C-N	-10.15	106.47	122.70
1	A	351	LYS	O-C-N	-10.14	106.48	122.70
1	C	351	LYS	O-C-N	-10.13	106.49	122.70
1	C	84	ILE	C-N-CA	-8.87	99.52	121.70
1	A	84	ILE	C-N-CA	-8.87	99.52	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	84	ILE	C-N-CA	-8.87	99.53	121.70
4	L	8	PRO	O-C-N	-8.71	108.77	122.70
4	J	8	PRO	O-C-N	-8.69	108.79	122.70
4	K	8	PRO	O-C-N	-8.68	108.81	122.70
1	D	393	SER	CA-C-N	-8.37	98.78	117.20
1	C	393	SER	CA-C-N	-8.37	98.79	117.20
1	A	393	SER	CA-C-N	-8.36	98.80	117.20
1	C	348	GLN	CA-C-N	-8.03	99.55	117.20
1	D	348	GLN	CA-C-N	-8.02	99.55	117.20
1	A	348	GLN	CA-C-N	-8.02	99.56	117.20
4	K	8	PRO	C-N-CA	-7.99	101.72	121.70
4	J	8	PRO	C-N-CA	-7.99	101.73	121.70
2	B	658	GLN	CA-C-N	-7.97	99.65	117.20
2	F	658	GLN	CA-C-N	-7.97	99.66	117.20
4	L	8	PRO	C-N-CA	-7.97	101.77	121.70
2	E	658	GLN	CA-C-N	-7.96	99.68	117.20
1	C	351	LYS	CA-C-N	7.25	133.16	117.20
1	A	351	LYS	CA-C-N	7.25	133.14	117.20
1	D	351	LYS	CA-C-N	7.23	133.10	117.20
2	F	648	GLU	N-CA-CB	-6.99	98.01	110.60
2	B	648	GLU	N-CA-CB	-6.99	98.01	110.60
2	E	648	GLU	N-CA-CB	-6.99	98.02	110.60
1	D	86	LEU	CA-C-N	6.77	132.10	117.20
1	A	86	LEU	CA-C-N	6.77	132.10	117.20
1	C	86	LEU	CA-C-N	6.76	132.06	117.20
1	C	348	GLN	C-N-CA	-6.73	104.86	121.70
1	D	348	GLN	C-N-CA	-6.73	104.87	121.70
1	A	348	GLN	C-N-CA	-6.73	104.88	121.70
1	D	86	LEU	C-N-CA	6.63	138.27	121.70
1	A	86	LEU	C-N-CA	6.61	138.22	121.70
1	C	86	LEU	C-N-CA	6.58	138.15	121.70
4	J	8	PRO	CA-C-N	6.22	130.88	117.20
4	L	8	PRO	CA-C-N	6.21	130.87	117.20
4	K	8	PRO	CA-C-N	6.21	130.85	117.20
1	C	393	SER	C-N-CA	-5.85	107.08	121.70
1	A	393	SER	C-N-CA	-5.84	107.10	121.70
1	D	393	SER	C-N-CA	-5.84	107.11	121.70
2	B	653	GLN	N-CA-C	5.70	126.40	111.00
2	F	653	GLN	N-CA-C	5.70	126.39	111.00
2	E	653	GLN	N-CA-C	5.68	126.35	111.00
1	C	351	LYS	C-N-CA	5.50	135.45	121.70
1	A	351	LYS	C-N-CA	5.50	135.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	351	LYS	C-N-CA	5.48	135.40	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	LEU	Mainchain
1	C	86	LEU	Mainchain
1	D	86	LEU	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	7	39
1	C	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	7	39
1	D	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	7	39
2	B	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	31
2	E	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	31
2	F	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	31
3	G	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	H	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
3	I	130/239 (54%)	121 (93%)	9 (7%)	0	100	100
4	J	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	7	40
4	K	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	101/211 (48%)	91 (90%)	8 (8%)	2 (2%)	7 40
All	All	2361/3237 (73%)	2100 (89%)	216 (9%)	45 (2%)	11 41

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	A	396	ILE
1	C	167	ASP
1	C	396	ILE
1	D	167	ASP
1	D	396	ILE
4	J	26	THR
4	K	26	THR
4	L	26	THR
1	A	464	THR
2	B	597	GLY
2	B	649	SER
1	C	464	THR
1	D	464	THR
2	E	597	GLY
2	E	649	SER
2	F	597	GLY
2	F	649	SER
1	A	166	ARG
2	B	548	ILE
1	C	166	ARG
1	D	166	ARG
2	E	548	ILE
2	F	548	ILE
1	A	70	ALA
1	A	321	GLY
2	B	656	ASN
1	C	70	ALA
1	C	321	GLY
1	D	70	ALA
1	D	321	GLY
2	E	656	ASN
2	F	656	ASN
1	A	84	ILE
1	A	351	LYS
1	C	84	ILE

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Mol	Chain	Res	Type
1	C	351	LYS
1	D	84	ILE
1	D	351	LYS
1	A	326	ILE
1	C	326	ILE
1	D	326	ILE
4	J	25	GLY
4	K	25	GLY
4	L	25	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/423 (93%)	392 (100%)	1 (0%)	92	95
1	C	393/423 (93%)	392 (100%)	1 (0%)	92	95
1	D	393/423 (93%)	392 (100%)	1 (0%)	92	95
2	B	114/129 (88%)	114 (100%)	0	100	100
2	E	114/129 (88%)	114 (100%)	0	100	100
2	F	114/129 (88%)	114 (100%)	0	100	100
3	G	110/203 (54%)	110 (100%)	0	100	100
3	H	110/203 (54%)	110 (100%)	0	100	100
3	I	110/203 (54%)	110 (100%)	0	100	100
4	J	84/177 (48%)	84 (100%)	0	100	100
4	K	84/177 (48%)	84 (100%)	0	100	100
4	L	84/177 (48%)	84 (100%)	0	100	100
All	All	2103/2796 (75%)	2100 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN

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Mol	Chain	Res	Type
1	C	197	ASN
1	D	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	C	279	ASN
1	D	279	ASN
3	G	59	HIS
3	H	59	HIS
3	I	59	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

183 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	$\#\|Z\| > 2$
5	NAG	0	1	1,5	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	0	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	BMA	0	3	5	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
8	NAG	1	1	1,8	14,14,15	0.49	0	17,19,21	2.24	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	1	2	8	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
8	BMA	1	3	8	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	MAN	1	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	1	5	8	11,11,12	0.63	0	15,15,17	2.53	4 (26%)
7	NAG	2	1	1,7	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
7	NAG	2	2	7	14,14,15	0.32	0	17,19,21	2.40	4 (23%)
7	BMA	2	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	2	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
7	MAN	2	5	7	11,11,12	0.44	0	15,15,17	0.88	1 (6%)
7	MAN	2	6	7	11,11,12	0.49	0	15,15,17	0.82	1 (6%)
7	MAN	2	7	7	11,11,12	0.34	0	15,15,17	1.31	2 (13%)
9	NAG	3	1	1,9	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
9	MAN	3	10	9	11,11,12	0.34	0	15,15,17	0.92	2 (13%)
9	NAG	3	2	9	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
9	BMA	3	3	9	11,11,12	0.42	0	15,15,17	0.63	0
9	MAN	3	4	9	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
9	MAN	3	5	9	11,11,12	0.47	0	15,15,17	1.05	2 (13%)
9	MAN	3	6	9	11,11,12	0.49	0	15,15,17	1.19	1 (6%)
9	MAN	3	7	9	11,11,12	0.29	0	15,15,17	1.12	1 (6%)
9	MAN	3	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	3	9	9	11,11,12	0.34	0	15,15,17	0.78	0
6	NAG	4	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	4	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	5	1	1,5	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	5	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	5	3	5	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
5	NAG	6	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	6	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	6	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	7	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	7	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	8	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	8	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	9	1	6,2	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
6	NAG	9	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	AA	1	6,2	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	AA	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	M	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	M	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	BMA	M	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
6	NAG	N	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	N	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	NAG	O	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	O	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	O	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	P	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	P	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	BMA	P	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	Q	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	Q	2	6	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
6	NAG	R	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	R	2	6	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
7	NAG	S	1	1,7	14,14,15	0.60	0	17,19,21	0.68	0
7	NAG	S	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	S	3	7	11,11,12	0.66	0	15,15,17	0.86	0
7	MAN	S	4	7	11,11,12	0.62	0	15,15,17	0.67	0
7	MAN	S	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	S	6	7	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
7	MAN	S	7	7	11,11,12	0.62	0	15,15,17	0.62	0
5	NAG	T	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	T	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
8	NAG	U	1	1,8	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
8	NAG	U	2	8	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
8	BMA	U	3	8	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	MAN	U	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	U	5	8	11,11,12	0.62	0	15,15,17	2.53	4 (26%)
7	NAG	V	1	1,7	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
7	NAG	V	2	7	14,14,15	0.32	0	17,19,21	2.40	4 (23%)
7	BMA	V	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	V	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MAN	V	5	7	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
7	MAN	V	6	7	11,11,12	0.48	0	15,15,17	0.82	1 (6%)
7	MAN	V	7	7	11,11,12	0.33	0	15,15,17	1.30	2 (13%)
9	NAG	W	1	1,9	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
9	MAN	W	10	9	11,11,12	0.34	0	15,15,17	0.92	2 (13%)
9	NAG	W	2	9	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
9	BMA	W	3	9	11,11,12	0.42	0	15,15,17	0.62	0
9	MAN	W	4	9	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
9	MAN	W	5	9	11,11,12	0.47	0	15,15,17	1.04	2 (13%)
9	MAN	W	6	9	11,11,12	0.49	0	15,15,17	1.20	1 (6%)
9	MAN	W	7	9	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
9	MAN	W	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	W	9	9	11,11,12	0.33	0	15,15,17	0.77	0
6	NAG	X	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	X	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	NAG	Y	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	Y	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	Y	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	Z	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	Z	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	Z	3	5	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
6	NAG	a	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	a	2	6	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
6	NAG	b	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	b	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	c	1	6,2	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
6	NAG	c	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	d	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	d	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	d	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
6	NAG	e	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	e	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	NAG	f	1	1,5	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
5	NAG	f	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	f	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	g	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	g	2	5	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
5	BMA	g	3	5	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
6	NAG	h	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	h	2	6	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
6	NAG	i	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	i	2	6	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
7	NAG	j	1	1,7	14,14,15	0.60	0	17,19,21	0.67	0
7	NAG	j	2	7	14,14,15	0.57	0	17,19,21	0.90	0
7	BMA	j	3	7	11,11,12	0.66	0	15,15,17	0.87	0
7	MAN	j	4	7	11,11,12	0.61	0	15,15,17	0.67	0
7	MAN	j	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	j	6	7	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
7	MAN	j	7	7	11,11,12	0.63	0	15,15,17	0.63	0
5	NAG	k	1	1,5	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	k	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	k	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
8	NAG	l	1	1,8	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
8	NAG	l	2	8	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
8	BMA	l	3	8	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
8	MAN	l	4	8	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
8	MAN	l	5	8	11,11,12	0.64	0	15,15,17	2.52	4 (26%)
7	NAG	m	1	1,7	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
7	NAG	m	2	7	14,14,15	0.32	0	17,19,21	2.39	4 (23%)
7	BMA	m	3	7	11,11,12	0.44	0	15,15,17	1.22	2 (13%)
7	MAN	m	4	7	11,11,12	0.44	0	15,15,17	0.90	1 (6%)
7	MAN	m	5	7	11,11,12	0.45	0	15,15,17	0.86	1 (6%)
7	MAN	m	6	7	11,11,12	0.48	0	15,15,17	0.82	1 (6%)
7	MAN	m	7	7	11,11,12	0.33	0	15,15,17	1.31	2 (13%)
9	NAG	n	1	1,9	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
9	MAN	n	10	9	11,11,12	0.33	0	15,15,17	0.93	2 (13%)
9	NAG	n	2	9	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
9	BMA	n	3	9	11,11,12	0.41	0	15,15,17	0.62	0
9	MAN	n	4	9	11,11,12	0.44	0	15,15,17	1.07	1 (6%)
9	MAN	n	5	9	11,11,12	0.47	0	15,15,17	1.04	2 (13%)
9	MAN	n	6	9	11,11,12	0.49	0	15,15,17	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	MAN	n	7	9	11,11,12	0.29	0	15,15,17	1.13	1 (6%)
9	MAN	n	8	9	11,11,12	0.39	0	15,15,17	1.27	1 (6%)
9	MAN	n	9	9	11,11,12	0.33	0	15,15,17	0.78	0
6	NAG	o	1	1,6	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	o	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	NAG	p	1	1,5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	p	2	5	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
5	BMA	p	3	5	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	q	1	1,5	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	q	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	BMA	q	3	5	11,11,12	0.65	0	15,15,17	1.48	3 (20%)
6	NAG	r	1	1,6	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	r	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	NAG	s	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	s	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	t	1	1,5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	t	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	BMA	t	3	5	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
6	NAG	u	1	1,6	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
6	NAG	u	2	6	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	NAG	v	1	1,5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	v	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	BMA	v	3	5	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	w	1	1,5	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	w	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	BMA	w	3	5	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
6	NAG	x	1	1,6	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	x	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	NAG	y	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	y	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
7	NAG	z	1	1,7	14,14,15	0.60	0	17,19,21	0.68	0
7	NAG	z	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	z	3	7	11,11,12	0.67	0	15,15,17	0.86	0
7	MAN	z	4	7	11,11,12	0.60	0	15,15,17	0.68	0
7	MAN	z	5	7	11,11,12	0.53	0	15,15,17	0.74	0
7	MAN	z	6	7	11,11,12	0.67	0	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MAN	z	7	7	11,11,12	0.62	0	15,15,17	0.63	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
5	NAG	0	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	2/2/19/22	0/1/1/1
8	NAG	1	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	BMA	1	3	8	-	2/2/19/22	0/1/1/1
8	MAN	1	4	8	-	0/2/19/22	0/1/1/1
8	MAN	1	5	8	-	0/2/19/22	0/1/1/1
7	NAG	2	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	2	2	7	-	1/6/23/26	0/1/1/1
7	BMA	2	3	7	-	0/2/19/22	0/1/1/1
7	MAN	2	4	7	-	2/2/19/22	0/1/1/1
7	MAN	2	5	7	-	0/2/19/22	0/1/1/1
7	MAN	2	6	7	-	2/2/19/22	0/1/1/1
7	MAN	2	7	7	-	1/2/19/22	0/1/1/1
9	NAG	3	1	1,9	-	0/6/23/26	0/1/1/1
9	MAN	3	10	9	-	1/2/19/22	0/1/1/1
9	NAG	3	2	9	-	1/6/23/26	0/1/1/1
9	BMA	3	3	9	-	0/2/19/22	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	-	0/2/19/22	0/1/1/1
9	MAN	3	7	9	-	0/2/19/22	0/1/1/1
9	MAN	3	8	9	-	0/2/19/22	0/1/1/1
9	MAN	3	9	9	-	1/2/19/22	0/1/1/1
6	NAG	4	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	4	2	6	-	0/6/23/26	0/1/1/1
5	NAG	5	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
5	BMA	5	3	5	-	2/2/19/22	0/1/1/1
5	NAG	6	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	2/2/19/22	0/1/1/1

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

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

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

There are no bond length outliers.

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2	2	NAG	C1-C2-N2	8.39	124.82	110.49
7	V	2	NAG	C1-C2-N2	8.39	124.81	110.49
7	m	2	NAG	C1-C2-N2	8.38	124.80	110.49
6	u	1	NAG	O5-C1-C2	-7.40	99.60	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	q	1	NAG	O5-C1-C2	-7.39	99.62	111.29
5	v	1	NAG	O5-C1-C2	-7.38	99.63	111.29
5	Z	1	NAG	O5-C1-C2	-7.38	99.63	111.29
5	6	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	0	1	NAG	O5-C1-C2	-7.38	99.64	111.29
6	x	1	NAG	O5-C1-C2	-7.38	99.64	111.29
6	h	1	NAG	O5-C1-C2	-7.38	99.64	111.29
6	8	1	NAG	O5-C1-C2	-7.37	99.65	111.29
6	b	1	NAG	O5-C1-C2	-7.37	99.65	111.29
6	s	1	NAG	O5-C1-C2	-7.37	99.65	111.29
6	AA	1	NAG	O5-C1-C2	-7.37	99.65	111.29
5	Y	1	NAG	O5-C1-C2	-7.37	99.65	111.29
6	N	1	NAG	O5-C1-C2	-7.37	99.65	111.29
6	c	1	NAG	O5-C1-C2	-7.37	99.66	111.29
6	e	1	NAG	O5-C1-C2	-7.37	99.66	111.29
6	4	1	NAG	O5-C1-C2	-7.37	99.66	111.29
6	X	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	t	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	p	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	5	1	NAG	O5-C1-C2	-7.36	99.66	111.29
6	i	1	NAG	O5-C1-C2	-7.36	99.66	111.29
6	y	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	O	1	NAG	O5-C1-C2	-7.36	99.66	111.29
6	Q	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	f	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	M	1	NAG	O5-C1-C2	-7.36	99.67	111.29
6	R	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	T	1	NAG	O5-C1-C2	-7.36	99.67	111.29
6	o	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	k	1	NAG	O5-C1-C2	-7.36	99.67	111.29
6	a	1	NAG	O5-C1-C2	-7.35	99.67	111.29
6	9	1	NAG	O5-C1-C2	-7.35	99.68	111.29
8	1	1	NAG	O5-C1-C2	-7.35	99.68	111.29
6	r	1	NAG	O5-C1-C2	-7.35	99.69	111.29
5	w	1	NAG	O5-C1-C2	-7.34	99.69	111.29
8	U	1	NAG	O5-C1-C2	-7.34	99.69	111.29
6	7	1	NAG	O5-C1-C2	-7.34	99.70	111.29
8	l	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	d	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	P	1	NAG	O5-C1-C2	-7.33	99.71	111.29
5	g	1	NAG	O5-C1-C2	-7.33	99.72	111.29
8	U	5	MAN	C1-C2-C3	6.94	118.20	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	5	MAN	C1-C2-C3	6.94	118.19	109.67
8	l	5	MAN	C1-C2-C3	6.90	118.14	109.67
9	n	8	MAN	C1-O5-C5	4.51	118.30	112.19
9	3	8	MAN	C1-O5-C5	4.50	118.29	112.19
9	W	8	MAN	C1-O5-C5	4.50	118.28	112.19
8	U	5	MAN	C2-C3-C4	-4.07	103.85	110.89
8	l	5	MAN	C2-C3-C4	-4.07	103.86	110.89
8	1	5	MAN	C2-C3-C4	-4.05	103.88	110.89
9	n	4	MAN	C1-O5-C5	3.86	117.42	112.19
9	W	4	MAN	C1-O5-C5	3.85	117.41	112.19
9	3	4	MAN	C1-O5-C5	3.83	117.38	112.19
9	W	6	MAN	C1-C2-C3	3.61	114.11	109.67
9	3	6	MAN	C1-C2-C3	3.61	114.10	109.67
9	n	6	MAN	C1-C2-C3	3.61	114.10	109.67
9	n	7	MAN	C1-O5-C5	3.55	117.01	112.19
5	t	2	NAG	O5-C5-C6	-3.54	101.65	107.20
9	3	7	MAN	C1-O5-C5	3.54	116.99	112.19
6	Q	2	NAG	O5-C5-C6	-3.54	101.65	107.20
6	x	2	NAG	O5-C5-C6	-3.54	101.66	107.20
6	h	2	NAG	O5-C5-C6	-3.54	101.66	107.20
5	M	2	NAG	O5-C5-C6	-3.54	101.66	107.20
8	1	2	NAG	O5-C5-C6	-3.54	101.66	107.20
5	p	2	NAG	O5-C5-C6	-3.53	101.67	107.20
9	W	7	MAN	C1-O5-C5	3.53	116.98	112.19
6	o	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	T	2	NAG	O5-C5-C6	-3.52	101.68	107.20
6	R	2	NAG	O5-C5-C6	-3.52	101.68	107.20
6	X	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	Y	2	NAG	O5-C5-C6	-3.52	101.68	107.20
6	r	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	6	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	k	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	w	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	d	2	NAG	O5-C5-C6	-3.52	101.69	107.20
8	U	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	5	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	O	2	NAG	O5-C5-C6	-3.52	101.69	107.20
6	i	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	0	2	NAG	O5-C5-C6	-3.51	101.69	107.20
5	Z	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	g	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	f	2	NAG	O5-C5-C6	-3.51	101.70	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	4	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	P	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	v	2	NAG	O5-C5-C6	-3.51	101.70	107.20
6	b	2	NAG	O5-C5-C6	-3.51	101.71	107.20
6	s	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	8	2	NAG	O5-C5-C6	-3.50	101.72	107.20
5	q	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	AA	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	c	2	NAG	O5-C5-C6	-3.50	101.72	107.20
8	l	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	y	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	N	2	NAG	O5-C5-C6	-3.49	101.72	107.20
6	a	2	NAG	O5-C5-C6	-3.49	101.73	107.20
6	9	2	NAG	O5-C5-C6	-3.49	101.73	107.20
6	e	2	NAG	O5-C5-C6	-3.49	101.73	107.20
6	7	2	NAG	O5-C5-C6	-3.47	101.76	107.20
6	u	2	NAG	O5-C5-C6	-3.47	101.76	107.20
8	U	5	MAN	O5-C1-C2	-3.44	105.47	110.77
8	l	5	MAN	O5-C1-C2	-3.43	105.48	110.77
8	1	5	MAN	O5-C1-C2	-3.43	105.48	110.77
7	2	7	MAN	C1-O5-C5	3.42	116.83	112.19
7	m	7	MAN	C1-O5-C5	3.42	116.82	112.19
7	V	7	MAN	C1-O5-C5	3.40	116.80	112.19
8	1	4	MAN	O5-C5-C6	3.38	112.50	107.20
8	l	4	MAN	O5-C5-C6	3.36	112.48	107.20
8	U	4	MAN	O5-C5-C6	3.36	112.47	107.20
7	2	4	MAN	C1-O5-C5	3.01	116.27	112.19
7	V	4	MAN	C1-O5-C5	3.01	116.27	112.19
7	m	4	MAN	C1-O5-C5	3.01	116.27	112.19
5	q	3	BMA	O2-C2-C3	2.98	116.10	110.14
5	t	3	BMA	O2-C2-C3	2.98	116.10	110.14
5	k	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	d	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	0	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	6	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	T	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	M	3	BMA	O2-C2-C3	2.97	116.09	110.14
5	5	3	BMA	O2-C2-C3	2.97	116.08	110.14
5	Z	3	BMA	O2-C2-C3	2.96	116.06	110.14
8	U	3	BMA	O2-C2-C3	2.95	116.06	110.14
5	Y	3	BMA	O2-C2-C3	2.95	116.05	110.14
5	P	3	BMA	O2-C2-C3	2.95	116.05	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	w	3	BMA	O2-C2-C3	2.95	116.04	110.14
5	p	3	BMA	O2-C2-C3	2.94	116.03	110.14
8	l	3	BMA	O2-C2-C3	2.94	116.03	110.14
5	g	3	BMA	O2-C2-C3	2.94	116.02	110.14
5	O	3	BMA	O2-C2-C3	2.94	116.02	110.14
5	f	3	BMA	O2-C2-C3	2.92	116.00	110.14
8	1	3	BMA	O2-C2-C3	2.92	116.00	110.14
5	v	3	BMA	O2-C2-C3	2.92	115.98	110.14
7	S	6	MAN	O5-C5-C6	2.84	111.65	107.20
7	z	6	MAN	O5-C5-C6	2.84	111.65	107.20
7	j	6	MAN	O5-C5-C6	2.84	111.65	107.20
5	5	1	NAG	O7-C7-C8	-2.81	116.84	122.06
5	w	1	NAG	O7-C7-C8	-2.81	116.84	122.06
5	g	1	NAG	O7-C7-C8	-2.81	116.85	122.06
6	9	1	NAG	O7-C7-C8	-2.80	116.85	122.06
7	V	3	BMA	O3-C3-C2	2.80	115.35	109.99
5	f	1	NAG	O7-C7-C8	-2.79	116.87	122.06
5	P	1	NAG	O7-C7-C8	-2.79	116.87	122.06
5	Y	1	NAG	O7-C7-C8	-2.79	116.87	122.06
7	2	3	BMA	O3-C3-C2	2.79	115.34	109.99
6	c	1	NAG	O7-C7-C8	-2.79	116.88	122.06
6	8	1	NAG	O7-C7-C8	-2.78	116.89	122.06
5	M	1	NAG	O7-C7-C8	-2.78	116.89	122.06
5	v	1	NAG	O7-C7-C8	-2.78	116.89	122.06
6	h	1	NAG	O7-C7-C8	-2.78	116.89	122.06
6	x	1	NAG	O7-C7-C8	-2.78	116.90	122.06
5	O	1	NAG	O7-C7-C8	-2.77	116.90	122.06
8	l	1	NAG	O7-C7-C8	-2.77	116.90	122.06
8	U	1	NAG	O7-C7-C8	-2.77	116.91	122.06
5	0	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	Q	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	AA	1	NAG	O7-C7-C8	-2.77	116.91	122.06
5	t	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	b	1	NAG	O7-C7-C8	-2.77	116.92	122.06
6	o	1	NAG	O7-C7-C8	-2.77	116.92	122.06
5	d	1	NAG	O7-C7-C8	-2.77	116.92	122.06
6	R	1	NAG	O7-C7-C8	-2.76	116.92	122.06
6	a	1	NAG	O7-C7-C8	-2.76	116.92	122.06
8	1	1	NAG	O7-C7-C8	-2.76	116.92	122.06
7	m	3	BMA	O3-C3-C2	2.76	115.29	109.99
6	r	1	NAG	O7-C7-C8	-2.76	116.92	122.06
5	p	1	NAG	O7-C7-C8	-2.76	116.93	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	i	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	Z	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	k	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	T	1	NAG	O7-C7-C8	-2.76	116.93	122.06
6	X	1	NAG	O7-C7-C8	-2.76	116.93	122.06
6	s	1	NAG	O7-C7-C8	-2.76	116.93	122.06
6	y	1	NAG	O7-C7-C8	-2.76	116.94	122.06
6	7	1	NAG	O7-C7-C8	-2.75	116.94	122.06
6	4	1	NAG	O7-C7-C8	-2.75	116.94	122.06
6	N	1	NAG	O7-C7-C8	-2.74	116.96	122.06
5	q	1	NAG	O7-C7-C8	-2.74	116.97	122.06
6	e	1	NAG	O7-C7-C8	-2.74	116.97	122.06
5	6	1	NAG	O7-C7-C8	-2.74	116.97	122.06
9	3	2	NAG	O5-C1-C2	-2.73	106.98	111.29
6	u	1	NAG	O7-C7-C8	-2.72	117.00	122.06
9	W	2	NAG	O5-C1-C2	-2.72	106.99	111.29
9	n	2	NAG	O5-C1-C2	-2.71	107.01	111.29
6	i	1	NAG	C4-C3-C2	-2.70	107.06	111.02
5	f	1	NAG	C4-C3-C2	-2.70	107.06	111.02
6	4	1	NAG	C4-C3-C2	-2.70	107.06	111.02
6	u	1	NAG	C4-C3-C2	-2.70	107.06	111.02
6	h	1	NAG	C4-C3-C2	-2.69	107.07	111.02
6	y	1	NAG	C4-C3-C2	-2.69	107.07	111.02
5	v	1	NAG	C4-C3-C2	-2.69	107.07	111.02
6	R	1	NAG	C4-C3-C2	-2.69	107.07	111.02
6	o	1	NAG	C4-C3-C2	-2.69	107.08	111.02
6	X	1	NAG	C4-C3-C2	-2.69	107.08	111.02
5	O	1	NAG	C4-C3-C2	-2.68	107.08	111.02
6	Q	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	N	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	c	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	9	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	s	1	NAG	C4-C3-C2	-2.68	107.09	111.02
8	1	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	8	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	AA	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	k	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	e	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	b	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	x	1	NAG	C4-C3-C2	-2.66	107.11	111.02
6	r	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	w	1	NAG	C4-C3-C2	-2.66	107.12	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	p	1	NAG	C4-C3-C2	-2.66	107.12	111.02
9	n	1	NAG	C1-O5-C5	2.66	115.80	112.19
8	U	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	5	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	T	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	0	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	P	1	NAG	C4-C3-C2	-2.65	107.14	111.02
8	l	1	NAG	C4-C3-C2	-2.65	107.14	111.02
5	0	3	BMA	O4-C4-C5	-2.65	102.73	109.30
5	P	3	BMA	O4-C4-C5	-2.65	102.73	109.30
5	M	1	NAG	C4-C3-C2	-2.64	107.14	111.02
5	T	3	BMA	O4-C4-C5	-2.64	102.74	109.30
5	Z	3	BMA	O4-C4-C5	-2.64	102.74	109.30
5	g	3	BMA	O4-C4-C5	-2.64	102.74	109.30
5	t	3	BMA	O4-C4-C5	-2.64	102.74	109.30
5	Z	1	NAG	C4-C3-C2	-2.64	107.15	111.02
5	g	1	NAG	C4-C3-C2	-2.64	107.15	111.02
5	q	1	NAG	C4-C3-C2	-2.64	107.15	111.02
5	t	1	NAG	C4-C3-C2	-2.64	107.15	111.02
5	d	3	BMA	O4-C4-C5	-2.64	102.75	109.30
5	w	3	BMA	O4-C4-C5	-2.64	102.75	109.30
5	k	3	BMA	O4-C4-C5	-2.64	102.75	109.30
5	d	1	NAG	C4-C3-C2	-2.64	107.16	111.02
5	6	3	BMA	O4-C4-C5	-2.64	102.75	109.30
5	O	3	BMA	O4-C4-C5	-2.63	102.76	109.30
5	q	3	BMA	O4-C4-C5	-2.63	102.76	109.30
5	Y	3	BMA	O4-C4-C5	-2.63	102.77	109.30
6	a	1	NAG	C4-C3-C2	-2.63	107.17	111.02
5	5	3	BMA	O4-C4-C5	-2.63	102.77	109.30
6	7	1	NAG	C4-C3-C2	-2.63	107.17	111.02
9	3	1	NAG	C1-O5-C5	2.63	115.75	112.19
5	M	3	BMA	O4-C4-C5	-2.62	102.78	109.30
5	f	3	BMA	O4-C4-C5	-2.62	102.78	109.30
8	l	3	BMA	O4-C4-C5	-2.62	102.79	109.30
5	6	1	NAG	C4-C3-C2	-2.62	107.18	111.02
8	1	3	BMA	O4-C4-C5	-2.62	102.79	109.30
8	U	3	BMA	O4-C4-C5	-2.62	102.80	109.30
7	2	2	NAG	C1-O5-C5	2.61	115.73	112.19
5	p	3	BMA	O4-C4-C5	-2.61	102.81	109.30
5	v	3	BMA	O4-C4-C5	-2.61	102.81	109.30
9	W	1	NAG	C1-O5-C5	2.61	115.73	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	2	NAG	C1-O5-C5	2.59	115.71	112.19
8	U	4	MAN	O5-C1-C2	2.58	114.75	110.77
7	m	2	NAG	C1-O5-C5	2.58	115.68	112.19
8	1	4	MAN	O5-C1-C2	2.57	114.74	110.77
8	l	4	MAN	O5-C1-C2	2.55	114.70	110.77
7	2	5	MAN	C1-C2-C3	2.54	112.78	109.67
7	V	5	MAN	C1-C2-C3	2.49	112.73	109.67
7	2	2	NAG	O5-C1-C2	-2.49	107.36	111.29
7	V	2	NAG	O5-C1-C2	-2.47	107.38	111.29
7	m	2	NAG	O5-C1-C2	-2.46	107.40	111.29
9	n	5	MAN	O2-C2-C3	-2.46	105.20	110.14
9	3	5	MAN	O2-C2-C3	-2.46	105.22	110.14
9	W	5	MAN	O2-C2-C3	-2.46	105.22	110.14
7	m	5	MAN	C1-C2-C3	2.45	112.68	109.67
5	v	3	BMA	C6-C5-C4	-2.44	107.29	113.00
5	q	3	BMA	C6-C5-C4	-2.44	107.30	113.00
5	6	3	BMA	C6-C5-C4	-2.43	107.30	113.00
5	p	3	BMA	C6-C5-C4	-2.43	107.31	113.00
5	5	3	BMA	C6-C5-C4	-2.43	107.31	113.00
5	Z	3	BMA	C6-C5-C4	-2.43	107.32	113.00
5	P	3	BMA	C6-C5-C4	-2.42	107.33	113.00
5	O	3	BMA	C6-C5-C4	-2.42	107.33	113.00
5	Y	3	BMA	C6-C5-C4	-2.42	107.33	113.00
5	w	3	BMA	C6-C5-C4	-2.42	107.33	113.00
5	d	3	BMA	C6-C5-C4	-2.42	107.34	113.00
5	0	3	BMA	C6-C5-C4	-2.42	107.34	113.00
5	t	3	BMA	C6-C5-C4	-2.42	107.35	113.00
5	g	3	BMA	C6-C5-C4	-2.41	107.35	113.00
5	M	3	BMA	C6-C5-C4	-2.41	107.35	113.00
5	T	3	BMA	C6-C5-C4	-2.41	107.36	113.00
7	m	7	MAN	O5-C1-C2	-2.41	107.05	110.77
7	m	3	BMA	O3-C3-C4	2.41	115.92	110.35
5	f	3	BMA	C6-C5-C4	-2.41	107.36	113.00
8	U	3	BMA	C6-C5-C4	-2.41	107.37	113.00
8	l	3	BMA	C6-C5-C4	-2.41	107.37	113.00
8	1	3	BMA	C6-C5-C4	-2.40	107.37	113.00
7	V	7	MAN	O5-C1-C2	-2.40	107.06	110.77
5	k	3	BMA	C6-C5-C4	-2.39	107.40	113.00
7	V	3	BMA	O3-C3-C4	2.39	115.88	110.35
7	2	7	MAN	O5-C1-C2	-2.39	107.08	110.77
7	2	3	BMA	O3-C3-C4	2.39	115.87	110.35
9	n	10	MAN	C1-O5-C5	2.35	115.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	10	MAN	C1-O5-C5	2.32	115.34	112.19
6	i	2	NAG	O5-C1-C2	-2.31	107.64	111.29
6	o	2	NAG	O5-C1-C2	-2.30	107.65	111.29
6	R	2	NAG	O5-C1-C2	-2.30	107.65	111.29
9	3	10	MAN	C1-O5-C5	2.30	115.31	112.19
6	y	2	NAG	O5-C1-C2	-2.30	107.66	111.29
6	r	2	NAG	O5-C1-C2	-2.29	107.67	111.29
5	O	2	NAG	O5-C1-C2	-2.28	107.68	111.29
5	q	2	NAG	O5-C1-C2	-2.28	107.69	111.29
6	X	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	d	2	NAG	O5-C1-C2	-2.28	107.69	111.29
6	e	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	v	2	NAG	O5-C1-C2	-2.28	107.69	111.29
6	a	2	NAG	O5-C1-C2	-2.27	107.70	111.29
6	s	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	Y	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	Z	2	NAG	O5-C1-C2	-2.27	107.71	111.29
5	g	2	NAG	O5-C1-C2	-2.27	107.71	111.29
5	k	2	NAG	O5-C1-C2	-2.27	107.71	111.29
6	7	2	NAG	O5-C1-C2	-2.27	107.71	111.29
5	t	2	NAG	O5-C1-C2	-2.26	107.71	111.29
8	U	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	M	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	T	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	6	2	NAG	O5-C1-C2	-2.26	107.72	111.29
6	N	2	NAG	O5-C1-C2	-2.26	107.72	111.29
6	b	2	NAG	O5-C1-C2	-2.26	107.73	111.29
6	h	2	NAG	O5-C1-C2	-2.26	107.73	111.29
6	9	2	NAG	O5-C1-C2	-2.26	107.73	111.29
8	l	2	NAG	O5-C1-C2	-2.25	107.73	111.29
5	f	2	NAG	O5-C1-C2	-2.25	107.73	111.29
6	x	2	NAG	O5-C1-C2	-2.25	107.73	111.29
6	4	2	NAG	O5-C1-C2	-2.25	107.73	111.29
5	0	2	NAG	O5-C1-C2	-2.25	107.73	111.29
7	V	2	NAG	C4-C3-C2	-2.25	107.72	111.02
6	c	2	NAG	O5-C1-C2	-2.25	107.73	111.29
5	5	2	NAG	O5-C1-C2	-2.25	107.73	111.29
6	Q	2	NAG	O5-C1-C2	-2.25	107.74	111.29
7	m	2	NAG	C4-C3-C2	-2.24	107.73	111.02
5	p	2	NAG	O5-C1-C2	-2.24	107.75	111.29
8	1	2	NAG	O5-C1-C2	-2.24	107.75	111.29
6	8	2	NAG	O5-C1-C2	-2.24	107.75	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AA	2	NAG	O5-C1-C2	-2.24	107.75	111.29
6	u	2	NAG	O5-C1-C2	-2.24	107.75	111.29
6	r	2	NAG	C4-C3-C2	-2.24	107.73	111.02
5	w	2	NAG	O5-C1-C2	-2.24	107.76	111.29
5	P	2	NAG	O5-C1-C2	-2.24	107.76	111.29
6	a	2	NAG	C4-C3-C2	-2.23	107.74	111.02
5	p	2	NAG	C4-C3-C2	-2.23	107.75	111.02
7	2	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	d	2	NAG	C4-C3-C2	-2.23	107.76	111.02
5	t	2	NAG	C4-C3-C2	-2.22	107.76	111.02
6	e	2	NAG	C4-C3-C2	-2.22	107.76	111.02
6	7	2	NAG	C4-C3-C2	-2.22	107.77	111.02
6	4	2	NAG	C4-C3-C2	-2.22	107.77	111.02
5	Y	2	NAG	C4-C3-C2	-2.22	107.77	111.02
8	1	2	NAG	C4-C3-C2	-2.22	107.77	111.02
5	M	2	NAG	C4-C3-C2	-2.22	107.77	111.02
5	q	2	NAG	C4-C3-C2	-2.21	107.77	111.02
5	v	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	6	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	f	2	NAG	C4-C3-C2	-2.21	107.78	111.02
6	c	2	NAG	C4-C3-C2	-2.21	107.78	111.02
6	s	2	NAG	C4-C3-C2	-2.21	107.78	111.02
6	X	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	O	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	Z	2	NAG	C4-C3-C2	-2.21	107.79	111.02
6	9	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	N	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	8	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	5	2	NAG	C4-C3-C2	-2.19	107.80	111.02
8	U	2	NAG	C4-C3-C2	-2.19	107.80	111.02
6	b	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	R	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	u	2	NAG	C4-C3-C2	-2.19	107.81	111.02
5	0	2	NAG	C4-C3-C2	-2.19	107.81	111.02
8	l	4	MAN	O3-C3-C4	2.19	115.41	110.35
6	i	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	AA	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	o	2	NAG	C4-C3-C2	-2.18	107.82	111.02
9	3	5	MAN	C1-O5-C5	2.18	115.15	112.19
5	k	2	NAG	C4-C3-C2	-2.18	107.82	111.02
8	l	2	NAG	C4-C3-C2	-2.18	107.82	111.02
8	U	4	MAN	O3-C3-C4	2.18	115.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	x	2	NAG	C4-C3-C2	-2.18	107.83	111.02
5	T	2	NAG	C4-C3-C2	-2.18	107.83	111.02
6	h	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	y	2	NAG	C4-C3-C2	-2.17	107.84	111.02
9	W	5	MAN	C1-O5-C5	2.17	115.13	112.19
8	1	4	MAN	O3-C3-C4	2.16	115.35	110.35
7	m	1	NAG	C1-C2-N2	2.16	114.18	110.49
6	Q	2	NAG	C4-C3-C2	-2.16	107.86	111.02
9	n	5	MAN	C1-O5-C5	2.15	115.10	112.19
5	P	2	NAG	C4-C3-C2	-2.14	107.89	111.02
7	V	1	NAG	C1-C2-N2	2.13	114.13	110.49
5	g	2	NAG	C4-C3-C2	-2.13	107.89	111.02
9	n	10	MAN	C1-C2-C3	2.13	112.28	109.67
5	w	2	NAG	C4-C3-C2	-2.12	107.91	111.02
7	2	1	NAG	C1-C2-N2	2.12	114.11	110.49
9	3	10	MAN	C1-C2-C3	2.12	112.27	109.67
9	W	10	MAN	C1-C2-C3	2.11	112.26	109.67
7	V	6	MAN	C1-O5-C5	2.08	115.01	112.19
8	1	5	MAN	O5-C5-C6	-2.08	103.95	107.20
7	m	6	MAN	C1-O5-C5	2.06	114.99	112.19
8	l	4	MAN	O4-C4-C3	-2.06	105.58	110.35
8	l	5	MAN	O5-C5-C6	-2.06	103.98	107.20
7	2	6	MAN	C1-O5-C5	2.06	114.98	112.19
8	U	5	MAN	O5-C5-C6	-2.05	103.99	107.20
8	U	4	MAN	O4-C4-C3	-2.04	105.63	110.35
8	1	4	MAN	O4-C4-C3	-2.04	105.63	110.35
7	j	6	MAN	C1-O5-C5	-2.03	109.45	112.19
7	S	6	MAN	C1-O5-C5	-2.01	109.46	112.19

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
5	0	1	NAG	O5-C5-C6-O6
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
7	m	1	NAG	C8-C7-N2-C2
7	m	1	NAG	O7-C7-N2-C2
7	2	1	NAG	C8-C7-N2-C2
7	2	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	S	5	MAN	O5-C5-C6-O6
7	j	5	MAN	O5-C5-C6-O6
7	z	5	MAN	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	0	1	NAG	C4-C5-C6-O6
7	V	6	MAN	O5-C5-C6-O6
7	m	6	MAN	O5-C5-C6-O6
7	2	6	MAN	O5-C5-C6-O6
7	S	2	NAG	C8-C7-N2-C2
7	j	2	NAG	C8-C7-N2-C2
7	z	2	NAG	C8-C7-N2-C2
7	V	1	NAG	C1-C2-N2-C7
7	V	2	NAG	C1-C2-N2-C7
7	m	1	NAG	C1-C2-N2-C7
7	m	2	NAG	C1-C2-N2-C7
7	2	1	NAG	C1-C2-N2-C7
7	2	2	NAG	C1-C2-N2-C7
7	z	3	BMA	C4-C5-C6-O6
7	S	3	BMA	C4-C5-C6-O6
7	S	6	MAN	C4-C5-C6-O6
7	j	3	BMA	C4-C5-C6-O6
7	j	6	MAN	C4-C5-C6-O6
7	z	6	MAN	C4-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6
9	n	4	MAN	O5-C5-C6-O6
9	3	4	MAN	O5-C5-C6-O6
7	S	6	MAN	O5-C5-C6-O6
7	j	6	MAN	O5-C5-C6-O6
7	z	6	MAN	O5-C5-C6-O6
7	S	2	NAG	O7-C7-N2-C2
7	j	2	NAG	O7-C7-N2-C2
7	z	2	NAG	O7-C7-N2-C2
9	W	10	MAN	O5-C5-C6-O6
9	n	10	MAN	O5-C5-C6-O6
9	3	10	MAN	O5-C5-C6-O6
7	V	7	MAN	O5-C5-C6-O6
7	m	7	MAN	O5-C5-C6-O6
7	2	7	MAN	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
9	3	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	S	3	BMA	O5-C5-C6-O6
7	j	3	BMA	O5-C5-C6-O6
7	z	3	BMA	O5-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	f	3	BMA	C4-C5-C6-O6
5	p	3	BMA	C4-C5-C6-O6
5	v	3	BMA	C4-C5-C6-O6
5	w	3	BMA	C4-C5-C6-O6
5	0	3	BMA	C4-C5-C6-O6
5	5	3	BMA	C4-C5-C6-O6
8	U	3	BMA	C4-C5-C6-O6
8	l	3	BMA	C4-C5-C6-O6
8	1	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
5	d	3	BMA	C4-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6
5	k	3	BMA	C4-C5-C6-O6
5	t	3	BMA	C4-C5-C6-O6
5	q	3	BMA	C4-C5-C6-O6
5	6	3	BMA	C4-C5-C6-O6
7	2	4	MAN	C4-C5-C6-O6
7	V	4	MAN	C4-C5-C6-O6
6	b	1	NAG	C4-C5-C6-O6
6	s	1	NAG	C4-C5-C6-O6
6	8	1	NAG	C4-C5-C6-O6
7	m	4	MAN	C4-C5-C6-O6
5	5	3	BMA	O5-C5-C6-O6
5	p	3	BMA	O5-C5-C6-O6
5	v	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	q	3	BMA	O5-C5-C6-O6
5	0	3	BMA	O5-C5-C6-O6
5	6	3	BMA	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6

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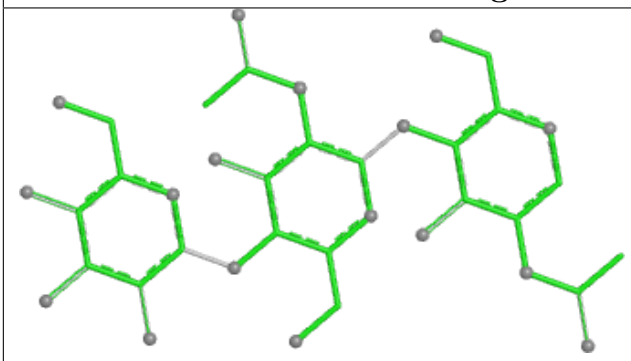
Mol	Chain	Res	Type	Atoms
5	f	3	BMA	O5-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
5	w	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	t	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
8	U	3	BMA	O5-C5-C6-O6
8	l	3	BMA	O5-C5-C6-O6
8	1	3	BMA	O5-C5-C6-O6
7	z	5	MAN	C4-C5-C6-O6
7	S	5	MAN	C4-C5-C6-O6
7	j	5	MAN	C4-C5-C6-O6
6	s	1	NAG	O5-C5-C6-O6
6	8	1	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
7	V	4	MAN	O5-C5-C6-O6
7	m	4	MAN	O5-C5-C6-O6
7	2	4	MAN	O5-C5-C6-O6
7	2	6	MAN	C4-C5-C6-O6
7	V	6	MAN	C4-C5-C6-O6
7	m	6	MAN	C4-C5-C6-O6
9	W	9	MAN	C4-C5-C6-O6
9	3	9	MAN	C4-C5-C6-O6
9	n	9	MAN	C4-C5-C6-O6
5	O	1	NAG	O7-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	f	1	NAG	O7-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	v	1	NAG	O7-C7-N2-C2
5	w	1	NAG	O7-C7-N2-C2
5	5	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	h	1	NAG	O7-C7-N2-C2
6	o	1	NAG	O7-C7-N2-C2
6	9	1	NAG	O7-C7-N2-C2

There are no ring outliers.

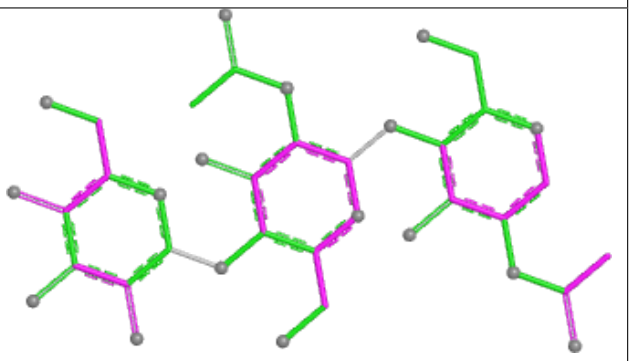
No monomer is involved in short contacts.

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

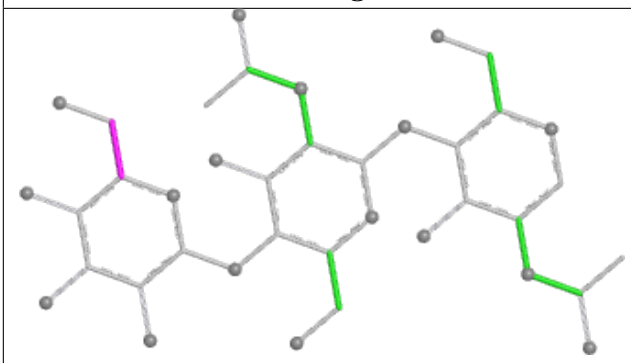
Oligosaccharide Chain M



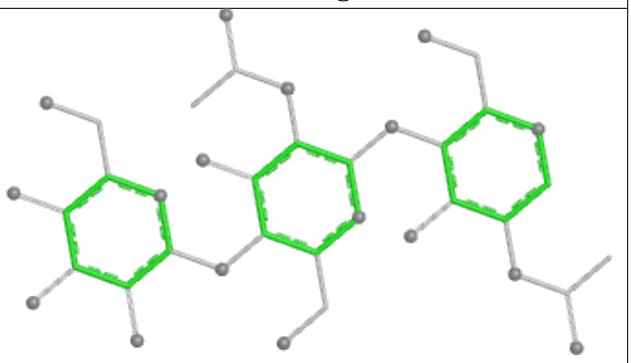
Bond lengths



Bond angles

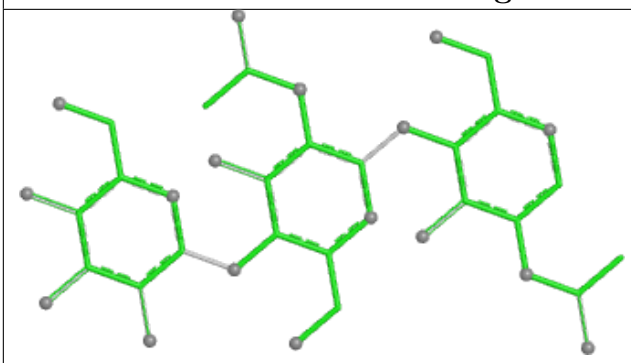


Torsions

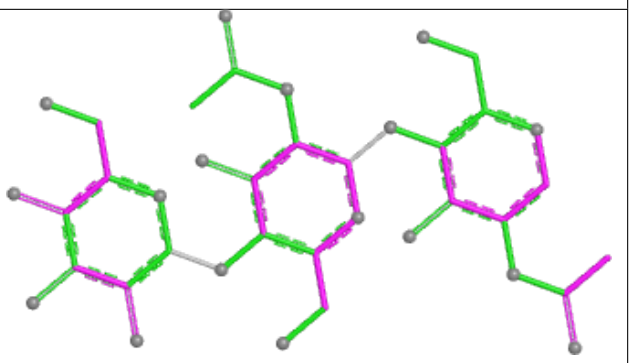


Rings

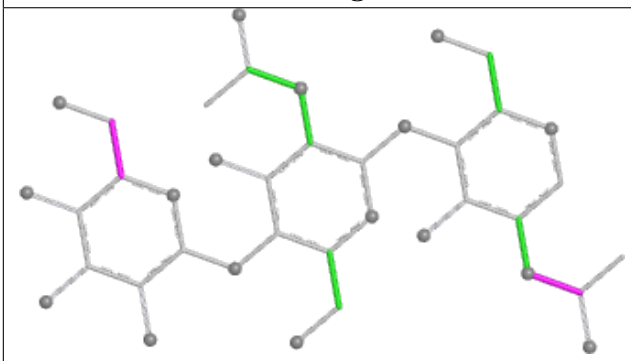
Oligosaccharide Chain O



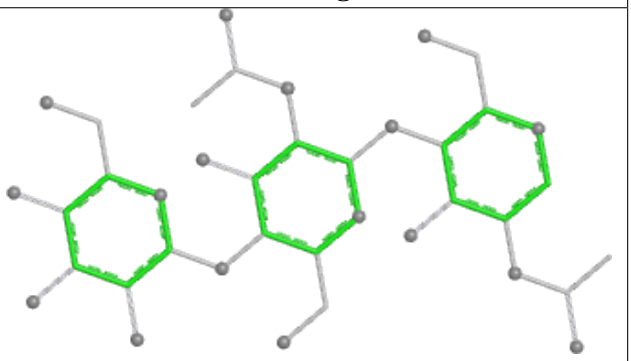
Bond lengths



Bond angles

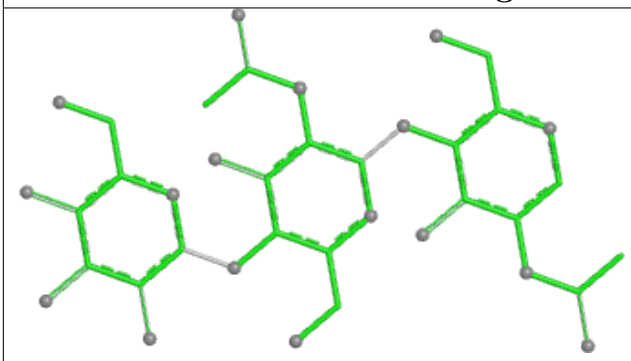


Torsions

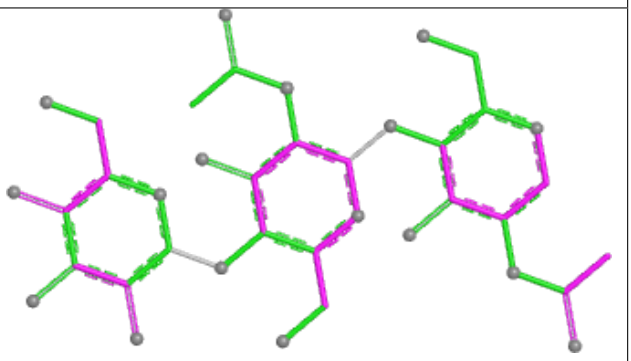


Rings

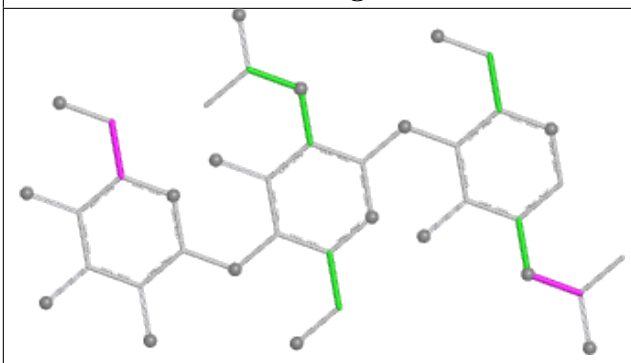
Oligosaccharide Chain P



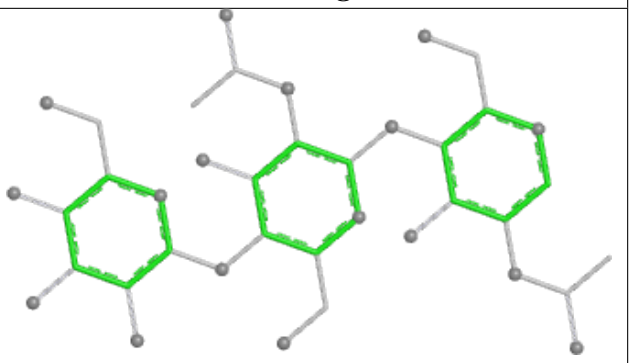
Bond lengths



Bond angles

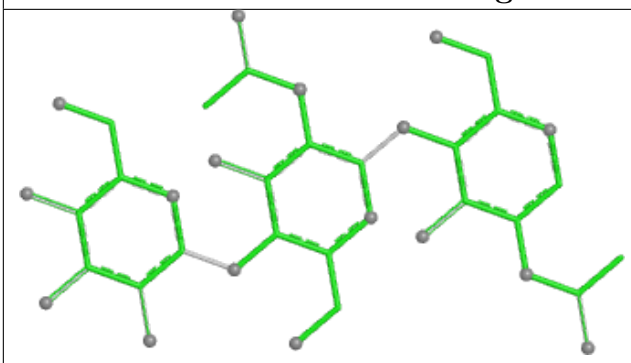


Torsions

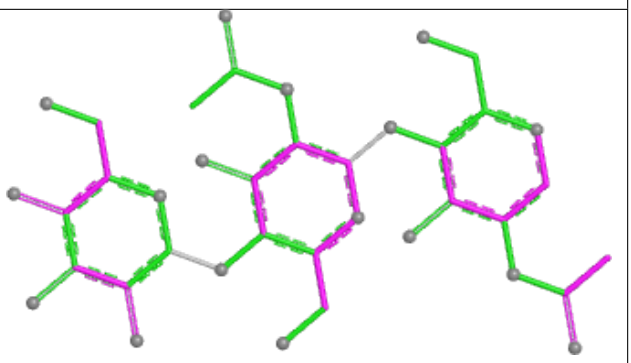


Rings

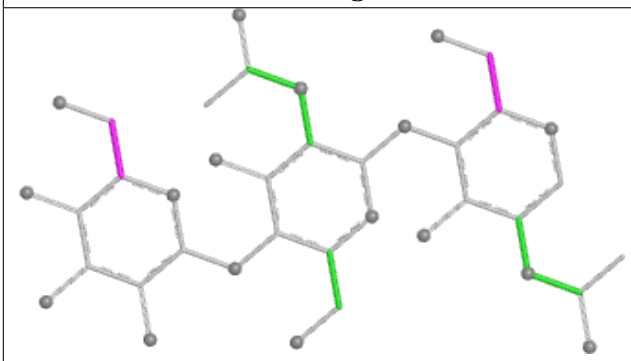
Oligosaccharide Chain T



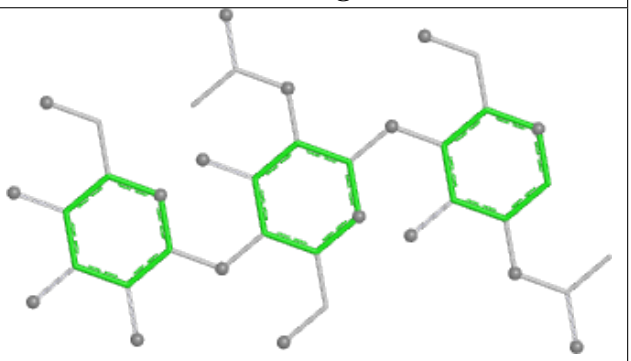
Bond lengths



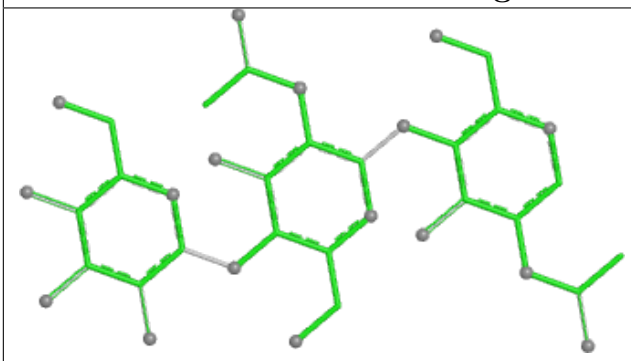
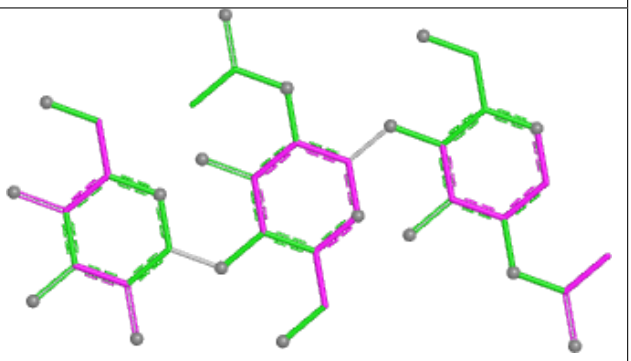
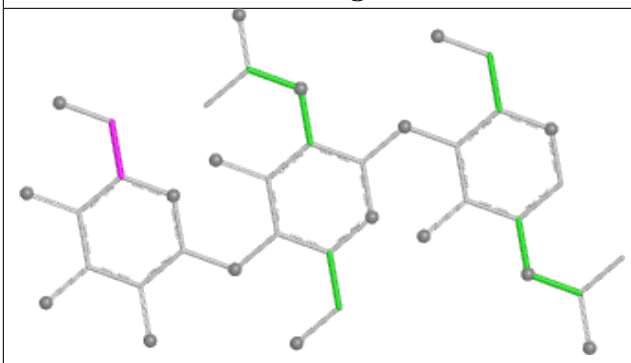
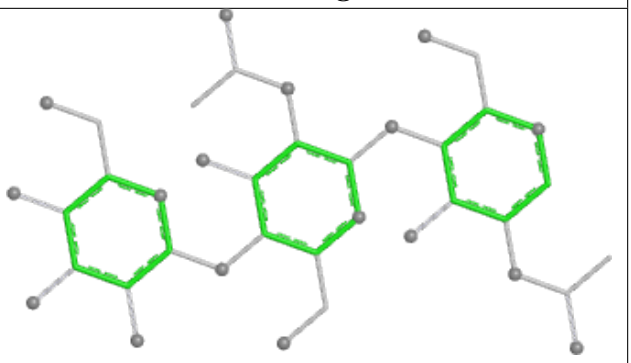
Bond angles

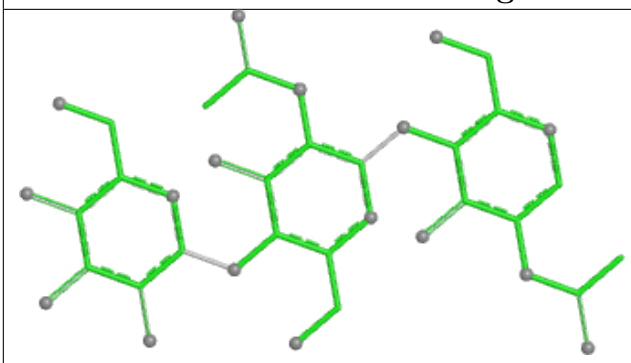
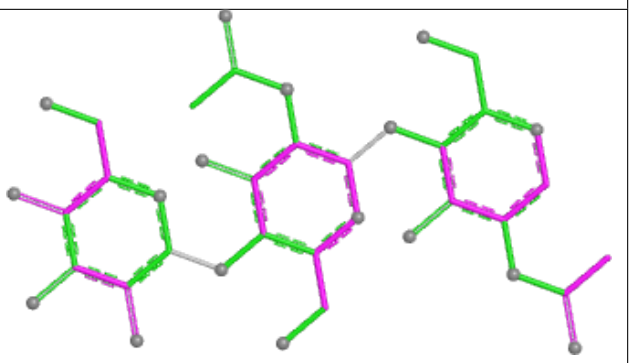
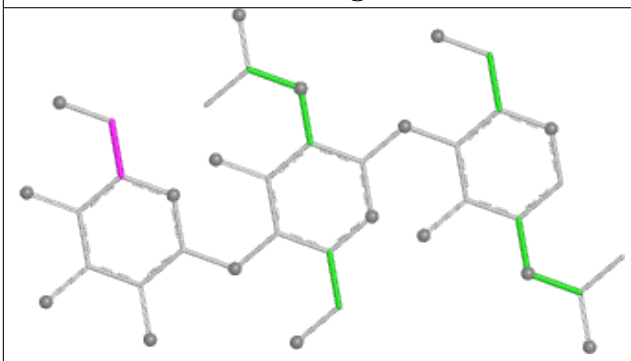
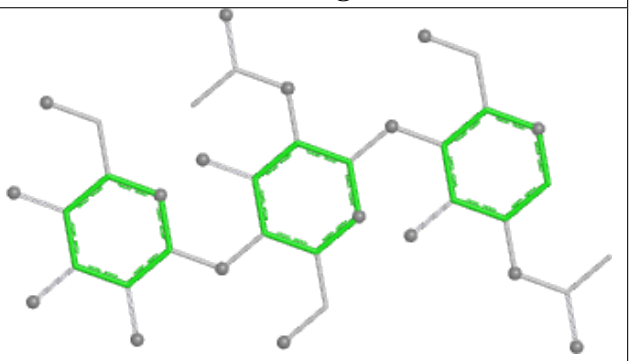


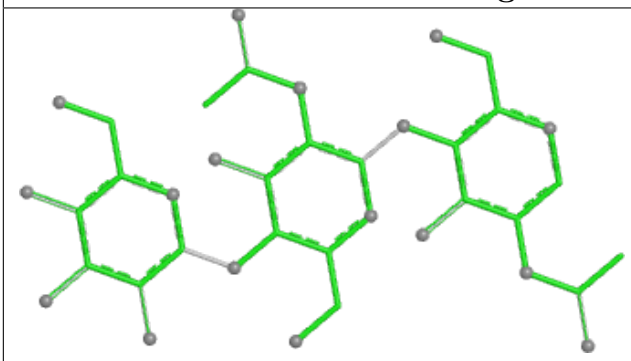
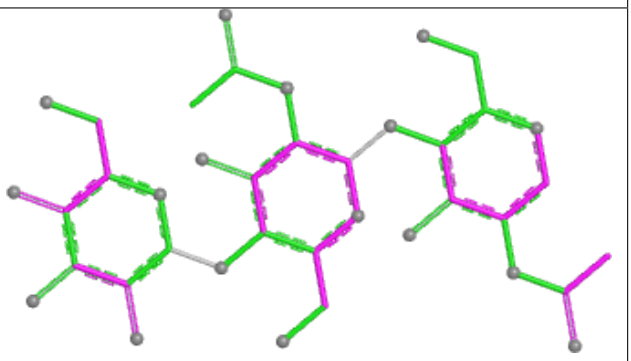
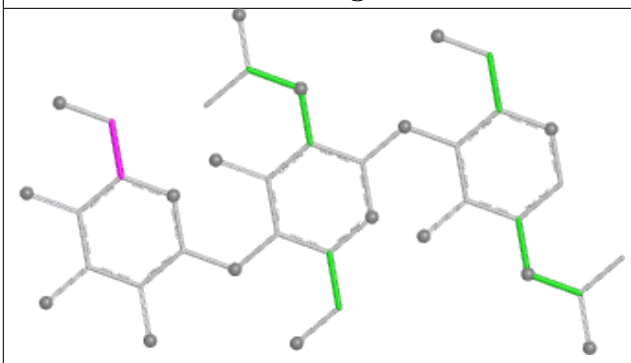
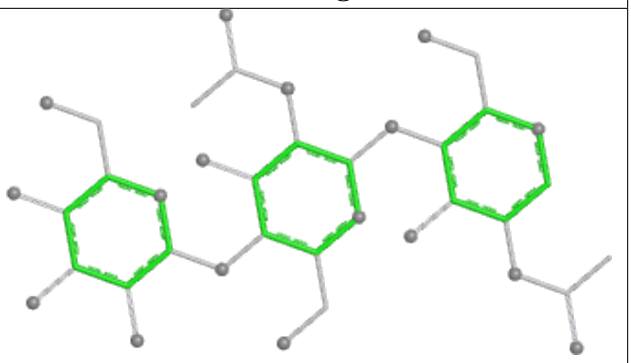
Torsions

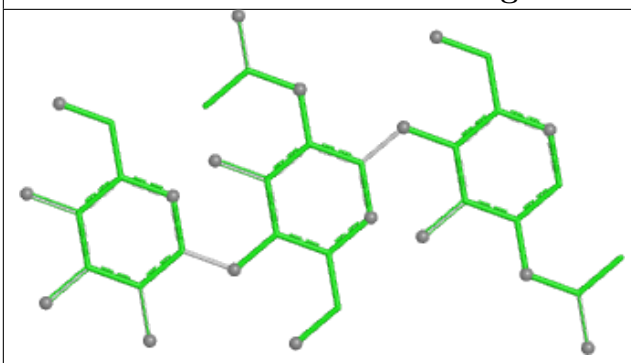
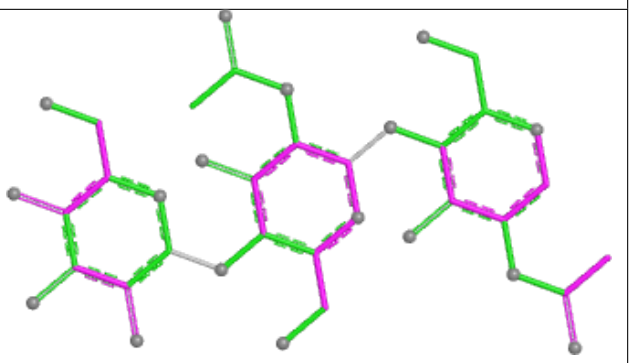
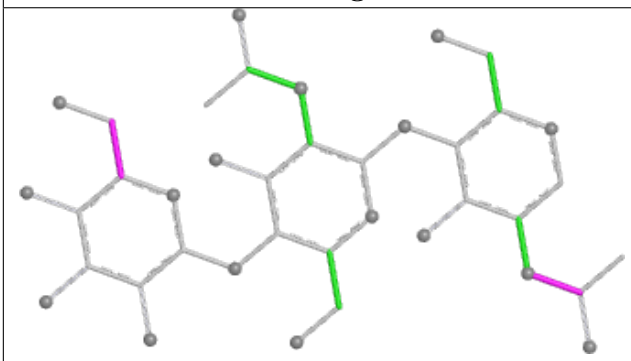
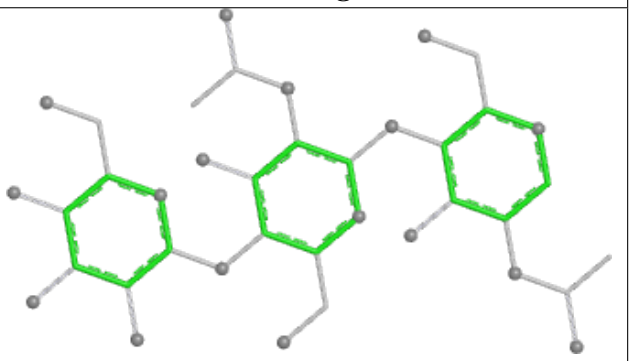


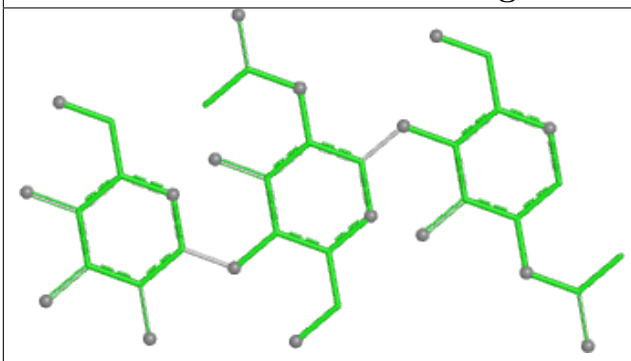
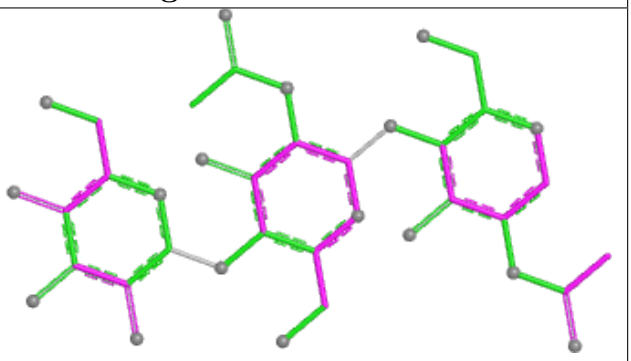
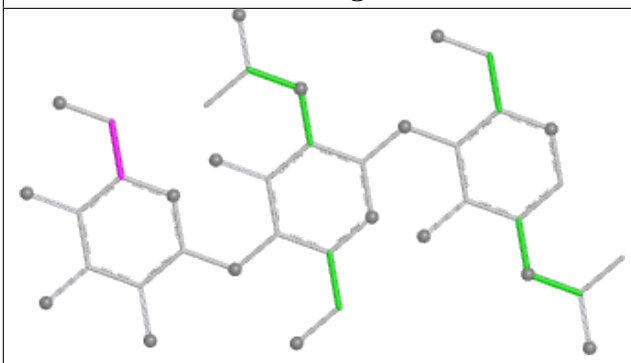
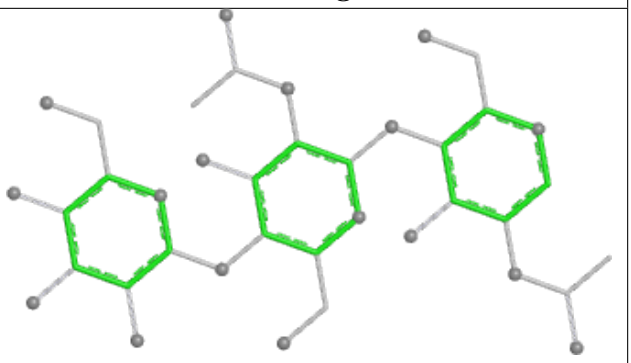
Rings

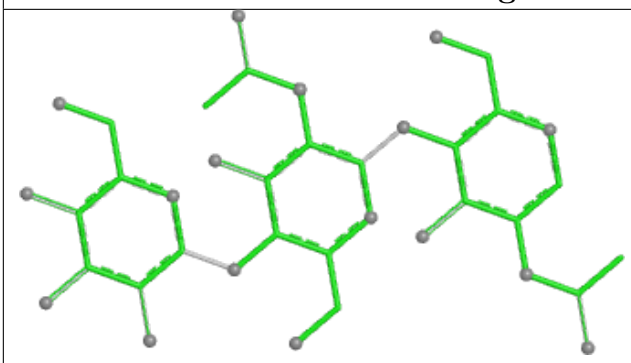
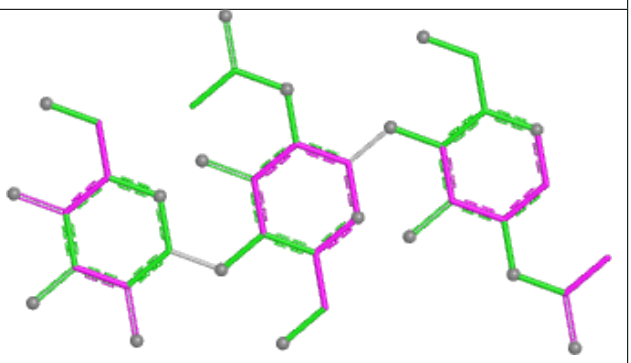
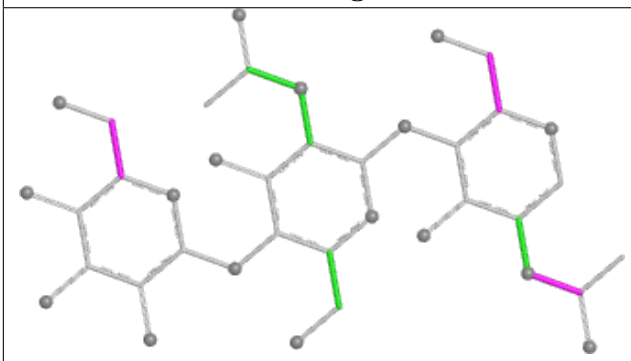
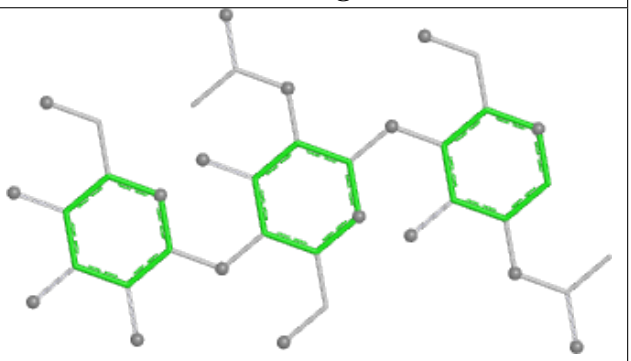
Oligosaccharide Chain Y	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

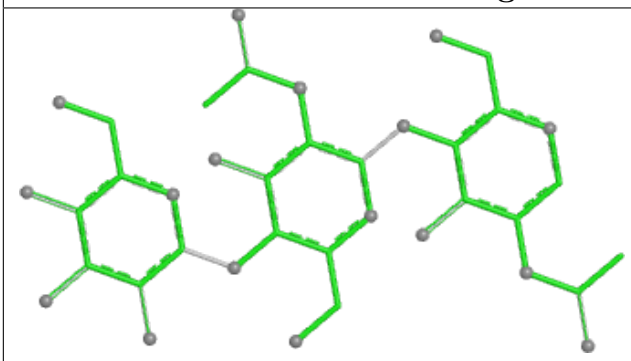
Oligosaccharide Chain d	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

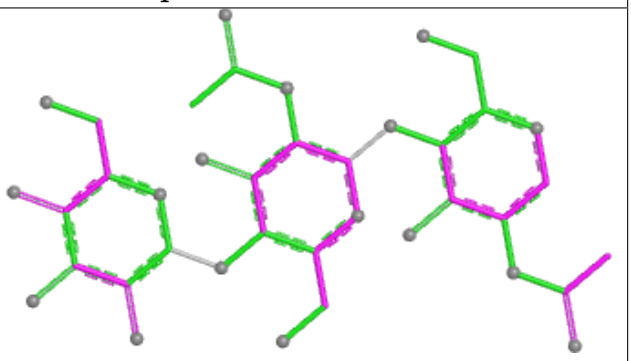
Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain k	
 Bond lengths	 Bond angles
 Torsions	 Rings

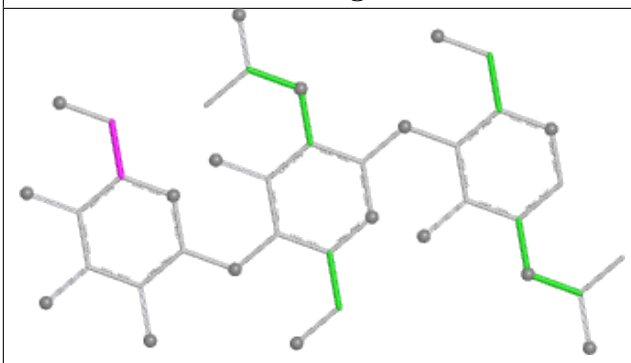
Oligosaccharide Chain p



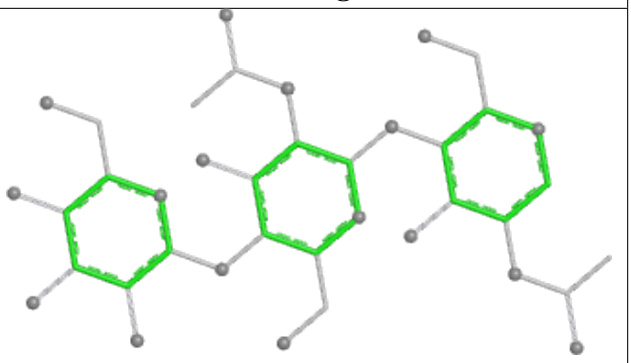
Bond lengths



Bond angles

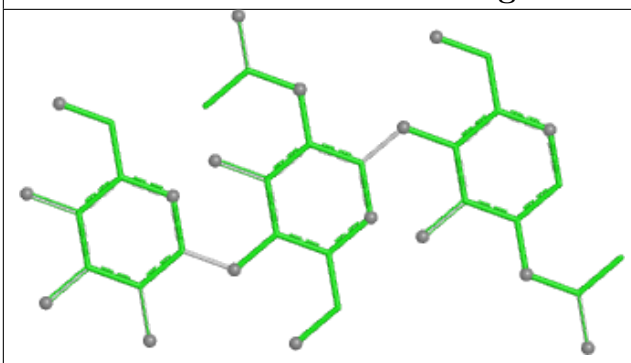


Torsions



Rings

Oligosaccharide Chain q



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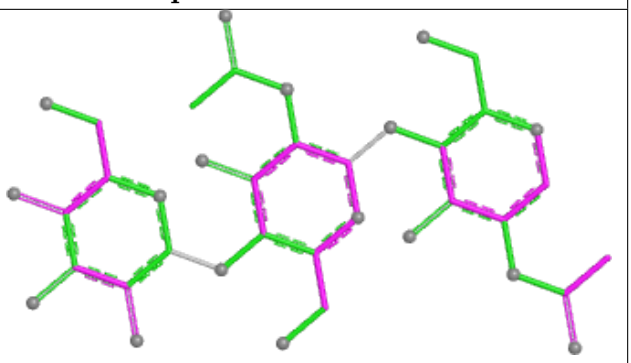

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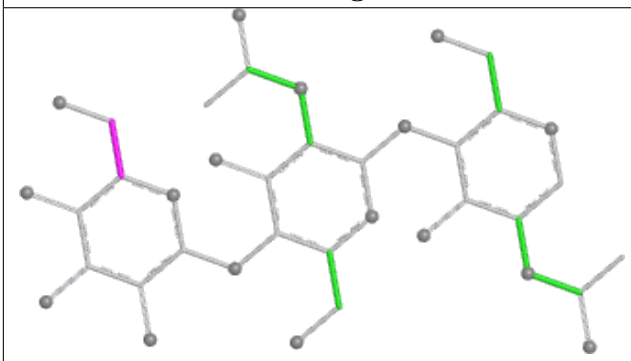

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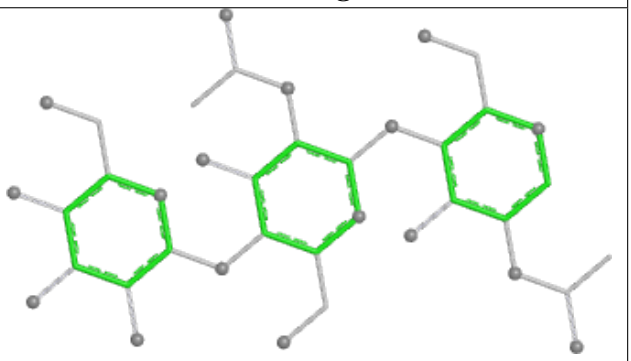
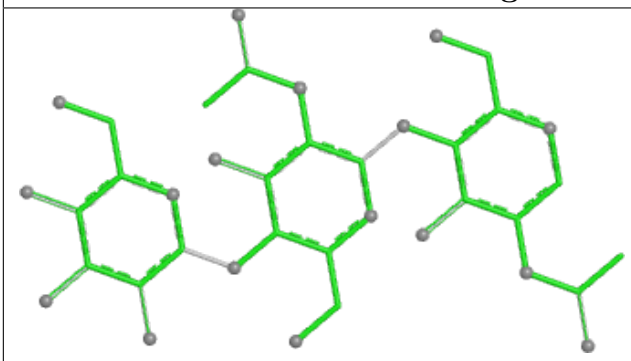
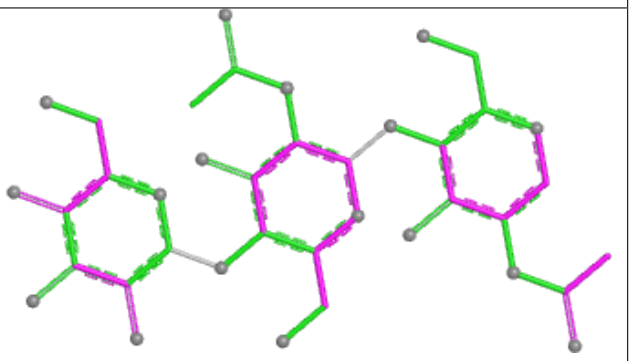
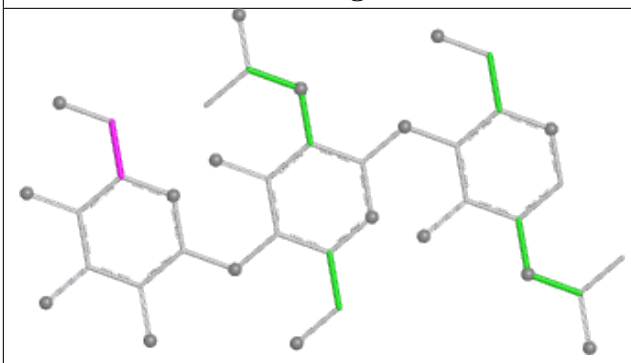
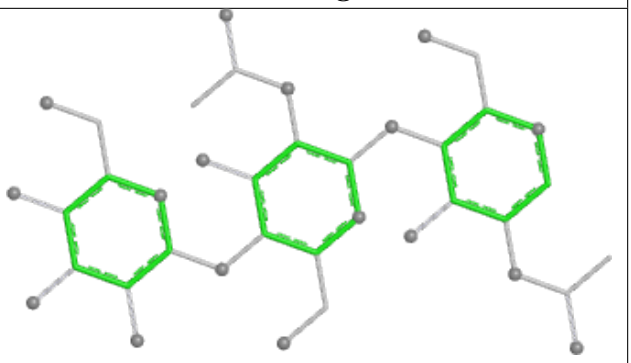
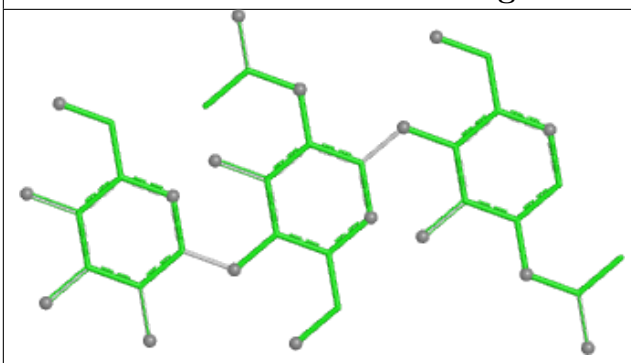
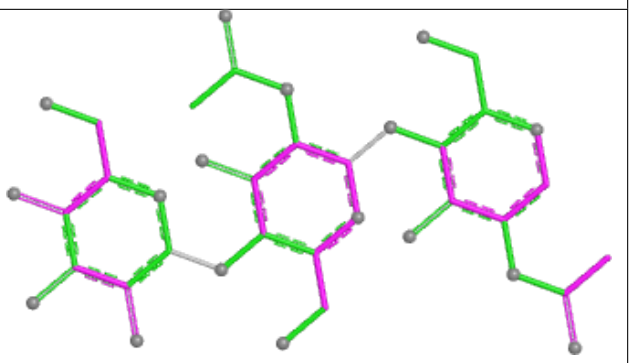
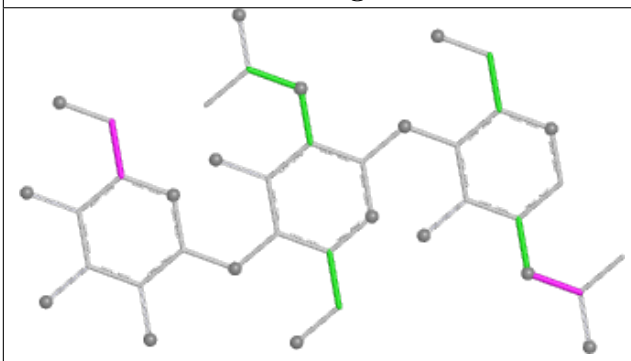
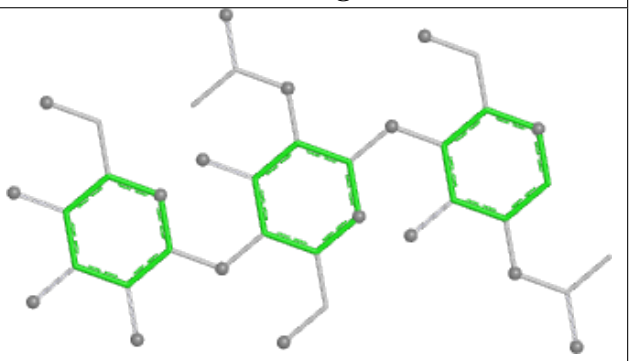
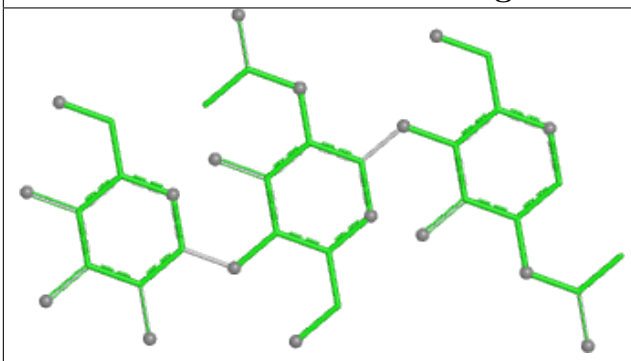
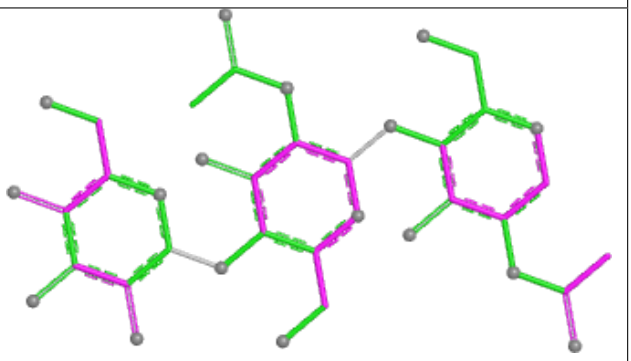
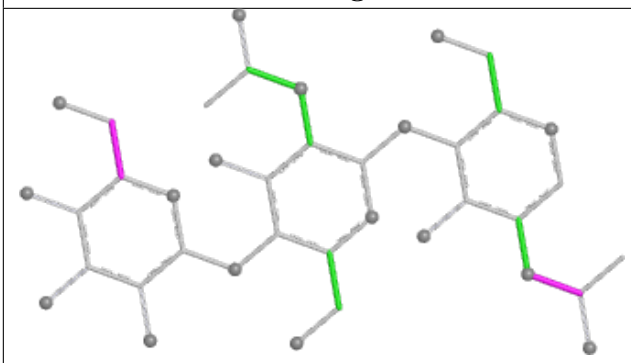
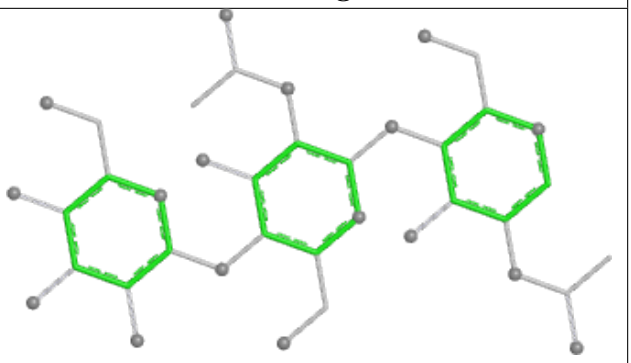
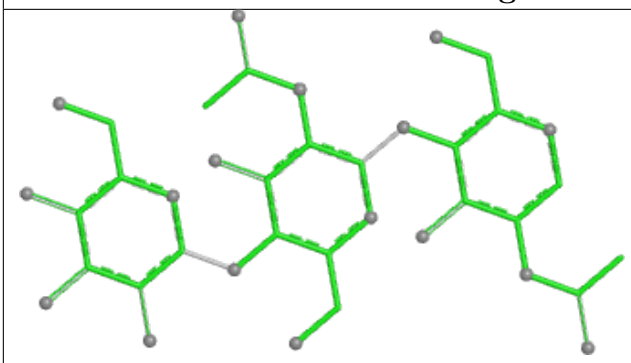
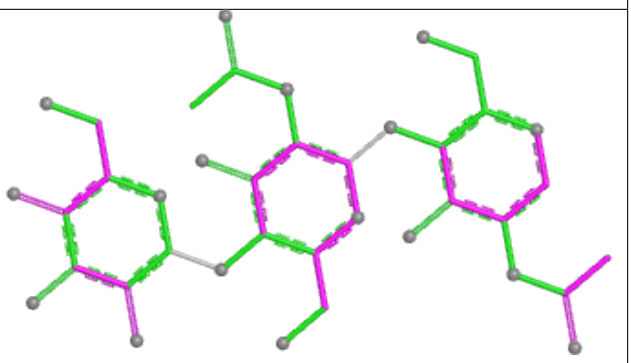
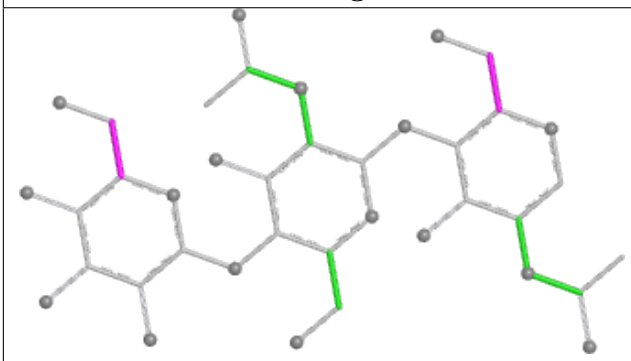
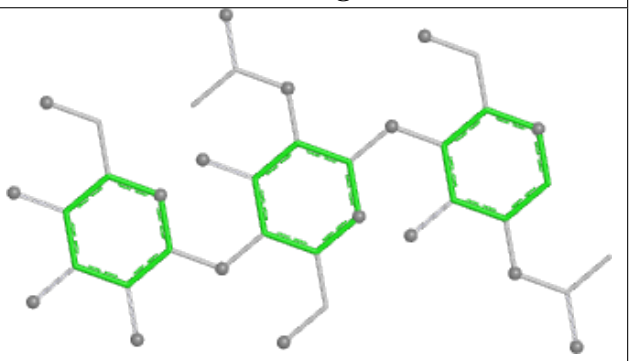


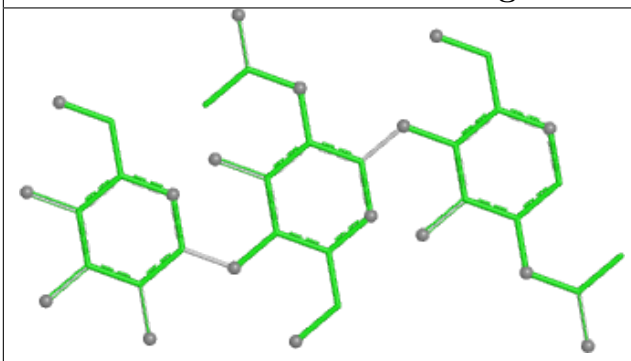
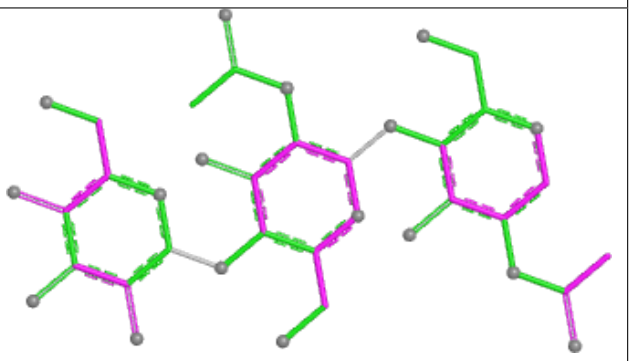
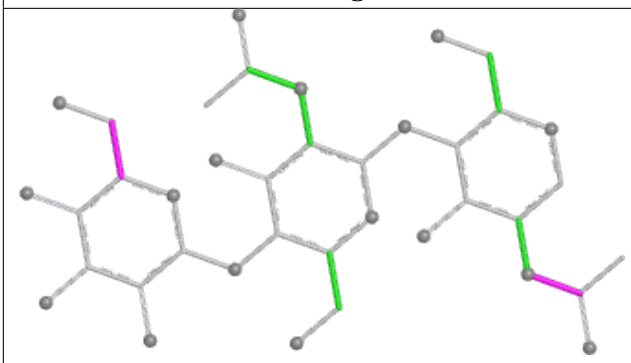
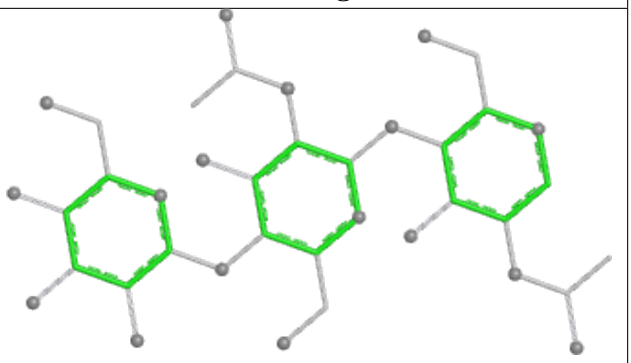
Rings

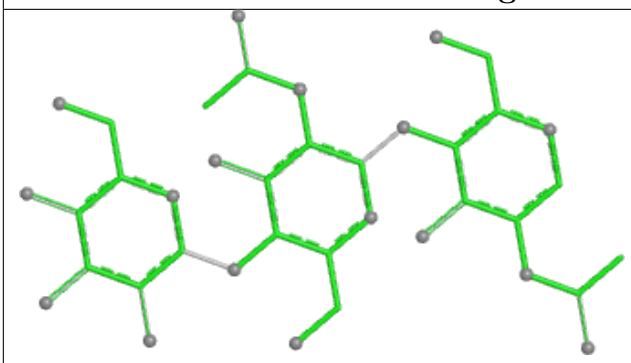
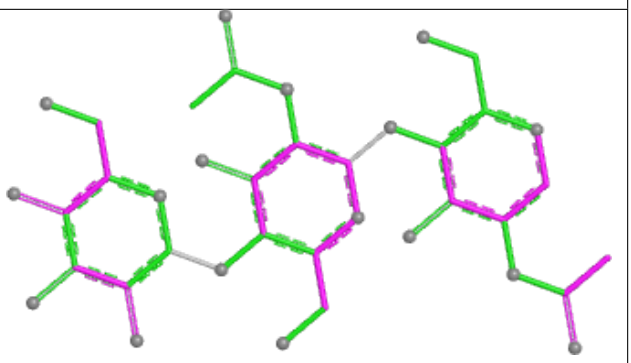
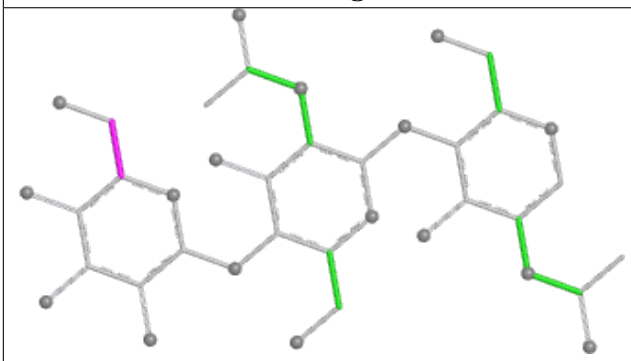
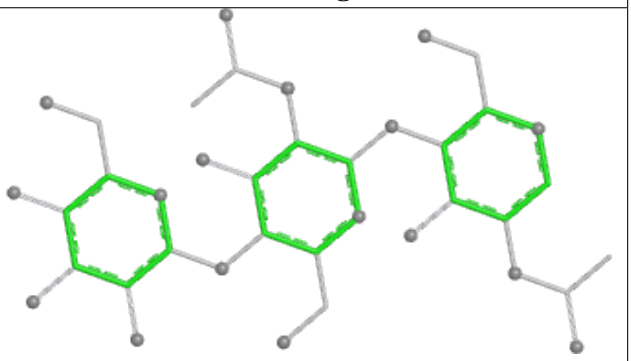
Oligosaccharide Chain t	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain v	
 Bond lengths	 Bond angles
 Torsions	 Rings

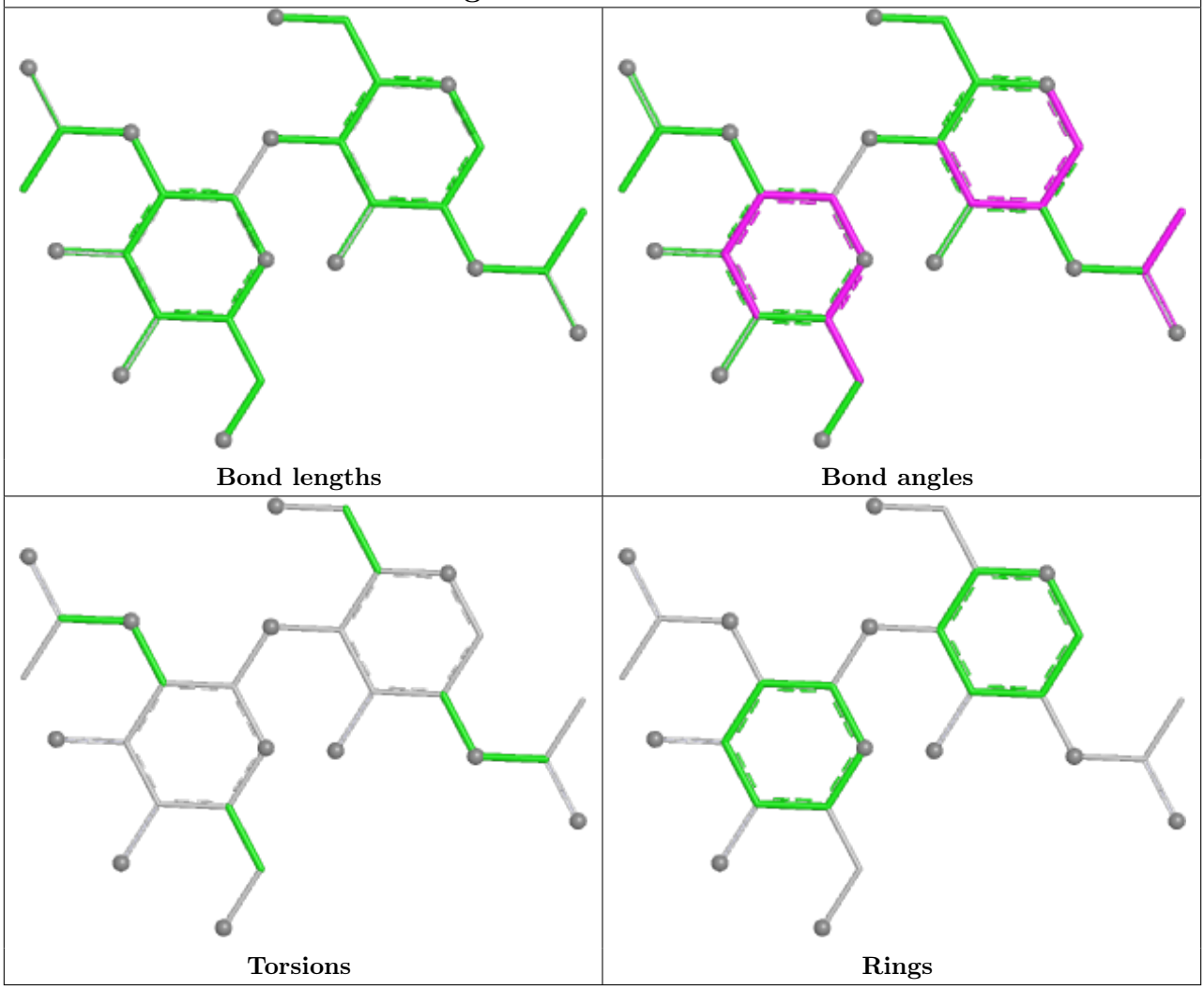
Oligosaccharide Chain w	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 0	
 Bond lengths	 Bond angles
 Torsions	 Rings

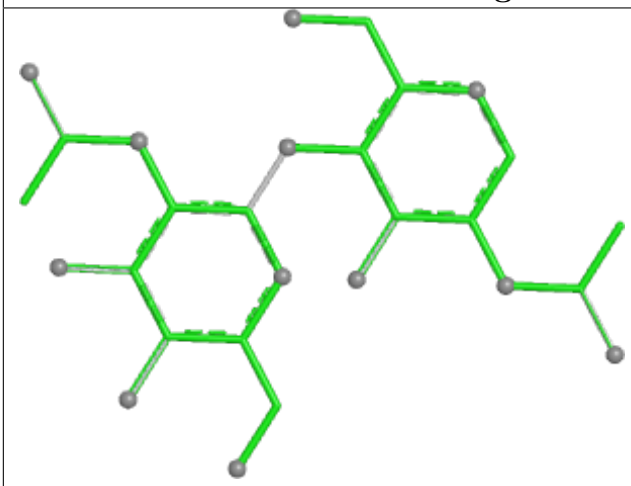
Oligosaccharide Chain 5	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 6	
 Bond lengths	 Bond angles
 Torsions	 Rings

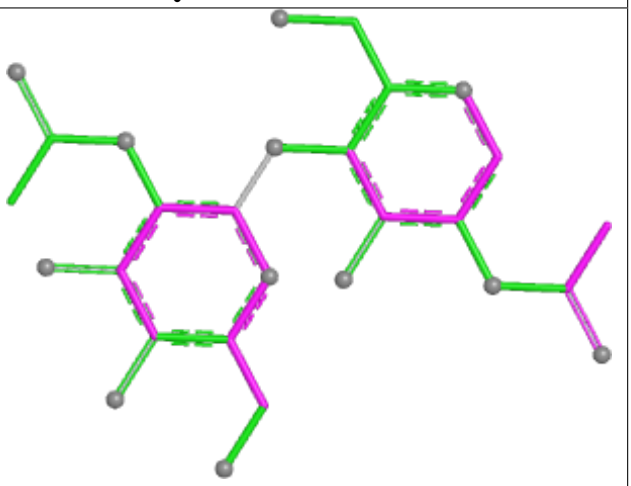
Oligosaccharide Chain N



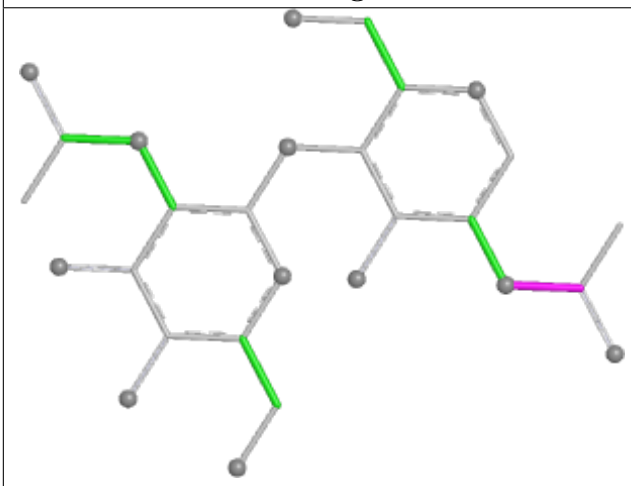
Oligosaccharide Chain Q



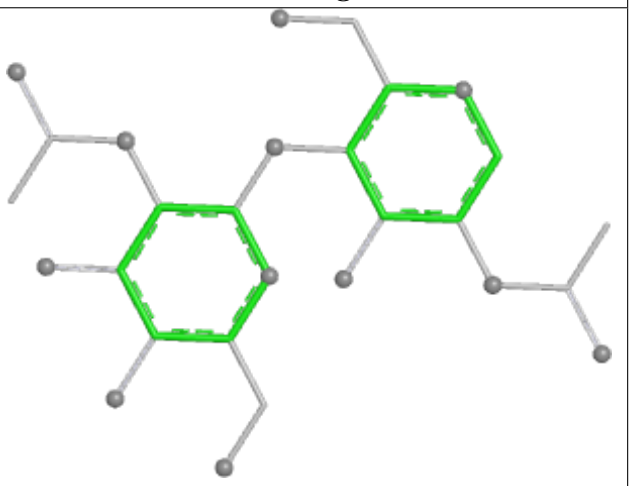
Bond lengths



Bond angles

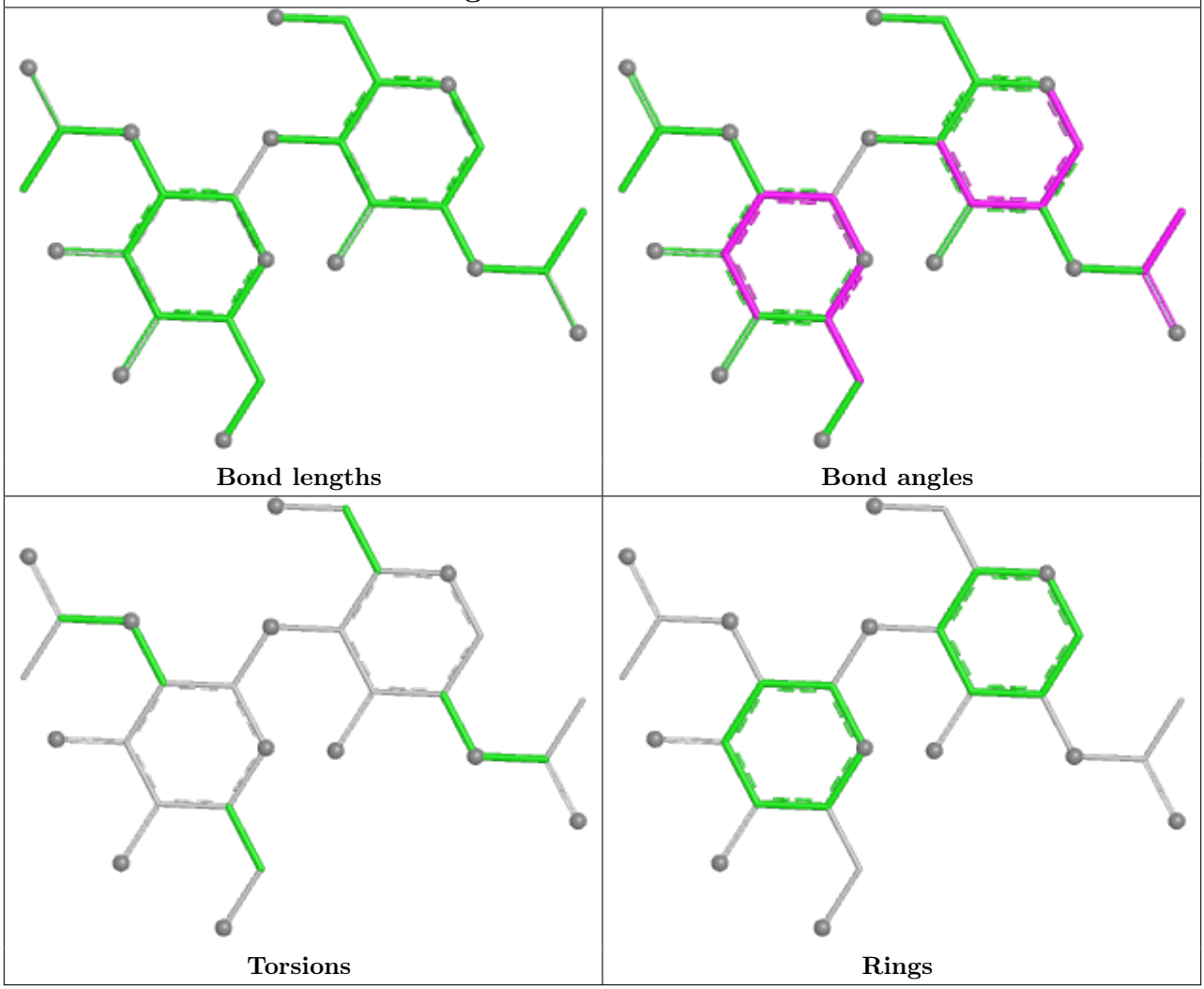


Torsions

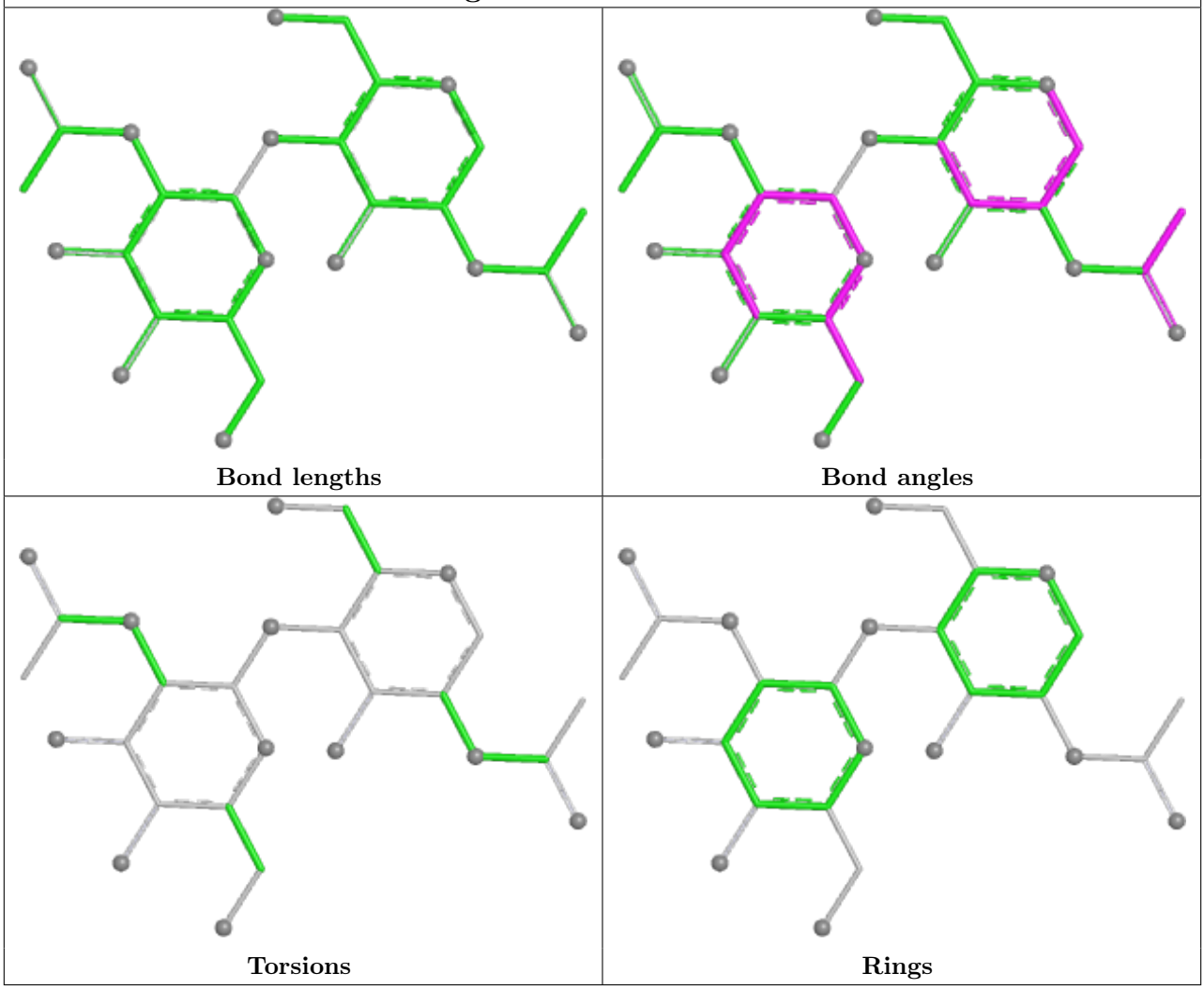


Rings

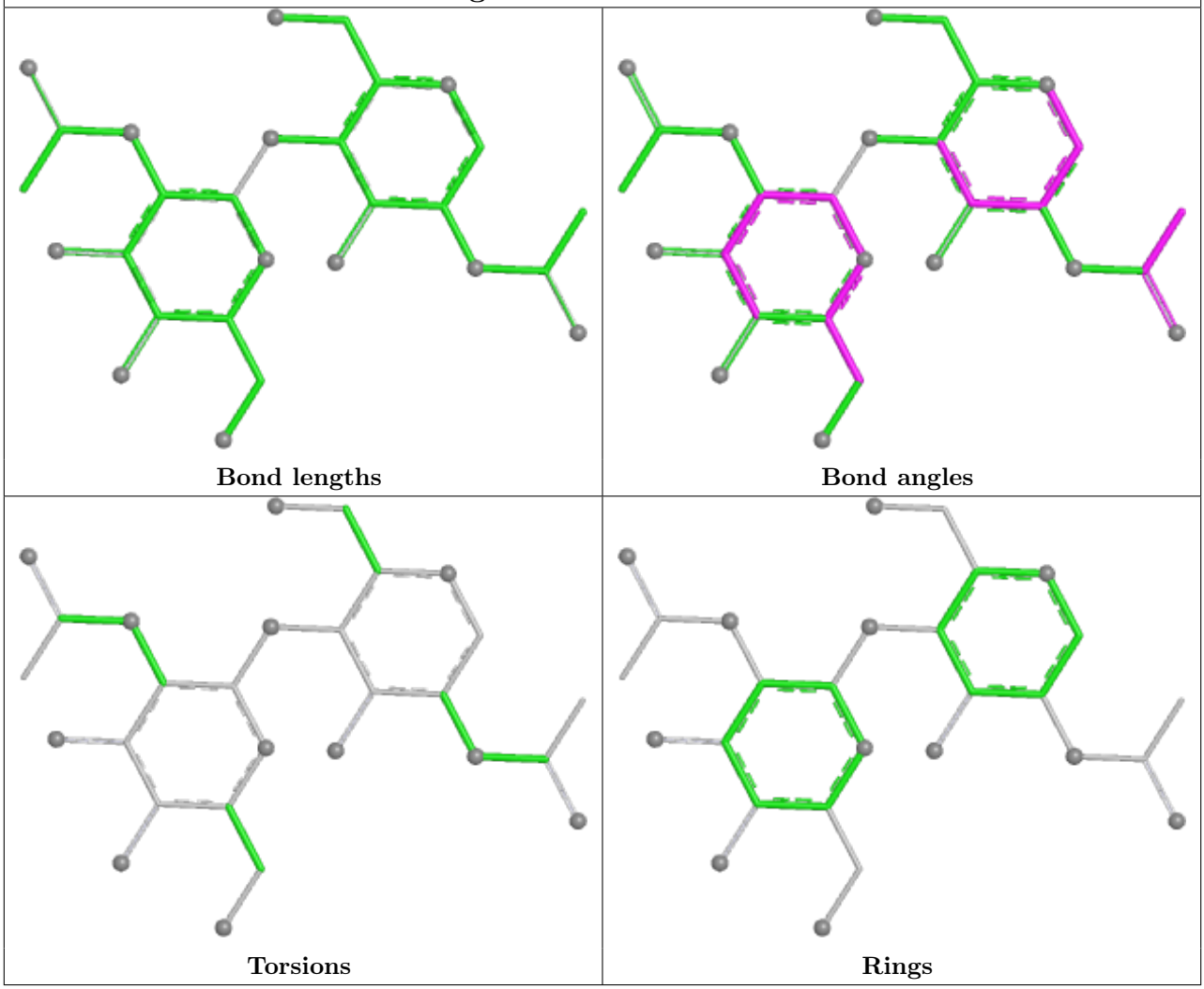
Oligosaccharide Chain R



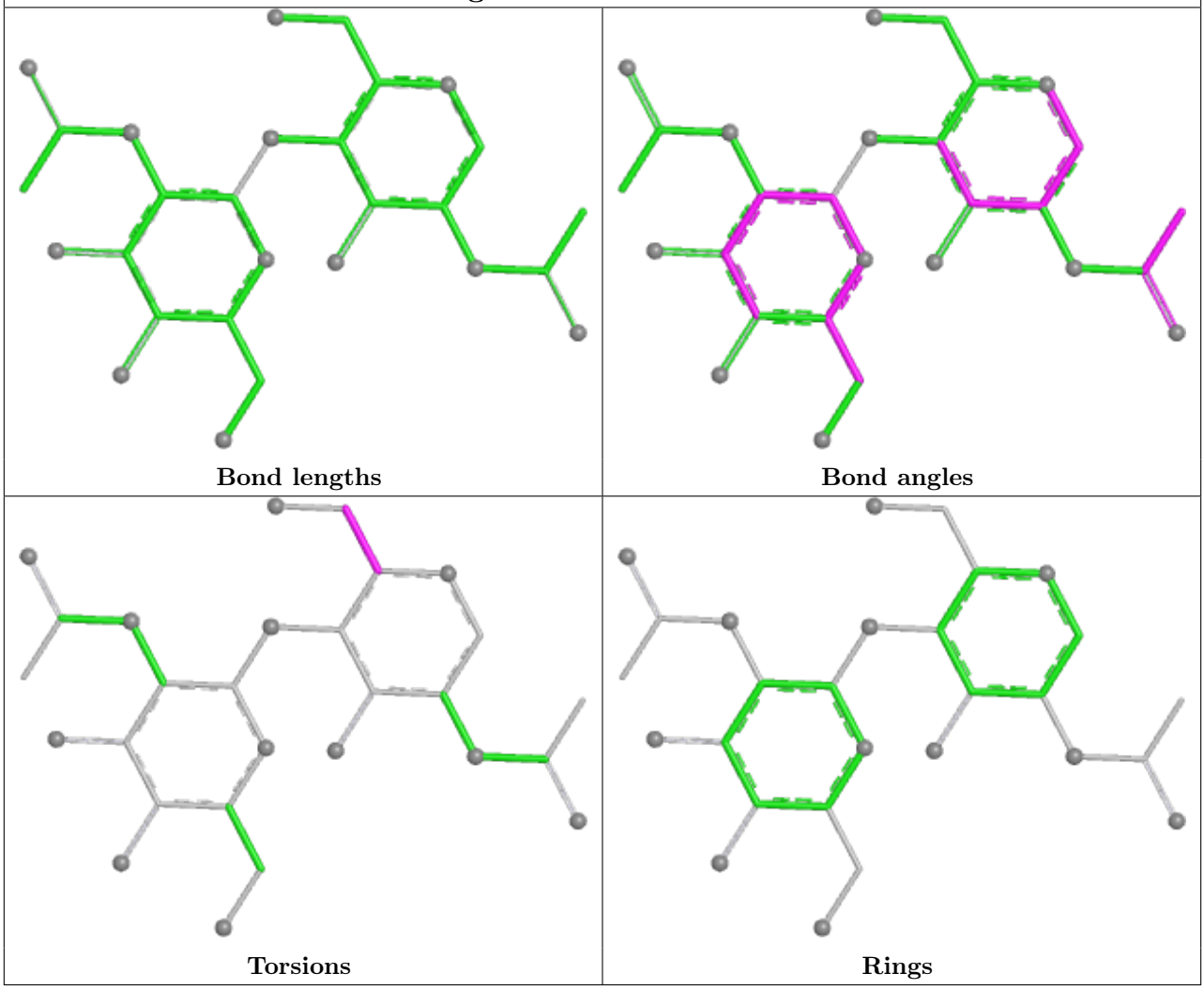
Oligosaccharide Chain X



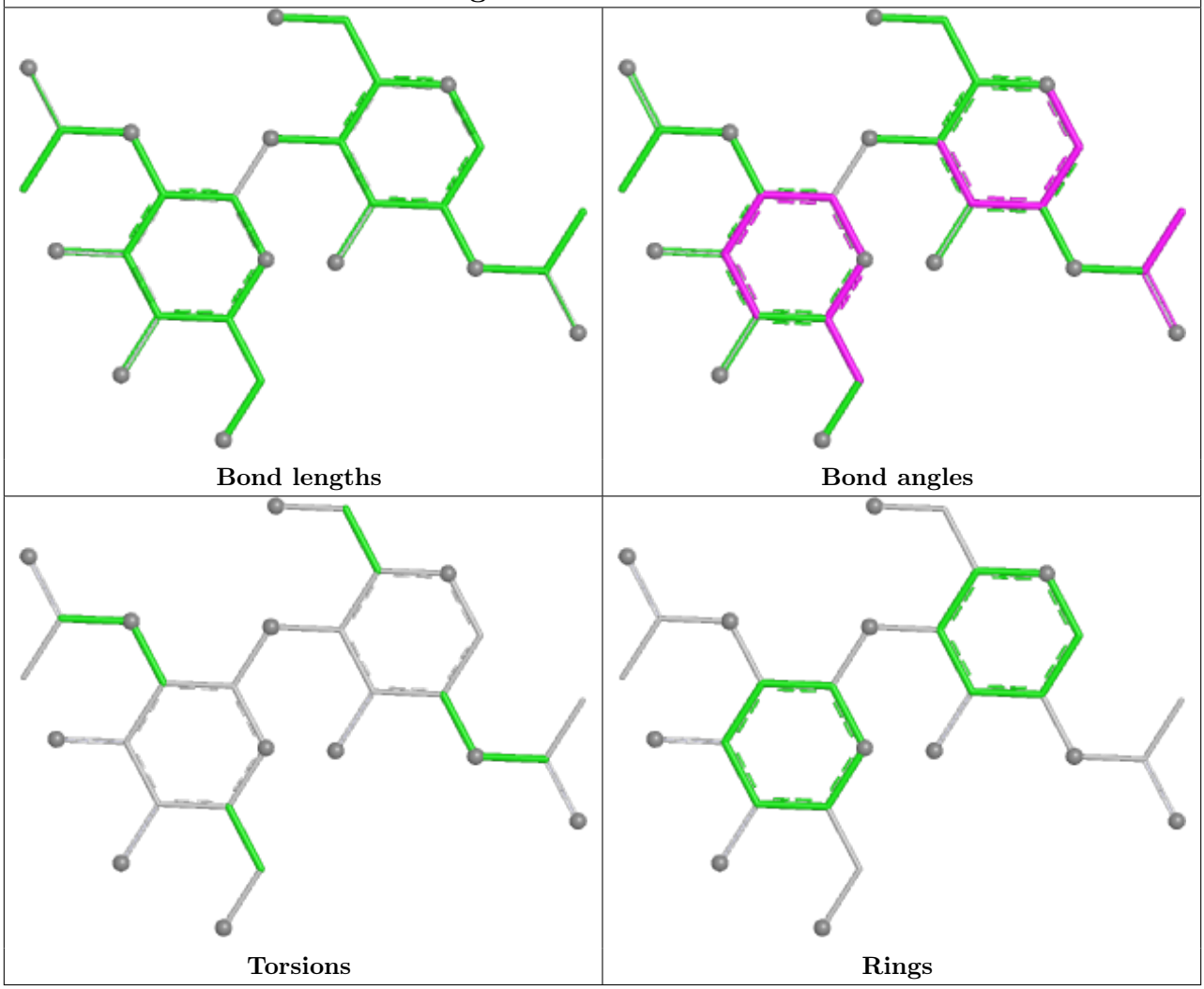
Oligosaccharide Chain a



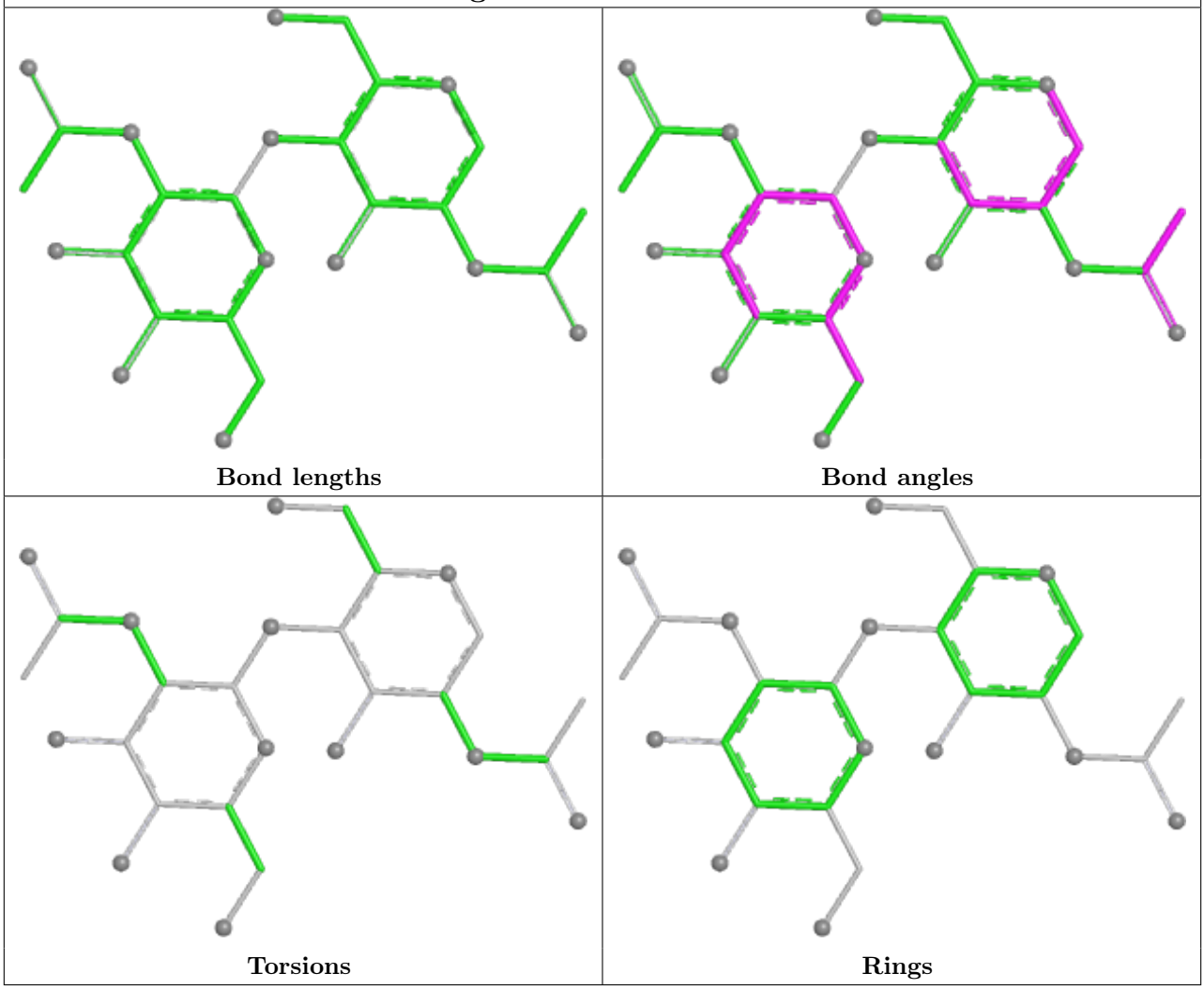
Oligosaccharide Chain b



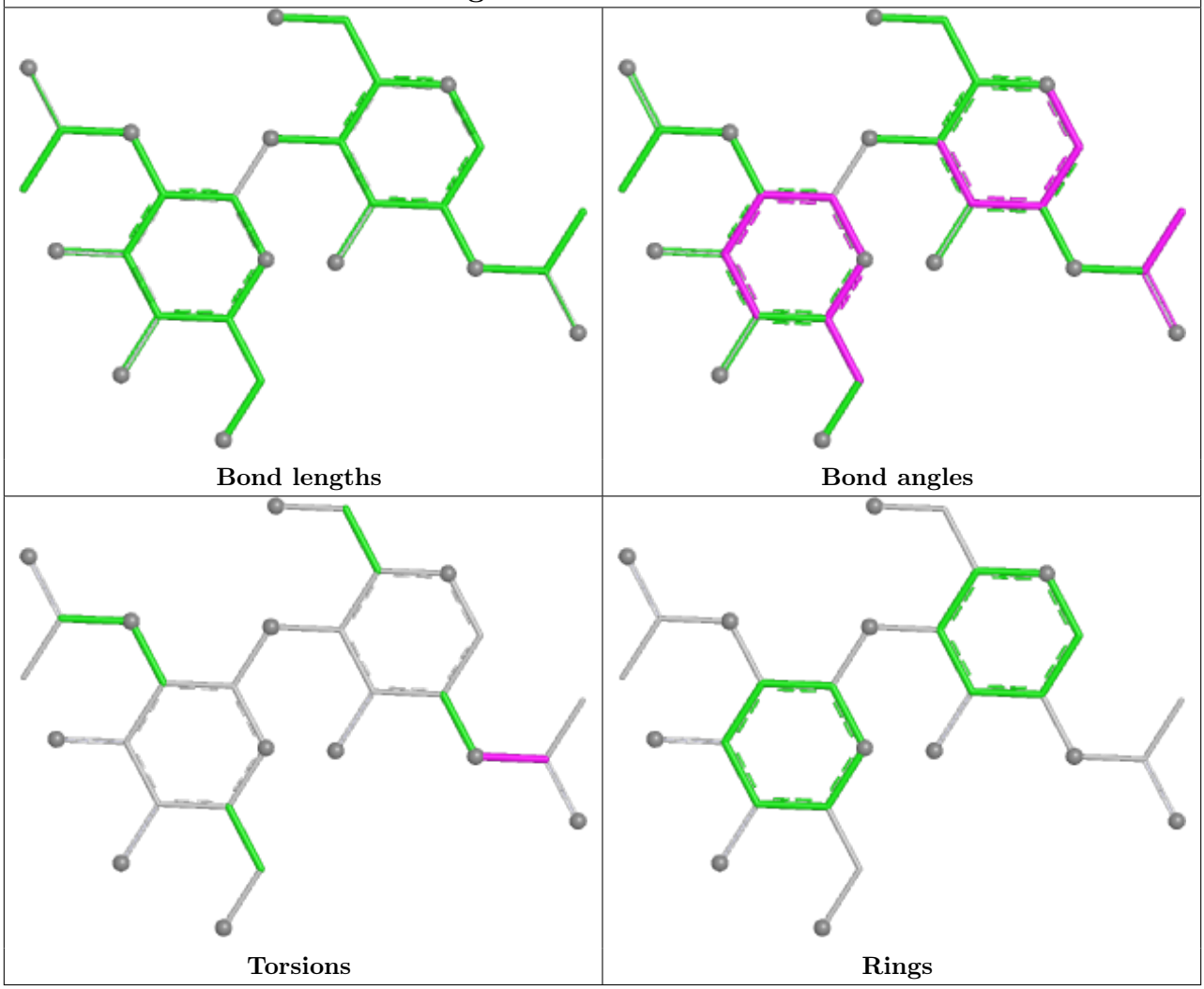
Oligosaccharide Chain c



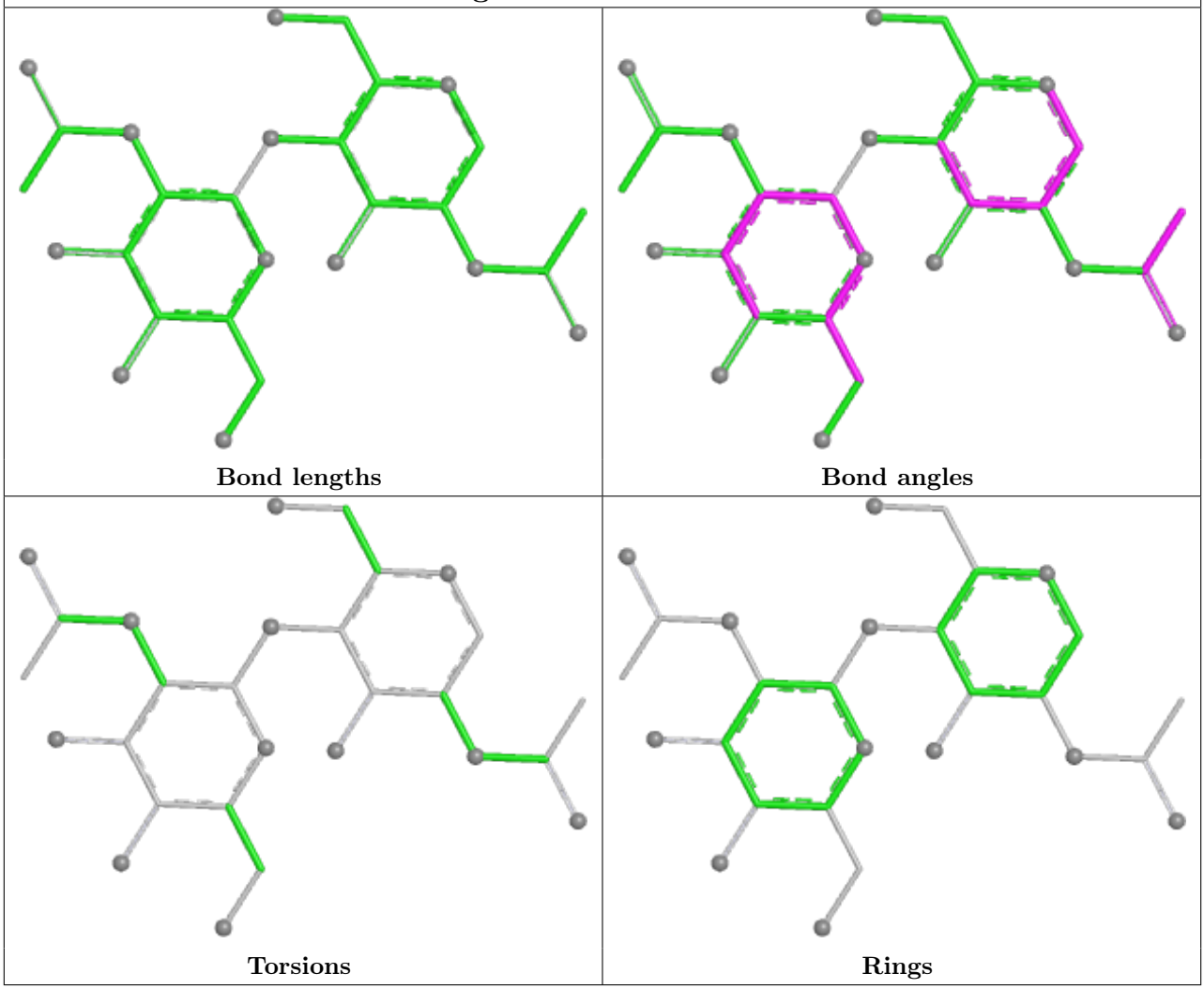
Oligosaccharide Chain e



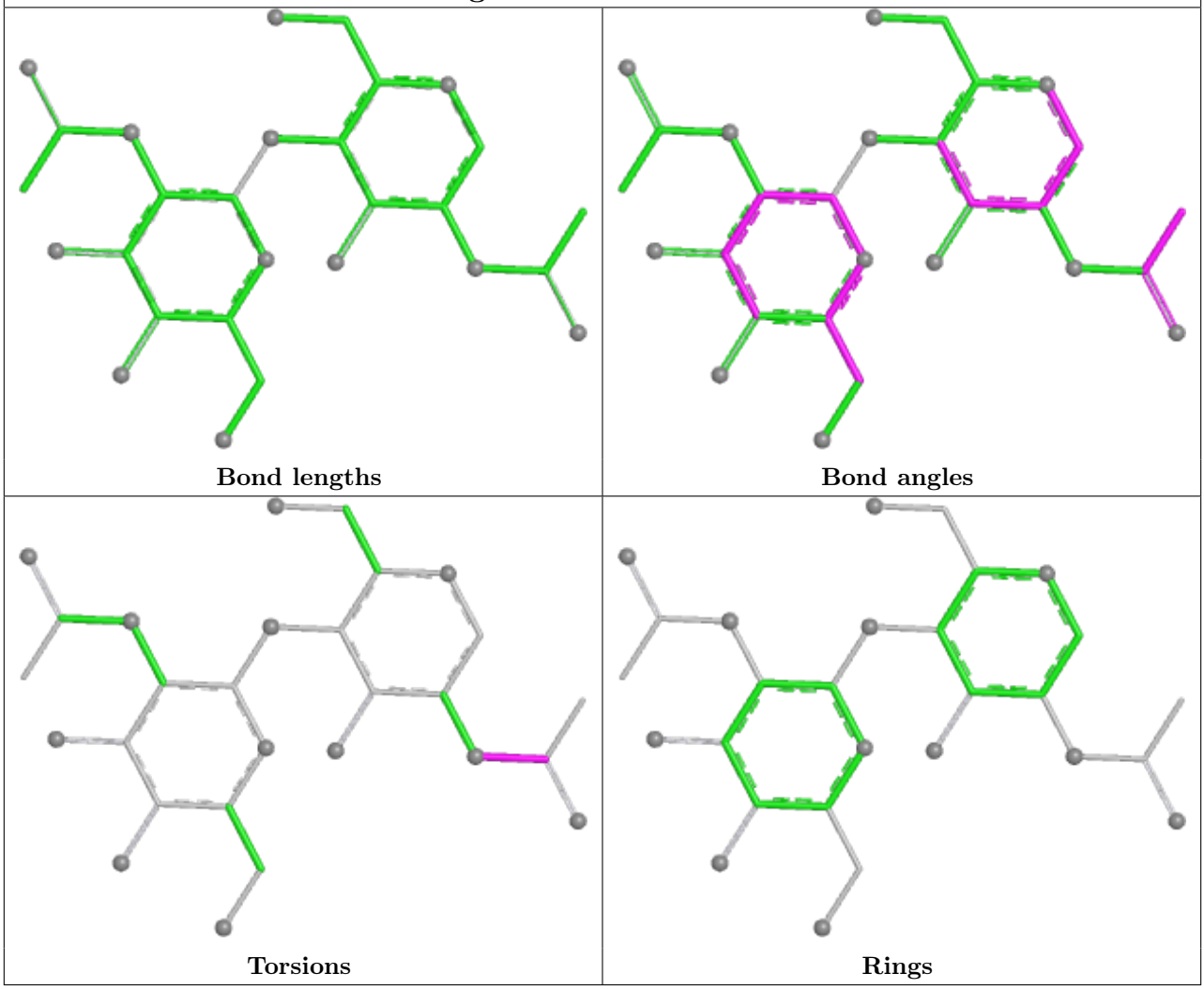
Oligosaccharide Chain h



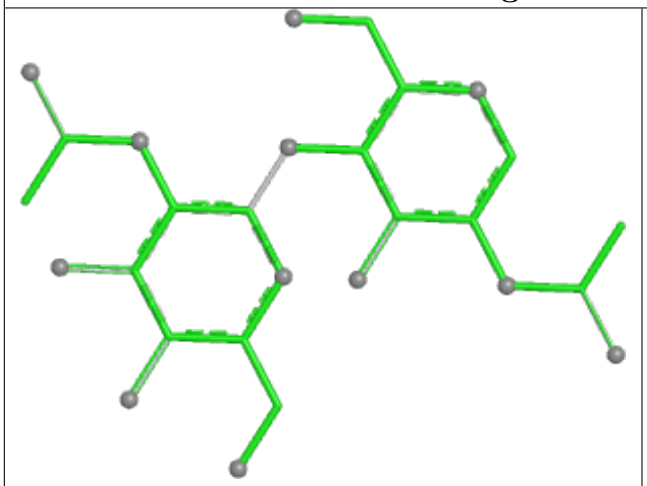
Oligosaccharide Chain i



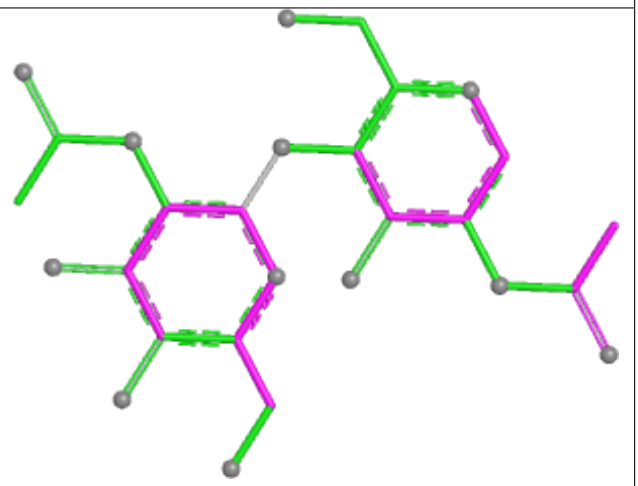
Oligosaccharide Chain o



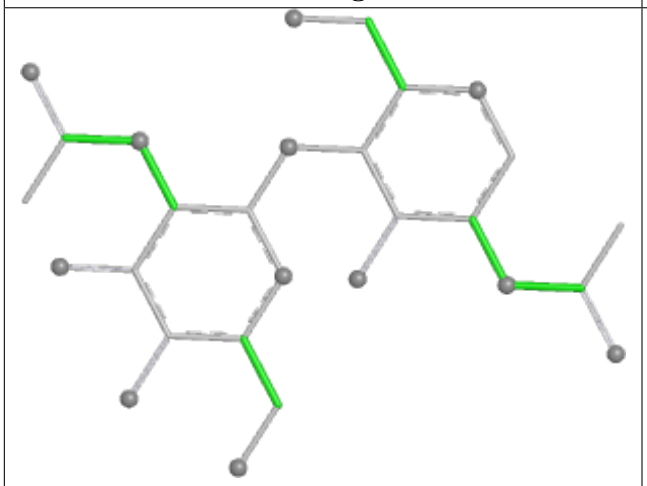
Oligosaccharide Chain r



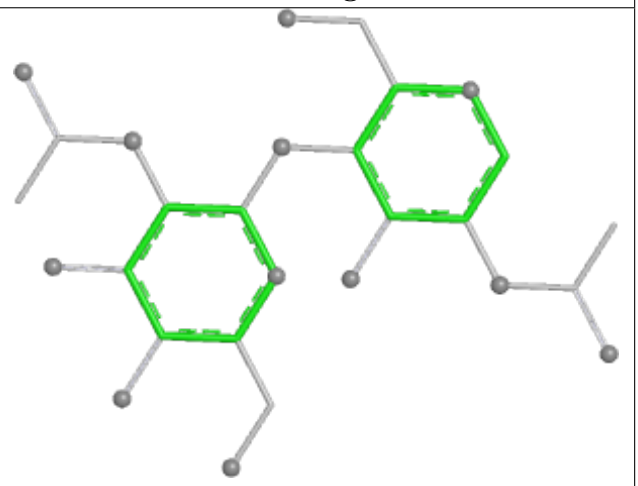
Bond lengths



Bond angles

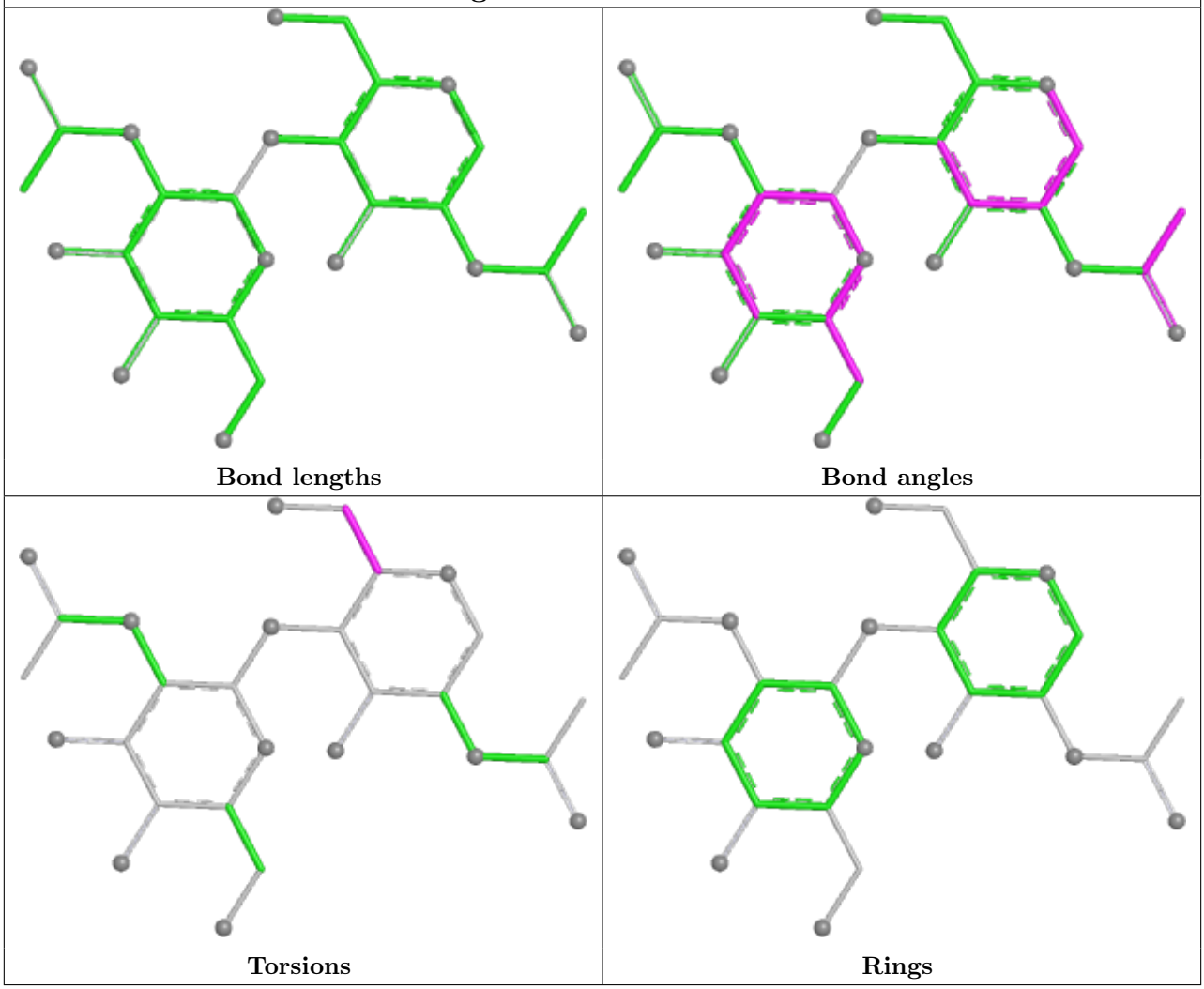


Torsions

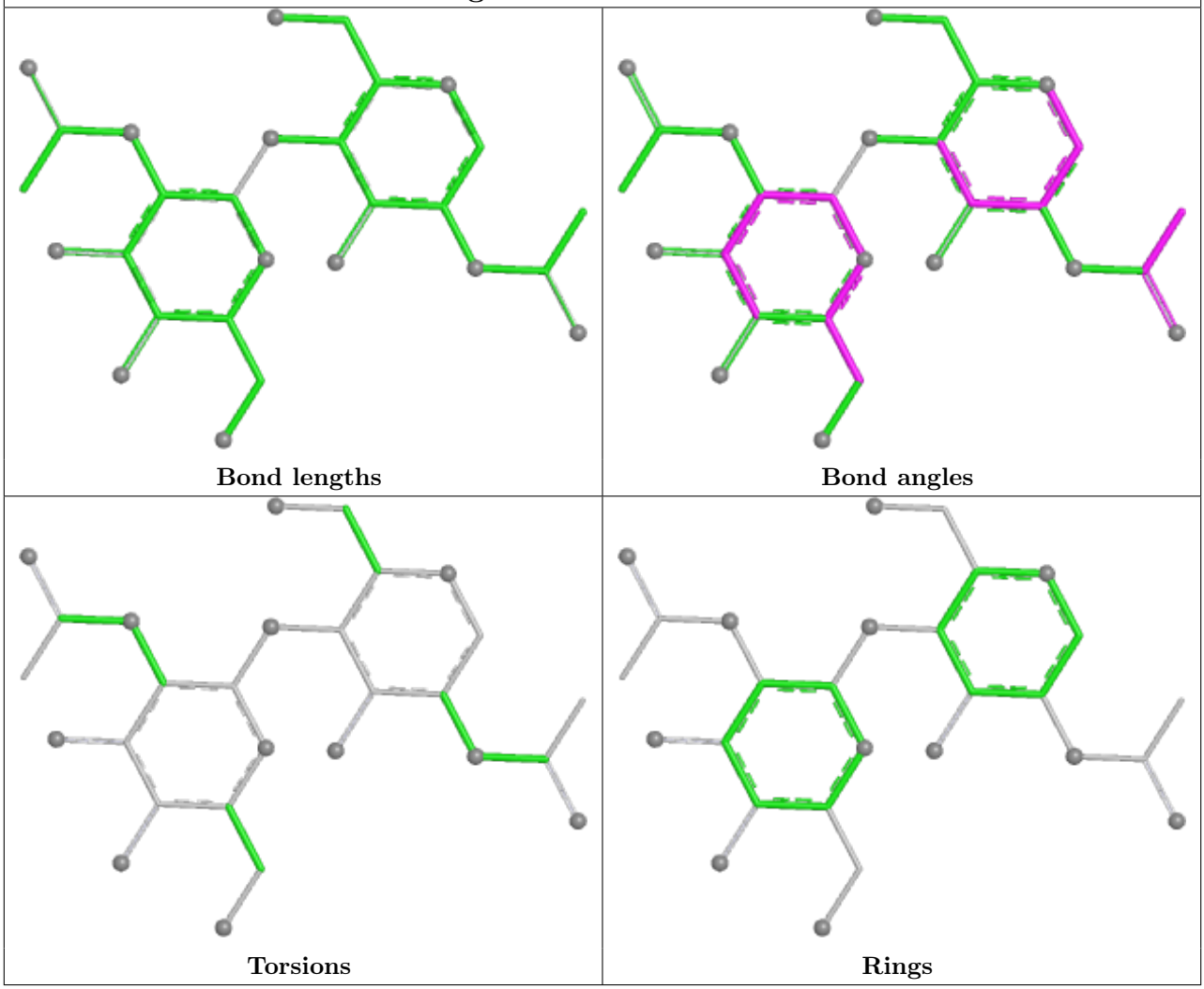


Rings

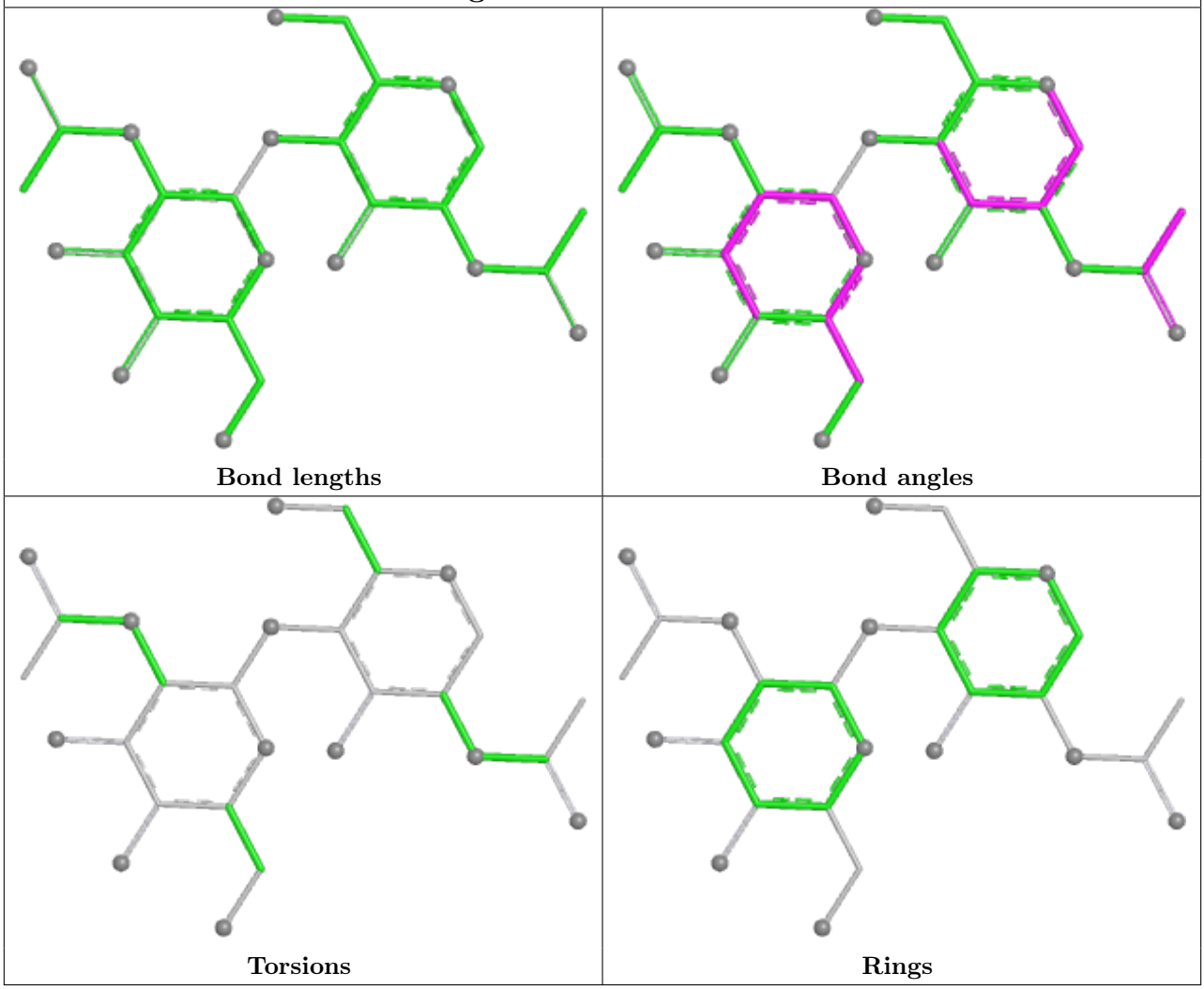
Oligosaccharide Chain s



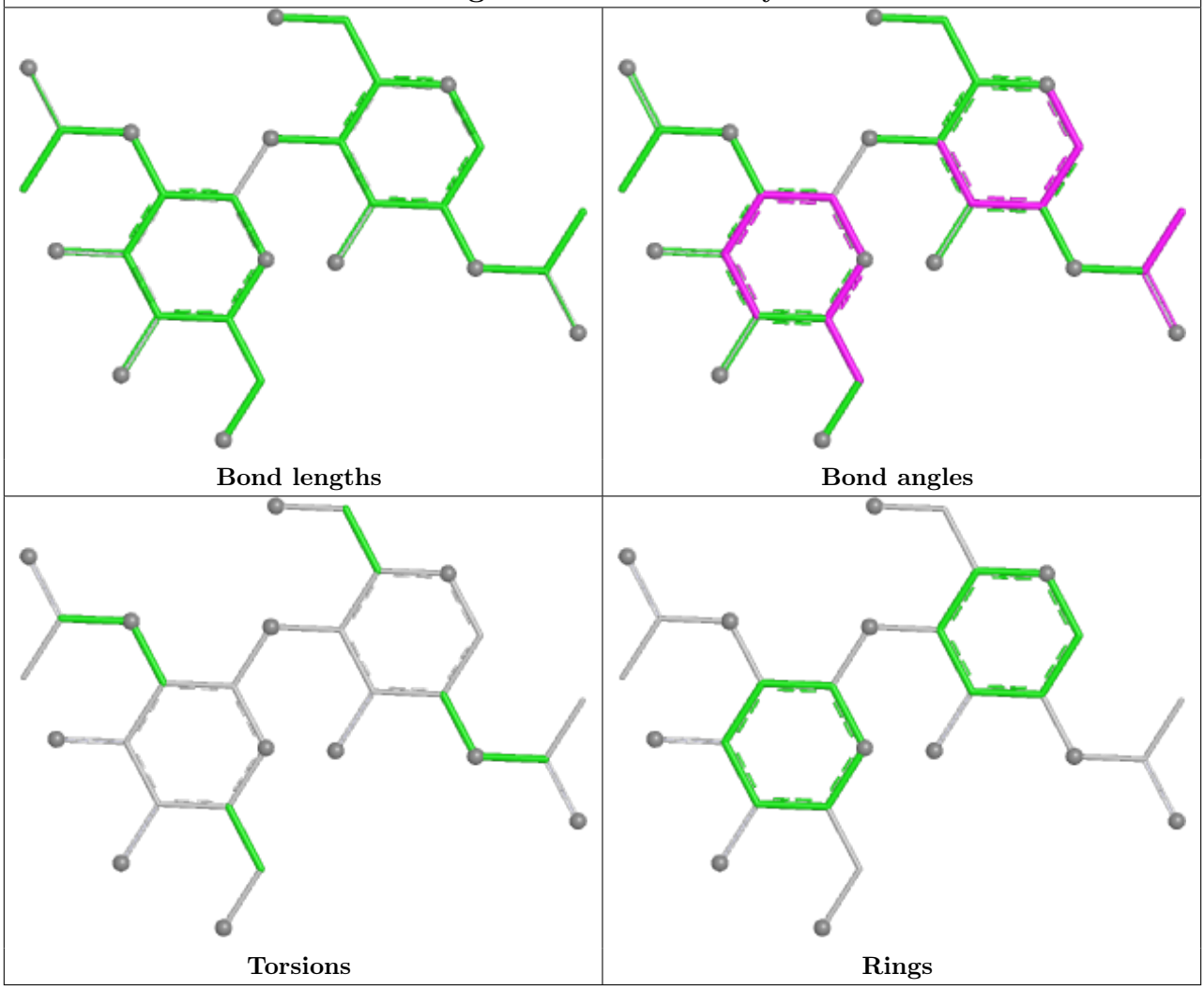
Oligosaccharide Chain u



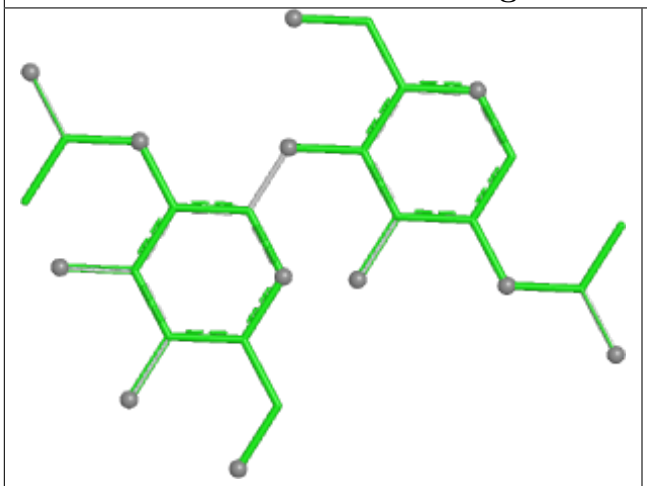
Oligosaccharide Chain x



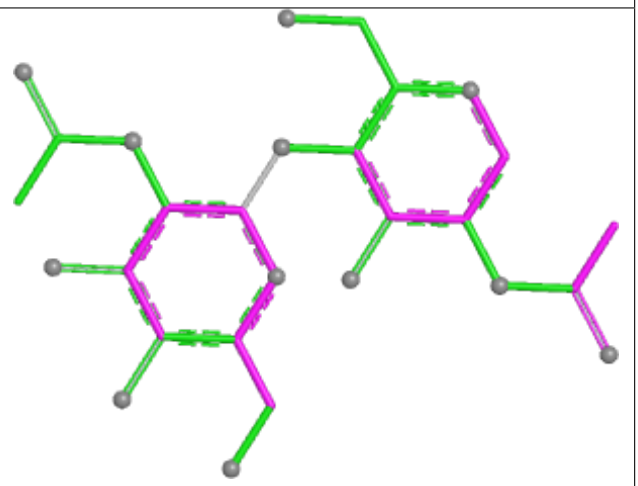
Oligosaccharide Chain y



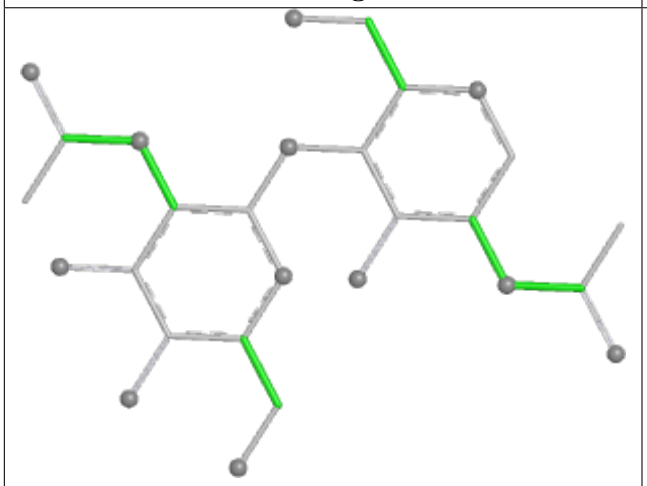
Oligosaccharide Chain 4



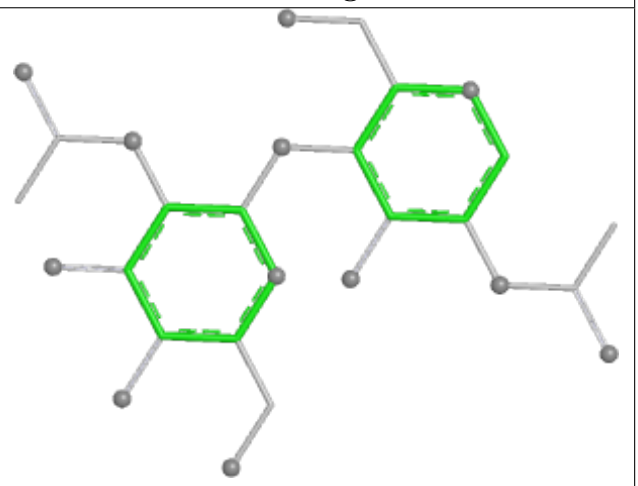
Bond lengths



Bond angles

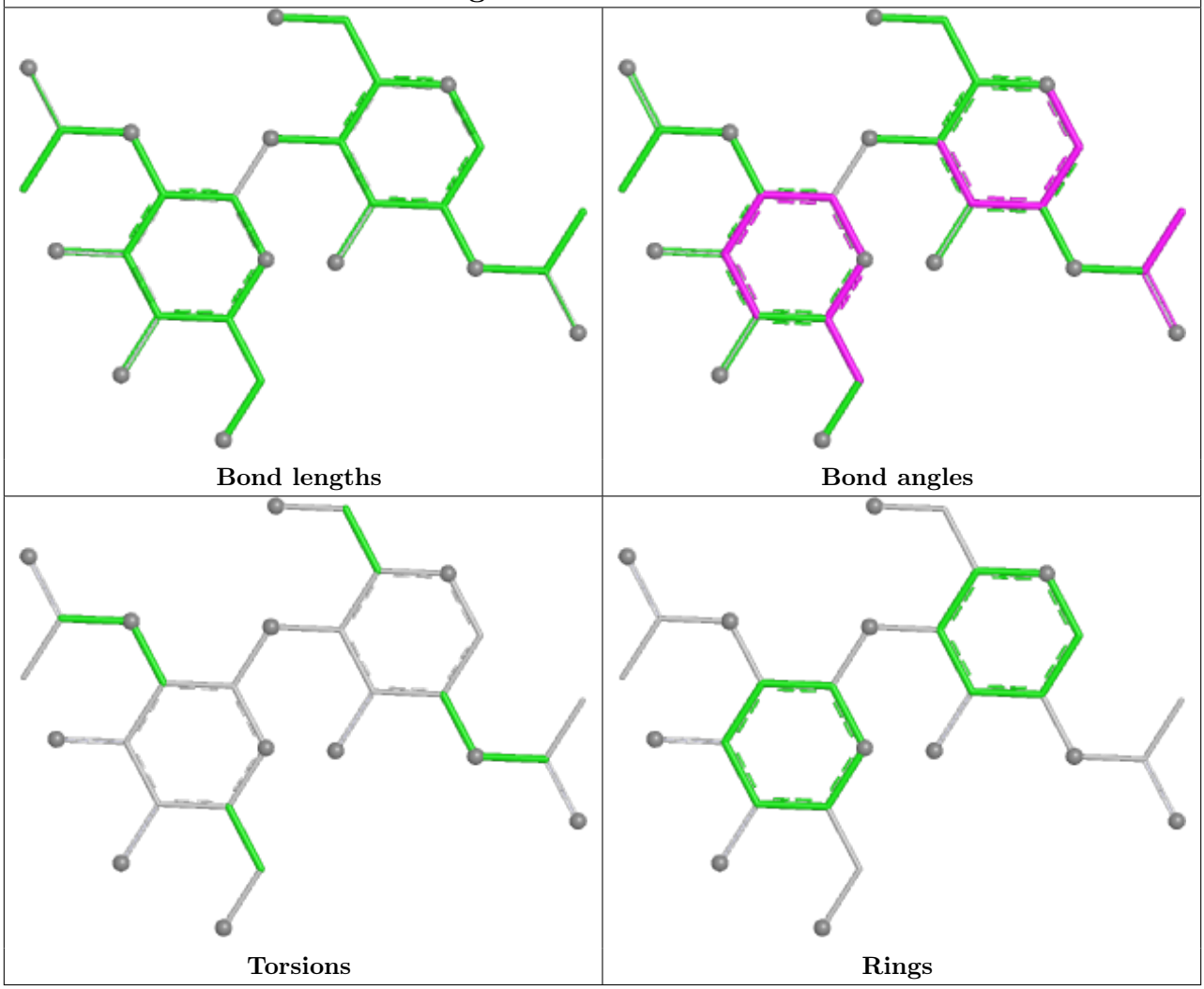


Torsions

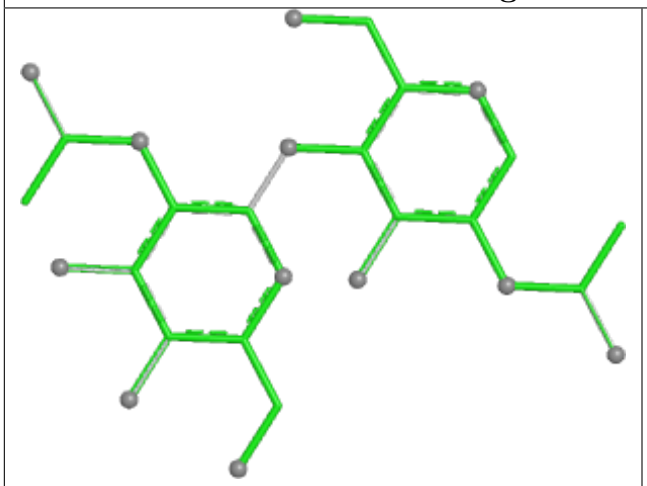


Rings

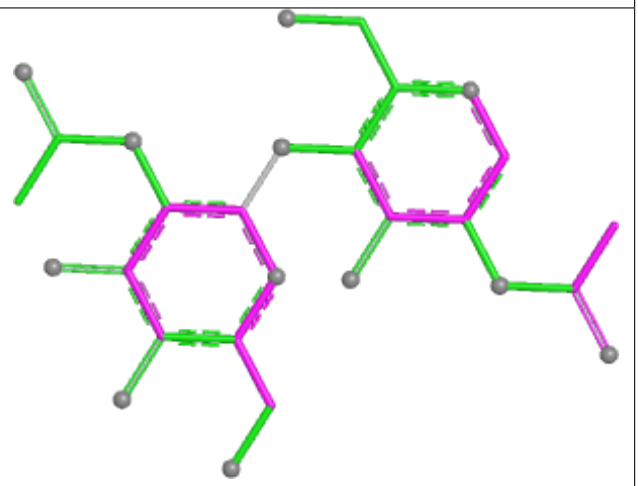
Oligosaccharide Chain 7



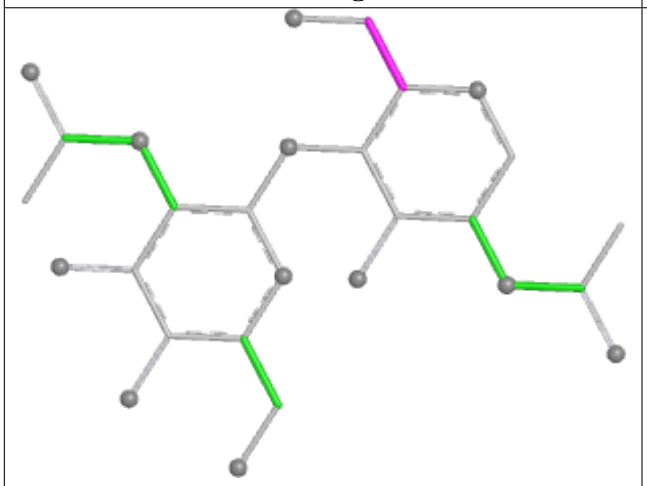
Oligosaccharide Chain 8



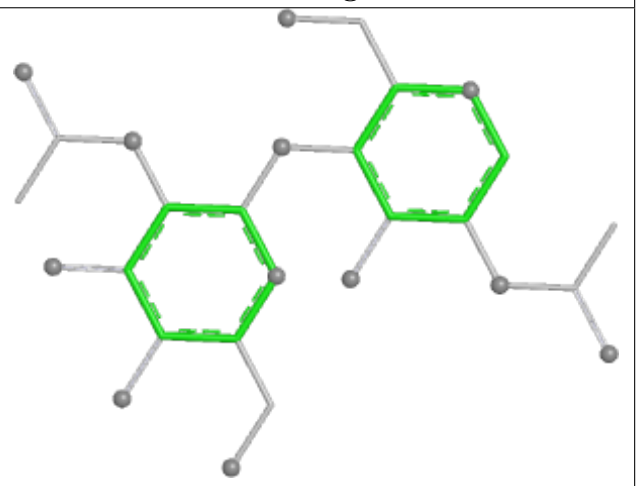
Bond lengths



Bond angles

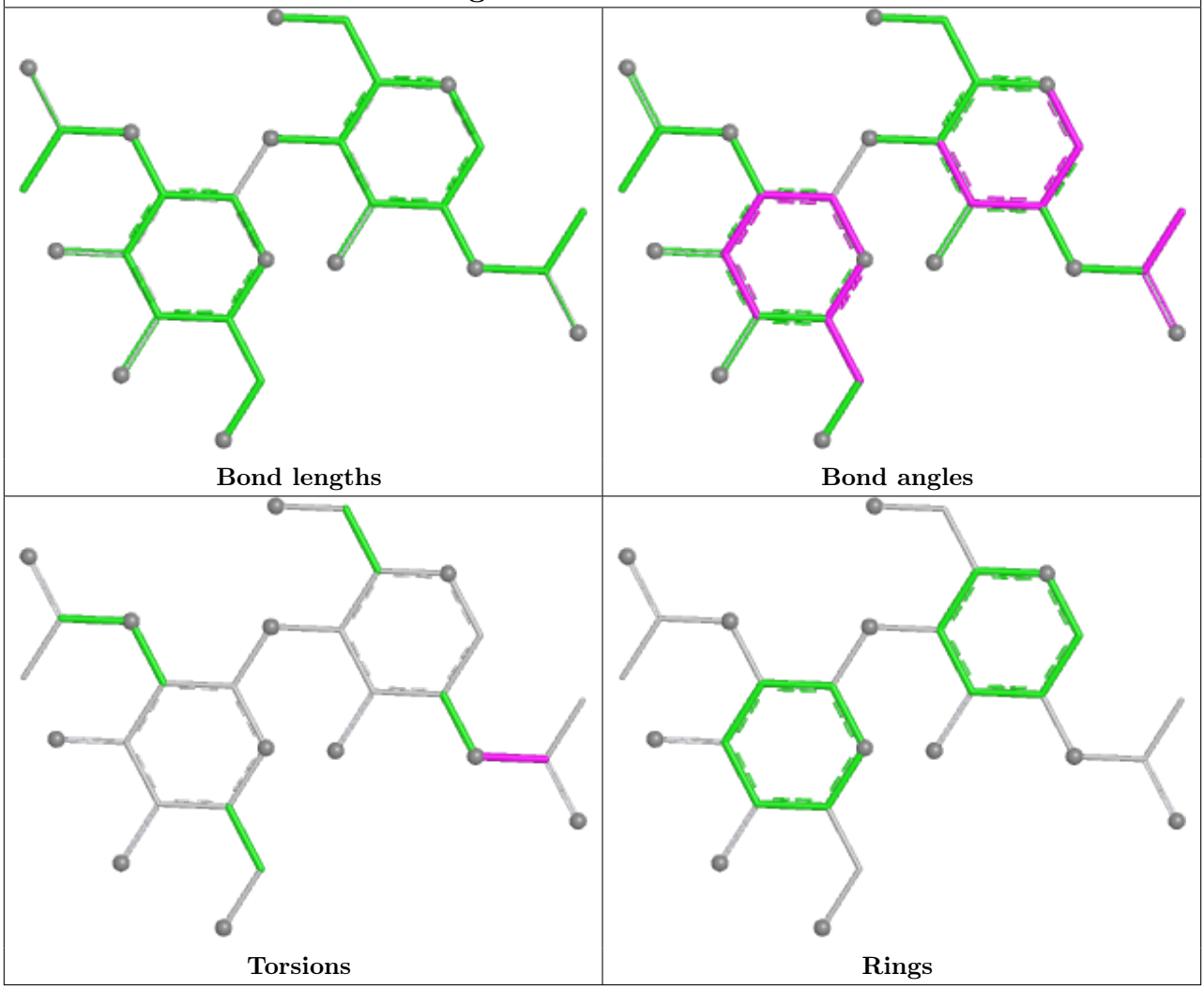


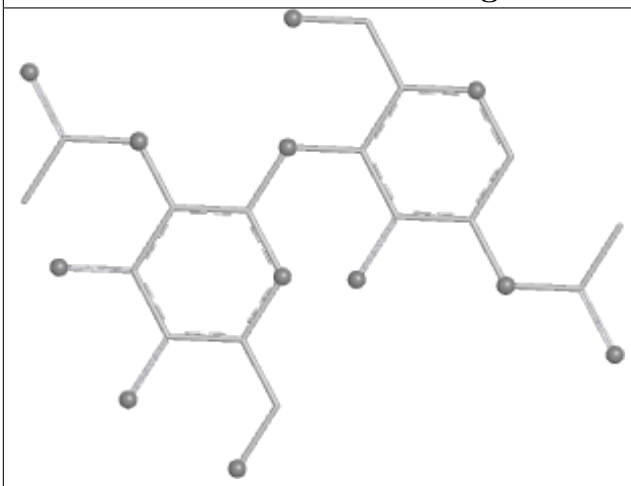
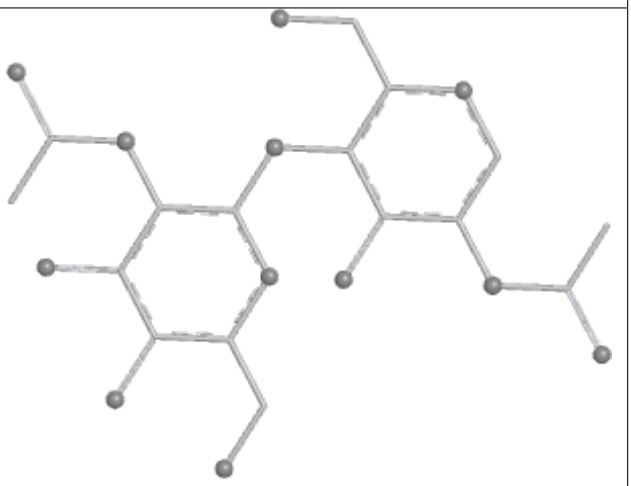
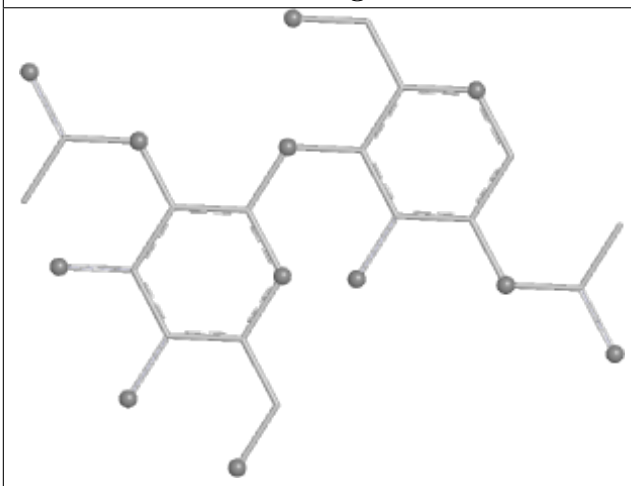
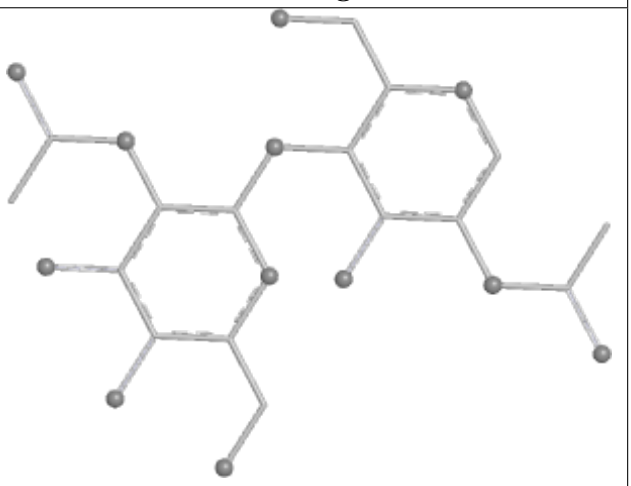
Torsions

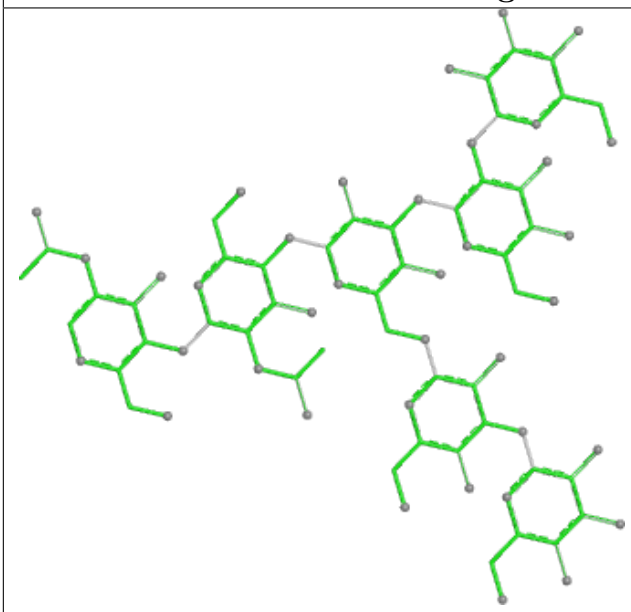
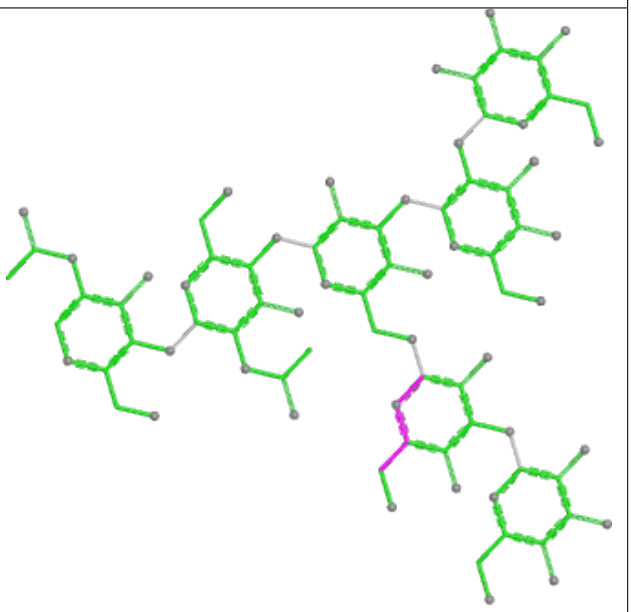
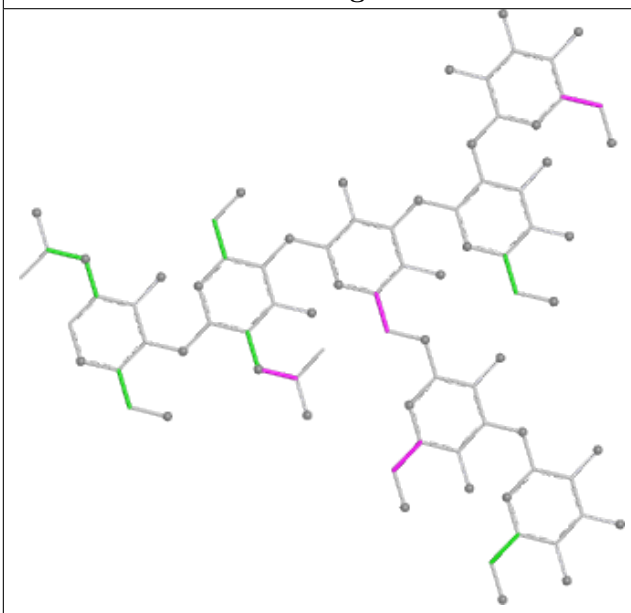
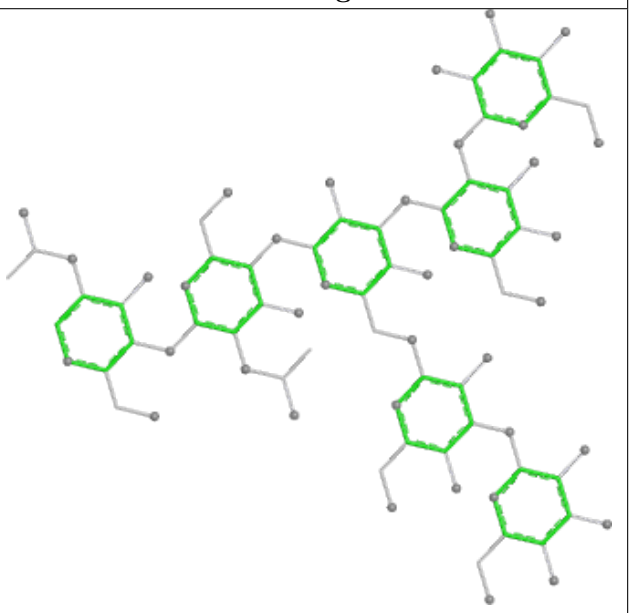


Rings

Oligosaccharide Chain 9



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

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

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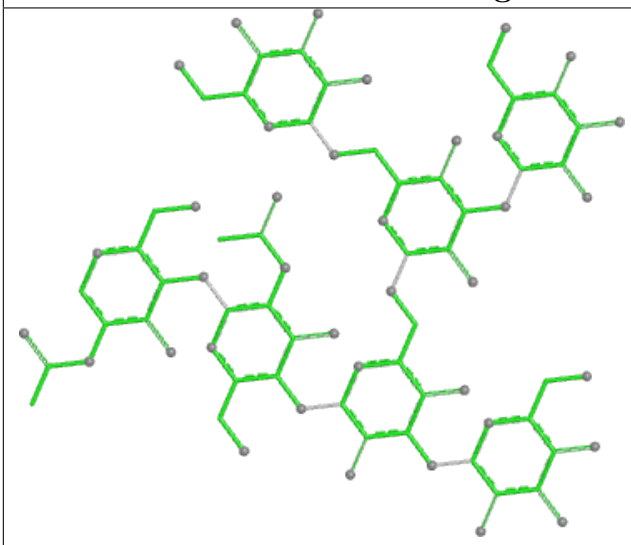
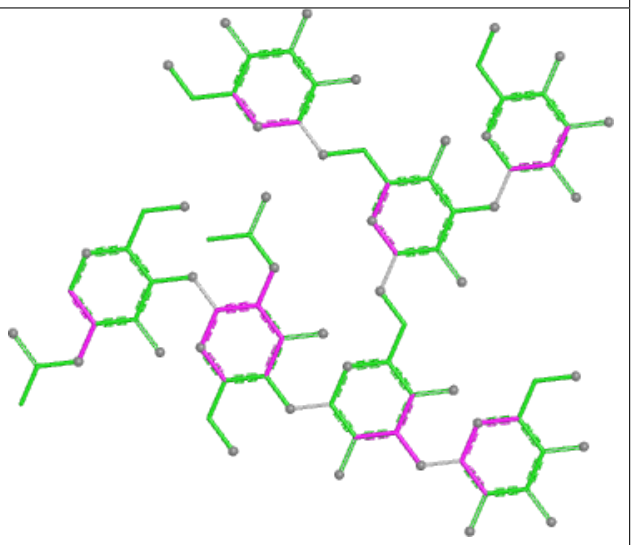
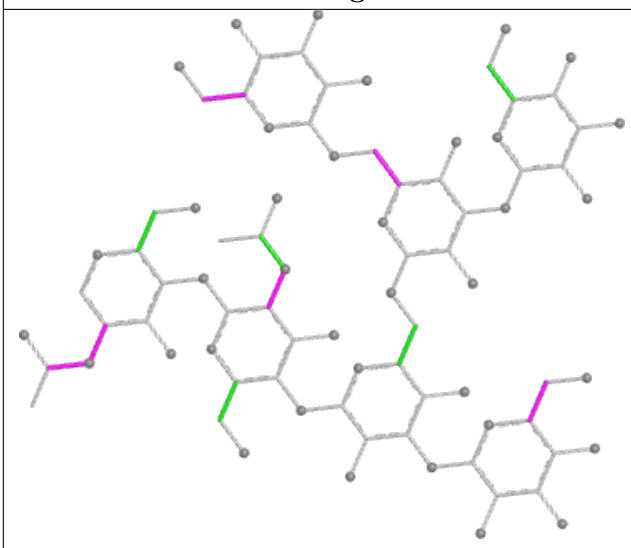
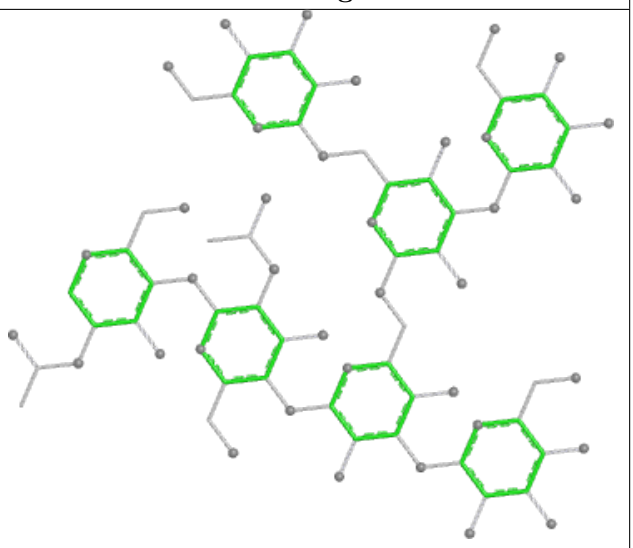
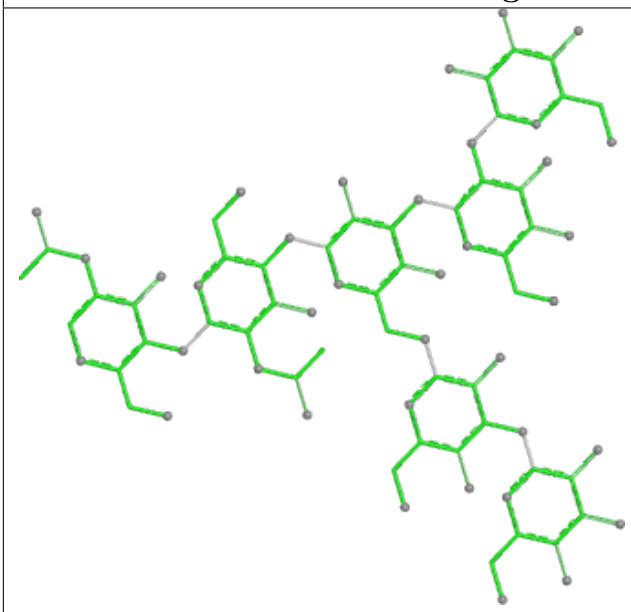
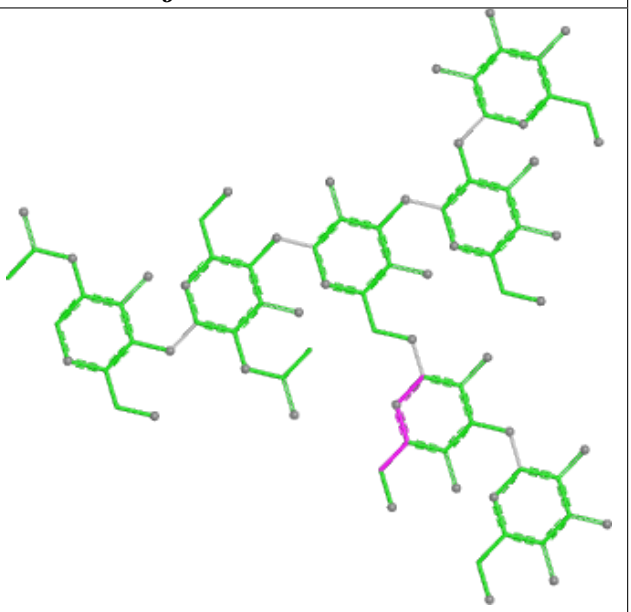
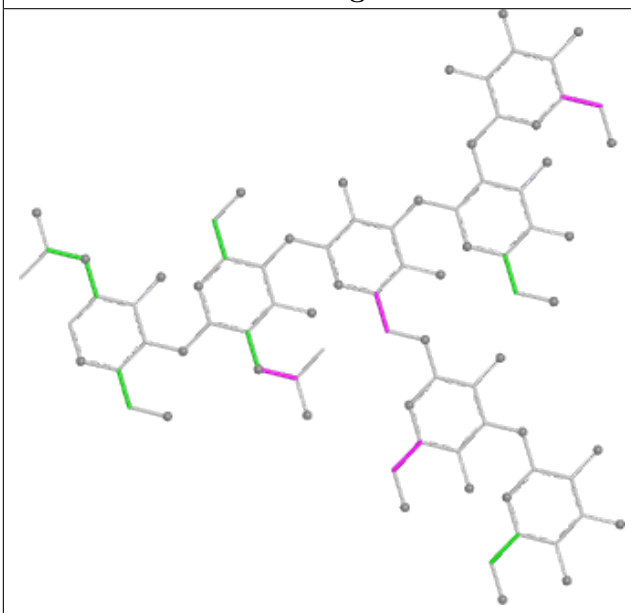
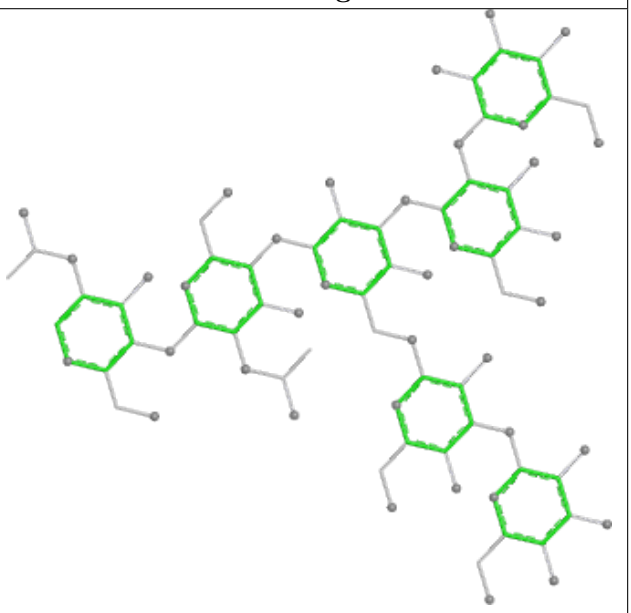
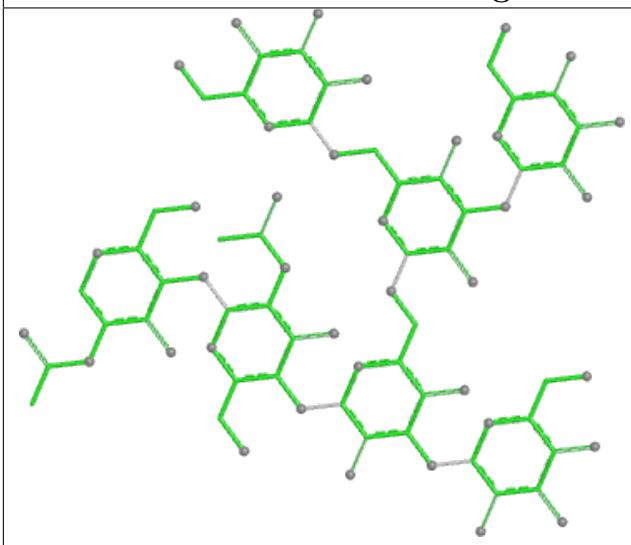
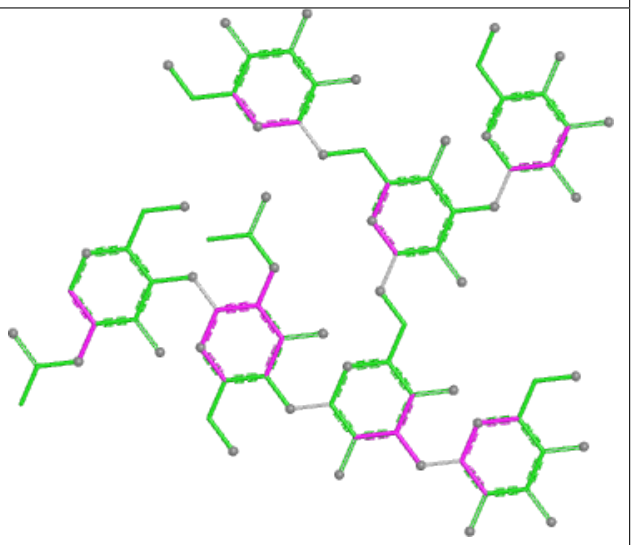
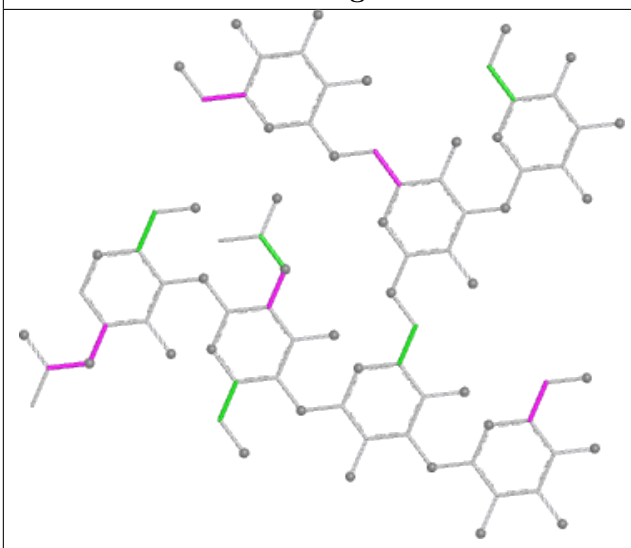
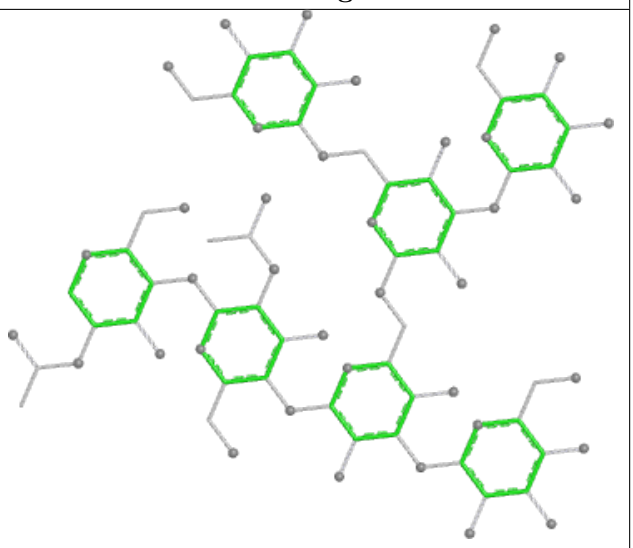
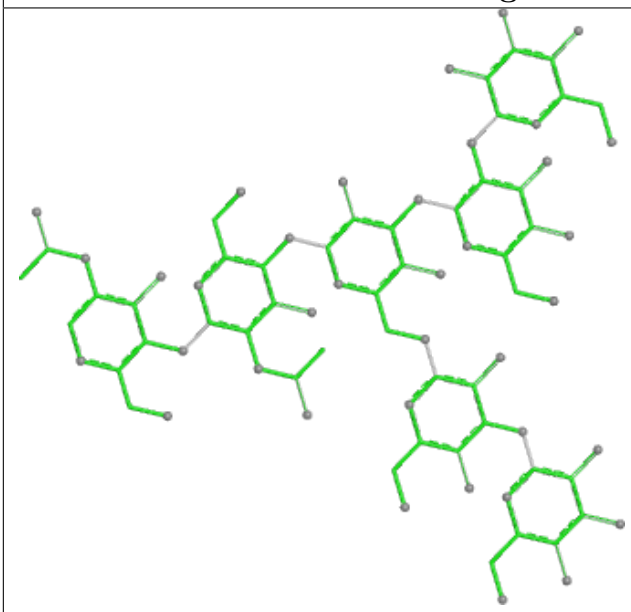
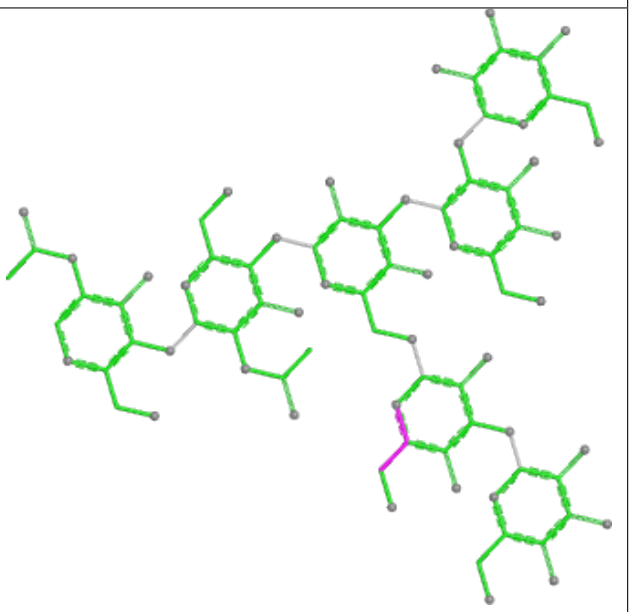
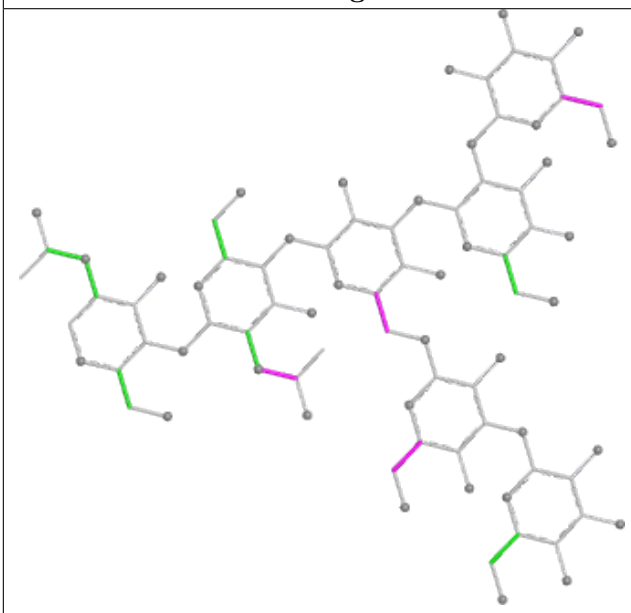
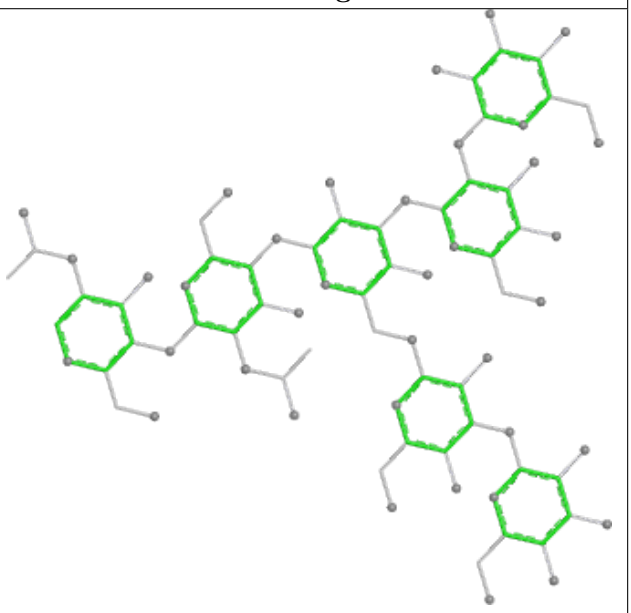
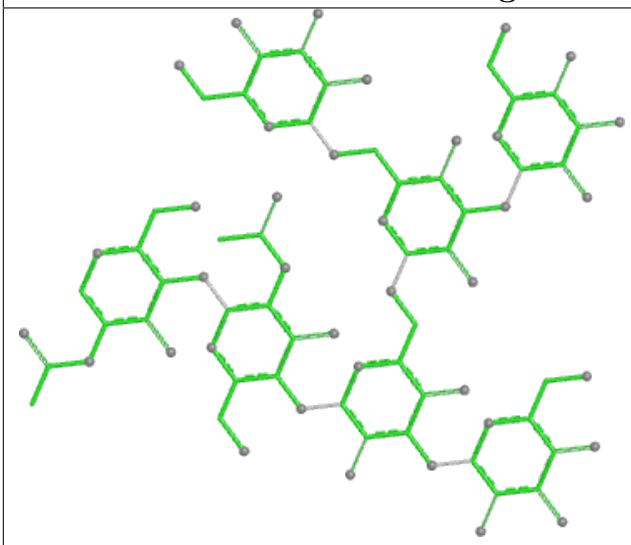
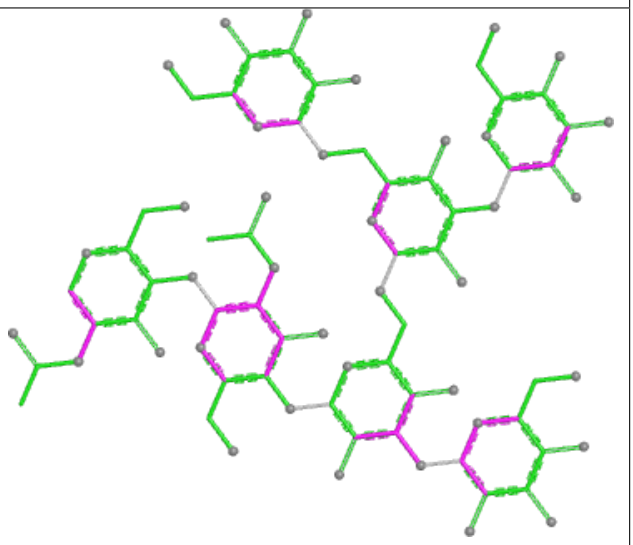
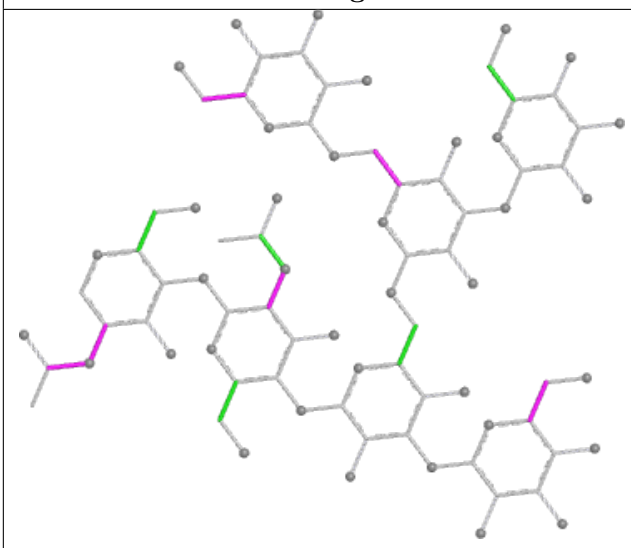
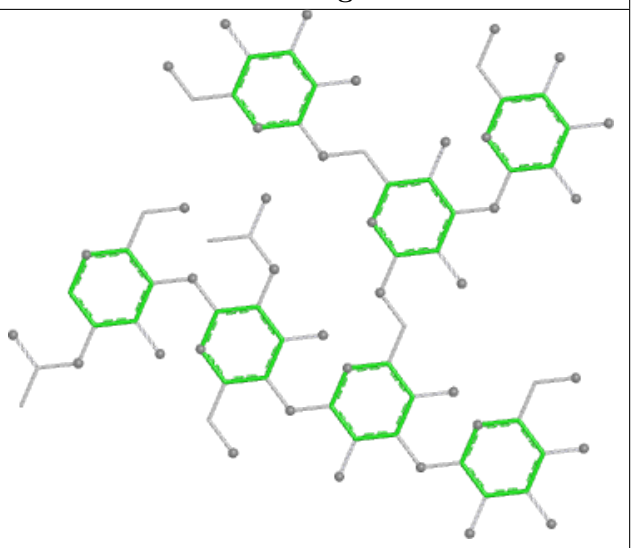
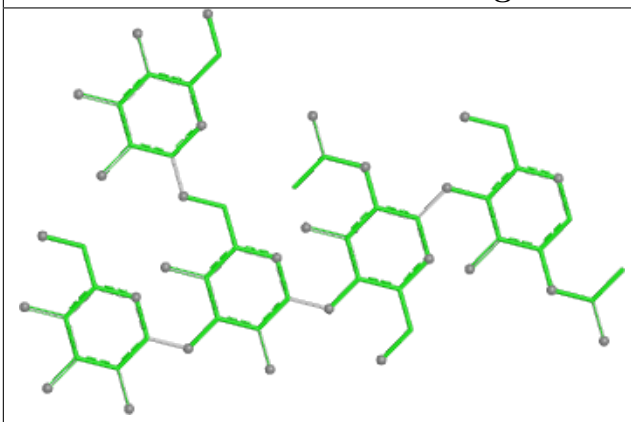
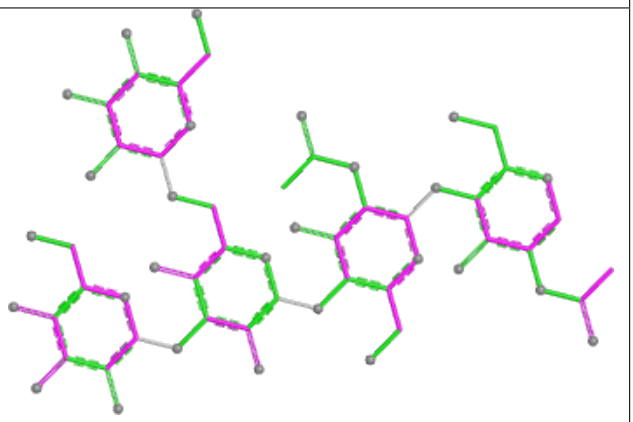
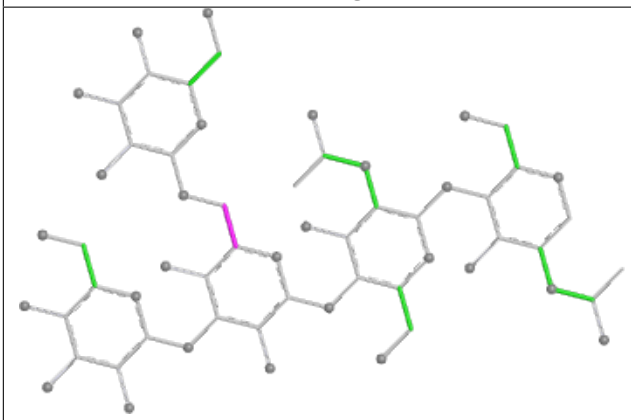
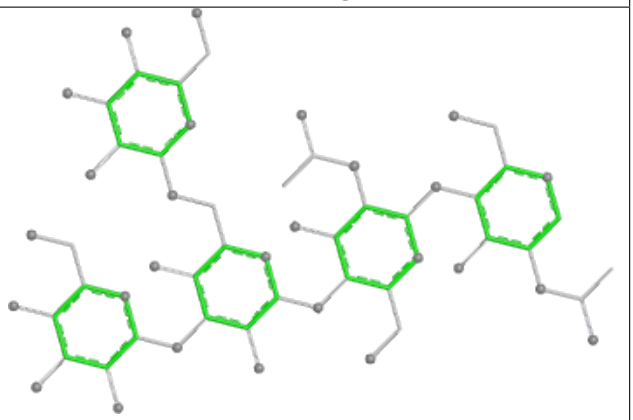
 Bond lengths	 Bond angles
 Torsions	 Rings

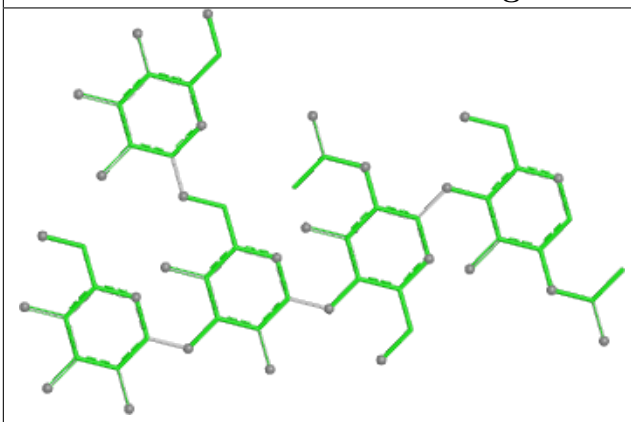
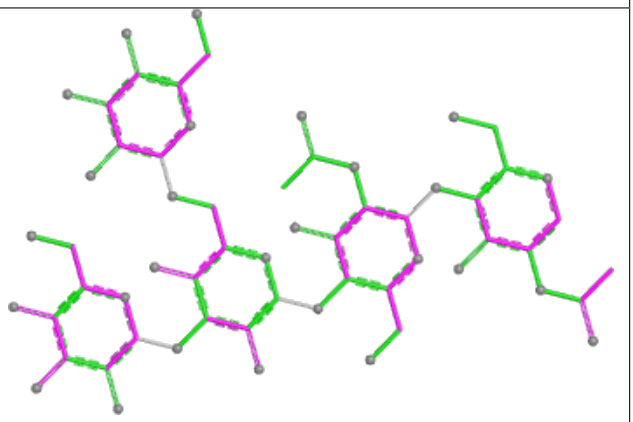
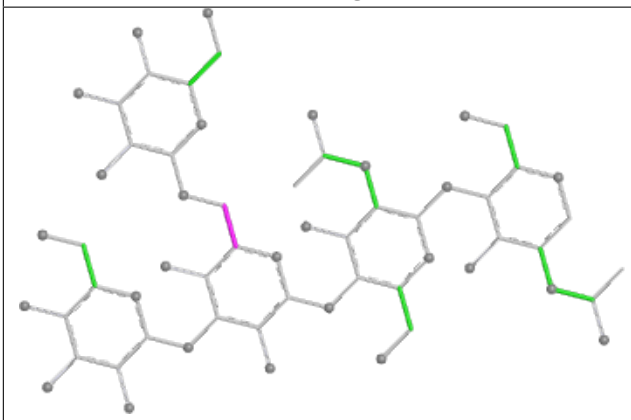
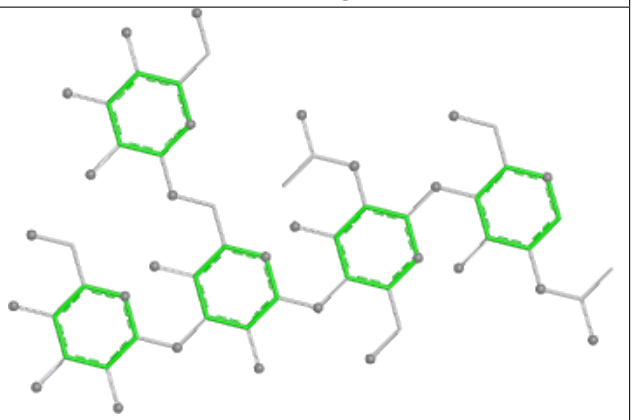
Oligosaccharide Chain j	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

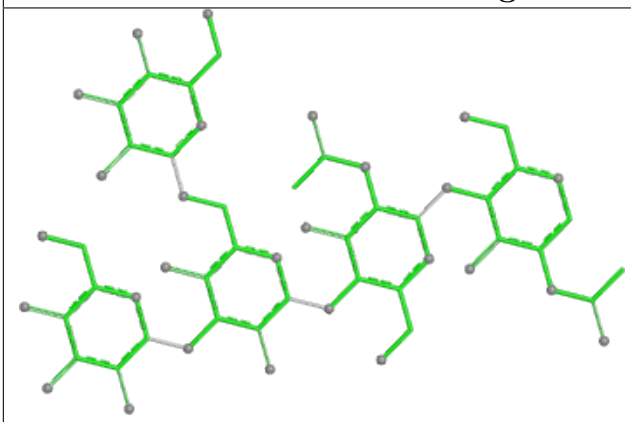
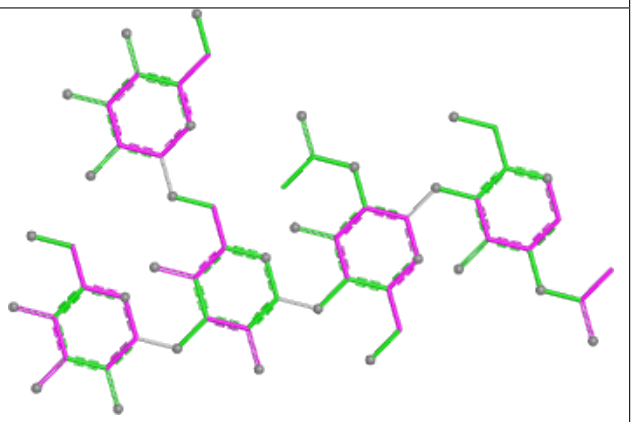
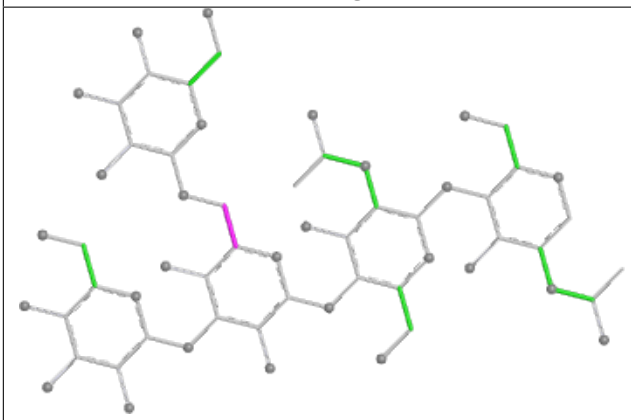
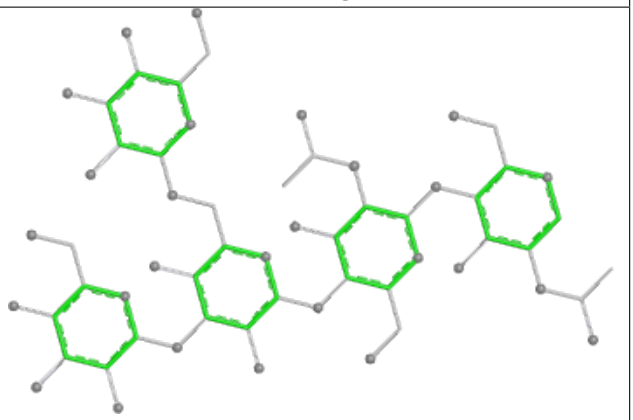
Oligosaccharide Chain m	
 Bond lengths	 Bond angles
 Torsions	 Rings

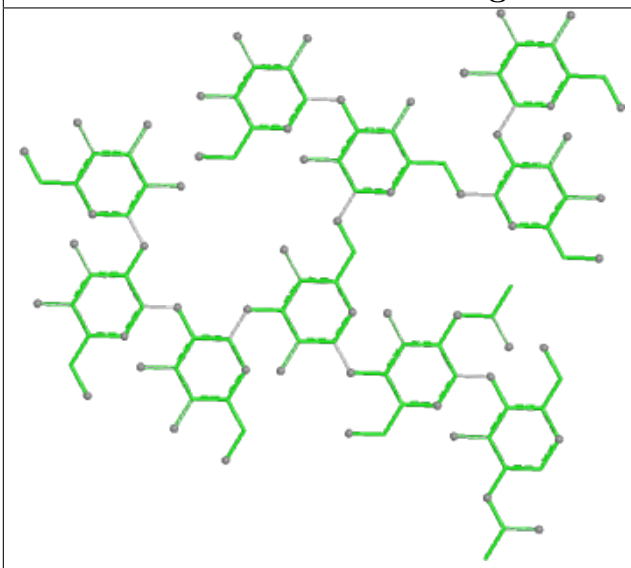
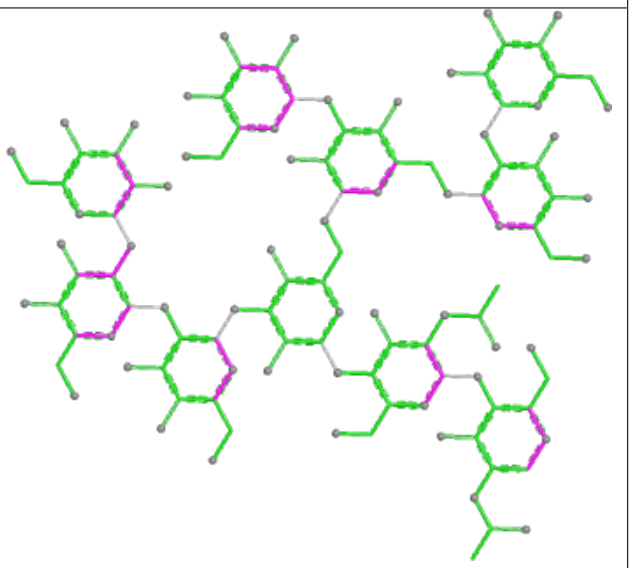
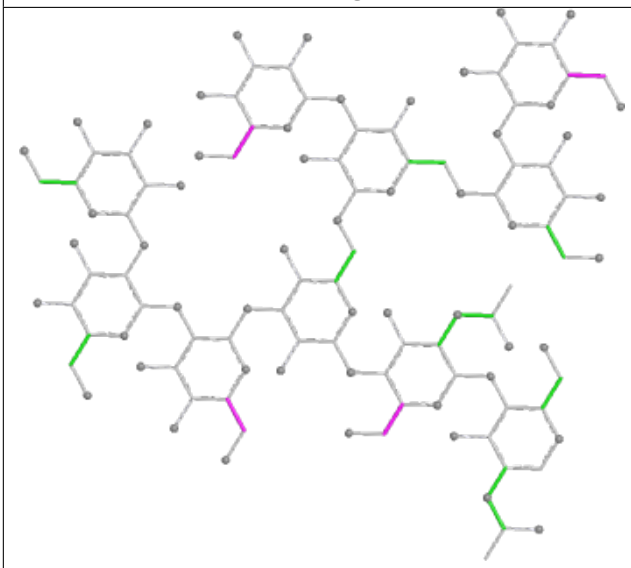
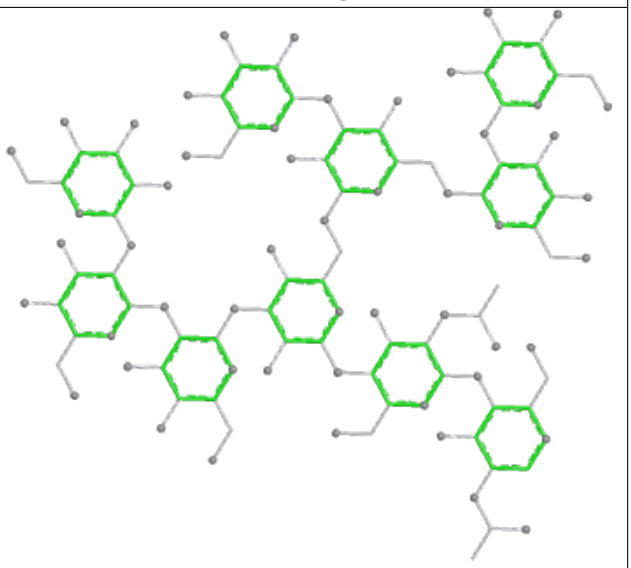
Oligosaccharide Chain z	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

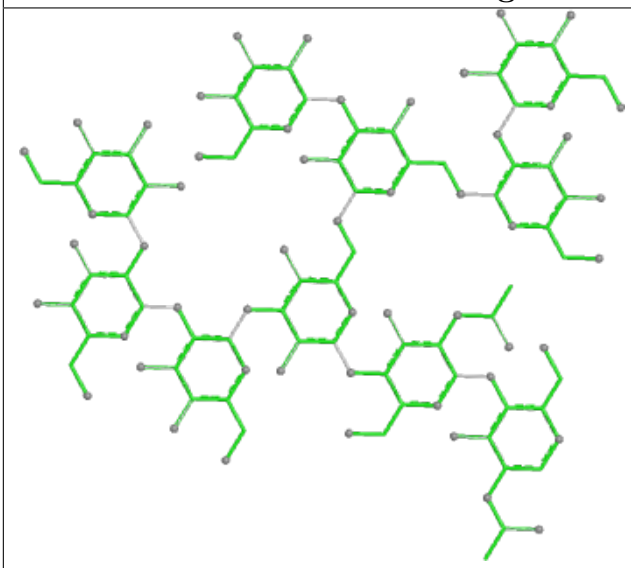
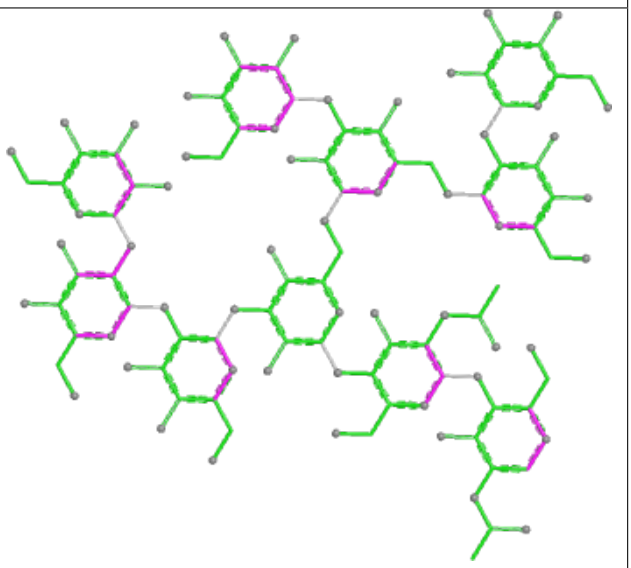
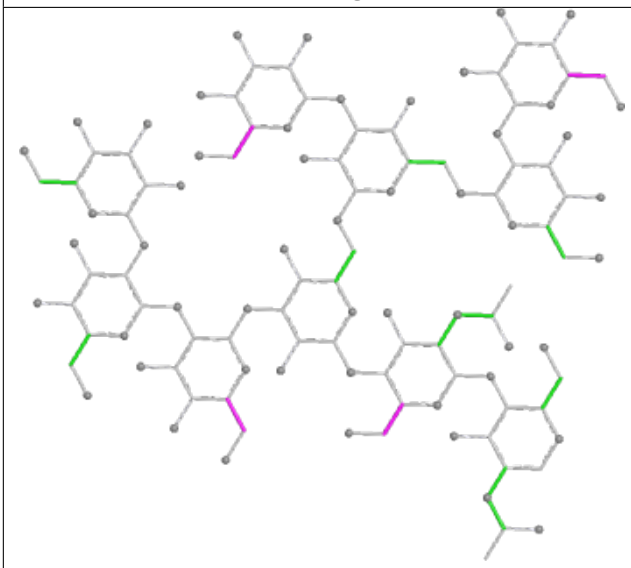
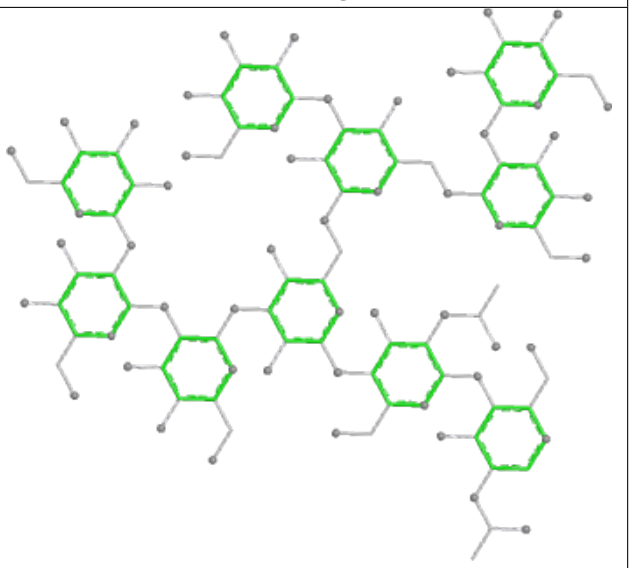
Oligosaccharide Chain 2	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain U	
 Bond lengths	 Bond angles
 Torsions	 Rings

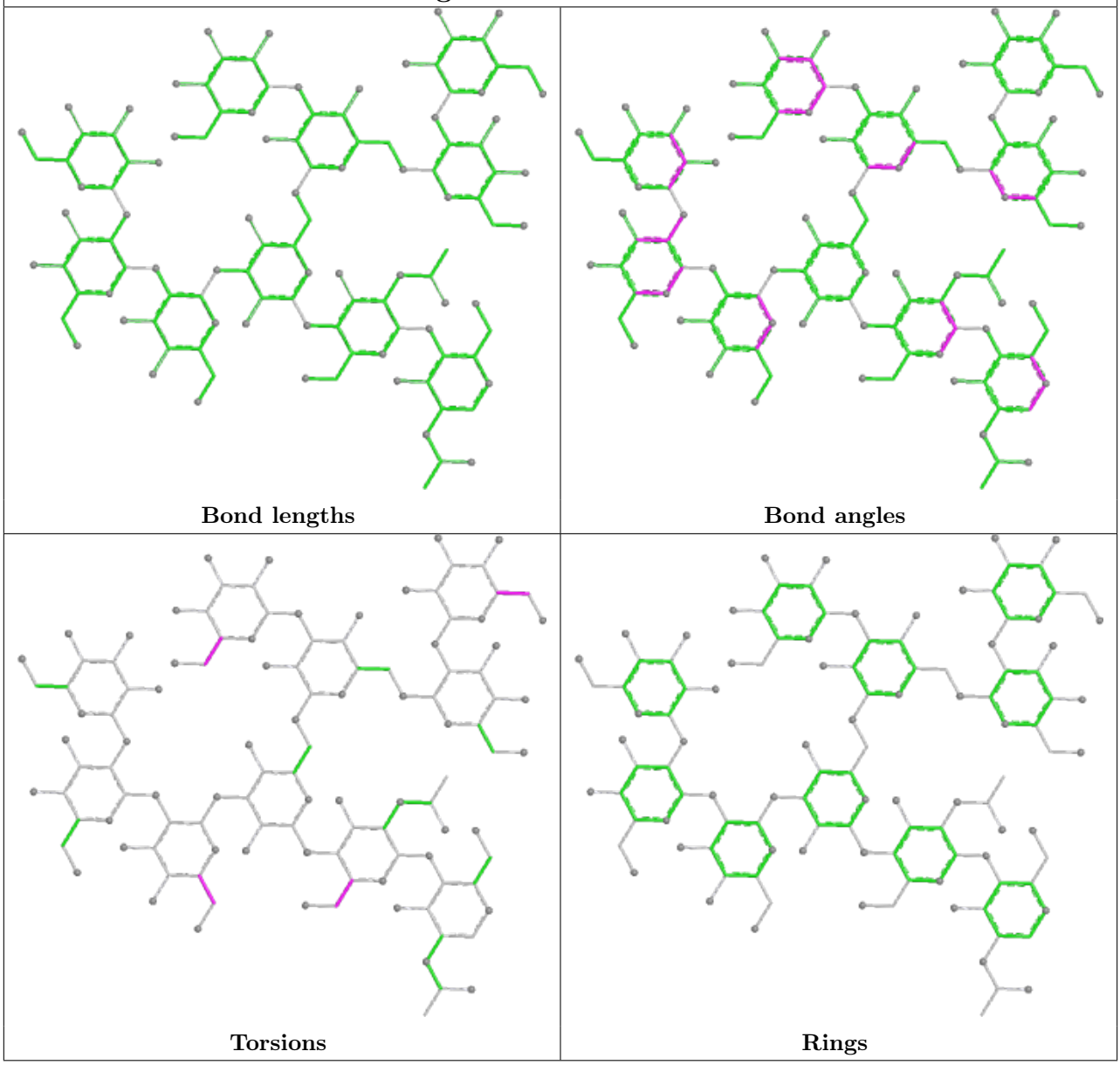
Oligosaccharide Chain l	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 1	
 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 3



5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	D	1343	1	14,14,15	0.53	0	17,19,21	2.23	3 (17%)
10	NAG	F	1637	2	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
10	NAG	B	1637	2	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
10	NAG	A	1343	1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	E	1637	2	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
10	NAG	B	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	C	1343	1	14,14,15	0.50	0	17,19,21	2.25	3 (17%)
10	NAG	E	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	F	1618	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	D	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	F	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	B	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	A	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	E	1637	2	-	0/6/23/26	0/1/1/1
10	NAG	B	1618	2	-	3/6/23/26	0/1/1/1
10	NAG	C	1343	1	-	0/6/23/26	0/1/1/1
10	NAG	E	1618	2	-	3/6/23/26	0/1/1/1
10	NAG	F	1618	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1343	NAG	O5-C1-C2	-7.39	99.61	111.29
10	B	1618	NAG	O5-C1-C2	-7.39	99.62	111.29
10	E	1637	NAG	O5-C1-C2	-7.38	99.63	111.29
10	F	1618	NAG	O5-C1-C2	-7.38	99.64	111.29
10	A	1343	NAG	O5-C1-C2	-7.38	99.64	111.29
10	F	1637	NAG	O5-C1-C2	-7.37	99.65	111.29
10	B	1637	NAG	O5-C1-C2	-7.37	99.66	111.29
10	E	1618	NAG	O5-C1-C2	-7.37	99.66	111.29
10	D	1343	NAG	O5-C1-C2	-7.36	99.67	111.29

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1343	NAG	O7-C7-C8	-2.80	116.86	122.06
10	B	1618	NAG	O7-C7-C8	-2.78	116.90	122.06
10	A	1343	NAG	O7-C7-C8	-2.77	116.91	122.06
10	E	1618	NAG	O7-C7-C8	-2.76	116.93	122.06
10	F	1637	NAG	O7-C7-C8	-2.76	116.93	122.06
10	B	1637	NAG	O7-C7-C8	-2.76	116.93	122.06
10	E	1637	NAG	O7-C7-C8	-2.76	116.94	122.06
10	F	1618	NAG	O7-C7-C8	-2.76	116.94	122.06
10	D	1343	NAG	O7-C7-C8	-2.75	116.96	122.06
10	C	1343	NAG	C4-C3-C2	-2.71	107.05	111.02
10	A	1343	NAG	C4-C3-C2	-2.69	107.07	111.02
10	B	1618	NAG	C4-C3-C2	-2.69	107.07	111.02
10	D	1343	NAG	C4-C3-C2	-2.69	107.07	111.02
10	E	1618	NAG	C4-C3-C2	-2.69	107.07	111.02
10	F	1618	NAG	C4-C3-C2	-2.69	107.08	111.02
10	B	1637	NAG	C4-C3-C2	-2.64	107.14	111.02
10	E	1637	NAG	C4-C3-C2	-2.64	107.15	111.02
10	F	1637	NAG	C4-C3-C2	-2.64	107.16	111.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1618	NAG	C1-C2-N2-C7
10	E	1618	NAG	C1-C2-N2-C7
10	F	1618	NAG	C1-C2-N2-C7
10	B	1618	NAG	C3-C2-N2-C7
10	E	1618	NAG	C3-C2-N2-C7
10	F	1618	NAG	C3-C2-N2-C7
10	B	1618	NAG	O7-C7-N2-C2
10	E	1618	NAG	O7-C7-N2-C2
10	F	1618	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	E	1
2	F	1
1	A	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	658:GLN	C	659:ASP	N	1.61
1	E	658:GLN	C	659:ASP	N	1.61
1	F	658:GLN	C	659:ASP	N	1.61
1	A	92:GLU	C	93:PHE	N	1.19
1	C	92:GLU	C	93:PHE	N	1.19
1	D	92:GLU	C	93:PHE	N	1.19

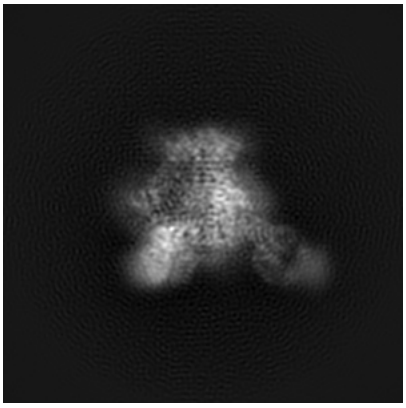
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3121. These allow visual inspection of the internal detail of the map and identification of artifacts.

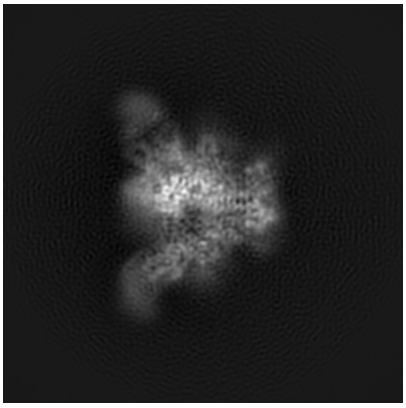
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

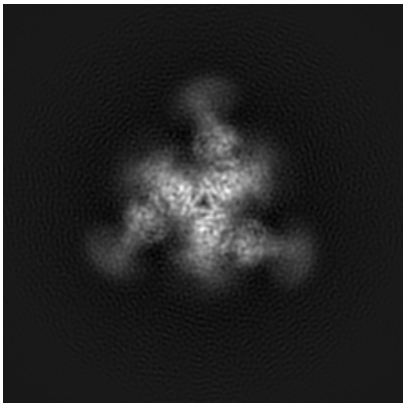
6.1.1 Primary map



X



Y

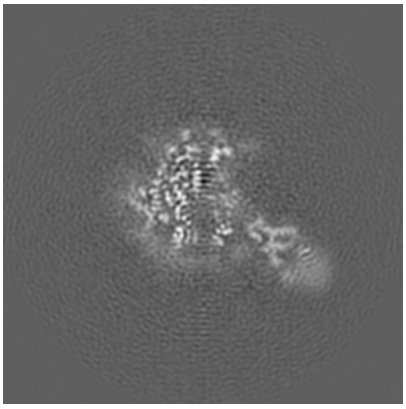


Z

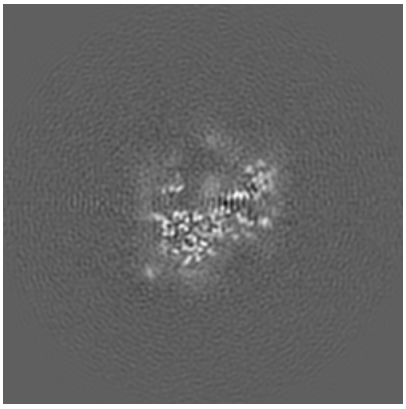
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

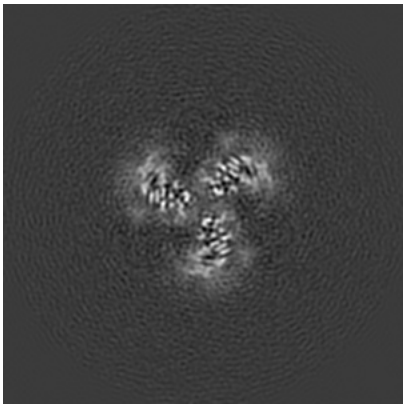
6.2.1 Primary map



X Index: 128



Y Index: 128

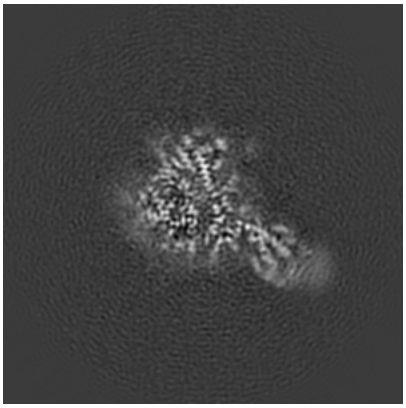


Z Index: 128

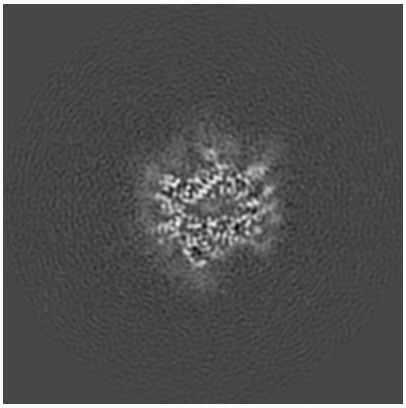
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

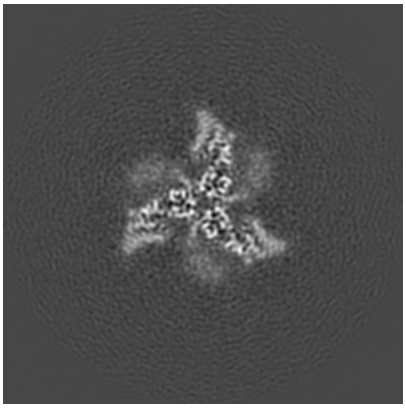
6.3.1 Primary map



X Index: 133



Y Index: 136

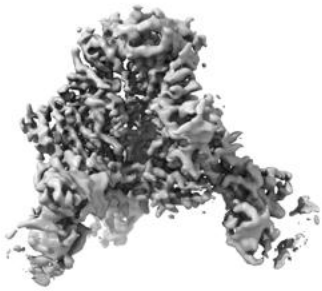


Z Index: 110

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

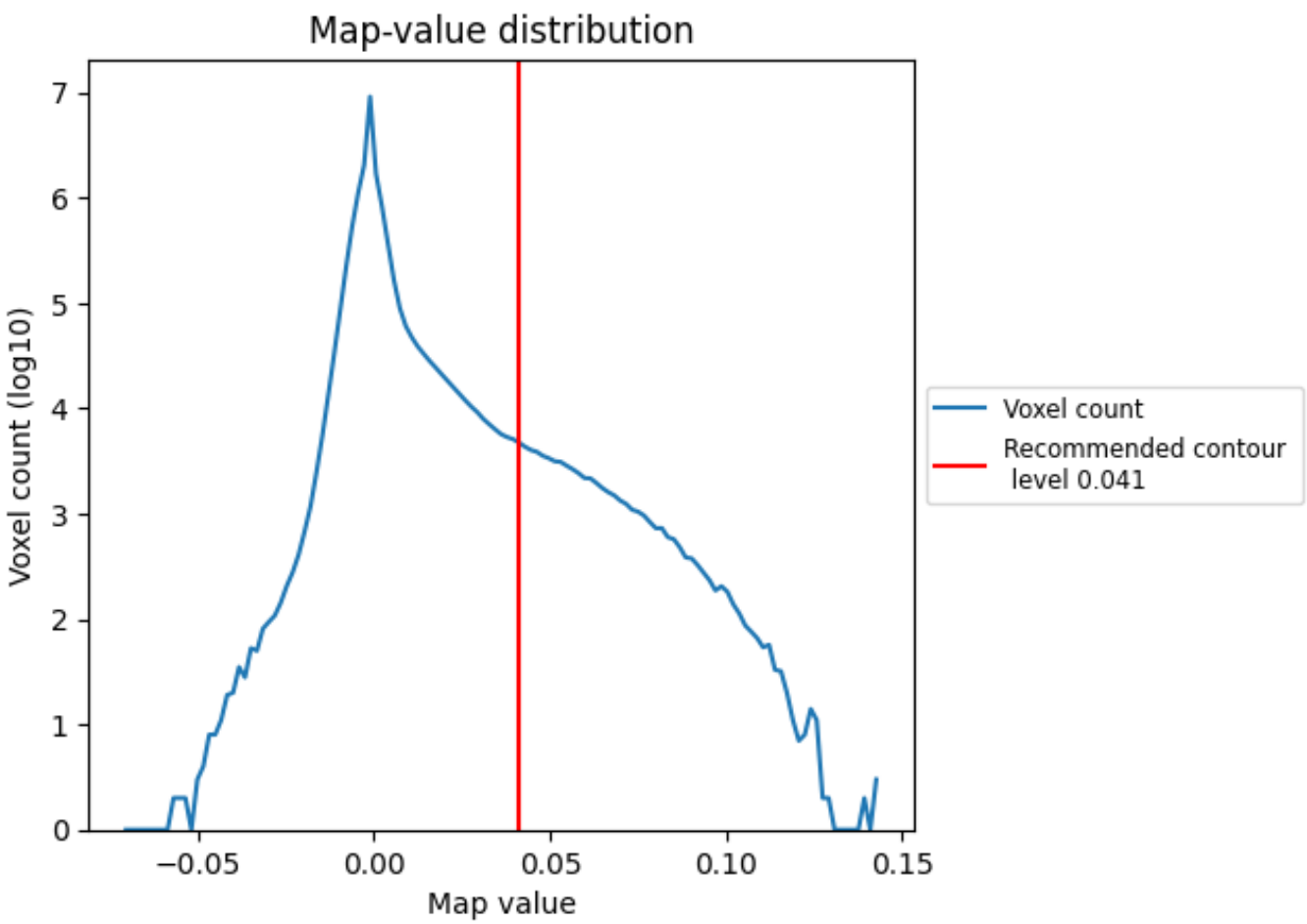
6.5 Mask visualisation (i)

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

7 Map analysis (i)

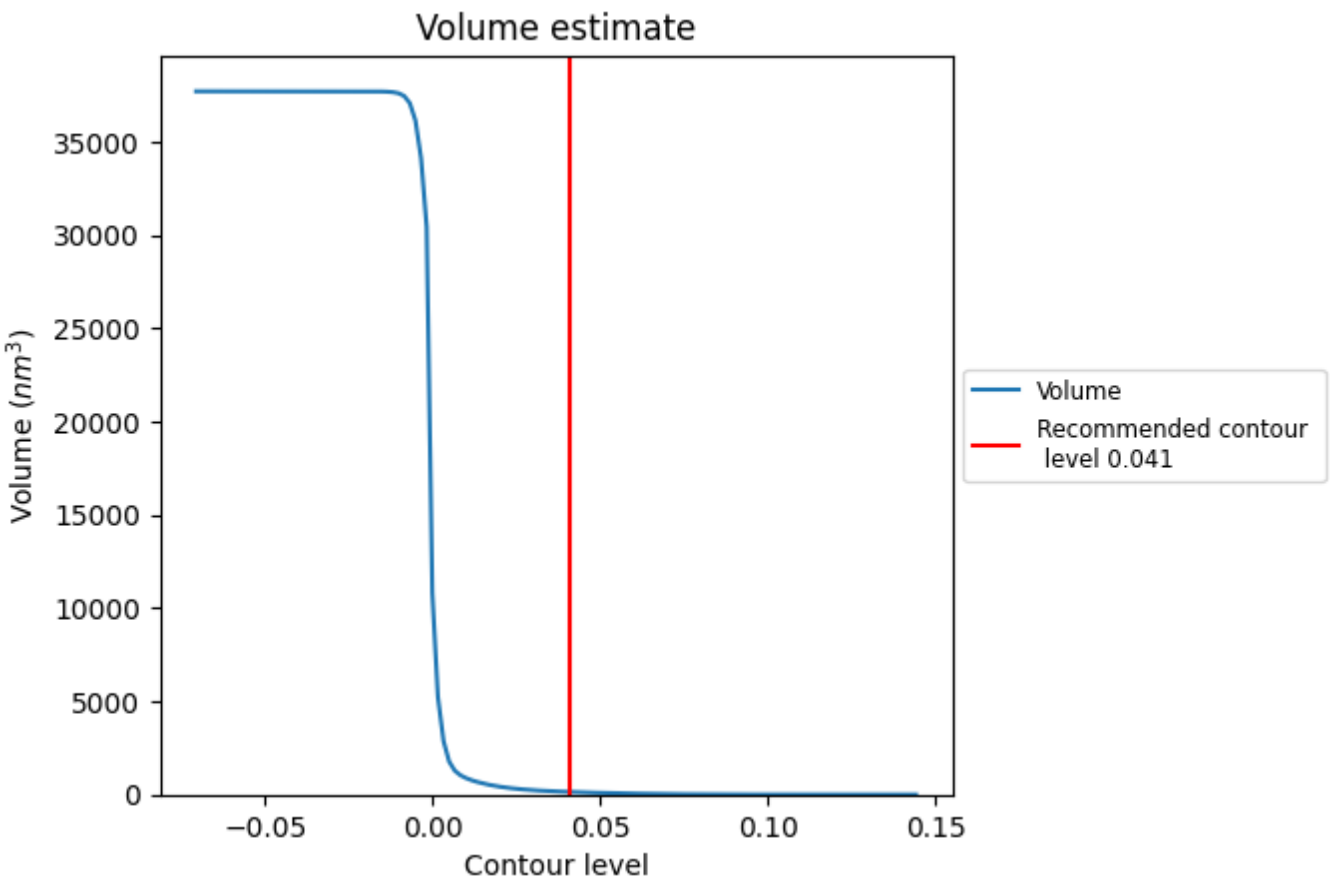
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

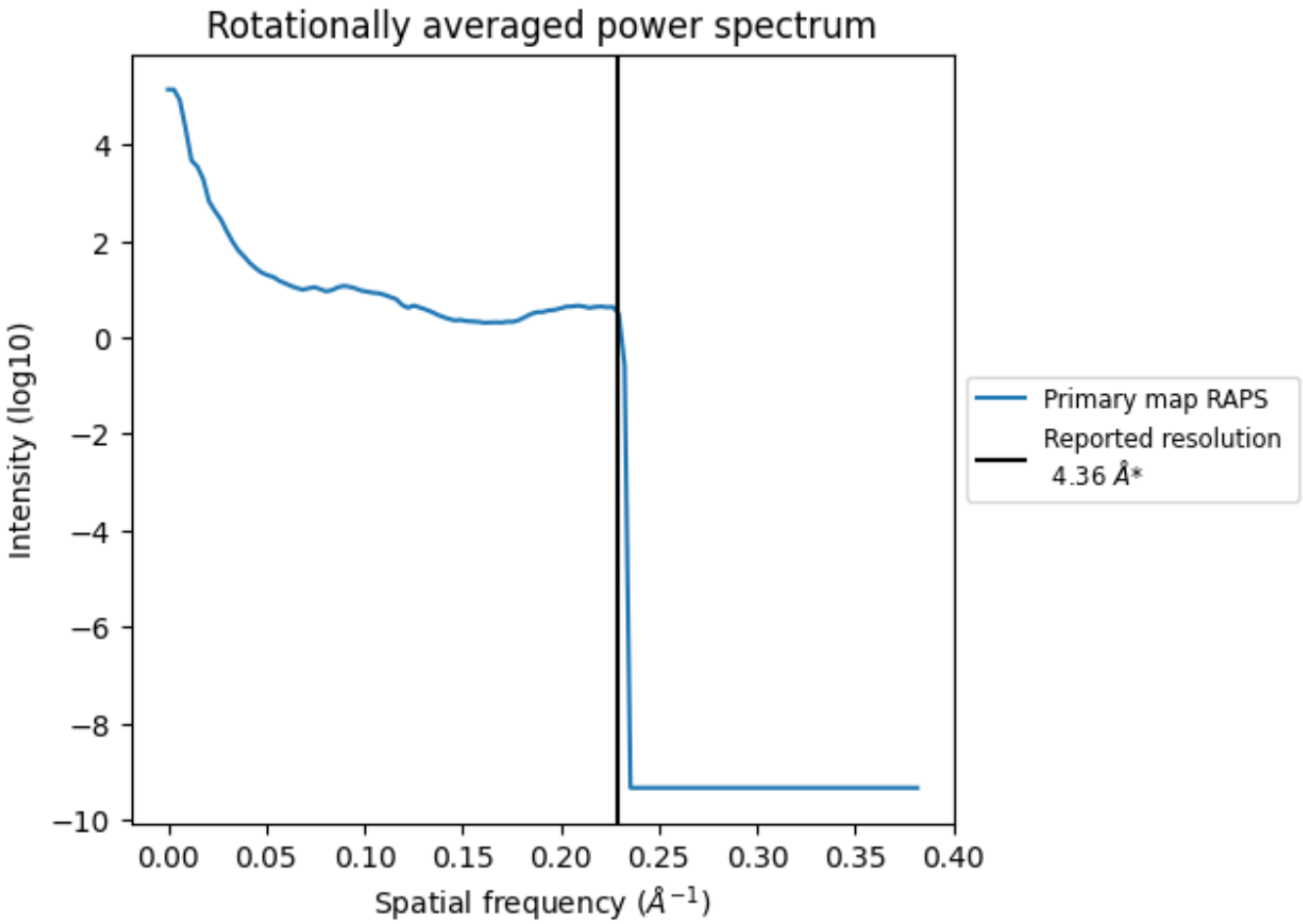
7.2 Volume estimate (i)



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 127 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.229 Å^{-1}

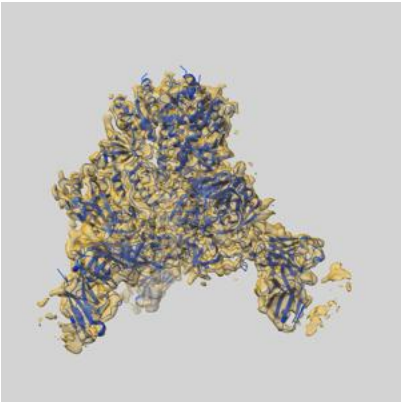
8 Fourier-Shell correlation (i)

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

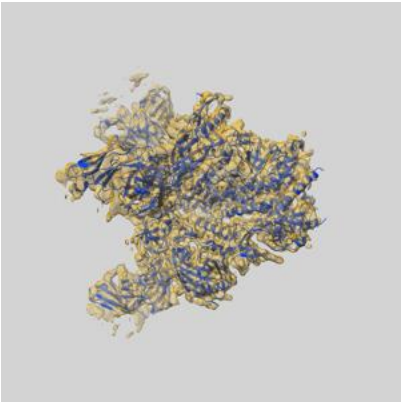
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3121 and PDB model 5ACO. Per-residue inclusion information can be found in section 3 on page 12.

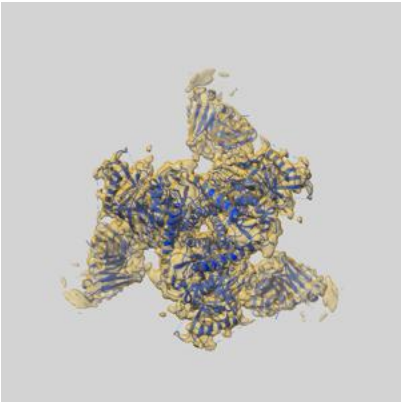
9.1 Map-model overlay (i)



X



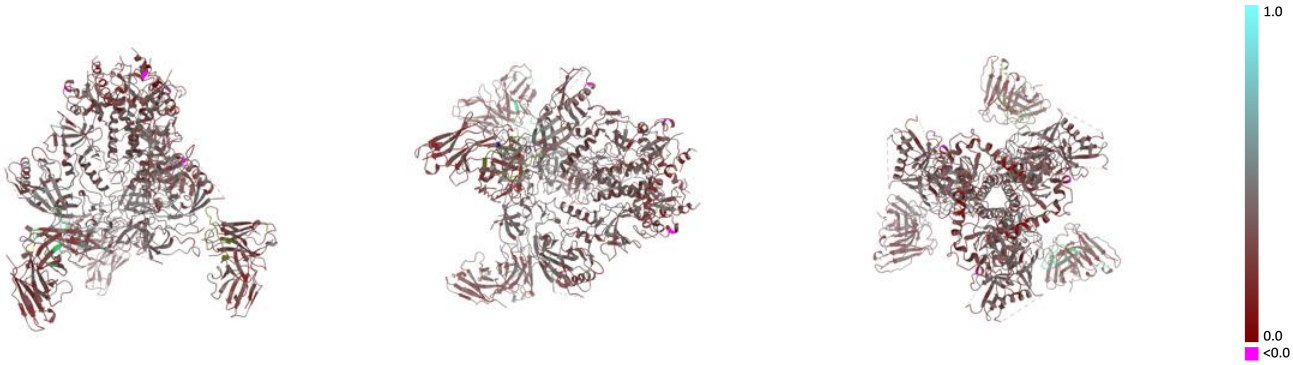
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.041 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

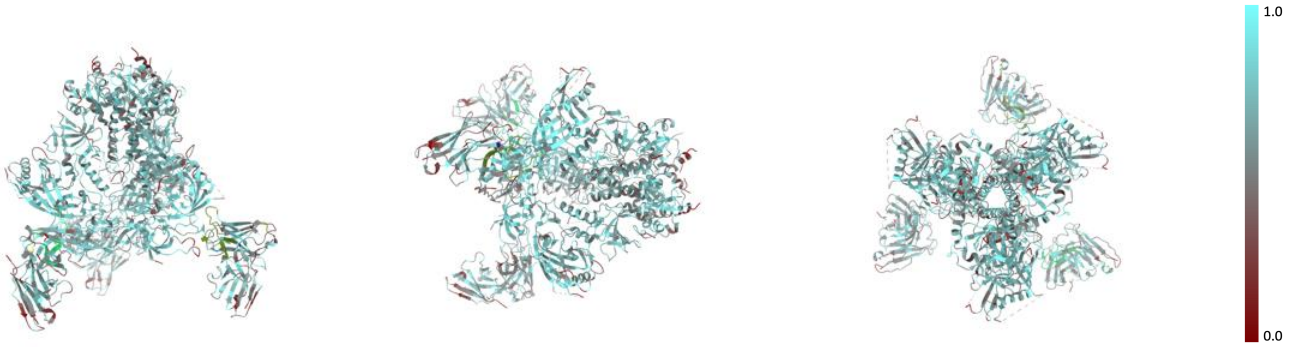
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

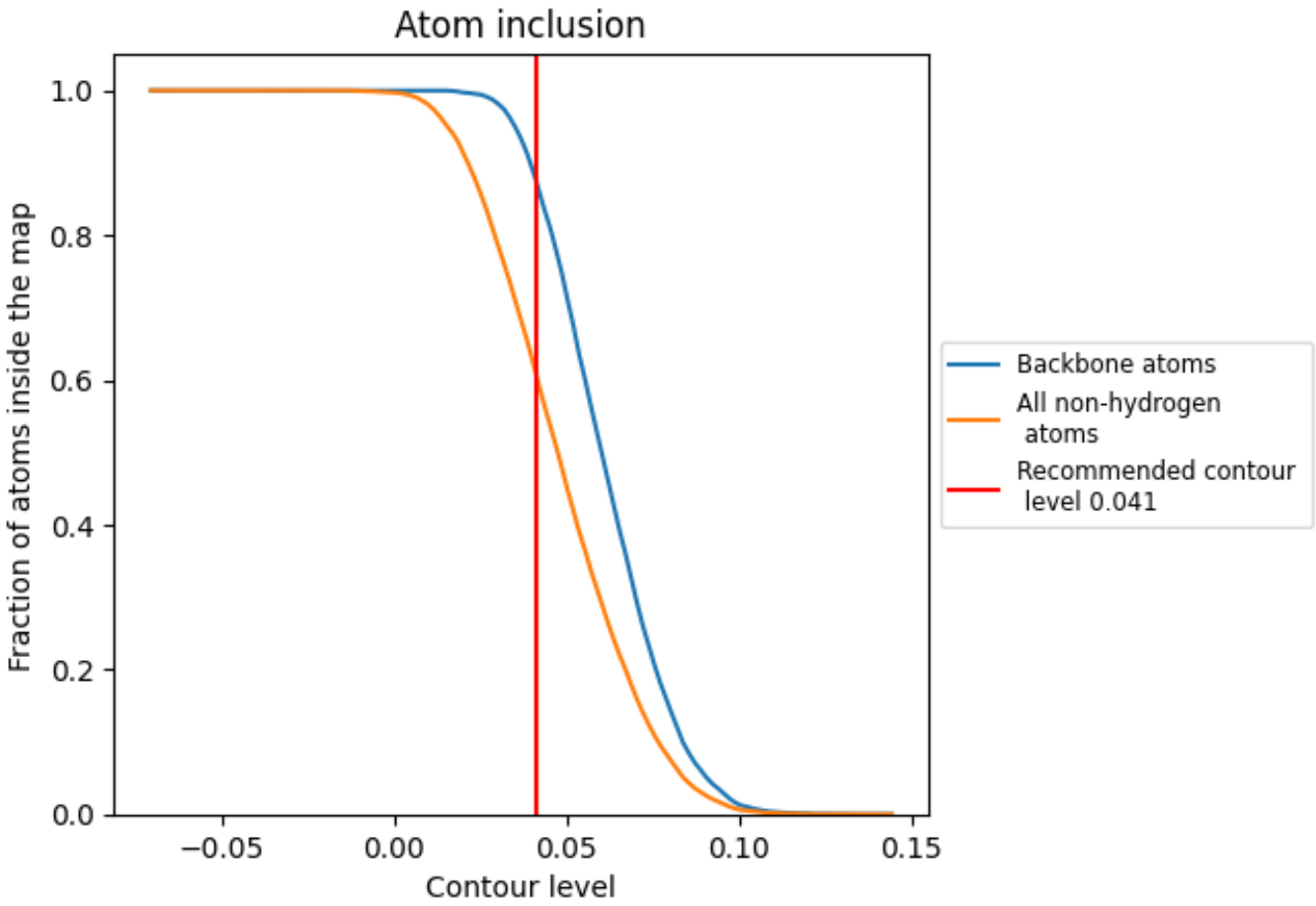
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.041).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6121	0.3320
0	0.1538	0.2740
1	0.2459	0.2430
2	0.4699	0.3210
3	0.6724	0.3810
4	0.0000	0.2270
5	0.2308	0.1350
6	0.3846	0.1600
7	0.0714	0.2440
8	0.3929	0.2610
9	0.1071	0.2370
A	0.6863	0.3690
AA	0.0714	0.2290
B	0.5836	0.2980
C	0.6858	0.3690
D	0.6843	0.3690
E	0.5902	0.3000
F	0.5883	0.2990
G	0.6291	0.3150
H	0.6321	0.3160
I	0.6321	0.3170
J	0.5782	0.2900
K	0.5768	0.2850
L	0.5755	0.2890
M	0.1282	0.2900
N	0.2143	0.2910
O	0.3333	0.2100
P	0.2564	0.3290
Q	0.3214	0.2740
R	0.2143	0.2670
S	0.3614	0.2860
T	0.1538	0.2570
U	0.2459	0.2370
V	0.4699	0.3220
W	0.6724	0.3740

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Chain	Atom inclusion	Q-score
X	0.0357	0.2450
Y	0.2308	0.1310
Z	0.3846	0.1680
a	0.0714	0.2230
b	0.3929	0.2500
c	0.0714	0.2230
d	0.1282	0.2750
e	0.2500	0.3020
f	0.3333	0.2020
g	0.2308	0.3240
h	0.3214	0.2760
i	0.2143	0.2970
j	0.3735	0.2830
k	0.1282	0.2610
l	0.2459	0.2380
m	0.4699	0.3210
n	0.6724	0.3670
o	0.0000	0.2280
p	0.2308	0.1450
q	0.4103	0.1620
r	0.0714	0.2330
s	0.3929	0.2440
t	0.1282	0.2900
u	0.2143	0.2980
v	0.3333	0.2120
w	0.2051	0.3370
x	0.3214	0.2700
y	0.2500	0.2800
z	0.3735	0.2830