Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:21 am GMT

PDB ID	:	5FUU
EMDB ID	:	EMD-3308
Title	:	Ectodomain of cleaved wild type JR-FL EnvdCT trimer in complex with PGT151 Fab
Authors	:	Lee, J.H.; Ward, A.B.
Deposited on	:	2016-01-29
Resolution	:	4.20 Å(reported)

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

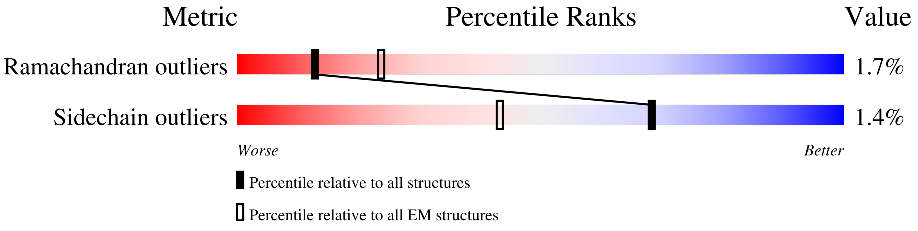
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

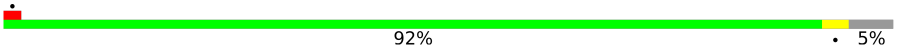
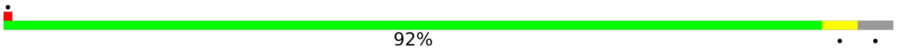
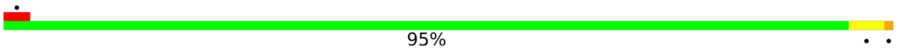
The reported resolution of this entry is 4.20 Å.

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	473	
1	C	473	
1	E	473	
2	B	153	
2	D	153	
2	F	153	
3	H	240	
3	M	240	
4	L	219	

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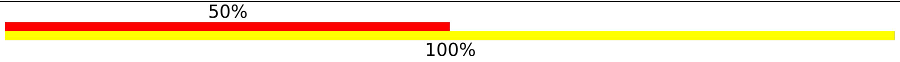
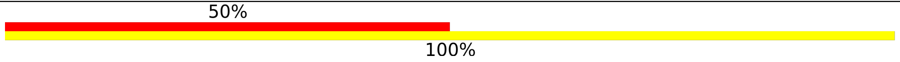
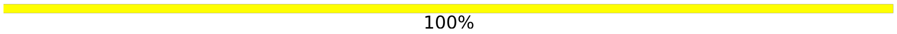
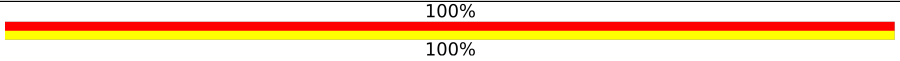
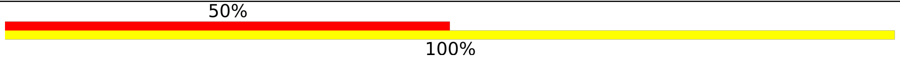
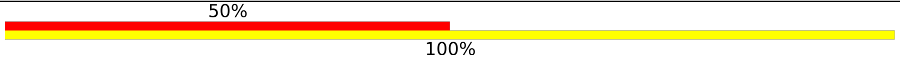
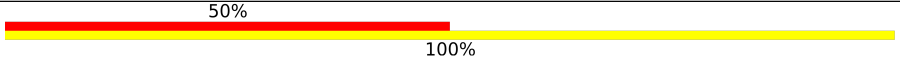
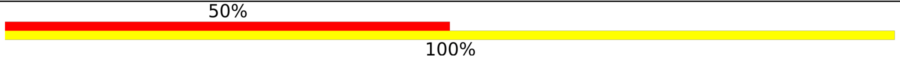
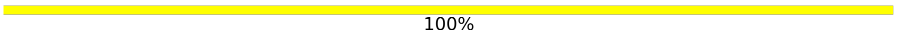
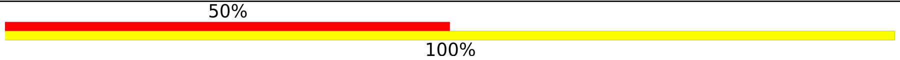
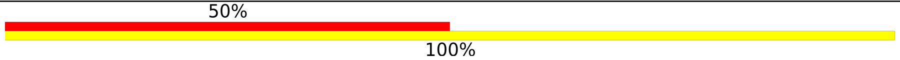
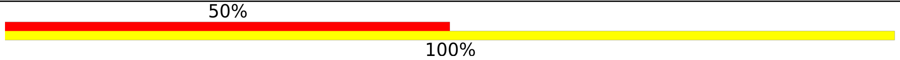
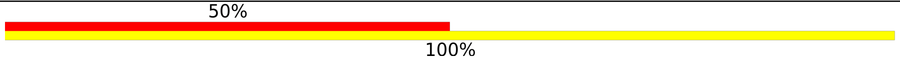
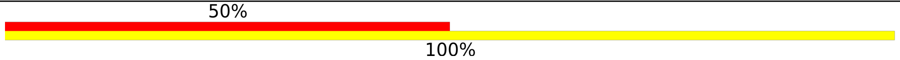
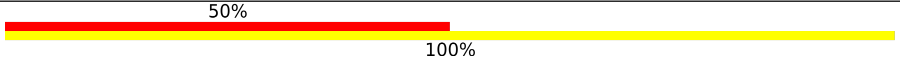
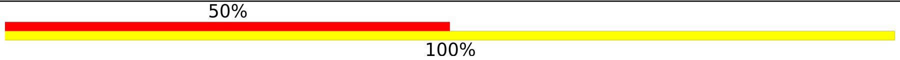
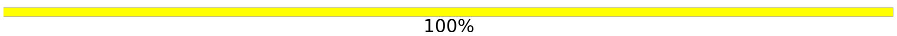
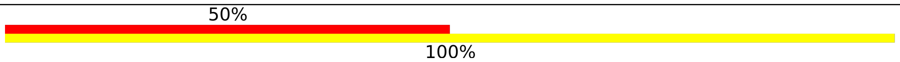
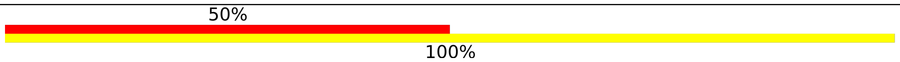
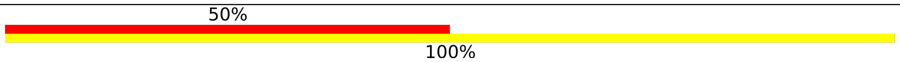
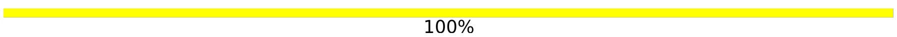
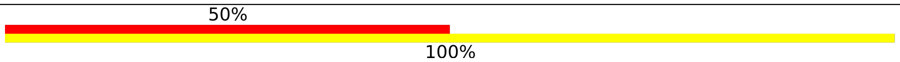
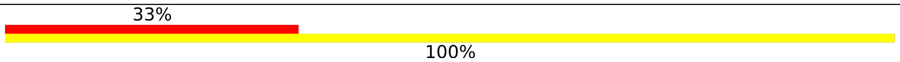
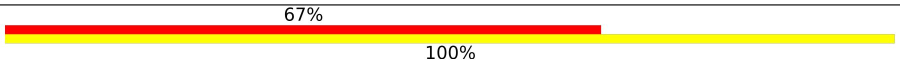
Mol	Chain	Length	Quality of chain
4	N	219	
5	0	2	
5	1	2	
5	3	2	
5	4	2	
5	5	2	
5	AA	2	
5	G	2	
5	Q	2	
5	R	2	
5	T	2	
5	X	2	
5	b	2	
5	c	2	
5	h	2	
5	k	2	
5	l	2	
5	o	2	
5	r	2	
5	s	2	
5	u	2	
5	w	2	
5	z	2	
6	2	3	
6	7	3	

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Mol	Chain	Length	Quality of chain
6	I	3	33% 100%
6	J	3	33% 100%
6	K	3	33% 100%
6	P	3	100%
6	S	3	33% 100%
6	U	3	67% 100%
6	V	3	100%
6	W	3	33% 100%
6	a	3	33% 100%
6	d	3	67% 100%
6	g	3	33% 100%
6	i	3	33% 100%
6	j	3	33% 100%
6	m	3	33% 100%
6	n	3	100%
6	t	3	100%
6	v	3	33% 100%
7	O	7	86% 14%
7	f	7	29% 86% 14%
7	y	7	86% 14%
8	9	11	18% 100%
8	Y	11	18% 100%
9	Z	13	15% 100%
10	e	5	100%
11	8	8	38% 100%

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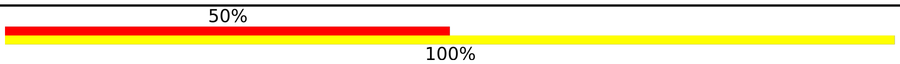
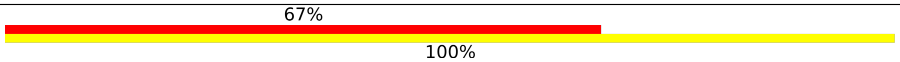
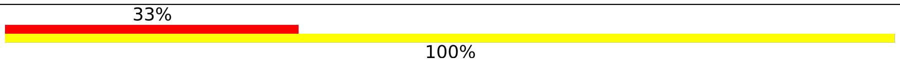
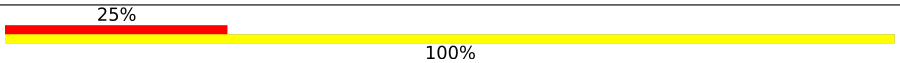
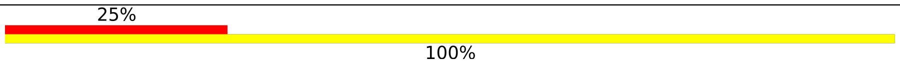
Mol	Chain	Length	Quality of chain
11	p	8	
12	q	3	
13	x	6	
14	6	4	
15	BA	12	

2 Entry composition ⓘ

There are 16 unique types of molecules in this entry. The entry contains 20735 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 GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3553	2233	624	671	25		
1	C	444	Total	C	N	O	S	0	0
			3506	2208	613	660	25		
1	E	448	Total	C	N	O	S	0	0
			3537	2224	620	668	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	THR	VAL	engineered mutation	UNP Q75760
C	31	THR	VAL	engineered mutation	UNP Q75760
E	31	THR	VAL	engineered mutation	UNP Q75760

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1150	722	200	221	7		
2	D	147	Total	C	N	O	S	0	0
			1159	731	203	218	7		
2	F	153	Total	C	N	O	S	0	0
			1209	763	209	230	7		

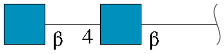
- Molecule 3 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	135	Total	C	N	O	S	0	0
			1073	682	188	197	6		
3	M	135	Total	C	N	O	S	0	0
			1067	679	185	197	6		

- Molecule 4 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	114	Total 881	C 553	N 151	O 173	S 4	0	0
4	N	112	Total 866	C 545	N 149	O 168	S 4	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total 28	C 16	N 2	O 10	0	0
5	Q	2	Total 28	C 16	N 2	O 10	0	0
5	R	2	Total 28	C 16	N 2	O 10	0	0
5	T	2	Total 28	C 16	N 2	O 10	0	0
5	X	2	Total 28	C 16	N 2	O 10	0	0
5	b	2	Total 28	C 16	N 2	O 10	0	0
5	c	2	Total 28	C 16	N 2	O 10	0	0
5	h	2	Total 28	C 16	N 2	O 10	0	0
5	k	2	Total 28	C 16	N 2	O 10	0	0
5	l	2	Total 28	C 16	N 2	O 10	0	0
5	o	2	Total 28	C 16	N 2	O 10	0	0
5	r	2	Total 28	C 16	N 2	O 10	0	0
5	s	2	Total 28	C 16	N 2	O 10	0	0
5	u	2	Total 28	C 16	N 2	O 10	0	0
5	w	2	Total 28	C 16	N 2	O 10	0	0

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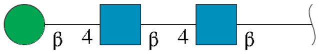
Mol	Chain	Residues	Atoms	AltConf	Trace
5	z	2	Total C N O 28 16 2 10	0	0
5	0	2	Total C N O 28 16 2 10	0	0
5	1	2	Total C N O 28 16 2 10	0	0
5	3	2	Total C N O 28 16 2 10	0	0
5	4	2	Total C N O 28 16 2 10	0	0
5	5	2	Total C N O 28 16 2 10	0	0
5	AA	2	Total C N O 28 16 2 10	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
6	I	3	Total C N O 39 22 2 15	0	0
6	J	3	Total C N O 39 22 2 15	0	0
6	K	3	Total C N O 39 22 2 15	0	0
6	P	3	Total C N O 39 22 2 15	0	0
6	S	3	Total C N O 39 22 2 15	0	0
6	U	3	Total C N O 39 22 2 15	0	0
6	V	3	Total C N O 39 22 2 15	0	0
6	W	3	Total C N O 39 22 2 15	0	0
6	a	3	Total C N O 39 22 2 15	0	0
6	d	3	Total C N O 39 22 2 15	0	0

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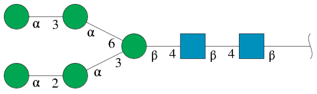
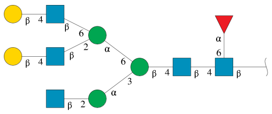
Mol	Chain	Residues	Atoms	AltConf	Trace
6	g	3	Total C N O 39 22 2 15	0	0
6	i	3	Total C N O 39 22 2 15	0	0
6	j	3	Total C N O 39 22 2 15	0	0
6	m	3	Total C N O 39 22 2 15	0	0
6	n	3	Total C N O 39 22 2 15	0	0
6	t	3	Total C N O 39 22 2 15	0	0
6	v	3	Total C N O 39 22 2 15	0	0
6	2	3	Total C N O 39 22 2 15	0	0
6	7	3	Total C N O 39 22 2 15	0	0

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



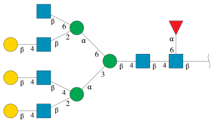
Mol	Chain	Residues	Atoms	AltConf	Trace
7	O	7	Total C N O 83 46 2 35	0	0
7	f	7	Total C N O 83 46 2 35	0	0
7	y	7	Total C N O 83 46 2 35	0	0

- Molecule 8 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



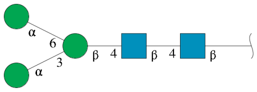
Mol	Chain	Residues	Atoms	AltConf	Trace
8	Y	11	Total C N O 135 76 5 54	0	0
8	9	11	Total C N O 135 76 5 54	0	0

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



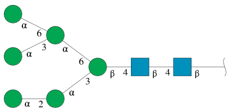
Mol	Chain	Residues	Atoms	AltConf	Trace
9	Z	13	Total C N O 160 90 6 64	0	0

- Molecule 10 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.



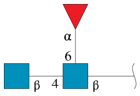
Mol	Chain	Residues	Atoms	AltConf	Trace
10	e	5	Total C N O 61 34 2 25	0	0

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



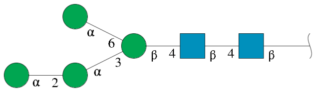
Mol	Chain	Residues	Atoms	AltConf	Trace
11	p	8	Total C N O 94 52 2 40	0	0
11	8	8	Total C N O 94 52 2 40	0	0

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



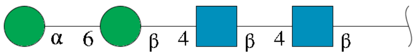
Mol	Chain	Residues	Atoms	AltConf	Trace
12	q	3	Total C N O 38 22 2 14	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



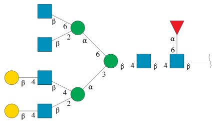
Mol	Chain	Residues	Atoms	AltConf	Trace
13	x	6	Total C N O 72 40 2 30	0	0

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



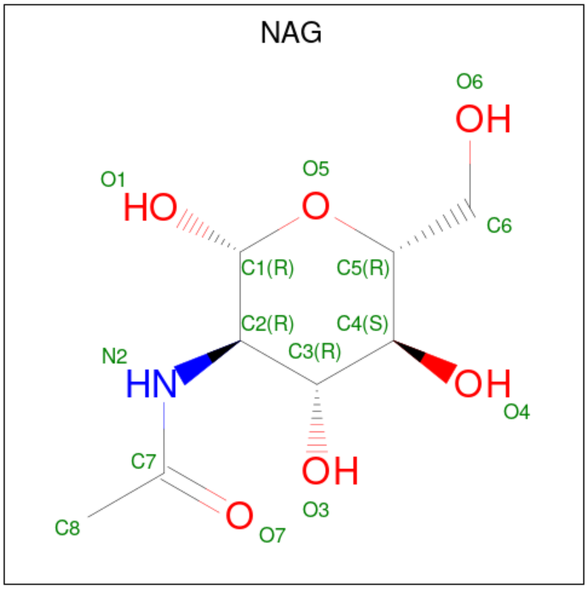
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	6	4	50	28	2	20	0	0

- Molecule 15 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	BA	12	149	84	6	59	0	0

- Molecule 16 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	
16	A	1	42	24	3	15	0
16	A	1	42	24	3	15	0

Continued on next page...

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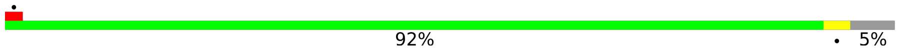
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	A	1	42	24	3	15	0
16	B	1	28	16	2	10	0
16	B	1	28	16	2	10	0
16	C	1	14	8	1	5	0
16	D	1	14	8	1	5	0
16	E	1	28	16	2	10	0
16	E	1	28	16	2	10	0
16	F	1	14	8	1	5	0

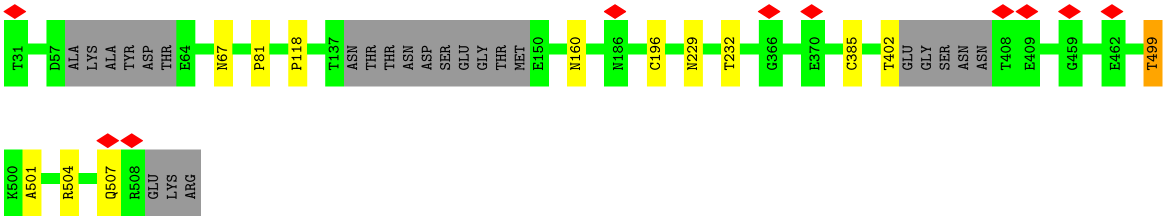
3 Residue-property plots

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

- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

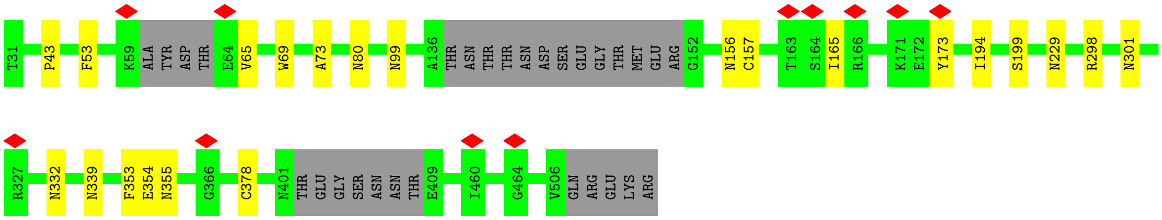
Chain A:





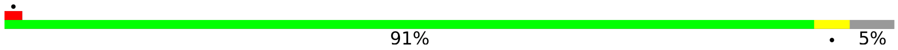
- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

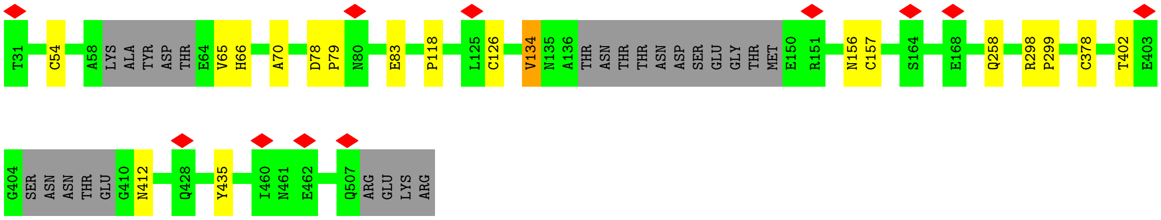
Chain C:



- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

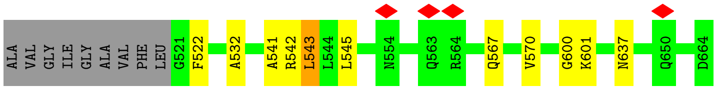
Chain E:



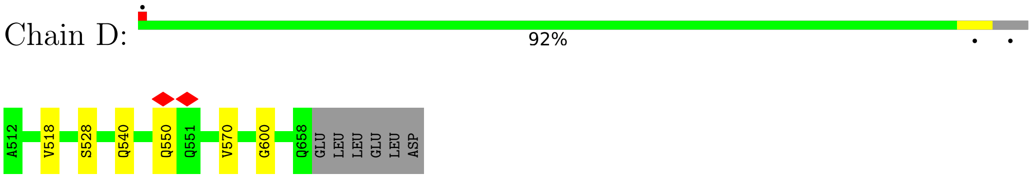


- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160

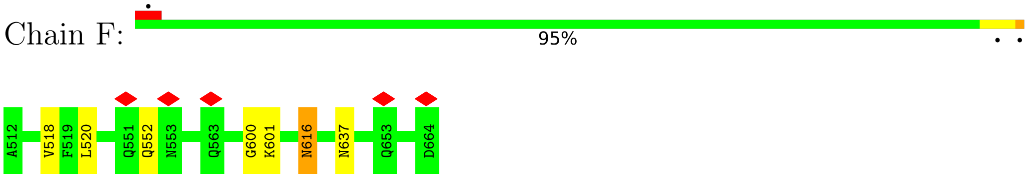
Chain B:



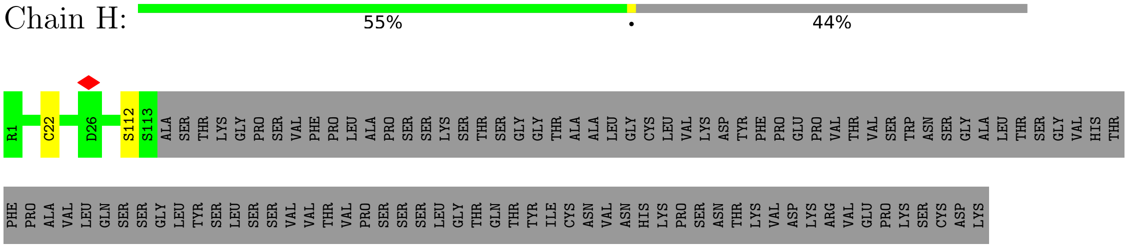
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160



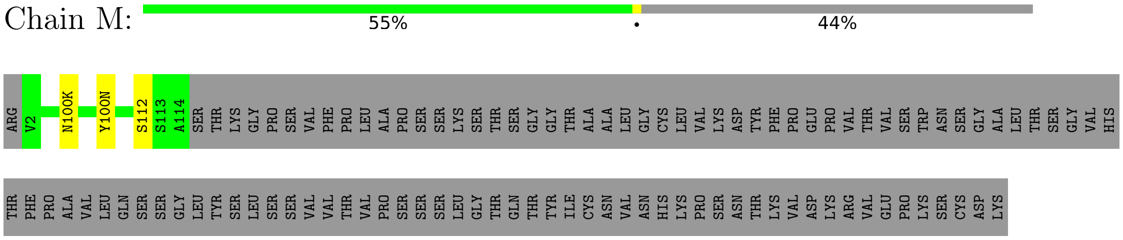
- Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160



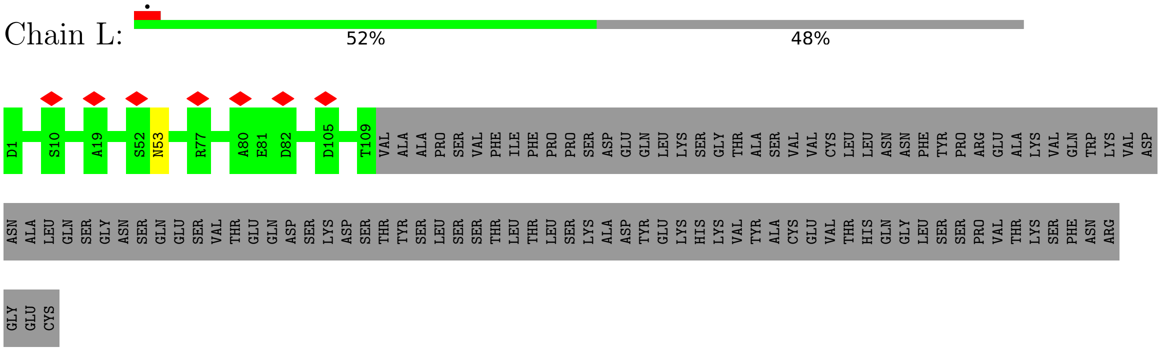
- Molecule 3: IMMUNOGLOBULIN G PGT151



- Molecule 3: IMMUNOGLOBULIN G PGT151

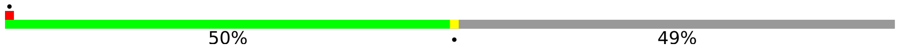


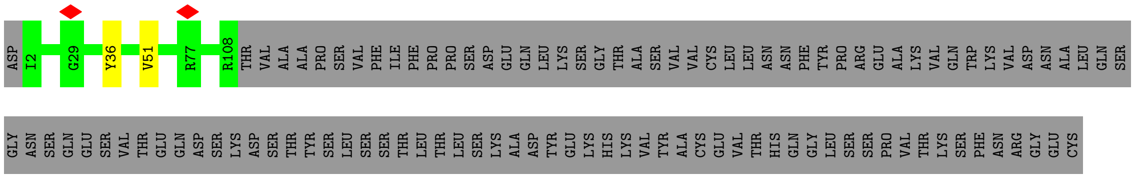
- Molecule 4: IMMUNOGLOBULIN G PGT151



- Molecule 4: IMMUNOGLOBULIN G PGT151

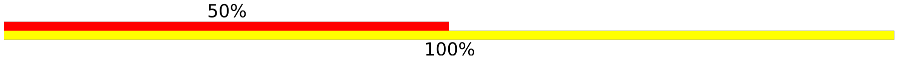
Chain N:





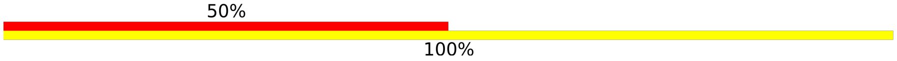
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



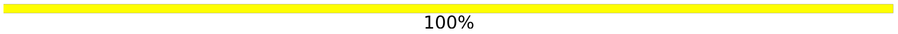
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



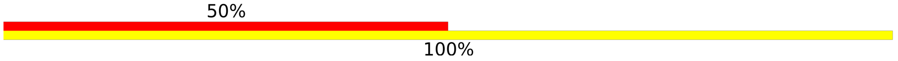
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



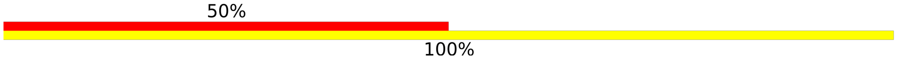
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



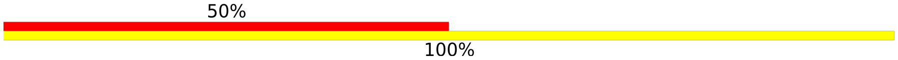
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



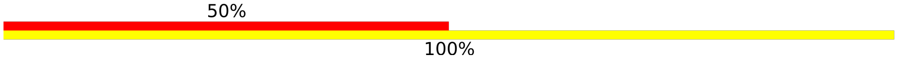
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



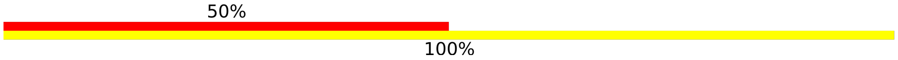
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



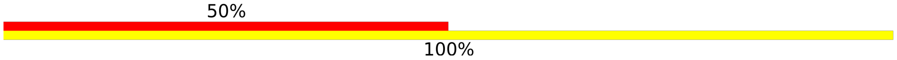
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



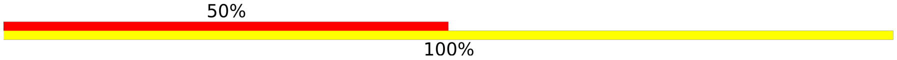
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



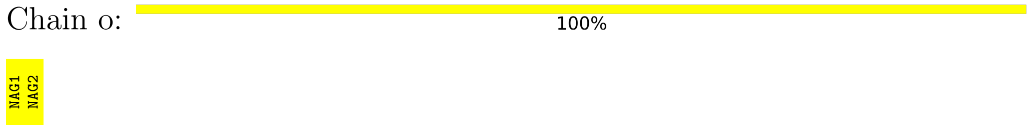
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



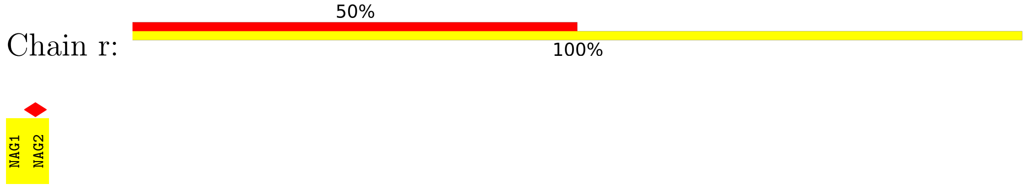
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



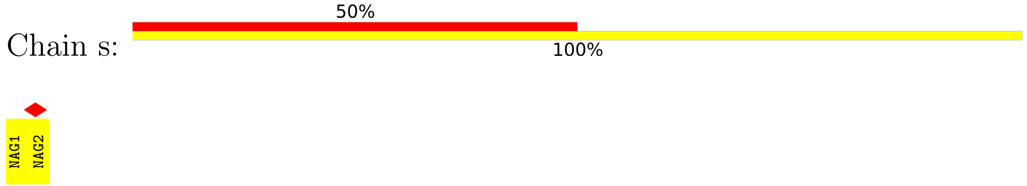
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



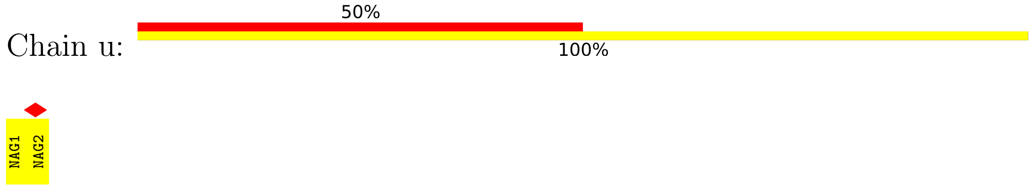
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



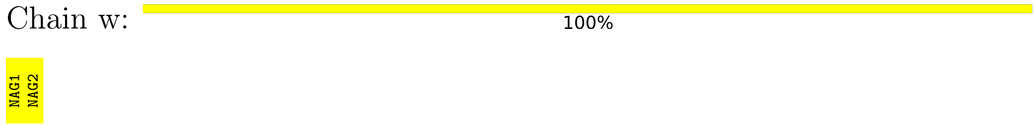
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



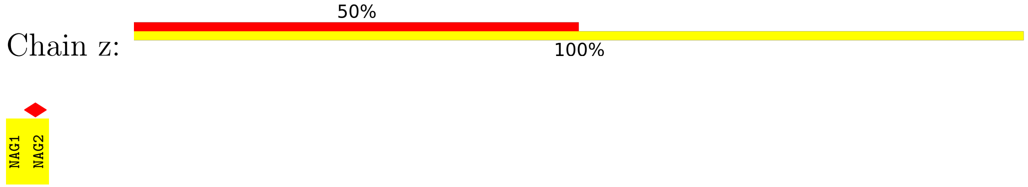
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



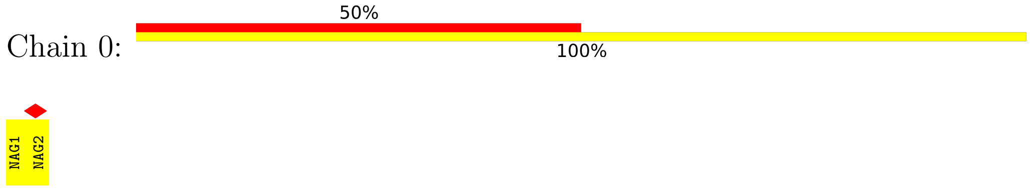
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



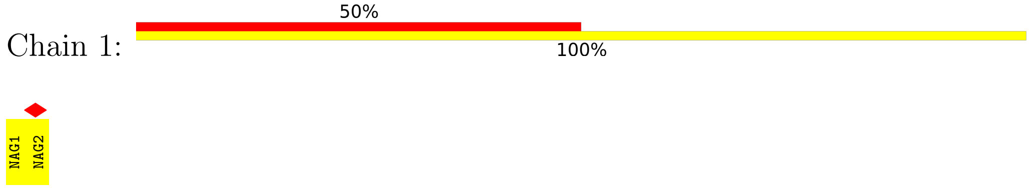
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



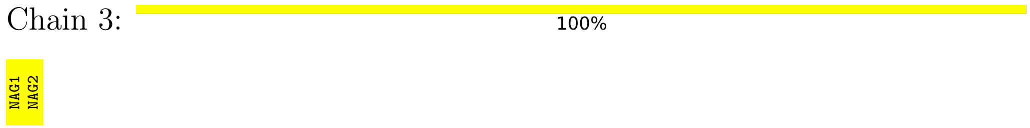
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



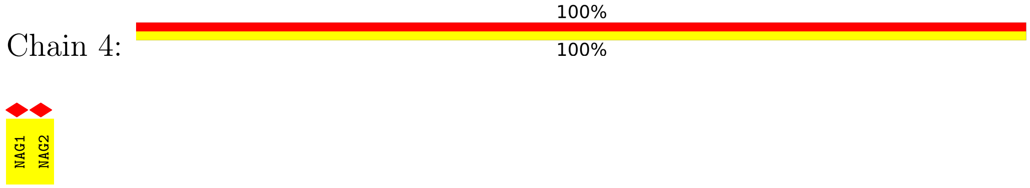
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



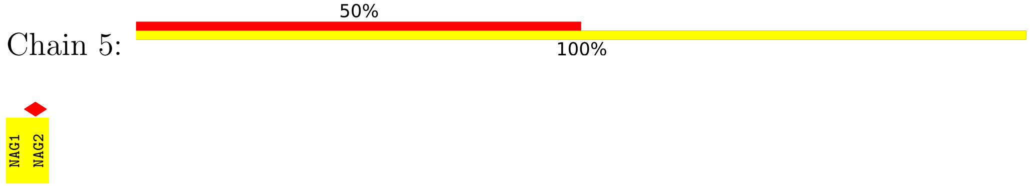
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:



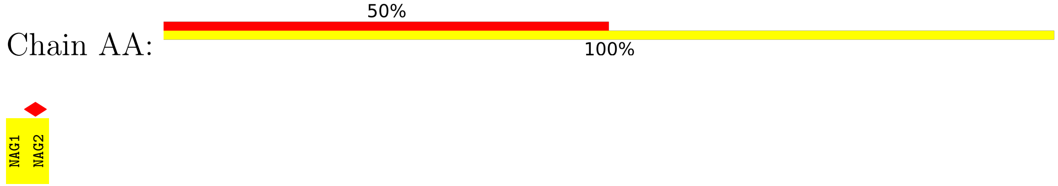
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



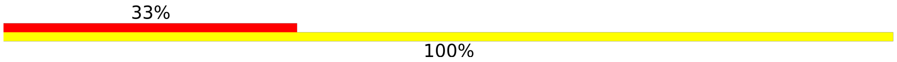
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



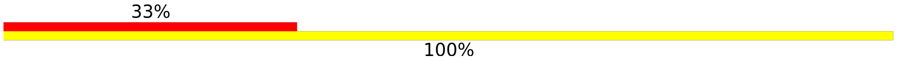
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



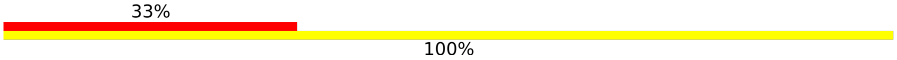
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



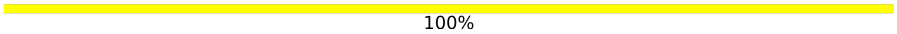
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



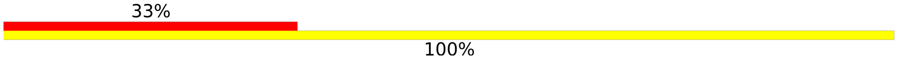
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



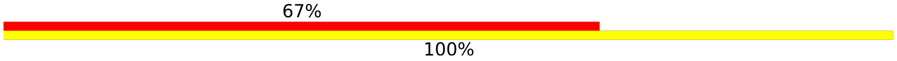
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



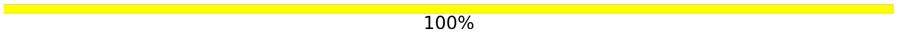
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



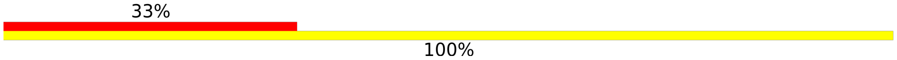
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



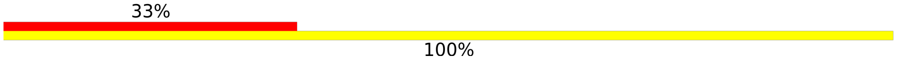
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



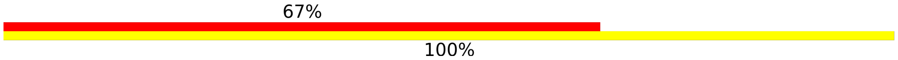
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

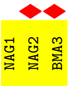
Chain a:



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

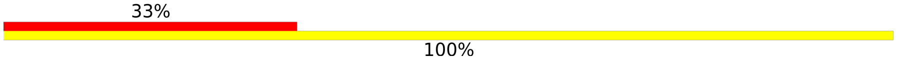
Chain d:





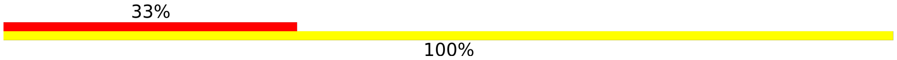
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



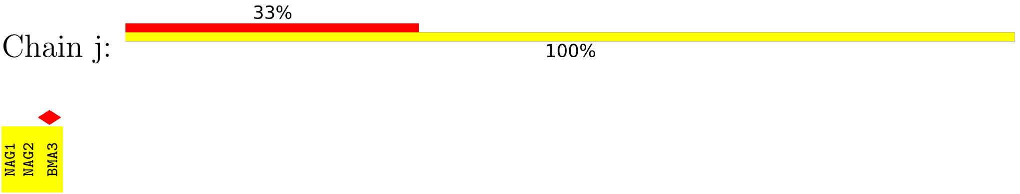
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



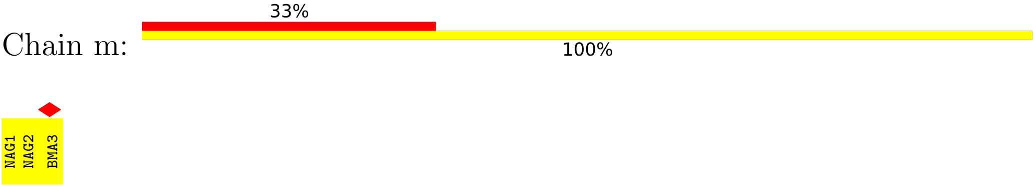
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



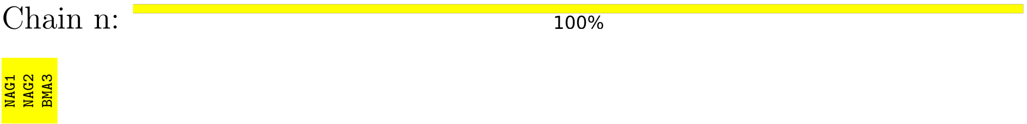
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



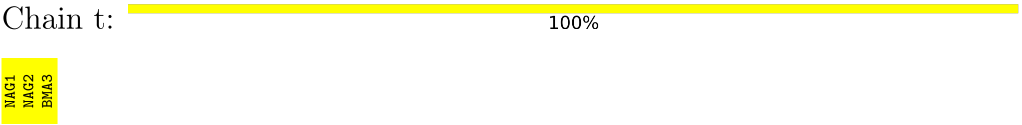
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



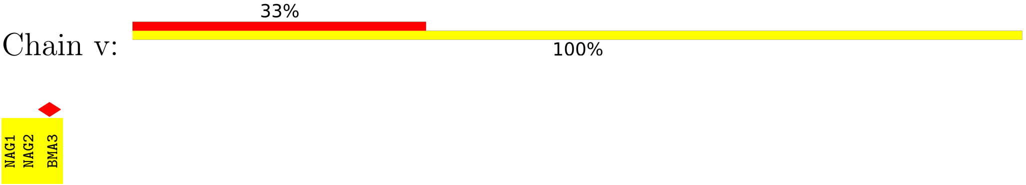
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



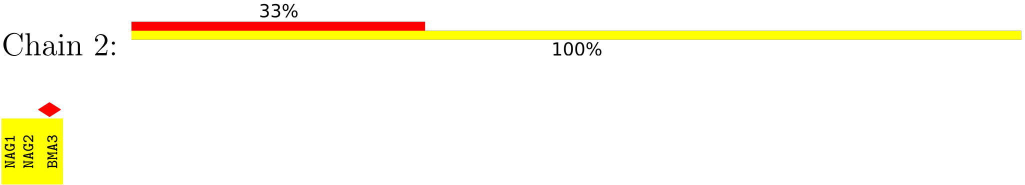
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



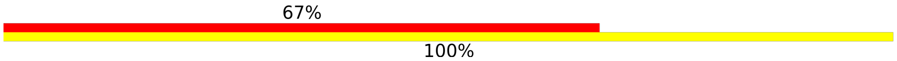
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



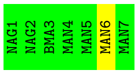
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:



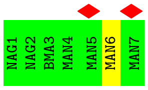
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



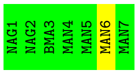
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



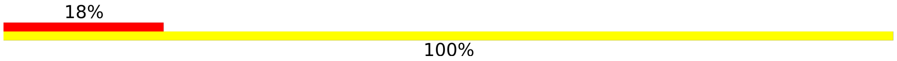
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

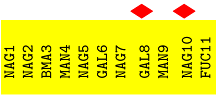
Chain y:



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

Chain Y:

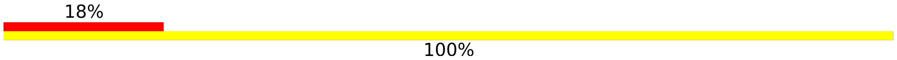


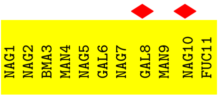


- Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D

-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

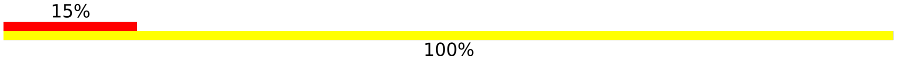
Chain 9:

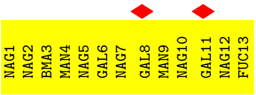




- Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyra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

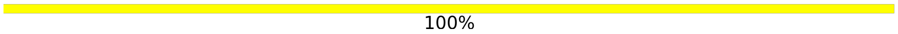
Chain Z:





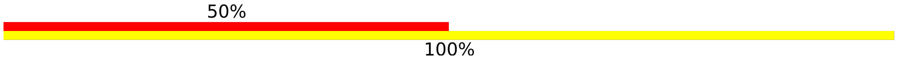
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

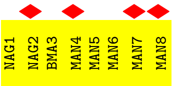
Chain e:



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

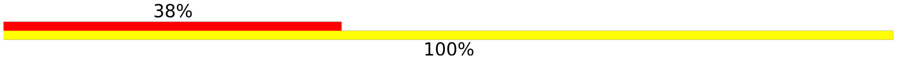
Chain p:

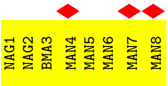




- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

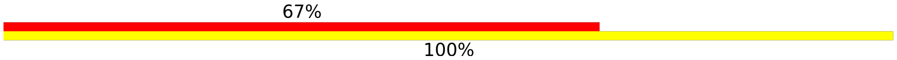
Chain 8:





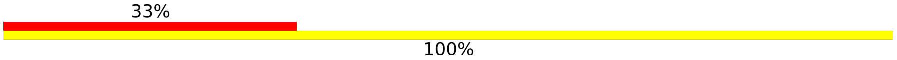
- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



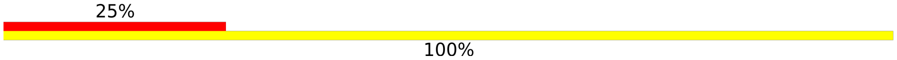
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



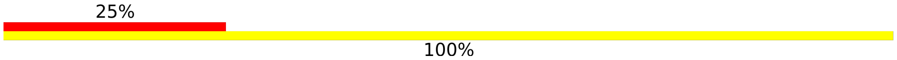
- Molecule 14: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

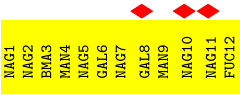
Chain 6:



- Molecule 15: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201386	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	32.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.034	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, BMA, GAL, 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	0.77	1/3625 (0.0%)	0.69	2/4921 (0.0%)
1	C	0.76	0/3578	0.70	2/4857 (0.0%)
1	E	0.76	1/3609 (0.0%)	0.72	1/4899 (0.0%)
2	B	0.81	0/1168	0.67	0/1583
2	D	0.75	0/1178	0.69	0/1597
2	F	0.81	0/1228	0.71	1/1665 (0.1%)
3	H	0.72	0/1102	0.70	1/1496 (0.1%)
3	M	0.73	0/1096	0.69	0/1489
4	L	0.71	0/899	0.67	0/1213
4	N	0.69	0/884	0.70	0/1192
All	All	0.76	2/18367 (0.0%)	0.70	7/24912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	2
1	E	0	5
2	B	0	1
2	D	0	3
2	F	0	2
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	PRO	N-CD	5.63	1.55	1.47
1	A	118	PRO	N-CD	5.33	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	PHE	N-CA-CB	-6.31	99.24	110.60
2	F	616	ASN	CB-CA-C	5.64	121.68	110.40
1	C	157	CYS	N-CA-CB	-5.41	100.86	110.60
1	A	385	CYS	N-CA-CB	-5.39	100.90	110.60
1	E	54	CYS	N-CA-CB	-5.10	101.42	110.60
1	A	196	CYS	N-CA-CB	-5.09	101.44	110.60
3	H	22	CYS	N-CA-CB	-5.04	101.53	110.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	THR	Mainchain
1	A	507	GLN	Mainchain
1	A	81	PRO	Mainchain,Peptide
2	B	600	GLY	Mainchain
1	C	65	VAL	Mainchain,Peptide
2	D	518	VAL	Mainchain
2	D	528	SER	Mainchain
2	D	600	GLY	Mainchain
1	E	157	CYS	Mainchain
1	E	412	ASN	Mainchain,Peptide
1	E	65	VAL	Mainchain
1	E	66	HIS	Mainchain
2	F	518	VAL	Mainchain
2	F	600	GLY	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	441/473 (93%)	409 (93%)	28 (6%)	4 (1%)	17	56
1	C	436/473 (92%)	395 (91%)	31 (7%)	10 (2%)	6	37
1	E	440/473 (93%)	405 (92%)	27 (6%)	8 (2%)	8	42
2	B	142/153 (93%)	127 (89%)	8 (6%)	7 (5%)	2	23
2	D	145/153 (95%)	136 (94%)	7 (5%)	2 (1%)	11	47
2	F	151/153 (99%)	137 (91%)	11 (7%)	3 (2%)	7	40
3	H	133/240 (55%)	125 (94%)	7 (5%)	1 (1%)	19	60
3	M	133/240 (55%)	124 (93%)	7 (5%)	2 (2%)	10	46
4	L	112/219 (51%)	105 (94%)	7 (6%)	0	100	100
4	N	110/219 (50%)	104 (94%)	5 (4%)	1 (1%)	17	56
All	All	2243/2796 (80%)	2067 (92%)	138 (6%)	38 (2%)	13	44

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
2	B	532	ALA
2	B	541	ALA
2	B	545	LEU
2	B	570	VAL
1	C	73	ALA
1	C	80	ASN
1	C	99	ASN
1	C	194	ILE
1	C	355	ASN
1	E	78	ASP
1	E	83	GLU
1	E	258	GLN
2	F	520	LEU
2	F	552	GLN
3	H	112	SER
3	M	112	SER
2	B	543	LEU
2	B	567	GLN
1	C	69	TRP
2	D	550	GLN
1	E	134	VAL

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Mol	Chain	Res	Type
1	E	402	THR
4	N	51	VAL
1	A	504	ARG
1	C	354	GLU
1	E	70	ALA
2	F	601	LYS
3	M	100(K)	ASN
2	B	601	LYS
1	C	199	SER
1	E	79	PRO
1	A	67	ASN
1	A	232	THR
1	C	165	ILE
1	E	299	PRO
1	C	43	PRO
2	D	570	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/424 (95%)	400 (99%)	4 (1%)	76	86
1	C	398/424 (94%)	389 (98%)	9 (2%)	50	70
1	E	401/424 (95%)	395 (98%)	6 (2%)	65	80
2	B	123/128 (96%)	119 (97%)	4 (3%)	38	61
2	D	122/128 (95%)	121 (99%)	1 (1%)	81	89
2	F	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	H	116/207 (56%)	116 (100%)	0	100	100
3	M	115/207 (56%)	114 (99%)	1 (1%)	78	87
4	L	101/195 (52%)	100 (99%)	1 (1%)	76	86
4	N	99/195 (51%)	98 (99%)	1 (1%)	76	86
All	All	2007/2460 (82%)	1978 (99%)	29 (1%)	68	80

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	229	ASN
1	A	402	THR
1	A	499	THR
2	B	522	PHE
2	B	542	ARG
2	B	543	LEU
2	B	637	ASN
1	C	53	PHE
1	C	156	ASN
1	C	173	TYR
1	C	229	ASN
1	C	298	ARG
1	C	301	ASN
1	C	332	ASN
1	C	339	ASN
1	C	378	CYS
2	D	540	GLN
1	E	126	CYS
1	E	134	VAL
1	E	156	ASN
1	E	298	ARG
1	E	378	CYS
1	E	435	TYR
2	F	616	ASN
2	F	637	ASN
4	L	53	ASN
3	M	100(N)	TYR
4	N	36	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	442	GLN
1	C	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

203 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	5,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
5	NAG	0	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
5	NAG	1	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	1	2	5	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
6	NAG	2	1	6,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	2	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	BMA	2	3	6	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	3	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	3	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	4	1	5,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	4	2	5	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
5	NAG	5	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	5	2	5	14,14,15	0.49	0	17,19,21	1.39	3 (17%)
14	NAG	6	1	14,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
14	NAG	6	2	14	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
14	BMA	6	3	14	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
14	MAN	6	4	14	11,11,12	0.61	0	15,15,17	2.53	4 (26%)
6	NAG	7	1	6,1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
6	NAG	7	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	BMA	7	3	6	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
11	NAG	8	1	11,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
11	NAG	8	2	11	14,14,15	0.52	0	17,19,21	1.39	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	BMA	8	3	11	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
11	MAN	8	4	11	11,11,12	0.56	0	15,15,17	1.71	4 (26%)
11	MAN	8	5	11	11,11,12	0.59	0	15,15,17	2.42	5 (33%)
11	MAN	8	6	11	11,11,12	0.62	0	15,15,17	2.54	3 (20%)
11	MAN	8	7	11	11,11,12	0.58	0	15,15,17	2.03	7 (46%)
11	MAN	8	8	11	11,11,12	0.60	0	15,15,17	2.41	7 (46%)
8	NAG	9	1	8,2	14,14,15	1.52	4 (28%)	17,19,21	1.10	1 (5%)
8	NAG	9	10	8	14,14,15	1.38	3 (21%)	17,19,21	1.21	1 (5%)
8	FUC	9	11	8	10,10,11	1.52	2 (20%)	14,14,16	0.95	0
8	NAG	9	2	8	14,14,15	1.34	2 (14%)	17,19,21	1.30	1 (5%)
8	BMA	9	3	8	11,11,12	1.36	2 (18%)	15,15,17	1.21	1 (6%)
8	MAN	9	4	8	11,11,12	1.53	3 (27%)	15,15,17	1.33	2 (13%)
8	NAG	9	5	8	14,14,15	1.44	3 (21%)	17,19,21	1.33	1 (5%)
8	GAL	9	6	8	11,11,12	1.35	2 (18%)	15,15,17	1.12	1 (6%)
8	NAG	9	7	8	14,14,15	1.43	3 (21%)	17,19,21	1.15	1 (5%)
8	GAL	9	8	8	11,11,12	1.36	2 (18%)	15,15,17	1.11	1 (6%)
8	MAN	9	9	8	11,11,12	1.72	4 (36%)	15,15,17	1.47	2 (13%)
5	NAG	AA	1	5,2	14,14,15	0.51	0	17,19,21	2.22	3 (17%)
5	NAG	AA	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
15	NAG	BA	1	15,2	14,14,15	1.53	3 (21%)	17,19,21	1.06	1 (5%)
15	NAG	BA	10	15	14,14,15	1.42	3 (21%)	17,19,21	1.30	1 (5%)
15	NAG	BA	11	15	14,14,15	1.40	3 (21%)	17,19,21	1.16	1 (5%)
15	FUC	BA	12	15	10,10,11	1.51	2 (20%)	14,14,16	0.95	1 (7%)
15	NAG	BA	2	15	14,14,15	1.35	2 (14%)	17,19,21	1.30	1 (5%)
15	BMA	BA	3	15	11,11,12	1.36	2 (18%)	15,15,17	1.22	1 (6%)
15	MAN	BA	4	15	11,11,12	1.73	4 (36%)	15,15,17	1.46	2 (13%)
15	NAG	BA	5	15	14,14,15	1.37	3 (21%)	17,19,21	1.18	1 (5%)
15	GAL	BA	6	15	11,11,12	1.35	2 (18%)	15,15,17	1.11	1 (6%)
15	NAG	BA	7	15	14,14,15	1.37	3 (21%)	17,19,21	1.29	1 (5%)
15	GAL	BA	8	15	11,11,12	1.32	2 (18%)	15,15,17	1.15	1 (6%)
15	MAN	BA	9	15	11,11,12	1.54	3 (27%)	15,15,17	1.35	2 (13%)
5	NAG	G	1	5,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	G	2	5	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
6	NAG	I	1	6,1	14,14,15	0.51	0	17,19,21	2.22	3 (17%)
6	NAG	I	2	6	14,14,15	0.50	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	BMA	I	3	6	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
6	NAG	J	1	6,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	J	2	6	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
6	BMA	J	3	6	11,11,12	0.66	0	15,15,17	1.46	3 (20%)
6	NAG	K	1	6,1	14,14,15	0.51	0	17,19,21	2.25	3 (17%)
6	NAG	K	2	6	14,14,15	0.48	0	17,19,21	1.42	3 (17%)
6	BMA	K	3	6	11,11,12	0.64	0	15,15,17	1.48	3 (20%)
7	NAG	O	1	7,1	14,14,15	0.62	0	17,19,21	0.66	0
7	NAG	O	2	7	14,14,15	0.56	0	17,19,21	0.90	0
7	BMA	O	3	7	11,11,12	0.66	0	15,15,17	0.86	0
7	MAN	O	4	7	11,11,12	0.60	0	15,15,17	0.70	0
7	MAN	O	5	7	11,11,12	0.52	0	15,15,17	0.73	0
7	MAN	O	6	7	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
7	MAN	O	7	7	11,11,12	0.65	0	15,15,17	0.64	0
6	NAG	P	1	6,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
6	NAG	P	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	BMA	P	3	6	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	Q	1	5,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
5	NAG	Q	2	5	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
5	NAG	R	1	5,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	R	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	NAG	S	1	6,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	S	2	6	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
6	BMA	S	3	6	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	T	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	T	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	NAG	U	1	6,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
6	NAG	U	2	6	14,14,15	0.49	0	17,19,21	1.38	3 (17%)
6	BMA	U	3	6	11,11,12	0.64	0	15,15,17	1.45	3 (20%)
6	NAG	V	1	6,1	14,14,15	0.52	0	17,19,21	2.25	3 (17%)
6	NAG	V	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	BMA	V	3	6	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
6	NAG	W	1	6,1	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
6	NAG	W	2	6	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	BMA	W	3	6	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
5	NAG	X	1	5,1	14,14,15	0.49	0	17,19,21	2.21	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	X	2	5	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
8	NAG	Y	1	8,2	14,14,15	1.52	3 (21%)	17,19,21	1.10	1 (5%)
8	NAG	Y	10	8	14,14,15	1.38	3 (21%)	17,19,21	1.22	1 (5%)
8	FUC	Y	11	8	10,10,11	1.52	2 (20%)	14,14,16	0.94	0
8	NAG	Y	2	8	14,14,15	1.34	2 (14%)	17,19,21	1.29	1 (5%)
8	BMA	Y	3	8	11,11,12	1.36	2 (18%)	15,15,17	1.20	1 (6%)
8	MAN	Y	4	8	11,11,12	1.53	3 (27%)	15,15,17	1.34	2 (13%)
8	NAG	Y	5	8	14,14,15	1.43	3 (21%)	17,19,21	1.33	1 (5%)
8	GAL	Y	6	8	11,11,12	1.34	2 (18%)	15,15,17	1.11	1 (6%)
8	NAG	Y	7	8	14,14,15	1.44	3 (21%)	17,19,21	1.14	1 (5%)
8	GAL	Y	8	8	11,11,12	1.34	2 (18%)	15,15,17	1.11	1 (6%)
8	MAN	Y	9	8	11,11,12	1.72	4 (36%)	15,15,17	1.47	2 (13%)
9	NAG	Z	1	9,2	14,14,15	1.53	3 (21%)	17,19,21	1.07	1 (5%)
9	NAG	Z	10	9	14,14,15	1.41	3 (21%)	17,19,21	1.32	1 (5%)
9	GAL	Z	11	9	11,11,12	1.34	2 (18%)	15,15,17	1.12	1 (6%)
9	NAG	Z	12	9	14,14,15	1.41	3 (21%)	17,19,21	1.17	2 (11%)
9	FUC	Z	13	9	10,10,11	1.51	2 (20%)	14,14,16	0.96	1 (7%)
9	NAG	Z	2	9	14,14,15	1.35	2 (14%)	17,19,21	1.30	1 (5%)
9	BMA	Z	3	9	11,11,12	1.37	2 (18%)	15,15,17	1.22	1 (6%)
9	MAN	Z	4	9	11,11,12	1.73	4 (36%)	15,15,17	1.45	2 (13%)
9	NAG	Z	5	9	14,14,15	1.36	3 (21%)	17,19,21	1.19	1 (5%)
9	GAL	Z	6	9	11,11,12	1.35	2 (18%)	15,15,17	1.10	1 (6%)
9	NAG	Z	7	9	14,14,15	1.36	3 (21%)	17,19,21	1.29	1 (5%)
9	GAL	Z	8	9	11,11,12	1.32	2 (18%)	15,15,17	1.13	1 (6%)
9	MAN	Z	9	9	11,11,12	1.55	3 (27%)	15,15,17	1.34	2 (13%)
6	NAG	a	1	6,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	a	2	6	14,14,15	0.53	0	17,19,21	1.36	3 (17%)
6	BMA	a	3	6	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
5	NAG	b	1	5,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	b	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
5	NAG	c	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	c	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	NAG	d	1	6,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	d	2	6	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
6	BMA	d	3	6	11,11,12	0.64	0	15,15,17	1.47	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	NAG	e	1	10,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
10	NAG	e	2	10	14,14,15	0.49	0	17,19,21	1.42	3 (17%)
10	BMA	e	3	10	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
10	MAN	e	4	10	11,11,12	0.56	0	15,15,17	1.70	4 (26%)
10	MAN	e	5	10	11,11,12	0.58	0	15,15,17	2.55	4 (26%)
7	NAG	f	1	7,1	14,14,15	0.61	0	17,19,21	0.66	0
7	NAG	f	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	f	3	7	11,11,12	0.65	0	15,15,17	0.85	0
7	MAN	f	4	7	11,11,12	0.61	0	15,15,17	0.69	0
7	MAN	f	5	7	11,11,12	0.53	0	15,15,17	0.73	0
7	MAN	f	6	7	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
7	MAN	f	7	7	11,11,12	0.65	0	15,15,17	0.63	0
6	NAG	g	1	6,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
6	NAG	g	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	BMA	g	3	6	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	h	1	5,1	14,14,15	0.49	0	17,19,21	2.22	3 (17%)
5	NAG	h	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	NAG	i	1	6,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	i	2	6	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
6	BMA	i	3	6	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
6	NAG	j	1	6,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	j	2	6	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
6	BMA	j	3	6	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	k	1	5,1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
5	NAG	k	2	5	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
5	NAG	l	1	5,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	l	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	NAG	m	1	6,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
6	NAG	m	2	6	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
6	BMA	m	3	6	11,11,12	0.62	0	15,15,17	1.45	3 (20%)
6	NAG	n	1	6,1	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
6	NAG	n	2	6	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
6	BMA	n	3	6	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
5	NAG	o	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	o	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
11	NAG	p	1	11,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	NAG	p	2	11	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
11	BMA	p	3	11	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
11	MAN	p	4	11	11,11,12	0.54	0	15,15,17	1.70	3 (20%)
11	MAN	p	5	11	11,11,12	0.60	0	15,15,17	2.43	5 (33%)
11	MAN	p	6	11	11,11,12	0.62	0	15,15,17	2.54	3 (20%)
11	MAN	p	7	11	11,11,12	0.59	0	15,15,17	2.03	7 (46%)
11	MAN	p	8	11	11,11,12	0.59	0	15,15,17	2.41	7 (46%)
12	NAG	q	1	12,2	14,14,15	1.52	4 (28%)	17,19,21	1.10	1 (5%)
12	NAG	q	2	12	14,14,15	1.36	2 (14%)	17,19,21	1.29	1 (5%)
12	FUC	q	3	12	10,10,11	1.51	2 (20%)	14,14,16	0.95	0
5	NAG	r	1	5,2	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	r	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
5	NAG	s	1	5,2	14,14,15	1.53	3 (21%)	17,19,21	1.07	1 (5%)
5	NAG	s	2	5	14,14,15	1.35	2 (14%)	17,19,21	1.30	1 (5%)
6	NAG	t	1	6,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
6	NAG	t	2	6	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
6	BMA	t	3	6	11,11,12	0.62	0	15,15,17	1.47	3 (20%)
5	NAG	u	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	u	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
6	NAG	v	1	6,1	14,14,15	0.51	0	17,19,21	2.22	3 (17%)
6	NAG	v	2	6	14,14,15	0.53	0	17,19,21	1.37	3 (17%)
6	BMA	v	3	6	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
5	NAG	w	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	w	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
13	NAG	x	1	13,1	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
13	NAG	x	2	13	14,14,15	0.49	0	17,19,21	1.40	3 (17%)
13	BMA	x	3	13	11,11,12	0.64	0	15,15,17	1.48	3 (20%)
13	MAN	x	4	13	11,11,12	0.55	0	15,15,17	1.72	4 (26%)
13	MAN	x	5	13	11,11,12	0.58	0	15,15,17	2.44	5 (33%)
13	MAN	x	6	13	11,11,12	0.60	0	15,15,17	2.54	4 (26%)
7	NAG	y	1	7,1	14,14,15	0.62	0	17,19,21	0.66	0
7	NAG	y	2	7	14,14,15	0.58	0	17,19,21	0.89	0
7	BMA	y	3	7	11,11,12	0.66	0	15,15,17	0.86	0
7	MAN	y	4	7	11,11,12	0.61	0	15,15,17	0.69	0
7	MAN	y	5	7	11,11,12	0.53	0	15,15,17	0.73	0
7	MAN	y	6	7	11,11,12	0.66	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
7	MAN	y	7	7	11,11,12	0.64	0	15,15,17	0.63	0
5	NAG	z	1	5,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	z	2	5	14,14,15	0.51	0	17,19,21	1.39	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
5	NAG	0	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	NAG	1	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	1	2	5	-	0/6/23/26	0/1/1/1
6	NAG	2	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	2	2	6	-	0/6/23/26	0/1/1/1
6	BMA	2	3	6	-	2/2/19/22	0/1/1/1
5	NAG	3	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	3	2	5	-	0/6/23/26	0/1/1/1
5	NAG	4	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	NAG	5	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
14	NAG	6	1	14,1	-	0/6/23/26	0/1/1/1
14	NAG	6	2	14	-	0/6/23/26	0/1/1/1
14	BMA	6	3	14	-	2/2/19/22	0/1/1/1
14	MAN	6	4	14	-	0/2/19/22	0/1/1/1
6	NAG	7	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
6	BMA	7	3	6	-	2/2/19/22	0/1/1/1
11	NAG	8	1	11,1	-	1/6/23/26	0/1/1/1
11	NAG	8	2	11	-	0/6/23/26	0/1/1/1
11	BMA	8	3	11	-	0/2/19/22	0/1/1/1
11	MAN	8	4	11	-	0/2/19/22	0/1/1/1
11	MAN	8	5	11	-	0/2/19/22	0/1/1/1
11	MAN	8	6	11	-	0/2/19/22	0/1/1/1
11	MAN	8	7	11	-	0/2/19/22	0/1/1/1
11	MAN	8	8	11	-	0/2/19/22	0/1/1/1
8	NAG	9	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	9	10	8	-	0/6/23/26	0/1/1/1
8	FUC	9	11	8	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	9	2	8	-	0/6/23/26	0/1/1/1
8	BMA	9	3	8	-	2/2/19/22	0/1/1/1
8	MAN	9	4	8	-	0/2/19/22	0/1/1/1
8	NAG	9	5	8	-	0/6/23/26	0/1/1/1
8	GAL	9	6	8	-	0/2/19/22	0/1/1/1
8	NAG	9	7	8	-	0/6/23/26	0/1/1/1
8	GAL	9	8	8	-	0/2/19/22	0/1/1/1
8	MAN	9	9	8	-	0/2/19/22	0/1/1/1
5	NAG	AA	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	0/6/23/26	0/1/1/1
15	NAG	BA	1	15,2	-	1/6/23/26	0/1/1/1
15	NAG	BA	10	15	-	0/6/23/26	0/1/1/1
15	NAG	BA	11	15	-	0/6/23/26	0/1/1/1
15	FUC	BA	12	15	-	-	0/1/1/1
15	NAG	BA	2	15	-	0/6/23/26	0/1/1/1
15	BMA	BA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	BA	4	15	-	0/2/19/22	0/1/1/1
15	NAG	BA	5	15	-	0/6/23/26	0/1/1/1
15	GAL	BA	6	15	-	0/2/19/22	0/1/1/1
15	NAG	BA	7	15	-	0/6/23/26	0/1/1/1
15	GAL	BA	8	15	-	0/2/19/22	0/1/1/1
15	MAN	BA	9	15	-	1/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	MAN	O	5	7	-	2/2/19/22	0/1/1/1
7	MAN	O	6	7	-	2/2/19/22	0/1/1/1
7	MAN	O	7	7	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	NAG	W	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
8	NAG	Y	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	Y	10	8	-	0/6/23/26	0/1/1/1
8	FUC	Y	11	8	-	-	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	5	8	-	0/6/23/26	0/1/1/1
8	GAL	Y	6	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	7	8	-	0/6/23/26	0/1/1/1
8	GAL	Y	8	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	9	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	Z	10	9	-	0/6/23/26	0/1/1/1
9	GAL	Z	11	9	-	0/2/19/22	0/1/1/1
9	NAG	Z	12	9	-	0/6/23/26	0/1/1/1
9	FUC	Z	13	9	-	-	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	l	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
6	NAG	m	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	m	2	6	-	0/6/23/26	0/1/1/1
6	BMA	m	3	6	-	2/2/19/22	0/1/1/1
6	NAG	n	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
6	BMA	n	3	6	-	2/2/19/22	0/1/1/1
5	NAG	o	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	o	2	5	-	0/6/23/26	0/1/1/1
11	NAG	p	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	p	2	11	-	0/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	0/2/19/22	0/1/1/1
11	MAN	p	5	11	-	0/2/19/22	0/1/1/1
11	MAN	p	6	11	-	0/2/19/22	0/1/1/1
11	MAN	p	7	11	-	0/2/19/22	0/1/1/1
11	MAN	p	8	11	-	0/2/19/22	0/1/1/1
12	NAG	q	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	q	2	12	-	0/6/23/26	0/1/1/1
12	FUC	q	3	12	-	-	0/1/1/1
5	NAG	r	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	r	2	5	-	0/6/23/26	0/1/1/1
5	NAG	s	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	s	2	5	-	0/6/23/26	0/1/1/1
6	NAG	t	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	t	2	6	-	0/6/23/26	0/1/1/1
6	BMA	t	3	6	-	2/2/19/22	0/1/1/1
5	NAG	u	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	u	2	5	-	0/6/23/26	0/1/1/1
6	NAG	v	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	v	2	6	-	0/6/23/26	0/1/1/1
6	BMA	v	3	6	-	2/2/19/22	0/1/1/1
5	NAG	w	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	w	2	5	-	0/6/23/26	0/1/1/1
13	NAG	x	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	x	2	13	-	0/6/23/26	0/1/1/1
13	BMA	x	3	13	-	0/2/19/22	0/1/1/1
13	MAN	x	4	13	-	0/2/19/22	0/1/1/1
13	MAN	x	5	13	-	0/2/19/22	0/1/1/1
13	MAN	x	6	13	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	y	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	y	2	7	-	2/6/23/26	0/1/1/1
7	BMA	y	3	7	-	0/2/19/22	0/1/1/1
7	MAN	y	4	7	-	0/2/19/22	0/1/1/1
7	MAN	y	5	7	-	2/2/19/22	0/1/1/1
7	MAN	y	6	7	-	2/2/19/22	0/1/1/1
7	MAN	y	7	7	-	0/2/19/22	0/1/1/1
5	NAG	z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	z	2	5	-	0/6/23/26	0/1/1/1

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	9	MAN	O5-C1	3.59	1.49	1.43
8	Y	9	MAN	O5-C1	3.52	1.49	1.43
15	BA	4	MAN	O5-C1	3.49	1.49	1.43
9	Z	4	MAN	O5-C1	3.49	1.49	1.43
5	s	1	NAG	O5-C1	3.24	1.48	1.43
15	BA	1	NAG	O5-C1	3.21	1.48	1.43
9	Z	1	NAG	O5-C1	3.20	1.48	1.43
12	q	1	NAG	O5-C1	3.16	1.48	1.43
8	Y	1	NAG	O5-C1	3.15	1.48	1.43
8	9	1	NAG	O5-C1	3.14	1.48	1.43
15	BA	10	NAG	O5-C1	3.12	1.48	1.43
9	Z	10	NAG	O5-C1	3.05	1.48	1.43
8	9	5	NAG	O5-C1	3.03	1.48	1.43
12	q	2	NAG	O5-C1	3.02	1.48	1.43
9	Z	13	FUC	O5-C1	3.00	1.48	1.43
8	9	11	FUC	O5-C1	2.99	1.48	1.43
15	BA	12	FUC	O5-C1	2.98	1.48	1.43
8	Y	5	NAG	O5-C1	2.98	1.48	1.43
8	Y	11	FUC	O5-C1	2.97	1.48	1.43
8	Y	2	NAG	O5-C1	2.95	1.48	1.43
8	9	8	GAL	O5-C1	2.94	1.48	1.43
8	9	2	NAG	O5-C1	2.94	1.48	1.43
8	9	7	NAG	O5-C1	2.94	1.48	1.43
12	q	3	FUC	O5-C1	2.93	1.48	1.43
15	BA	11	NAG	O5-C1	2.92	1.48	1.43
8	Y	7	NAG	O5-C1	2.90	1.48	1.43
9	Z	12	NAG	O5-C1	2.90	1.48	1.43
8	9	10	NAG	O5-C1	2.90	1.48	1.43
8	Y	10	NAG	O5-C1	2.89	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	7	NAG	O5-C1	2.88	1.48	1.43
15	BA	6	GAL	O5-C1	2.88	1.48	1.43
15	BA	2	NAG	O5-C1	2.88	1.48	1.43
15	BA	5	NAG	O5-C1	2.87	1.48	1.43
8	Y	8	GAL	O5-C1	2.87	1.48	1.43
15	BA	7	NAG	O5-C1	2.86	1.48	1.43
9	Z	2	NAG	O5-C1	2.85	1.48	1.43
5	s	2	NAG	O5-C1	2.85	1.48	1.43
9	Z	6	GAL	O5-C1	2.85	1.48	1.43
9	Z	5	NAG	O5-C1	2.82	1.48	1.43
9	Z	9	MAN	O5-C1	2.82	1.48	1.43
8	9	6	GAL	O5-C1	2.81	1.48	1.43
15	BA	9	MAN	O5-C1	2.80	1.48	1.43
9	Z	11	GAL	O5-C1	2.80	1.48	1.43
15	BA	8	GAL	O5-C1	2.78	1.48	1.43
8	Y	6	GAL	O5-C1	2.76	1.48	1.43
8	Y	3	BMA	O5-C1	2.75	1.48	1.43
9	Z	3	BMA	O5-C1	2.74	1.48	1.43
9	Z	8	GAL	O5-C1	2.74	1.48	1.43
8	9	3	BMA	O5-C1	2.72	1.48	1.43
15	BA	3	BMA	O5-C1	2.68	1.48	1.43
8	Y	4	MAN	O5-C5	2.68	1.48	1.43
8	9	4	MAN	O5-C5	2.67	1.48	1.43
8	9	4	MAN	O5-C1	2.65	1.48	1.43
8	Y	4	MAN	O5-C1	2.64	1.47	1.43
15	BA	4	MAN	O5-C5	2.63	1.48	1.43
9	Z	4	MAN	O5-C5	2.62	1.48	1.43
5	s	1	NAG	O5-C5	2.60	1.48	1.43
8	Y	9	MAN	O5-C5	2.60	1.48	1.43
9	Z	1	NAG	O5-C5	2.57	1.48	1.43
8	9	9	MAN	O5-C5	2.56	1.48	1.43
9	Z	9	MAN	O5-C5	2.55	1.48	1.43
15	BA	1	NAG	O5-C5	2.55	1.48	1.43
12	q	1	NAG	O5-C5	2.54	1.48	1.43
15	BA	9	MAN	O5-C5	2.54	1.48	1.43
8	Y	1	NAG	O5-C5	2.52	1.48	1.43
15	BA	12	FUC	O5-C5	2.51	1.48	1.43
8	9	1	NAG	O5-C5	2.50	1.48	1.43
9	Z	13	FUC	O5-C5	2.49	1.48	1.43
8	Y	11	FUC	O5-C5	2.48	1.48	1.43
8	9	11	FUC	O5-C5	2.47	1.48	1.43
12	q	3	FUC	O5-C5	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	4	MAN	O2-C2	2.41	1.48	1.43
15	BA	11	NAG	O5-C5	2.41	1.48	1.43
15	BA	3	BMA	O5-C5	2.40	1.48	1.43
9	Z	3	BMA	O5-C5	2.39	1.48	1.43
15	BA	9	MAN	O2-C2	2.38	1.48	1.43
9	Z	4	MAN	O2-C2	2.38	1.48	1.43
9	Z	12	NAG	O5-C5	2.38	1.48	1.43
8	9	4	MAN	O2-C2	2.38	1.48	1.43
15	BA	4	MAN	O2-C2	2.38	1.48	1.43
8	Y	9	MAN	O2-C2	2.37	1.48	1.43
8	Y	7	NAG	O5-C5	2.37	1.48	1.43
9	Z	9	MAN	O2-C2	2.36	1.48	1.43
8	Y	6	GAL	O5-C5	2.36	1.48	1.43
9	Z	11	GAL	O5-C5	2.36	1.48	1.43
8	Y	3	BMA	O5-C5	2.35	1.48	1.43
8	9	3	BMA	O5-C5	2.35	1.48	1.43
8	9	9	MAN	O2-C2	2.34	1.48	1.43
8	9	6	GAL	O5-C5	2.34	1.48	1.43
9	Z	8	GAL	O5-C5	2.33	1.48	1.43
15	BA	4	MAN	O4-C4	2.32	1.48	1.43
15	BA	8	GAL	O5-C5	2.31	1.48	1.43
8	9	7	NAG	O5-C5	2.30	1.48	1.43
9	Z	4	MAN	O4-C4	2.30	1.48	1.43
8	Y	5	NAG	O4-C4	2.29	1.48	1.43
8	9	7	NAG	O4-C4	2.29	1.48	1.43
8	Y	5	NAG	O5-C5	2.29	1.48	1.43
8	Y	8	GAL	O5-C5	2.28	1.48	1.43
8	9	5	NAG	O4-C4	2.28	1.48	1.43
8	9	5	NAG	O5-C5	2.28	1.48	1.43
9	Z	5	NAG	O5-C5	2.27	1.48	1.43
8	Y	10	NAG	O5-C5	2.27	1.48	1.43
8	9	10	NAG	O5-C5	2.26	1.48	1.43
9	Z	6	GAL	O5-C5	2.26	1.48	1.43
15	BA	5	NAG	O5-C5	2.26	1.48	1.43
8	Y	7	NAG	O4-C4	2.25	1.48	1.43
8	9	10	NAG	O4-C4	2.25	1.48	1.43
8	9	8	GAL	O5-C5	2.25	1.48	1.43
15	BA	6	GAL	O5-C5	2.24	1.48	1.43
8	Y	10	NAG	O4-C4	2.23	1.48	1.43
15	BA	10	NAG	O4-C4	2.23	1.48	1.43
9	Z	10	NAG	O4-C4	2.23	1.48	1.43
5	s	2	NAG	O5-C5	2.20	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	2	NAG	O5-C5	2.20	1.47	1.43
5	s	1	NAG	O4-C4	2.19	1.48	1.43
15	BA	2	NAG	O5-C5	2.18	1.47	1.43
9	Z	12	NAG	O4-C4	2.18	1.48	1.43
15	BA	10	NAG	O5-C5	2.18	1.47	1.43
9	Z	10	NAG	O5-C5	2.18	1.47	1.43
8	Y	1	NAG	O4-C4	2.18	1.48	1.43
15	BA	7	NAG	O4-C4	2.18	1.48	1.43
15	BA	11	NAG	O4-C4	2.17	1.48	1.43
9	Z	7	NAG	O4-C4	2.17	1.48	1.43
8	Y	9	MAN	O4-C4	2.16	1.48	1.43
9	Z	1	NAG	O4-C4	2.16	1.48	1.43
15	BA	1	NAG	O4-C4	2.16	1.48	1.43
8	9	9	MAN	O4-C4	2.15	1.48	1.43
8	9	1	NAG	O4-C4	2.15	1.48	1.43
12	q	1	NAG	O4-C4	2.15	1.48	1.43
12	q	2	NAG	O5-C5	2.14	1.47	1.43
15	BA	7	NAG	O5-C5	2.12	1.47	1.43
9	Z	5	NAG	O4-C4	2.12	1.48	1.43
8	9	2	NAG	O5-C5	2.11	1.47	1.43
8	Y	2	NAG	O5-C5	2.11	1.47	1.43
15	BA	5	NAG	O4-C4	2.10	1.47	1.43
9	Z	7	NAG	O5-C5	2.07	1.47	1.43
8	9	1	NAG	C8-C7	2.05	1.54	1.50
12	q	1	NAG	C8-C7	2.03	1.54	1.50

All (482) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O5-C1-C2	-7.43	99.56	111.29
6	t	1	NAG	O5-C1-C2	-7.42	99.57	111.29
6	V	1	NAG	O5-C1-C2	-7.41	99.59	111.29
6	a	1	NAG	O5-C1-C2	-7.41	99.59	111.29
5	G	1	NAG	O5-C1-C2	-7.41	99.59	111.29
6	U	1	NAG	O5-C1-C2	-7.41	99.59	111.29
5	5	1	NAG	O5-C1-C2	-7.40	99.61	111.29
5	T	1	NAG	O5-C1-C2	-7.39	99.61	111.29
5	l	1	NAG	O5-C1-C2	-7.39	99.61	111.29
5	k	1	NAG	O5-C1-C2	-7.39	99.62	111.29
6	n	1	NAG	O5-C1-C2	-7.39	99.62	111.29
5	4	1	NAG	O5-C1-C2	-7.38	99.63	111.29
14	6	1	NAG	O5-C1-C2	-7.38	99.63	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	3	1	NAG	O5-C1-C2	-7.38	99.64	111.29
13	x	1	NAG	O5-C1-C2	-7.37	99.64	111.29
6	d	1	NAG	O5-C1-C2	-7.37	99.65	111.29
5	u	1	NAG	O5-C1-C2	-7.37	99.66	111.29
5	w	1	NAG	O5-C1-C2	-7.37	99.66	111.29
11	p	1	NAG	O5-C1-C2	-7.37	99.66	111.29
6	m	1	NAG	O5-C1-C2	-7.36	99.66	111.29
11	8	1	NAG	O5-C1-C2	-7.36	99.66	111.29
6	J	1	NAG	O5-C1-C2	-7.36	99.66	111.29
10	e	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	o	1	NAG	O5-C1-C2	-7.35	99.68	111.29
5	1	1	NAG	O5-C1-C2	-7.35	99.68	111.29
6	2	1	NAG	O5-C1-C2	-7.35	99.68	111.29
5	c	1	NAG	O5-C1-C2	-7.35	99.68	111.29
5	R	1	NAG	O5-C1-C2	-7.34	99.69	111.29
6	j	1	NAG	O5-C1-C2	-7.34	99.69	111.29
6	7	1	NAG	O5-C1-C2	-7.34	99.70	111.29
6	W	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	r	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	b	1	NAG	O5-C1-C2	-7.34	99.70	111.29
6	S	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	z	1	NAG	O5-C1-C2	-7.33	99.71	111.29
5	0	1	NAG	O5-C1-C2	-7.33	99.71	111.29
5	Q	1	NAG	O5-C1-C2	-7.33	99.72	111.29
6	P	1	NAG	O5-C1-C2	-7.32	99.72	111.29
6	g	1	NAG	O5-C1-C2	-7.32	99.73	111.29
5	h	1	NAG	O5-C1-C2	-7.31	99.74	111.29
6	v	1	NAG	O5-C1-C2	-7.31	99.74	111.29
5	AA	1	NAG	O5-C1-C2	-7.30	99.76	111.29
6	I	1	NAG	O5-C1-C2	-7.28	99.79	111.29
5	X	1	NAG	O5-C1-C2	-7.24	99.85	111.29
11	p	6	MAN	C1-C2-C3	7.03	118.31	109.67
10	e	5	MAN	C1-C2-C3	7.02	118.30	109.67
11	8	6	MAN	C1-C2-C3	7.00	118.27	109.67
13	x	6	MAN	C1-C2-C3	6.98	118.25	109.67
14	6	4	MAN	C1-C2-C3	6.95	118.22	109.67
11	8	5	MAN	O2-C2-C1	5.08	119.54	109.15
13	x	5	MAN	O2-C2-C1	5.07	119.53	109.15
11	p	5	MAN	O2-C2-C1	5.07	119.53	109.15
11	8	8	MAN	C6-C5-C4	-5.04	101.19	113.00
11	p	8	MAN	C6-C5-C4	-5.02	101.24	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	x	5	MAN	C1-O5-C5	4.88	118.81	112.19
11	p	5	MAN	C1-O5-C5	4.81	118.70	112.19
11	8	5	MAN	C1-O5-C5	4.79	118.69	112.19
8	Y	9	MAN	C1-O5-C5	4.54	118.34	112.19
8	9	9	MAN	C1-O5-C5	4.53	118.33	112.19
15	BA	4	MAN	C1-O5-C5	4.51	118.30	112.19
9	Z	4	MAN	C1-O5-C5	4.47	118.25	112.19
8	Y	5	NAG	C1-O5-C5	4.19	117.87	112.19
8	9	5	NAG	C1-O5-C5	4.19	117.86	112.19
13	x	5	MAN	O2-C2-C3	-4.16	101.80	110.14
9	Z	10	NAG	C1-O5-C5	4.14	117.80	112.19
13	x	6	MAN	C2-C3-C4	-4.13	103.75	110.89
10	e	5	MAN	C2-C3-C4	-4.12	103.77	110.89
11	p	5	MAN	O2-C2-C3	-4.12	101.89	110.14
11	8	6	MAN	C2-C3-C4	-4.11	103.79	110.89
11	8	5	MAN	O2-C2-C3	-4.10	101.93	110.14
14	6	4	MAN	C2-C3-C4	-4.09	103.81	110.89
11	p	6	MAN	C2-C3-C4	-4.09	103.82	110.89
15	BA	10	NAG	C1-O5-C5	4.09	117.73	112.19
8	9	2	NAG	C1-O5-C5	4.09	117.73	112.19
9	Z	2	NAG	C1-O5-C5	4.05	117.69	112.19
8	Y	2	NAG	C1-O5-C5	4.05	117.68	112.19
15	BA	2	NAG	C1-O5-C5	4.05	117.67	112.19
5	s	2	NAG	C1-O5-C5	4.03	117.66	112.19
12	q	2	NAG	C1-O5-C5	4.01	117.63	112.19
9	Z	7	NAG	C1-O5-C5	3.97	117.57	112.19
15	BA	7	NAG	C1-O5-C5	3.97	117.56	112.19
11	8	7	MAN	O4-C4-C3	-3.93	101.27	110.35
11	p	7	MAN	O4-C4-C3	-3.93	101.27	110.35
15	BA	3	BMA	C1-O5-C5	3.86	117.42	112.19
9	Z	3	BMA	C1-O5-C5	3.83	117.38	112.19
8	9	3	BMA	C1-O5-C5	3.77	117.30	112.19
8	Y	3	BMA	C1-O5-C5	3.75	117.28	112.19
8	Y	10	NAG	C1-O5-C5	3.62	117.09	112.19
8	9	10	NAG	C1-O5-C5	3.60	117.07	112.19
5	R	2	NAG	O5-C5-C6	-3.57	101.60	107.20
5	5	2	NAG	O5-C5-C6	-3.57	101.61	107.20
5	X	2	NAG	O5-C5-C6	-3.56	101.62	107.20
11	8	2	NAG	O5-C5-C6	-3.56	101.62	107.20
5	Q	2	NAG	O5-C5-C6	-3.55	101.63	107.20
6	V	2	NAG	O5-C5-C6	-3.55	101.64	107.20
11	p	2	NAG	O5-C5-C6	-3.54	101.65	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BA	9	MAN	C1-O5-C5	3.54	116.99	112.19
11	8	8	MAN	O4-C4-C3	-3.54	102.17	110.35
11	p	8	MAN	O4-C4-C3	-3.54	102.18	110.35
6	P	2	NAG	O5-C5-C6	-3.53	101.67	107.20
5	z	2	NAG	O5-C5-C6	-3.53	101.67	107.20
5	b	2	NAG	O5-C5-C6	-3.53	101.67	107.20
5	u	2	NAG	O5-C5-C6	-3.53	101.67	107.20
9	Z	9	MAN	C1-O5-C5	3.53	116.97	112.19
6	W	2	NAG	O5-C5-C6	-3.52	101.68	107.20
9	Z	5	NAG	C1-O5-C5	3.52	116.97	112.19
6	U	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	1	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	AA	2	NAG	O5-C5-C6	-3.52	101.68	107.20
6	m	2	NAG	O5-C5-C6	-3.52	101.68	107.20
6	v	2	NAG	O5-C5-C6	-3.52	101.69	107.20
6	7	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	o	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	c	2	NAG	O5-C5-C6	-3.52	101.69	107.20
6	2	2	NAG	O5-C5-C6	-3.51	101.69	107.20
5	l	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	0	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	T	2	NAG	O5-C5-C6	-3.51	101.71	107.20
5	4	2	NAG	O5-C5-C6	-3.51	101.71	107.20
6	g	2	NAG	O5-C5-C6	-3.51	101.71	107.20
5	h	2	NAG	O5-C5-C6	-3.50	101.71	107.20
6	S	2	NAG	O5-C5-C6	-3.50	101.71	107.20
10	e	2	NAG	O5-C5-C6	-3.50	101.72	107.20
6	j	2	NAG	O5-C5-C6	-3.50	101.72	107.20
5	r	2	NAG	O5-C5-C6	-3.50	101.72	107.20
14	6	2	NAG	O5-C5-C6	-3.50	101.72	107.20
5	w	2	NAG	O5-C5-C6	-3.49	101.72	107.20
6	i	2	NAG	O5-C5-C6	-3.49	101.73	107.20
6	J	2	NAG	O5-C5-C6	-3.49	101.73	107.20
10	e	5	MAN	O5-C1-C2	-3.49	105.39	110.77
6	K	2	NAG	O5-C5-C6	-3.49	101.74	107.20
5	k	2	NAG	O5-C5-C6	-3.48	101.74	107.20
6	I	2	NAG	O5-C5-C6	-3.48	101.75	107.20
6	d	2	NAG	O5-C5-C6	-3.48	101.75	107.20
13	x	2	NAG	O5-C5-C6	-3.48	101.75	107.20
5	3	2	NAG	O5-C5-C6	-3.48	101.75	107.20
5	G	2	NAG	O5-C5-C6	-3.47	101.76	107.20
6	t	2	NAG	O5-C5-C6	-3.47	101.77	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	4	MAN	C1-O5-C5	3.47	116.89	112.19
6	n	2	NAG	O5-C5-C6	-3.47	101.77	107.20
15	BA	5	NAG	C1-O5-C5	3.46	116.88	112.19
11	p	6	MAN	O5-C1-C2	-3.46	105.43	110.77
14	6	4	MAN	O5-C1-C2	-3.46	105.44	110.77
6	a	2	NAG	O5-C5-C6	-3.44	101.81	107.20
8	9	4	MAN	C1-O5-C5	3.44	116.85	112.19
11	8	6	MAN	O5-C1-C2	-3.43	105.48	110.77
13	x	6	MAN	O5-C1-C2	-3.42	105.49	110.77
11	p	8	MAN	O5-C5-C6	3.41	112.54	107.20
11	8	8	MAN	O5-C5-C6	3.40	112.54	107.20
11	8	4	MAN	O5-C5-C6	3.38	112.50	107.20
8	Y	1	NAG	C1-O5-C5	3.37	116.76	112.19
12	q	1	NAG	C1-O5-C5	3.37	116.76	112.19
8	9	1	NAG	C1-O5-C5	3.36	116.75	112.19
11	p	4	MAN	O5-C5-C6	3.35	112.45	107.20
9	Z	12	NAG	C1-O5-C5	3.31	116.67	112.19
15	BA	11	NAG	C1-O5-C5	3.30	116.66	112.19
9	Z	1	NAG	C1-O5-C5	3.29	116.65	112.19
13	x	4	MAN	O5-C5-C6	3.28	112.35	107.20
10	e	4	MAN	O5-C5-C6	3.28	112.34	107.20
5	s	1	NAG	C1-O5-C5	3.27	116.62	112.19
15	BA	1	NAG	C1-O5-C5	3.25	116.60	112.19
8	9	7	NAG	C1-O5-C5	3.24	116.59	112.19
11	p	7	MAN	O4-C4-C5	3.24	117.34	109.30
11	8	7	MAN	O4-C4-C5	3.21	117.27	109.30
8	Y	7	NAG	C1-O5-C5	3.20	116.53	112.19
11	8	8	MAN	C3-C4-C5	-3.15	104.63	110.24
11	p	8	MAN	C3-C4-C5	-3.13	104.66	110.24
15	BA	8	GAL	C1-O5-C5	3.08	116.36	112.19
9	Z	11	GAL	C1-O5-C5	3.04	116.32	112.19
9	Z	8	GAL	C1-O5-C5	3.03	116.30	112.19
8	9	6	GAL	C1-O5-C5	3.02	116.29	112.19
8	Y	6	GAL	C1-O5-C5	3.01	116.27	112.19
6	I	3	BMA	O2-C2-C3	3.00	116.14	110.14
6	a	3	BMA	O2-C2-C3	2.98	116.11	110.14
6	v	3	BMA	O2-C2-C3	2.98	116.11	110.14
6	j	3	BMA	O2-C2-C3	2.98	116.11	110.14
6	t	3	BMA	O2-C2-C3	2.97	116.09	110.14
6	g	3	BMA	O2-C2-C3	2.97	116.09	110.14
6	7	3	BMA	O2-C2-C3	2.96	116.07	110.14
6	W	3	BMA	O2-C2-C3	2.96	116.07	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	3	BMA	O2-C2-C3	2.96	116.06	110.14
14	6	3	BMA	O2-C2-C3	2.96	116.06	110.14
15	BA	9	MAN	C1-C2-C3	2.95	113.30	109.67
6	P	3	BMA	O2-C2-C3	2.95	116.06	110.14
6	n	3	BMA	O2-C2-C3	2.95	116.06	110.14
15	BA	6	GAL	C1-O5-C5	2.95	116.19	112.19
6	d	3	BMA	O2-C2-C3	2.95	116.04	110.14
13	x	3	BMA	O2-C2-C3	2.94	116.04	110.14
6	J	3	BMA	O2-C2-C3	2.94	116.03	110.14
6	V	3	BMA	O2-C2-C3	2.94	116.03	110.14
11	8	3	BMA	O2-C2-C3	2.94	116.03	110.14
8	Y	8	GAL	C1-O5-C5	2.94	116.18	112.19
11	p	3	BMA	O2-C2-C3	2.94	116.03	110.14
9	Z	9	MAN	C1-C2-C3	2.94	113.28	109.67
11	8	8	MAN	O2-C2-C3	-2.94	104.25	110.14
6	K	3	BMA	O2-C2-C3	2.93	116.02	110.14
9	Z	6	GAL	C1-O5-C5	2.93	116.17	112.19
8	9	4	MAN	C1-C2-C3	2.93	113.27	109.67
6	2	3	BMA	O2-C2-C3	2.93	116.01	110.14
8	Y	4	MAN	C1-C2-C3	2.93	113.27	109.67
6	S	3	BMA	O2-C2-C3	2.93	116.01	110.14
8	9	8	GAL	C1-O5-C5	2.93	116.16	112.19
11	p	8	MAN	O2-C2-C3	-2.92	104.29	110.14
10	e	3	BMA	O2-C2-C3	2.92	115.99	110.14
6	U	3	BMA	O2-C2-C3	2.90	115.96	110.14
6	m	3	BMA	O2-C2-C3	2.90	115.95	110.14
11	p	7	MAN	O5-C5-C6	-2.84	102.75	107.20
11	8	7	MAN	O5-C5-C6	-2.83	102.77	107.20
6	V	1	NAG	O7-C7-C8	-2.82	116.83	122.06
7	O	6	MAN	O5-C5-C6	2.81	111.61	107.20
5	o	1	NAG	O7-C7-C8	-2.81	116.84	122.06
6	W	1	NAG	O7-C7-C8	-2.81	116.84	122.06
14	6	1	NAG	O7-C7-C8	-2.81	116.85	122.06
6	n	1	NAG	O7-C7-C8	-2.80	116.85	122.06
7	f	6	MAN	O5-C5-C6	2.79	111.58	107.20
6	j	1	NAG	O7-C7-C8	-2.79	116.87	122.06
6	7	1	NAG	O7-C7-C8	-2.79	116.87	122.06
5	Q	1	NAG	O7-C7-C8	-2.79	116.87	122.06
5	T	1	NAG	O7-C7-C8	-2.79	116.88	122.06
5	0	1	NAG	O7-C7-C8	-2.79	116.88	122.06
13	x	1	NAG	O7-C7-C8	-2.79	116.88	122.06
10	e	1	NAG	O7-C7-C8	-2.78	116.89	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O7-C7-C8	-2.78	116.90	122.06
6	J	1	NAG	O7-C7-C8	-2.78	116.90	122.06
11	8	5	MAN	O4-C4-C3	-2.77	103.94	110.35
5	u	1	NAG	O7-C7-C8	-2.77	116.91	122.06
5	b	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	d	1	NAG	O7-C7-C8	-2.77	116.91	122.06
7	y	6	MAN	O5-C5-C6	2.77	111.55	107.20
5	w	1	NAG	O7-C7-C8	-2.77	116.91	122.06
11	p	5	MAN	O4-C4-C3	-2.77	103.95	110.35
6	S	1	NAG	O7-C7-C8	-2.76	116.92	122.06
6	2	1	NAG	O7-C7-C8	-2.76	116.92	122.06
13	x	5	MAN	O4-C4-C3	-2.76	103.96	110.35
6	i	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	3	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	1	1	NAG	O7-C7-C8	-2.76	116.93	122.06
5	5	1	NAG	O7-C7-C8	-2.76	116.94	122.06
6	I	1	NAG	O7-C7-C8	-2.76	116.94	122.06
5	l	1	NAG	O7-C7-C8	-2.75	116.94	122.06
5	r	1	NAG	O7-C7-C8	-2.75	116.95	122.06
5	AA	1	NAG	O7-C7-C8	-2.75	116.95	122.06
5	c	1	NAG	O7-C7-C8	-2.75	116.96	122.06
5	z	1	NAG	O7-C7-C8	-2.75	116.96	122.06
5	h	1	NAG	O7-C7-C8	-2.74	116.96	122.06
5	X	1	NAG	O7-C7-C8	-2.74	116.97	122.06
6	v	1	NAG	O7-C7-C8	-2.74	116.97	122.06
6	P	1	NAG	O7-C7-C8	-2.74	116.97	122.06
5	4	1	NAG	O7-C7-C8	-2.74	116.98	122.06
11	8	1	NAG	O7-C7-C8	-2.73	116.98	122.06
5	k	1	NAG	O7-C7-C8	-2.73	116.99	122.06
5	R	1	NAG	O7-C7-C8	-2.73	116.99	122.06
5	G	1	NAG	O7-C7-C8	-2.72	117.00	122.06
6	m	1	NAG	O7-C7-C8	-2.72	117.01	122.06
6	g	1	NAG	O7-C7-C8	-2.72	117.01	122.06
6	t	1	NAG	O7-C7-C8	-2.72	117.01	122.06
5	c	1	NAG	C4-C3-C2	-2.72	107.04	111.02
11	p	1	NAG	O7-C7-C8	-2.72	117.01	122.06
6	W	1	NAG	C4-C3-C2	-2.71	107.04	111.02
6	v	1	NAG	C4-C3-C2	-2.71	107.05	111.02
6	a	1	NAG	O7-C7-C8	-2.71	117.03	122.06
6	U	1	NAG	O7-C7-C8	-2.70	117.04	122.06
5	R	1	NAG	C4-C3-C2	-2.70	107.06	111.02
8	9	9	MAN	C1-C2-C3	2.70	112.98	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C4-C3-C2	-2.70	107.06	111.02
5	5	1	NAG	C4-C3-C2	-2.70	107.07	111.02
5	o	1	NAG	C4-C3-C2	-2.69	107.07	111.02
6	7	1	NAG	C4-C3-C2	-2.69	107.08	111.02
5	h	1	NAG	C4-C3-C2	-2.69	107.08	111.02
6	m	1	NAG	C4-C3-C2	-2.69	107.08	111.02
8	Y	9	MAN	C1-C2-C3	2.67	112.95	109.67
6	t	1	NAG	C4-C3-C2	-2.67	107.10	111.02
11	8	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	u	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	4	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	t	3	BMA	O4-C4-C5	-2.67	102.67	109.30
6	V	1	NAG	C4-C3-C2	-2.67	107.11	111.02
6	n	1	NAG	C4-C3-C2	-2.67	107.11	111.02
6	a	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	0	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	G	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	l	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	k	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	U	1	NAG	C4-C3-C2	-2.66	107.12	111.02
13	x	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	2	3	BMA	O4-C4-C5	-2.66	102.69	109.30
5	AA	1	NAG	C4-C3-C2	-2.65	107.13	111.02
6	P	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	z	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	1	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	r	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	b	1	NAG	C4-C3-C2	-2.65	107.14	111.02
6	J	3	BMA	O4-C4-C5	-2.65	102.72	109.30
6	i	1	NAG	C4-C3-C2	-2.65	107.14	111.02
5	T	1	NAG	C4-C3-C2	-2.65	107.14	111.02
5	w	1	NAG	C4-C3-C2	-2.65	107.14	111.02
14	6	1	NAG	C4-C3-C2	-2.65	107.14	111.02
6	S	3	BMA	O4-C4-C5	-2.64	102.73	109.30
6	j	3	BMA	O4-C4-C5	-2.64	102.74	109.30
5	X	1	NAG	C4-C3-C2	-2.64	107.15	111.02
6	W	3	BMA	O4-C4-C5	-2.64	102.74	109.30
6	d	1	NAG	C4-C3-C2	-2.64	107.15	111.02
11	8	3	BMA	O4-C4-C5	-2.64	102.75	109.30
6	a	3	BMA	O4-C4-C5	-2.64	102.75	109.30
11	p	3	BMA	O4-C4-C5	-2.63	102.75	109.30
5	Q	1	NAG	C4-C3-C2	-2.63	107.16	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	j	1	NAG	C4-C3-C2	-2.63	107.16	111.02
11	p	1	NAG	C4-C3-C2	-2.63	107.16	111.02
6	V	3	BMA	O4-C4-C5	-2.63	102.77	109.30
5	3	1	NAG	C4-C3-C2	-2.63	107.16	111.02
6	d	3	BMA	O4-C4-C5	-2.63	102.77	109.30
10	e	1	NAG	C4-C3-C2	-2.63	107.17	111.02
6	7	3	BMA	O4-C4-C5	-2.63	102.77	109.30
6	i	3	BMA	O4-C4-C5	-2.63	102.78	109.30
6	g	1	NAG	C4-C3-C2	-2.63	107.17	111.02
6	g	3	BMA	O4-C4-C5	-2.62	102.78	109.30
6	I	3	BMA	O4-C4-C5	-2.62	102.78	109.30
6	m	3	BMA	O4-C4-C5	-2.62	102.79	109.30
6	2	1	NAG	C4-C3-C2	-2.62	107.18	111.02
6	S	1	NAG	C4-C3-C2	-2.62	107.18	111.02
14	6	3	BMA	O4-C4-C5	-2.62	102.80	109.30
6	v	3	BMA	O4-C4-C5	-2.62	102.80	109.30
6	n	3	BMA	O4-C4-C5	-2.62	102.80	109.30
6	K	1	NAG	C4-C3-C2	-2.61	107.19	111.02
6	P	3	BMA	O4-C4-C5	-2.61	102.82	109.30
6	J	1	NAG	C4-C3-C2	-2.61	107.19	111.02
6	U	3	BMA	O4-C4-C5	-2.60	102.83	109.30
6	K	3	BMA	O4-C4-C5	-2.59	102.87	109.30
13	x	3	BMA	O4-C4-C5	-2.59	102.87	109.30
10	e	3	BMA	O4-C4-C5	-2.58	102.89	109.30
13	x	4	MAN	O5-C1-C2	2.56	114.72	110.77
15	BA	4	MAN	C1-C2-C3	2.56	112.81	109.67
10	e	4	MAN	O5-C1-C2	2.52	114.66	110.77
9	Z	4	MAN	C1-C2-C3	2.52	112.76	109.67
11	8	4	MAN	O5-C1-C2	2.48	114.61	110.77
11	p	4	MAN	O5-C1-C2	2.47	114.58	110.77
6	K	3	BMA	C6-C5-C4	-2.46	107.23	113.00
13	x	3	BMA	C6-C5-C4	-2.46	107.24	113.00
10	e	3	BMA	C6-C5-C4	-2.45	107.27	113.00
6	J	3	BMA	C6-C5-C4	-2.44	107.30	113.00
6	7	3	BMA	C6-C5-C4	-2.43	107.31	113.00
6	W	3	BMA	C6-C5-C4	-2.43	107.31	113.00
6	j	3	BMA	C6-C5-C4	-2.43	107.31	113.00
6	K	2	NAG	O5-C1-C2	-2.43	107.45	111.29
6	P	3	BMA	C6-C5-C4	-2.42	107.33	113.00
6	d	3	BMA	C6-C5-C4	-2.42	107.33	113.00
6	n	3	BMA	C6-C5-C4	-2.42	107.33	113.00
11	8	8	MAN	O2-C2-C1	2.42	114.10	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	v	3	BMA	C6-C5-C4	-2.42	107.34	113.00
6	U	3	BMA	C6-C5-C4	-2.42	107.34	113.00
6	I	3	BMA	C6-C5-C4	-2.41	107.35	113.00
14	6	3	BMA	C6-C5-C4	-2.41	107.35	113.00
6	2	3	BMA	C6-C5-C4	-2.41	107.35	113.00
6	m	3	BMA	C6-C5-C4	-2.41	107.35	113.00
11	8	3	BMA	C6-C5-C4	-2.41	107.36	113.00
6	g	3	BMA	C6-C5-C4	-2.41	107.37	113.00
6	i	3	BMA	C6-C5-C4	-2.41	107.37	113.00
11	p	3	BMA	C6-C5-C4	-2.41	107.37	113.00
6	V	3	BMA	C6-C5-C4	-2.40	107.37	113.00
11	p	8	MAN	O2-C2-C1	2.40	114.07	109.15
6	S	3	BMA	C6-C5-C4	-2.40	107.39	113.00
6	a	3	BMA	C6-C5-C4	-2.39	107.40	113.00
6	t	3	BMA	C6-C5-C4	-2.39	107.41	113.00
13	x	2	NAG	O5-C1-C2	-2.37	107.54	111.29
10	e	2	NAG	O5-C1-C2	-2.35	107.57	111.29
10	e	2	NAG	C4-C3-C2	-2.35	107.57	111.02
5	G	2	NAG	O5-C1-C2	-2.31	107.64	111.29
5	3	2	NAG	O5-C1-C2	-2.31	107.64	111.29
6	n	2	NAG	O5-C1-C2	-2.30	107.66	111.29
11	8	5	MAN	O6-C6-C5	2.29	119.16	111.29
6	t	2	NAG	O5-C1-C2	-2.29	107.67	111.29
6	V	2	NAG	O5-C1-C2	-2.29	107.67	111.29
5	5	2	NAG	O5-C1-C2	-2.29	107.67	111.29
11	p	5	MAN	O6-C6-C5	2.29	119.14	111.29
5	Q	2	NAG	O5-C1-C2	-2.29	107.68	111.29
5	T	2	NAG	O5-C1-C2	-2.28	107.68	111.29
14	6	2	NAG	O5-C1-C2	-2.28	107.68	111.29
6	W	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	h	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	w	2	NAG	O5-C1-C2	-2.27	107.70	111.29
6	7	2	NAG	O5-C1-C2	-2.27	107.70	111.29
13	x	5	MAN	O6-C6-C5	2.27	119.09	111.29
5	b	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	k	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	0	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	o	2	NAG	O5-C1-C2	-2.27	107.71	111.29
6	K	2	NAG	C4-C3-C2	-2.27	107.69	111.02
6	I	2	NAG	O5-C1-C2	-2.26	107.71	111.29
6	d	2	NAG	O5-C1-C2	-2.26	107.71	111.29
5	c	2	NAG	O5-C1-C2	-2.26	107.72	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	r	2	NAG	C4-C3-C2	-2.26	107.70	111.02
13	x	2	NAG	C4-C3-C2	-2.26	107.70	111.02
6	m	2	NAG	O5-C1-C2	-2.26	107.72	111.29
11	p	2	NAG	O5-C1-C2	-2.26	107.72	111.29
11	8	7	MAN	O3-C3-C2	-2.26	105.67	109.99
6	U	2	NAG	O5-C1-C2	-2.25	107.73	111.29
5	z	2	NAG	O5-C1-C2	-2.25	107.73	111.29
6	7	2	NAG	C4-C3-C2	-2.25	107.72	111.02
5	u	2	NAG	O5-C1-C2	-2.25	107.74	111.29
6	J	2	NAG	O5-C1-C2	-2.25	107.74	111.29
11	8	2	NAG	O5-C1-C2	-2.25	107.74	111.29
5	l	2	NAG	O5-C1-C2	-2.24	107.75	111.29
5	X	2	NAG	O5-C1-C2	-2.24	107.75	111.29
5	1	2	NAG	O5-C1-C2	-2.24	107.75	111.29
5	4	2	NAG	O5-C1-C2	-2.24	107.76	111.29
6	g	2	NAG	O5-C1-C2	-2.24	107.76	111.29
6	i	2	NAG	O5-C1-C2	-2.23	107.76	111.29
5	u	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	R	2	NAG	O5-C1-C2	-2.23	107.77	111.29
5	r	2	NAG	O5-C1-C2	-2.23	107.77	111.29
5	l	2	NAG	C4-C3-C2	-2.23	107.75	111.02
6	P	2	NAG	O5-C1-C2	-2.23	107.77	111.29
11	p	7	MAN	O3-C3-C2	-2.23	105.73	109.99
5	AA	2	NAG	O5-C1-C2	-2.23	107.77	111.29
6	W	2	NAG	C4-C3-C2	-2.23	107.76	111.02
6	2	2	NAG	O5-C1-C2	-2.22	107.78	111.29
5	G	2	NAG	C4-C3-C2	-2.22	107.76	111.02
6	d	2	NAG	C4-C3-C2	-2.22	107.77	111.02
5	o	2	NAG	C4-C3-C2	-2.22	107.77	111.02
6	j	2	NAG	O5-C1-C2	-2.21	107.79	111.29
6	2	2	NAG	C4-C3-C2	-2.21	107.78	111.02
6	v	2	NAG	O5-C1-C2	-2.21	107.80	111.29
5	AA	2	NAG	C4-C3-C2	-2.21	107.78	111.02
6	S	2	NAG	O5-C1-C2	-2.21	107.80	111.29
11	8	7	MAN	C1-O5-C5	2.20	115.18	112.19
6	a	2	NAG	O5-C1-C2	-2.20	107.81	111.29
5	k	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	0	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	P	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	g	2	NAG	C4-C3-C2	-2.20	107.79	111.02
14	6	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	w	2	NAG	C4-C3-C2	-2.20	107.79	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	5	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	z	2	NAG	C4-C3-C2	-2.20	107.80	111.02
6	m	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	b	2	NAG	C4-C3-C2	-2.20	107.80	111.02
6	I	2	NAG	C4-C3-C2	-2.19	107.80	111.02
5	X	2	NAG	C4-C3-C2	-2.19	107.81	111.02
11	8	2	NAG	C4-C3-C2	-2.19	107.81	111.02
5	4	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	a	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	n	2	NAG	C4-C3-C2	-2.19	107.81	111.02
5	c	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	J	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	S	2	NAG	C4-C3-C2	-2.19	107.81	111.02
11	p	7	MAN	C1-O5-C5	2.18	115.15	112.19
11	p	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	V	2	NAG	C4-C3-C2	-2.18	107.82	111.02
5	T	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	t	2	NAG	C4-C3-C2	-2.18	107.82	111.02
13	x	4	MAN	O3-C3-C4	2.18	115.39	110.35
6	U	2	NAG	C4-C3-C2	-2.17	107.83	111.02
6	j	2	NAG	C4-C3-C2	-2.17	107.83	111.02
5	h	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	v	2	NAG	C4-C3-C2	-2.16	107.85	111.02
5	Q	2	NAG	C4-C3-C2	-2.16	107.86	111.02
5	1	2	NAG	C4-C3-C2	-2.14	107.88	111.02
6	i	2	NAG	C4-C3-C2	-2.14	107.88	111.02
10	e	4	MAN	O3-C3-C4	2.14	115.30	110.35
11	8	8	MAN	C2-C3-C4	2.13	114.58	110.89
11	p	8	MAN	C2-C3-C4	2.13	114.58	110.89
5	R	2	NAG	C4-C3-C2	-2.13	107.90	111.02
11	8	4	MAN	O3-C3-C4	2.12	115.26	110.35
11	p	4	MAN	O3-C3-C4	2.12	115.24	110.35
13	x	6	MAN	O5-C5-C6	-2.10	103.91	107.20
15	BA	12	FUC	C1-C2-C3	2.10	112.25	109.67
9	Z	13	FUC	C1-C2-C3	2.10	112.24	109.67
11	p	7	MAN	O5-C1-C2	2.08	113.97	110.77
7	y	6	MAN	C1-O5-C5	-2.06	109.40	112.19
14	6	4	MAN	O5-C5-C6	-2.06	103.98	107.20
13	x	4	MAN	O4-C4-C3	-2.05	105.61	110.35
11	8	7	MAN	O5-C1-C2	2.05	113.93	110.77
10	e	5	MAN	O5-C5-C6	-2.04	104.01	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	p	7	MAN	O3-C3-C4	2.02	115.03	110.35
10	e	4	MAN	O4-C4-C3	-2.02	105.68	110.35
11	8	7	MAN	O3-C3-C4	2.02	115.01	110.35
7	O	6	MAN	C1-O5-C5	-2.01	109.47	112.19
9	Z	12	NAG	O5-C1-C2	-2.01	108.12	111.29
7	f	6	MAN	C1-O5-C5	-2.00	109.48	112.19
11	8	4	MAN	O4-C4-C3	-2.00	105.72	110.35

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	1	NAG	C3-C2-N2-C7
5	s	1	NAG	C1-C2-N2-C7
9	Z	1	NAG	C1-C2-N2-C7
11	p	1	NAG	C3-C2-N2-C7
11	8	1	NAG	C3-C2-N2-C7
15	BA	1	NAG	C1-C2-N2-C7
8	Y	3	BMA	C4-C5-C6-O6
8	9	3	BMA	C4-C5-C6-O6
7	f	5	MAN	O5-C5-C6-O6
7	y	5	MAN	O5-C5-C6-O6
7	O	5	MAN	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	9	3	BMA	O5-C5-C6-O6
7	O	2	NAG	C8-C7-N2-C2
7	f	2	NAG	C8-C7-N2-C2
7	y	2	NAG	C8-C7-N2-C2
7	O	6	MAN	C4-C5-C6-O6
7	f	6	MAN	C4-C5-C6-O6
7	y	6	MAN	C4-C5-C6-O6
6	i	1	NAG	C1-C2-N2-C7
7	O	6	MAN	O5-C5-C6-O6
7	f	6	MAN	O5-C5-C6-O6
15	BA	9	MAN	O5-C5-C6-O6
7	y	6	MAN	O5-C5-C6-O6
7	y	2	NAG	O7-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	f	2	NAG	O7-C7-N2-C2
9	Z	9	MAN	O5-C5-C6-O6
5	c	1	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	v	1	NAG	C3-C2-N2-C7
6	U	3	BMA	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	g	3	BMA	C4-C5-C6-O6
6	v	3	BMA	C4-C5-C6-O6
6	7	3	BMA	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
6	W	3	BMA	C4-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
6	d	3	BMA	C4-C5-C6-O6
6	i	3	BMA	C4-C5-C6-O6
6	j	3	BMA	C4-C5-C6-O6
6	m	3	BMA	C4-C5-C6-O6
14	6	3	BMA	C4-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6
6	n	3	BMA	C4-C5-C6-O6
6	2	3	BMA	C4-C5-C6-O6
6	t	3	BMA	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	m	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
6	v	3	BMA	O5-C5-C6-O6
6	7	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
6	i	3	BMA	O5-C5-C6-O6
6	2	3	BMA	O5-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
6	d	3	BMA	O5-C5-C6-O6
6	j	3	BMA	O5-C5-C6-O6
6	t	3	BMA	O5-C5-C6-O6
14	6	3	BMA	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
6	n	3	BMA	O5-C5-C6-O6
7	f	5	MAN	C4-C5-C6-O6
7	y	5	MAN	C4-C5-C6-O6
7	O	5	MAN	C4-C5-C6-O6

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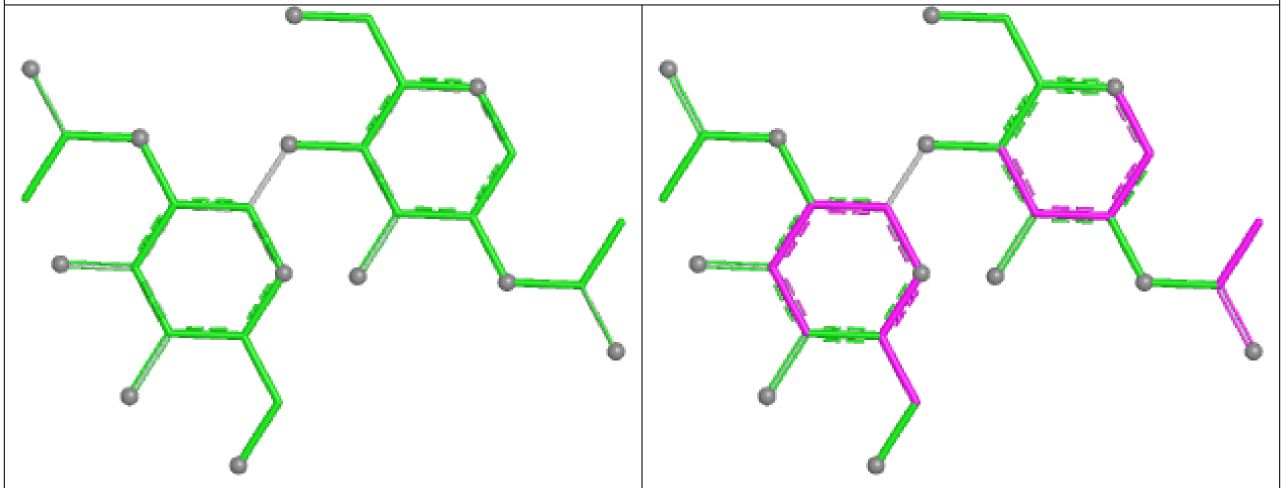
Mol	**Chain**	**Res**	**Type**	**Atoms**
6	i	1	NAG	C3-C2-N2-C7
10	e	1	NAG	O7-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	l	1	NAG	O7-C7-N2-C2
5	0	1	NAG	O7-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	g	1	NAG	O7-C7-N2-C2
6	t	1	NAG	O7-C7-N2-C2
6	7	1	NAG	O7-C7-N2-C2
11	p	1	NAG	O7-C7-N2-C2
13	x	1	NAG	O7-C7-N2-C2

There are no ring outliers.

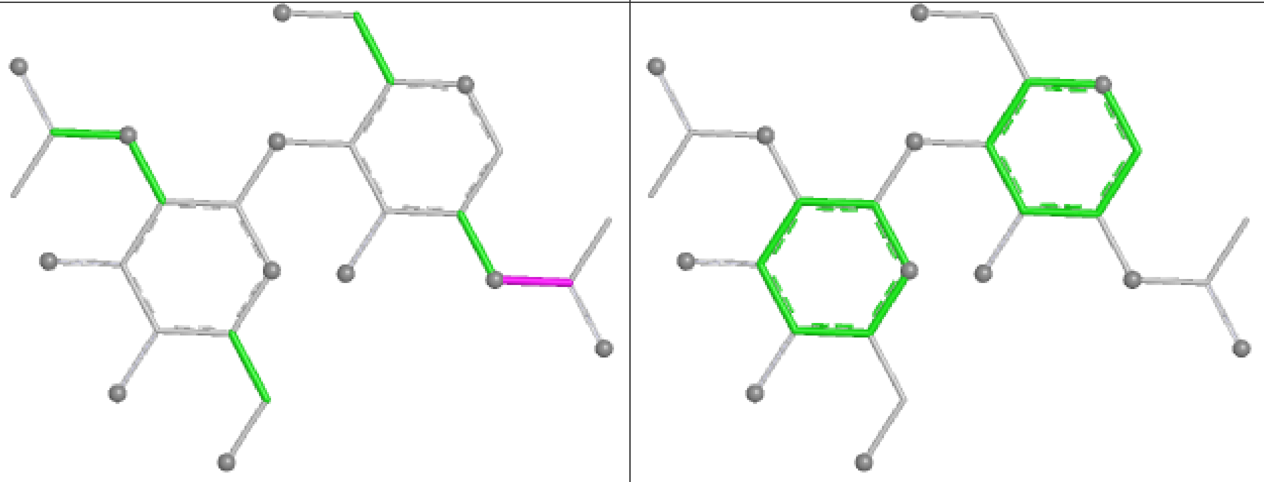
No monomer is involved in short contacts.

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 G

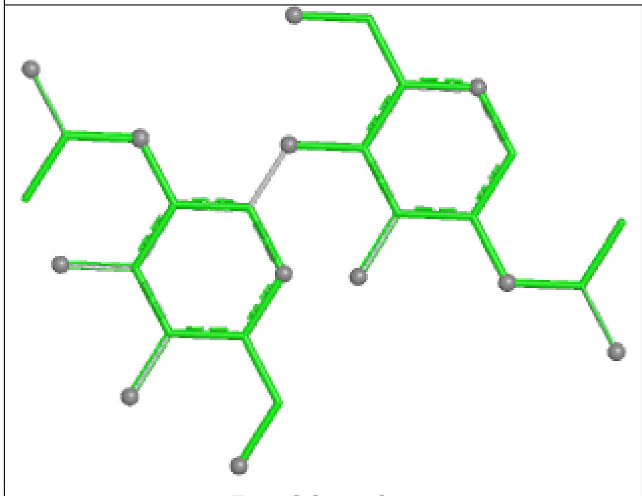


Bond lengths **Bond angles**

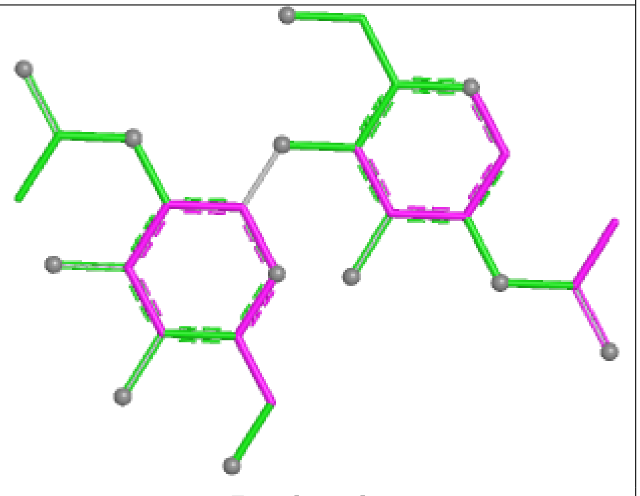


Torsions **Rings**

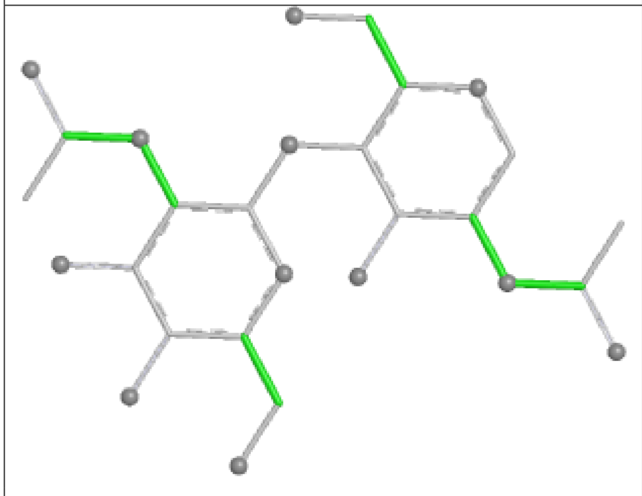
Oligosaccharide Chain Q



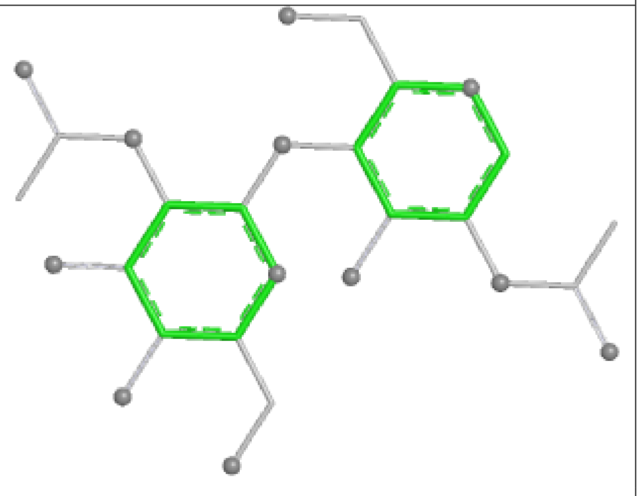
Bond lengths



Bond angles

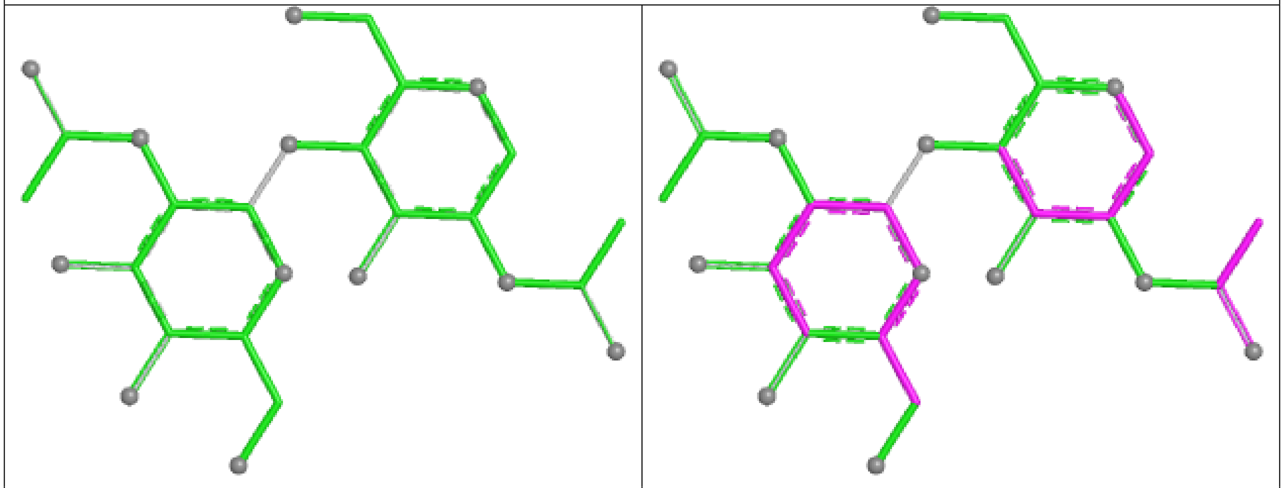


Torsions



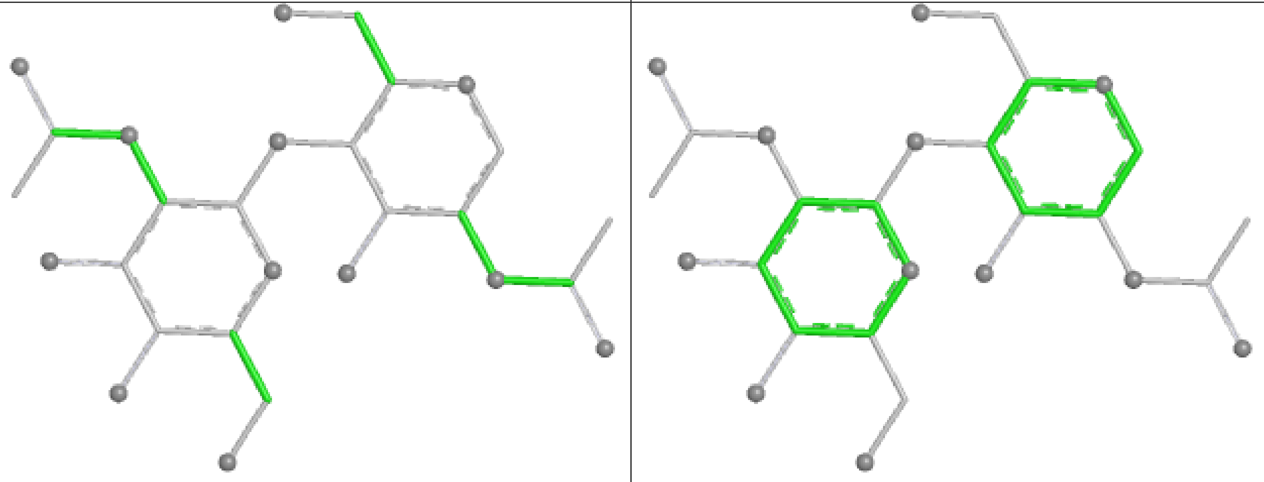
Rings

Oligosaccharide Chain R



Bond lengths

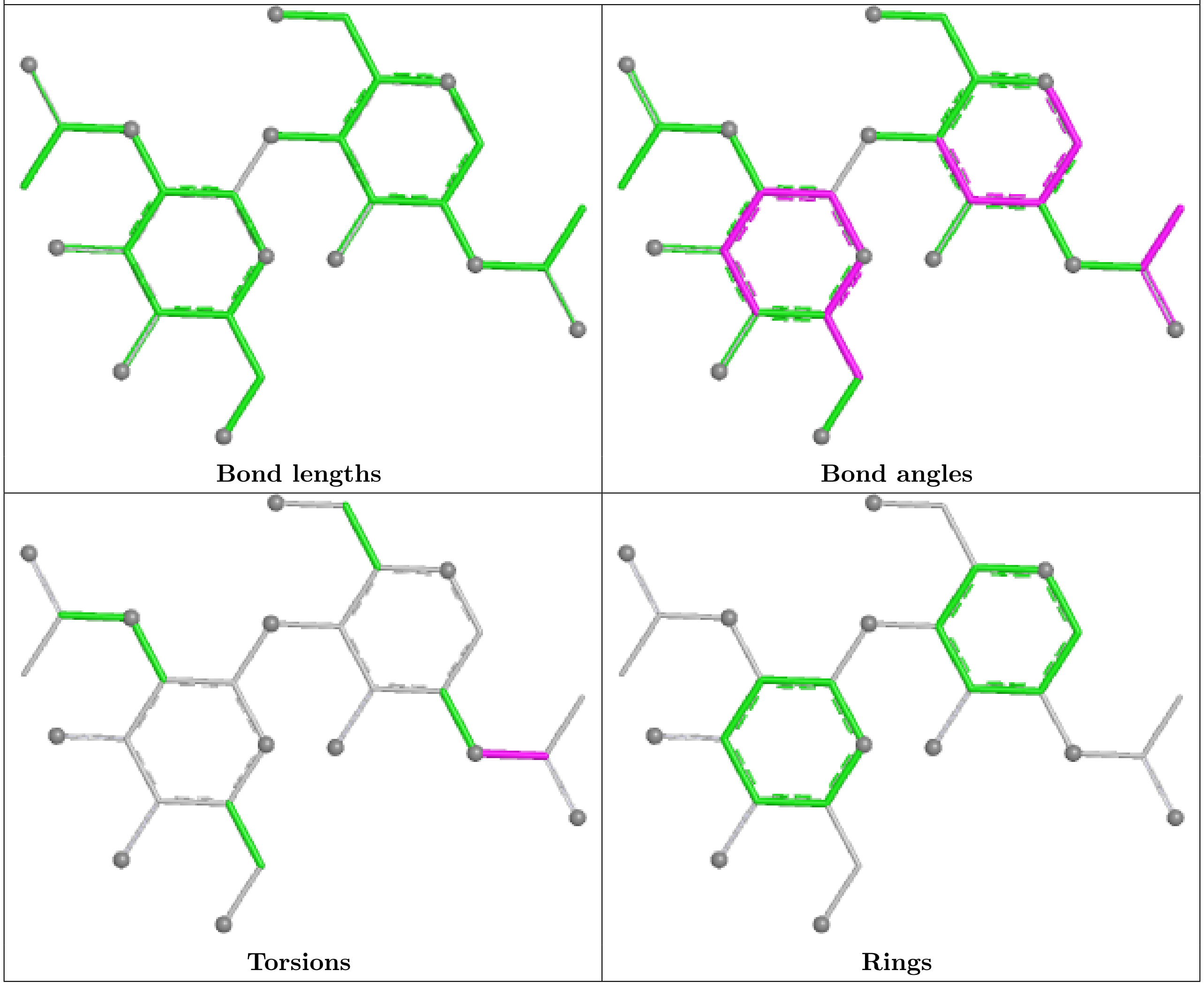
Bond angles



Torsions

Rings

Oligosaccharide Chain T



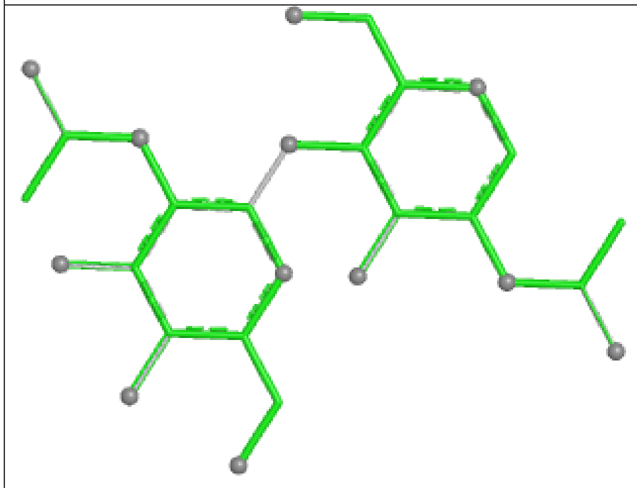
Bond lengths

Bond angles

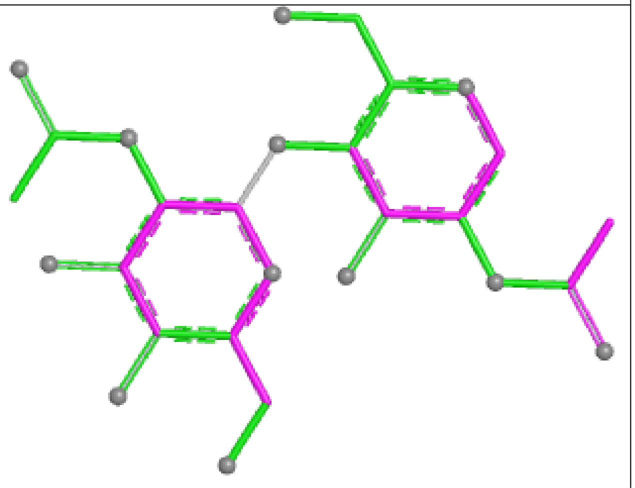
Torsions

Rings

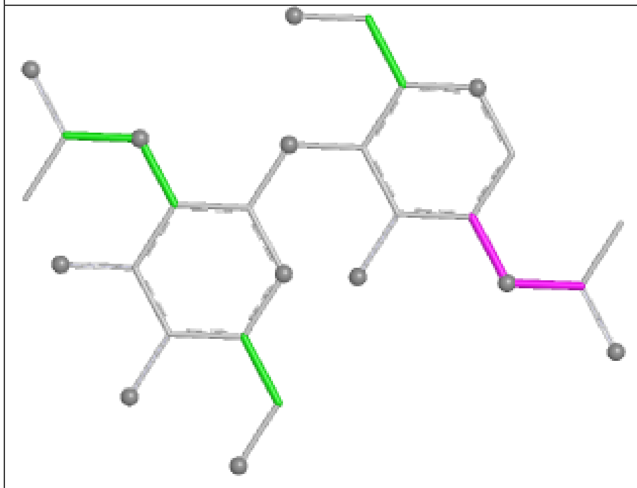
Oligosaccharide Chain X



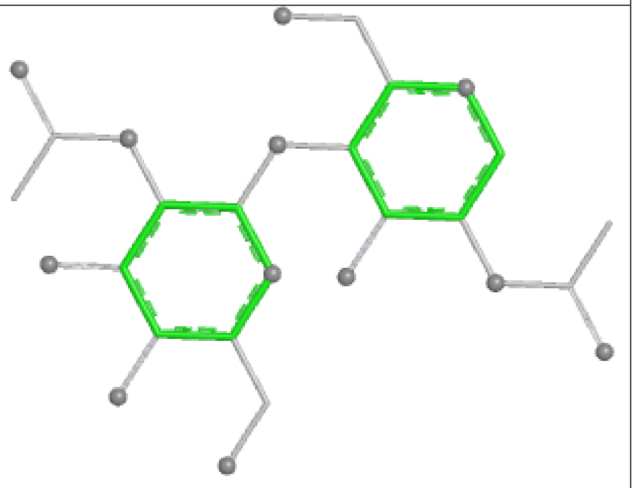
Bond lengths



Bond angles

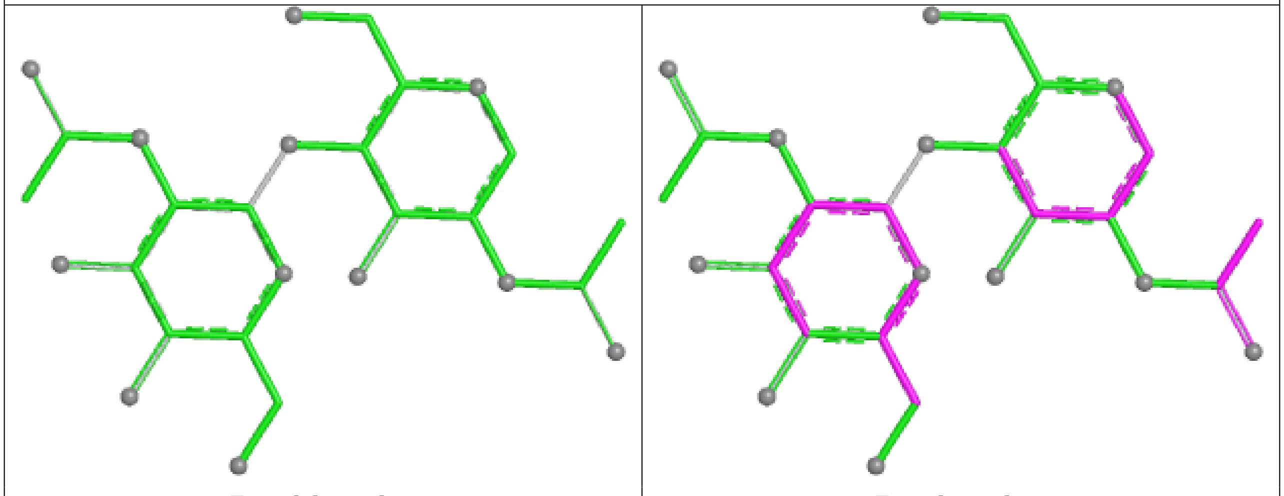


Torsions



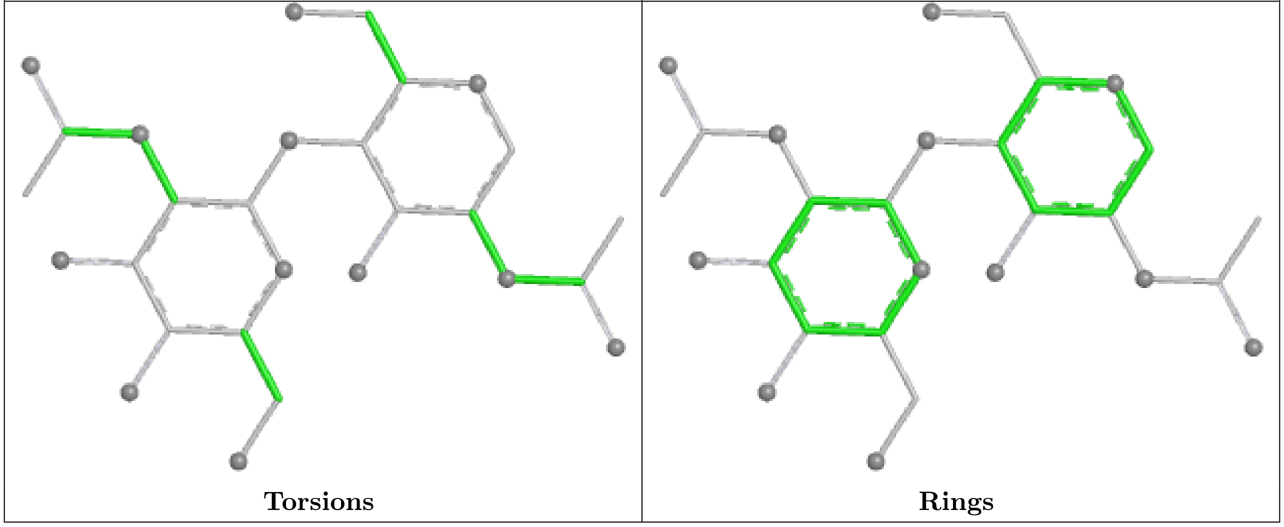
Rings

Oligosaccharide Chain b



Bond lengths

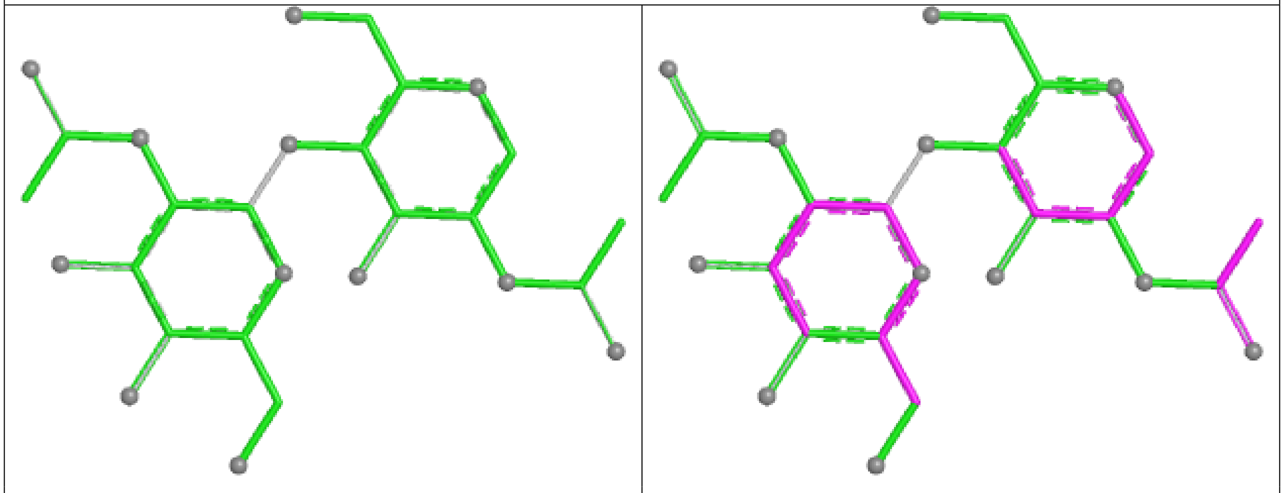
Bond angles



Torsions

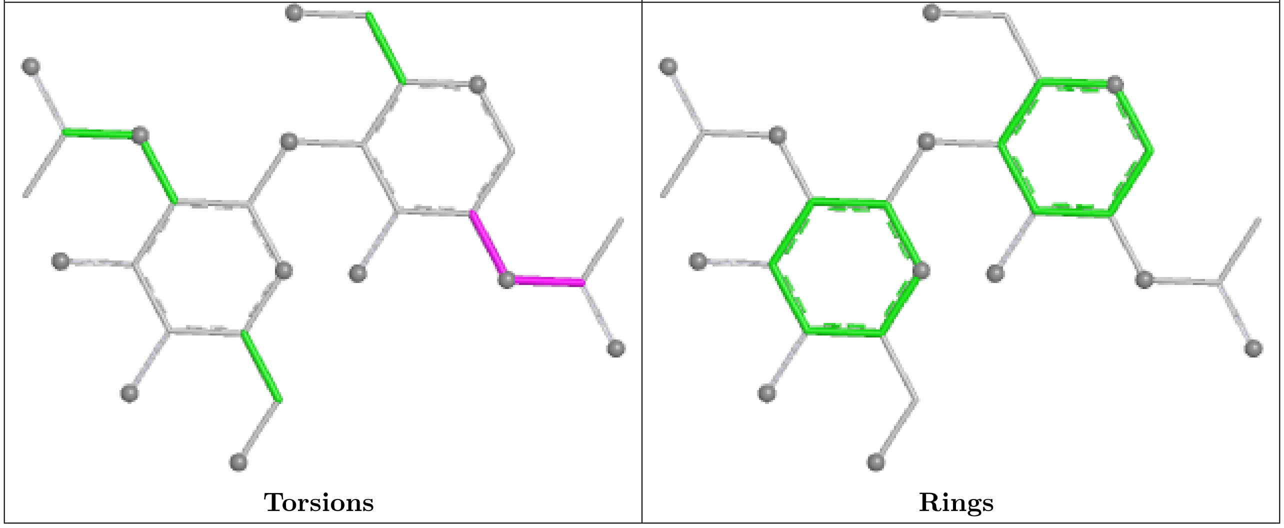
Rings

Oligosaccharide Chain c



Bond lengths

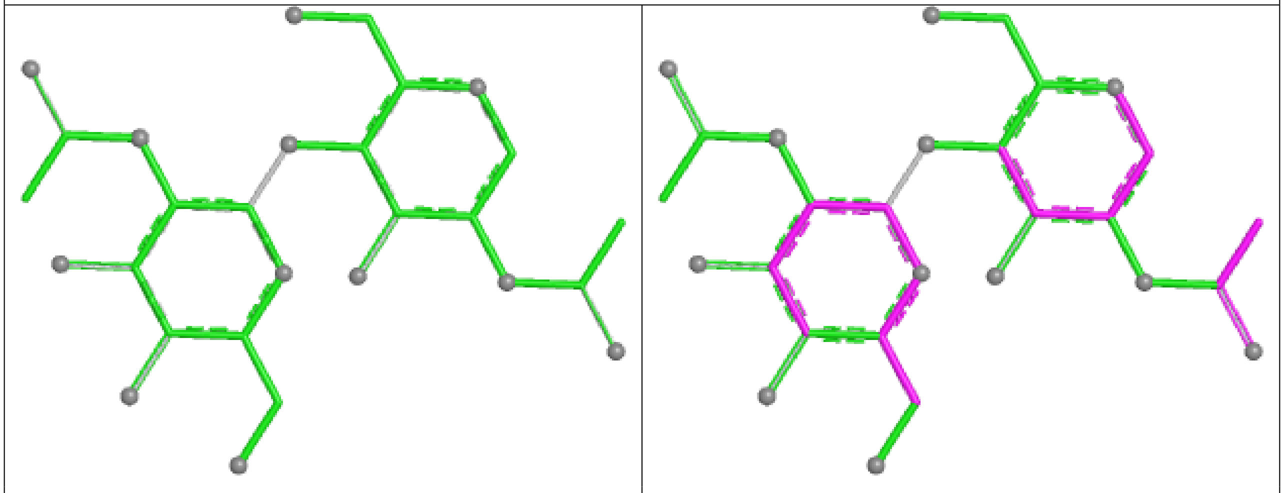
Bond angles



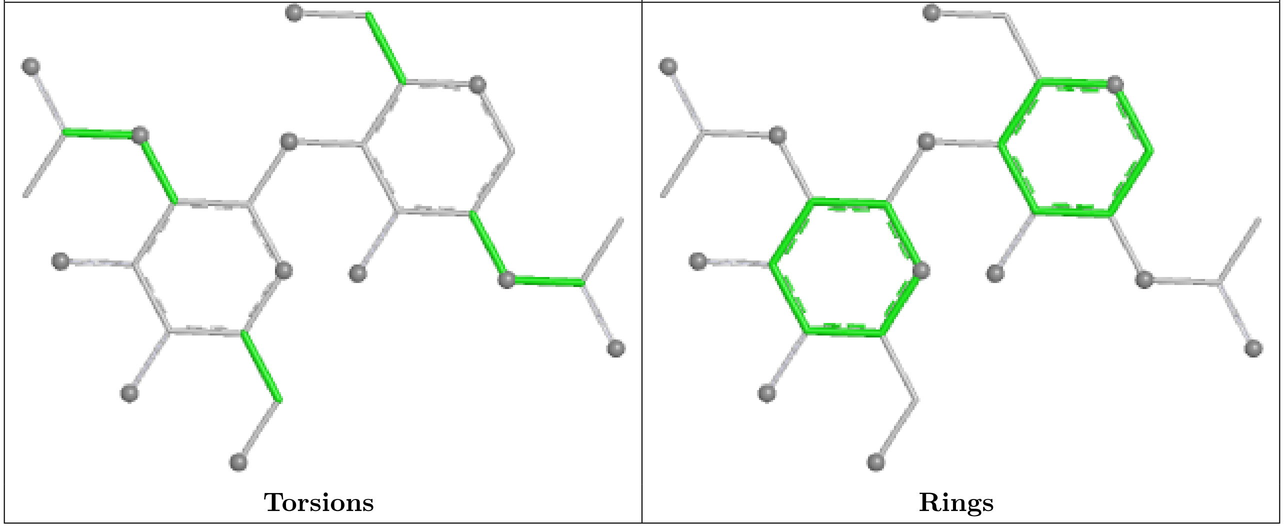
Torsions

Rings

Oligosaccharide Chain h

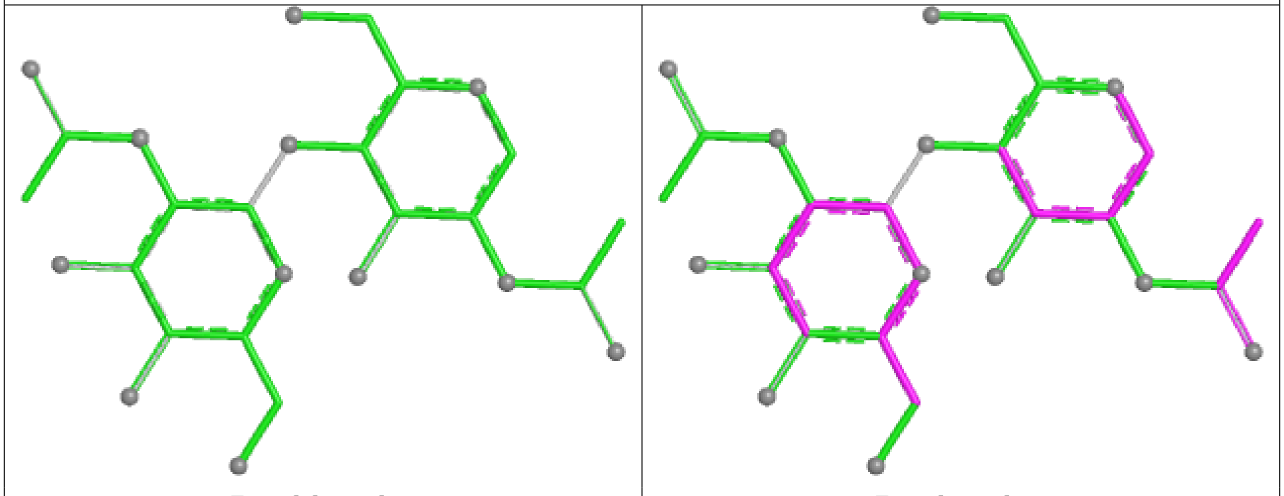


Bond lengths **Bond angles**



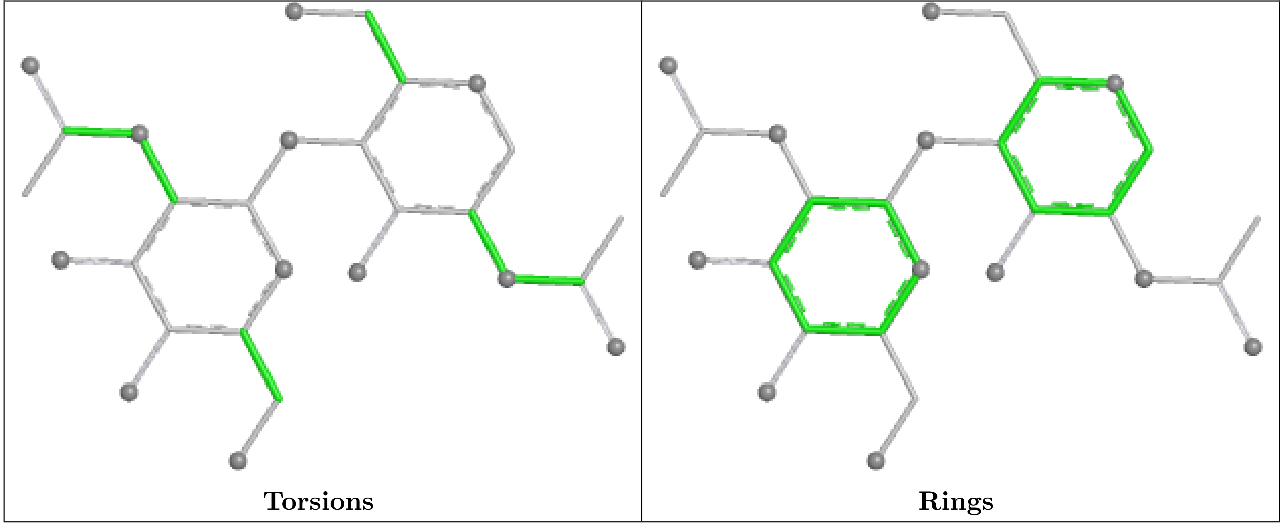
Torsions **Rings**

Oligosaccharide Chain k



Bond lengths

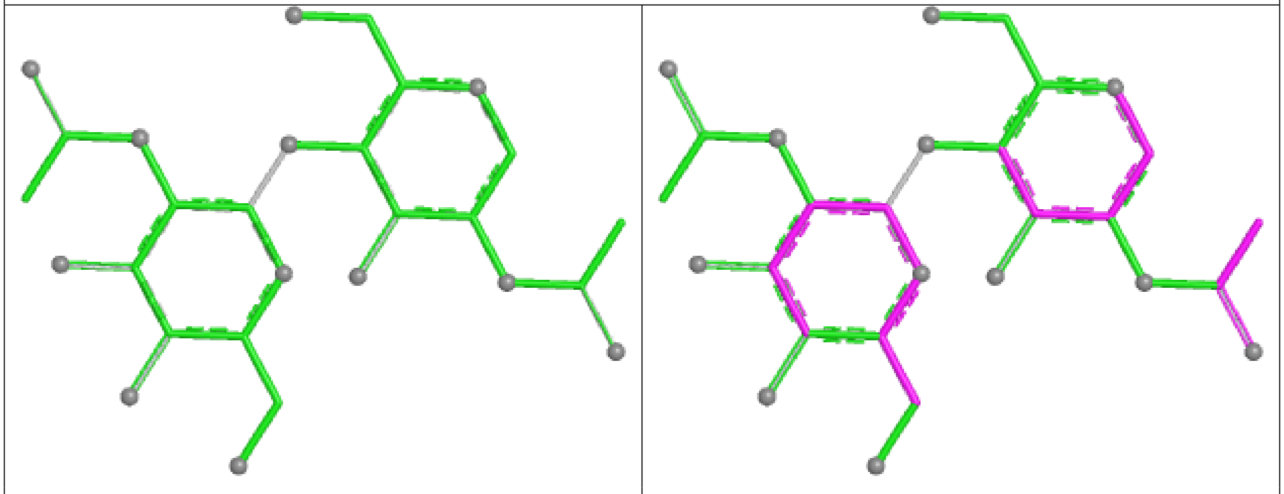
Bond angles



Torsions

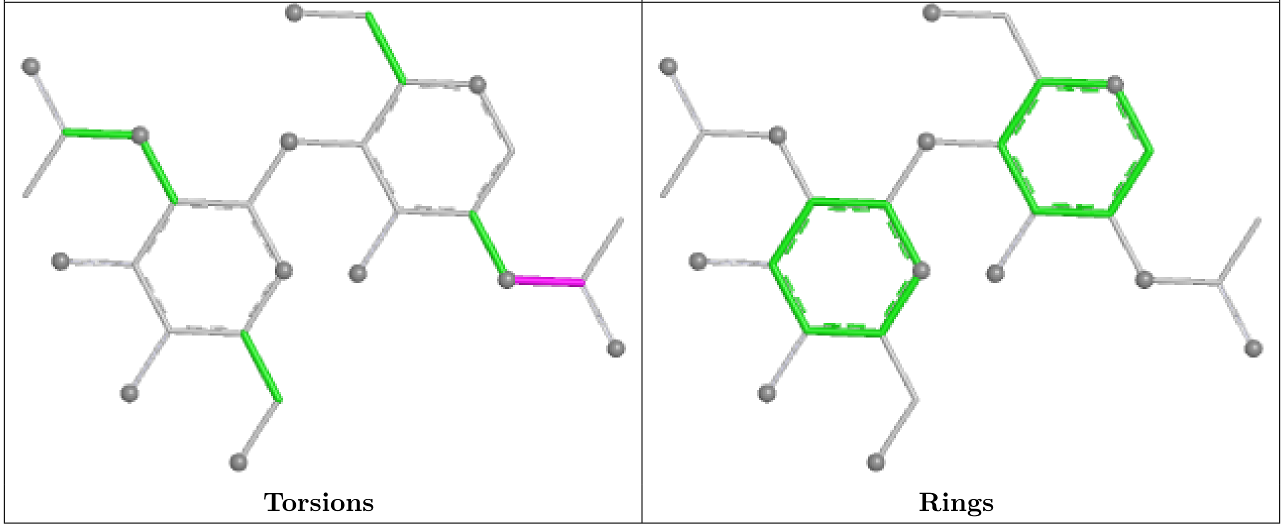
Rings

Oligosaccharide Chain l



Bond lengths

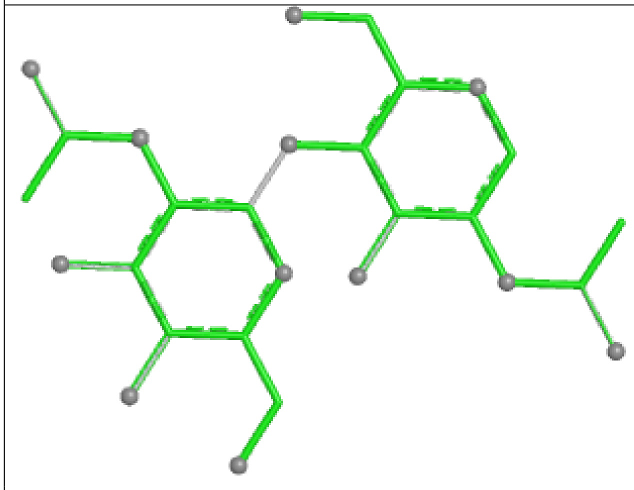
Bond angles



Torsions

Rings

Oligosaccharide Chain o



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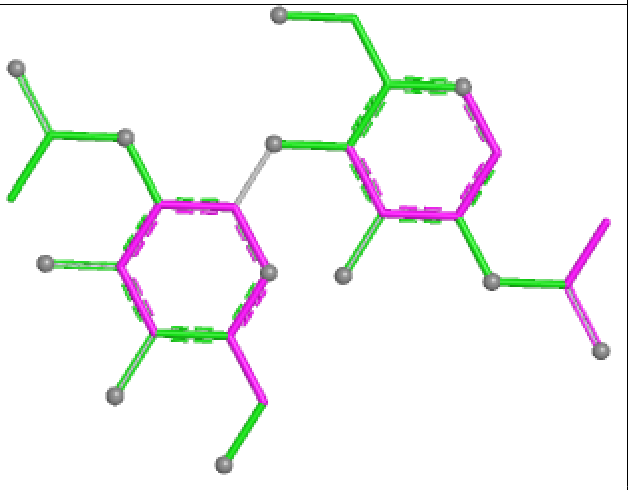
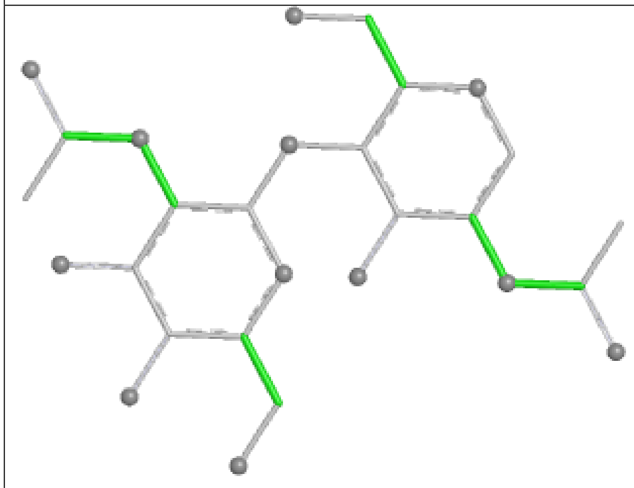


Bond angles



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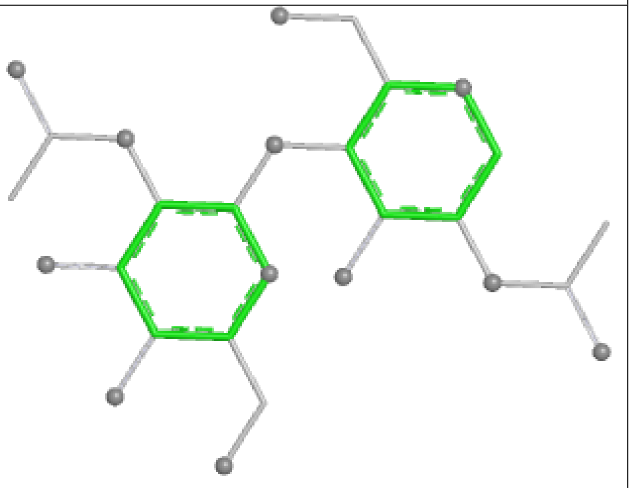
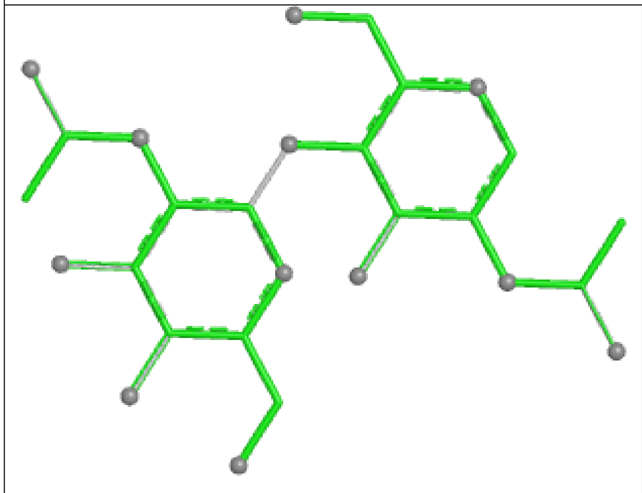


Rings

Oligosaccharide Chain r



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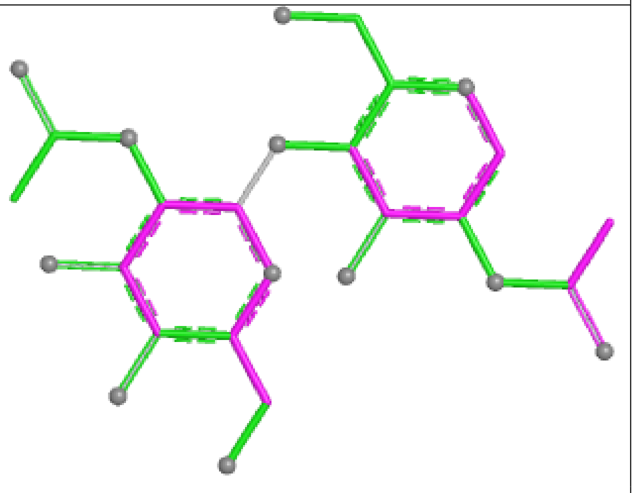
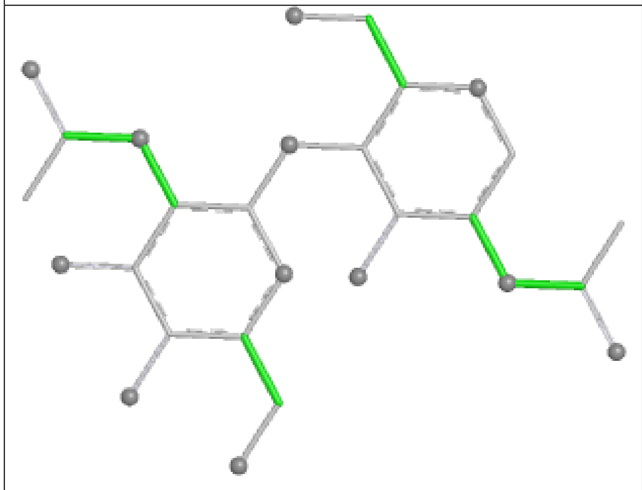


Bond angles



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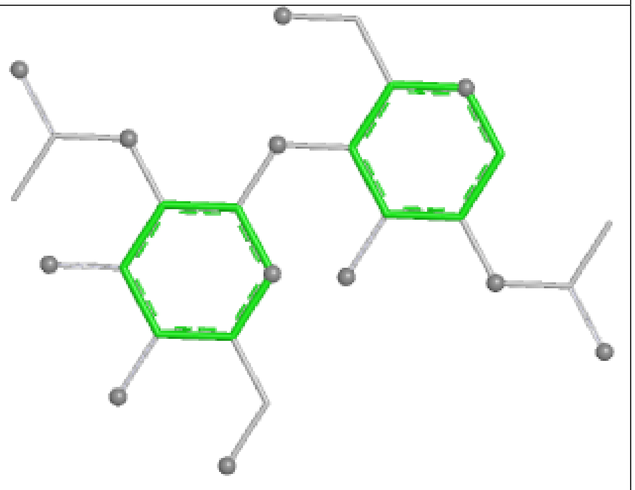
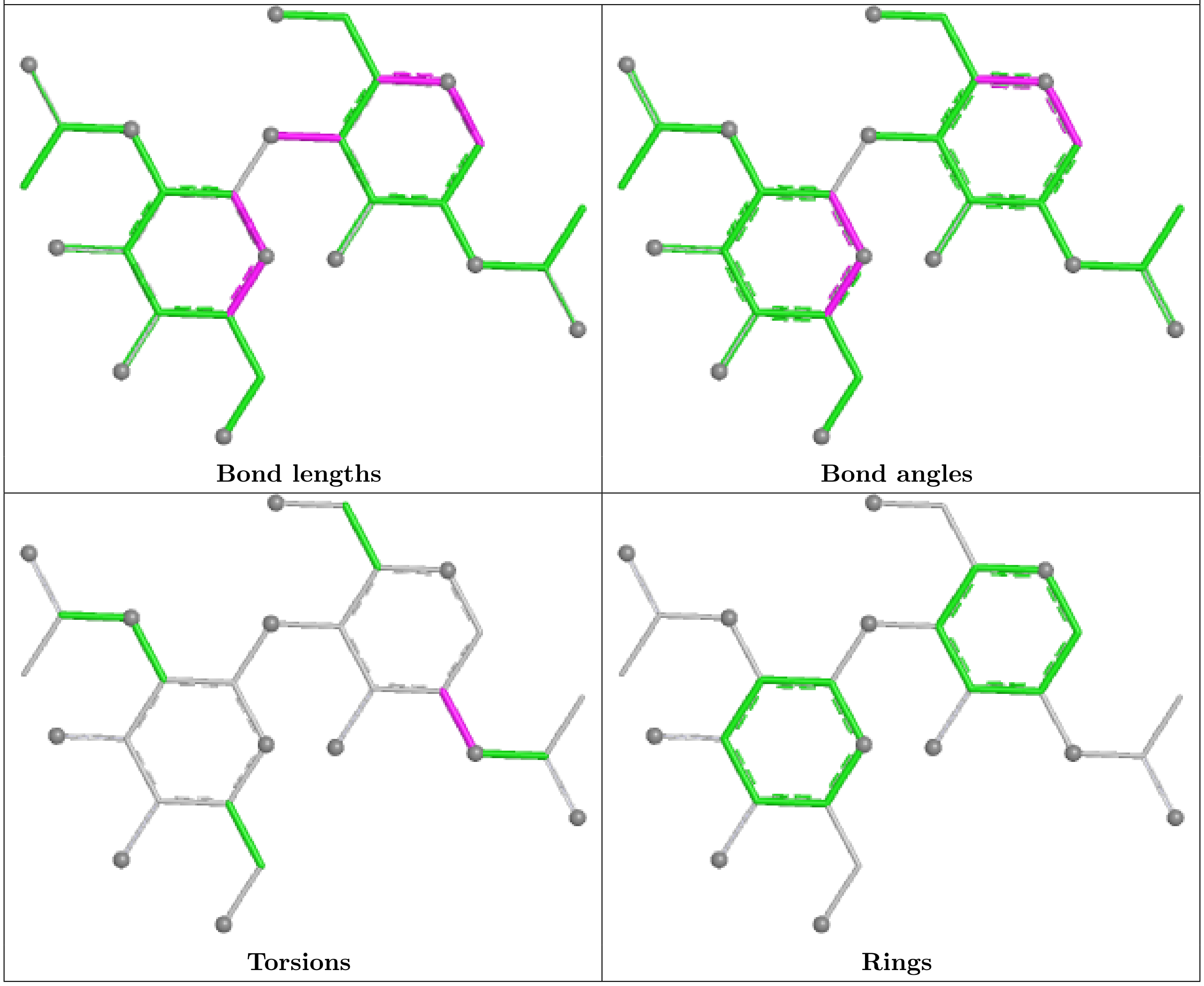


Rings

Oligosaccharide Chain s



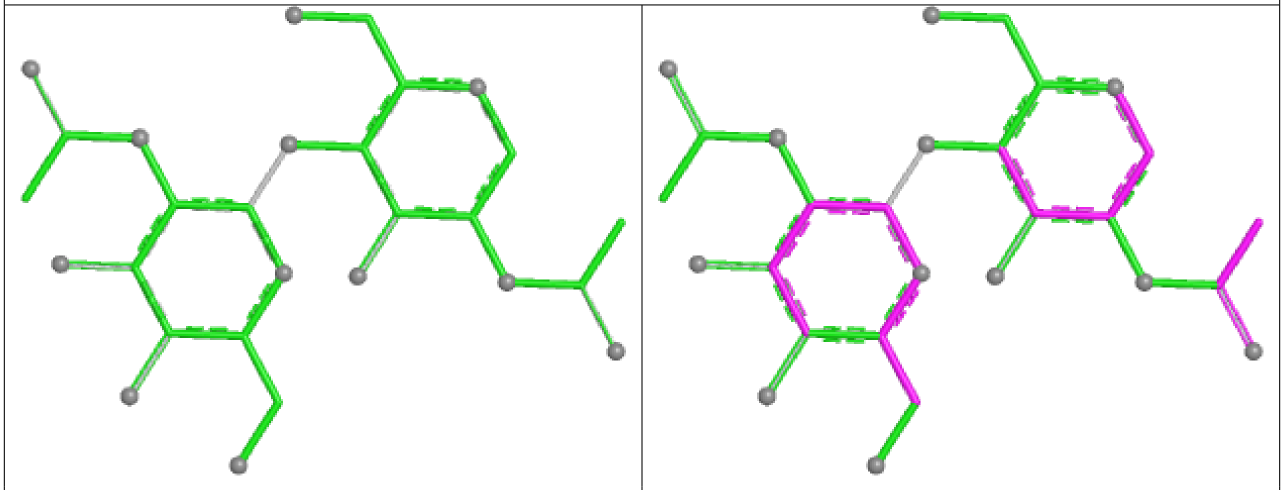
Bond lengths

Bond angles

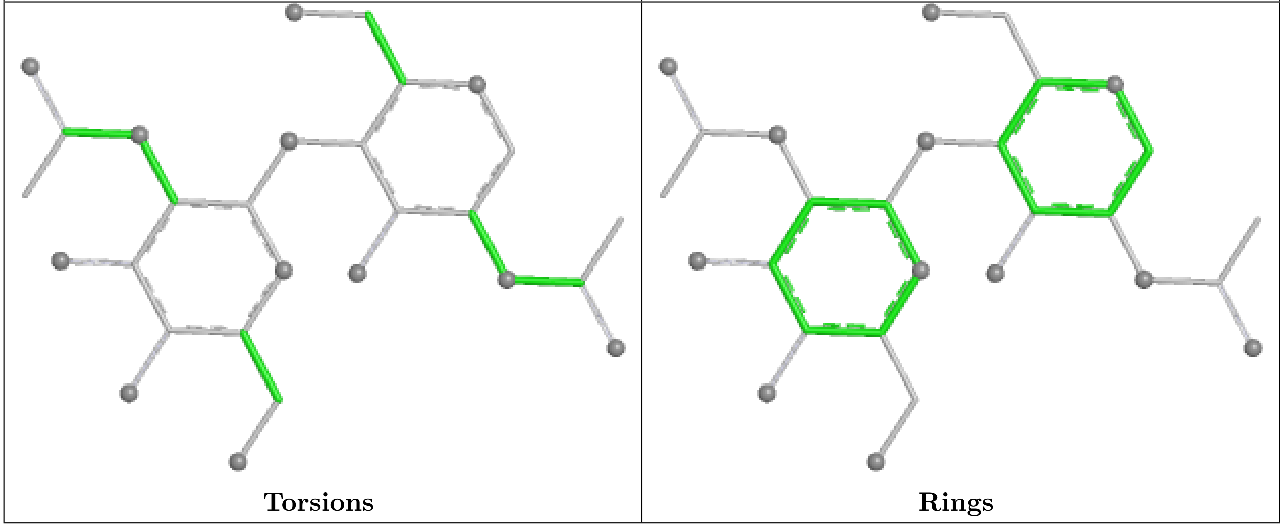
Torsions

Rings

Oligosaccharide Chain u

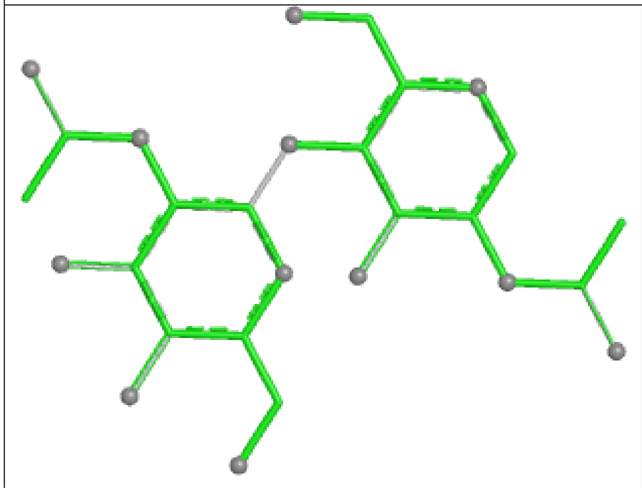


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain w



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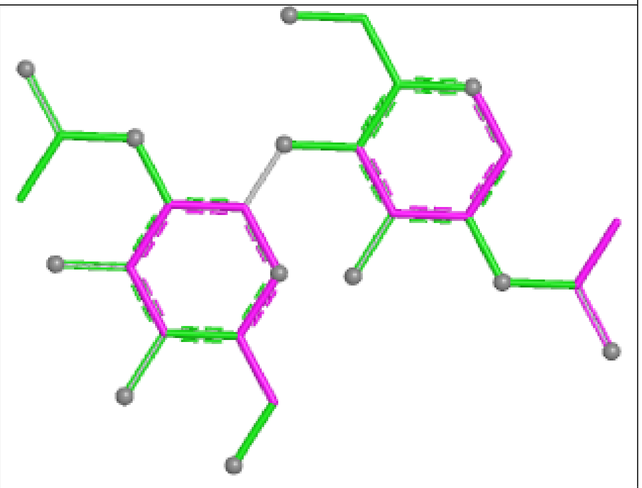
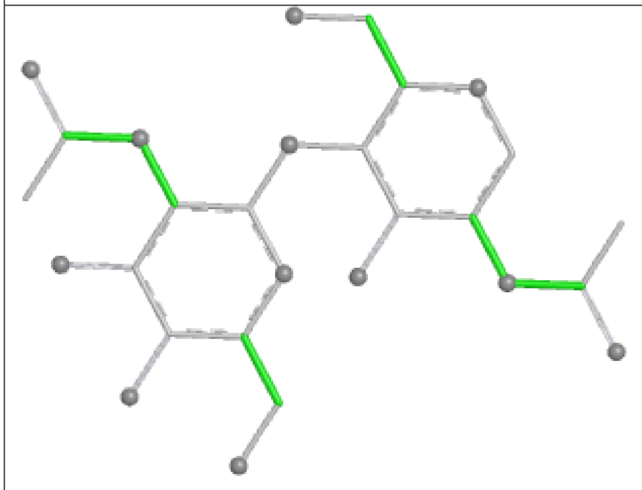


Bond angles



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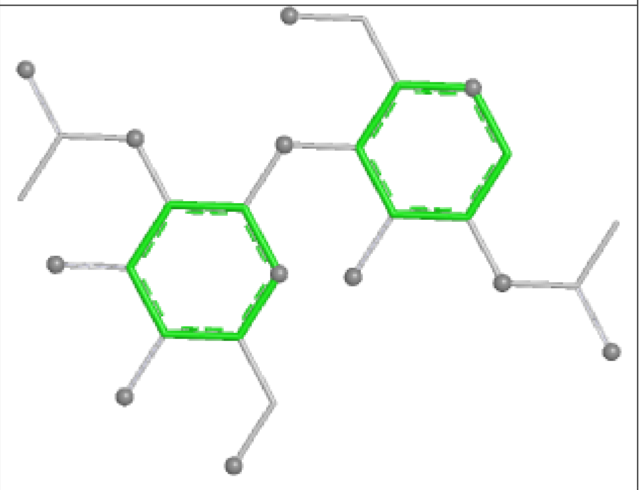

Rings

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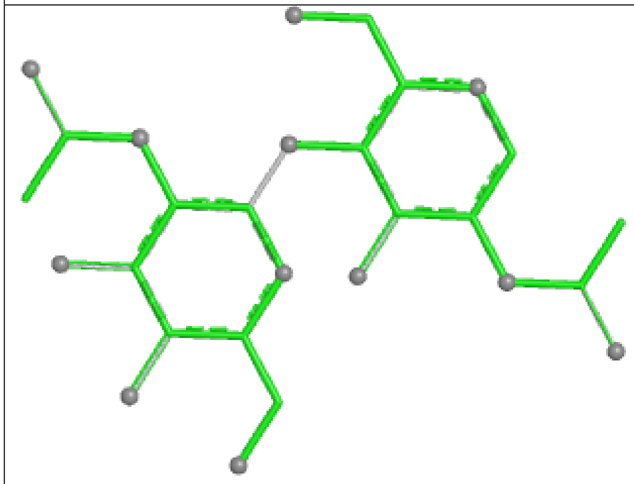
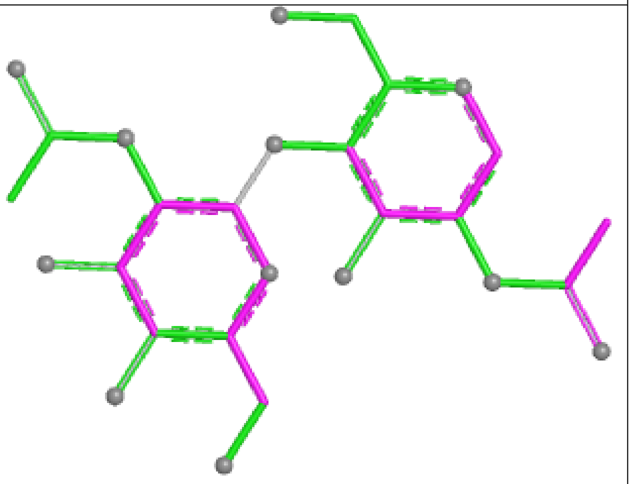
<tr><td>
Bond lengths</td><td>
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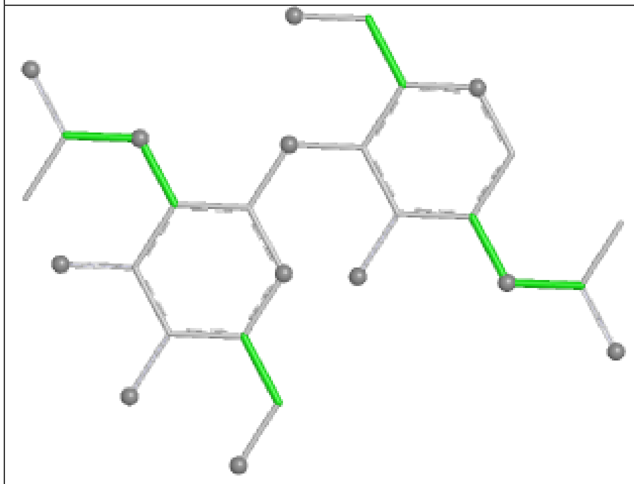
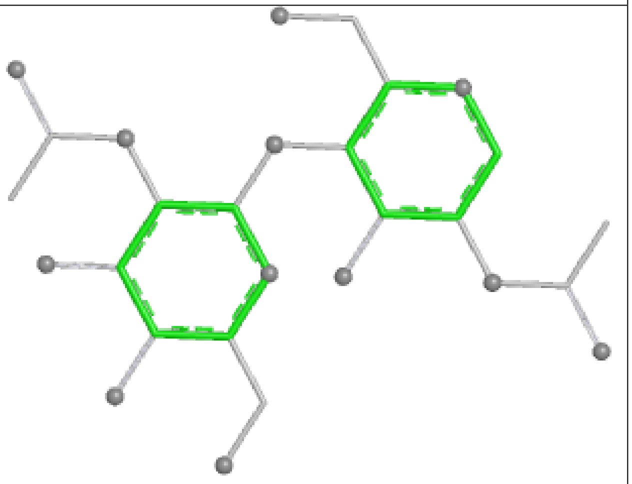
<tr><td>
Torsions</td><td>
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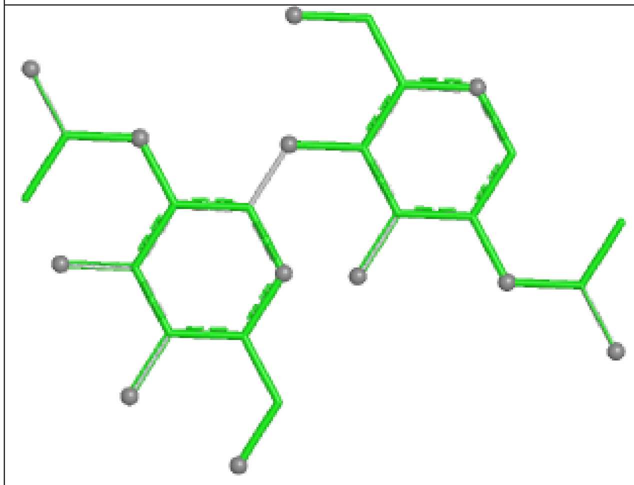
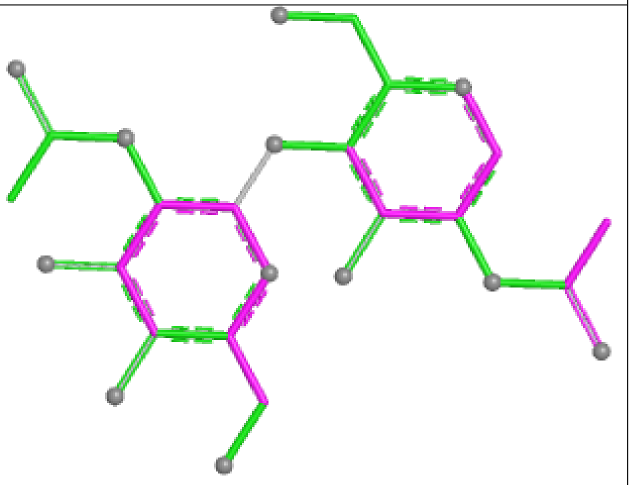
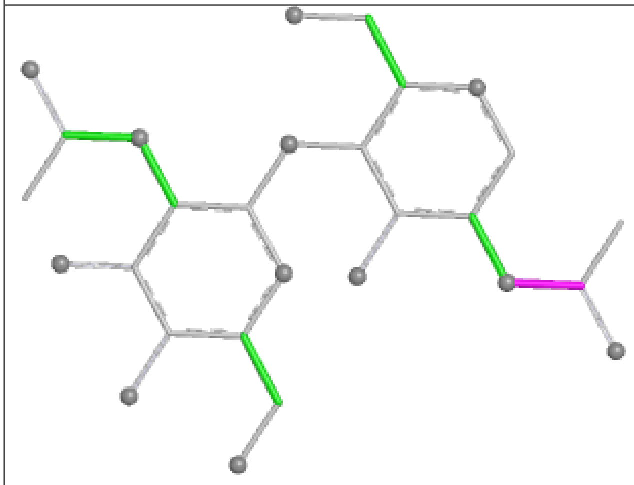
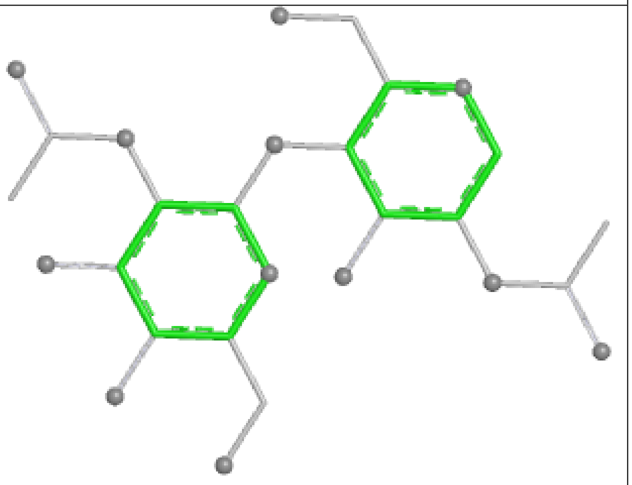
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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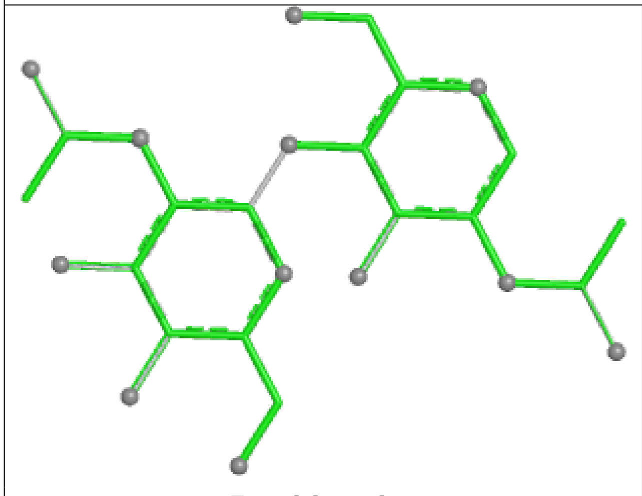

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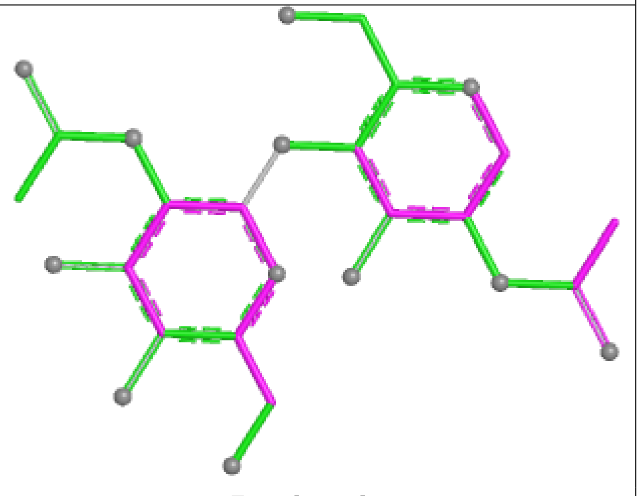

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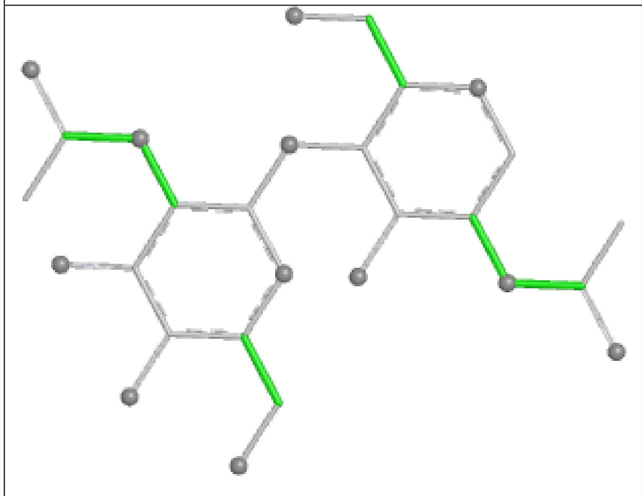

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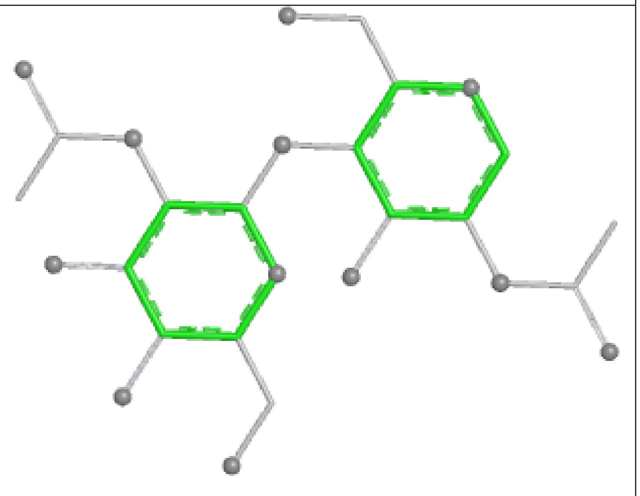

Rings

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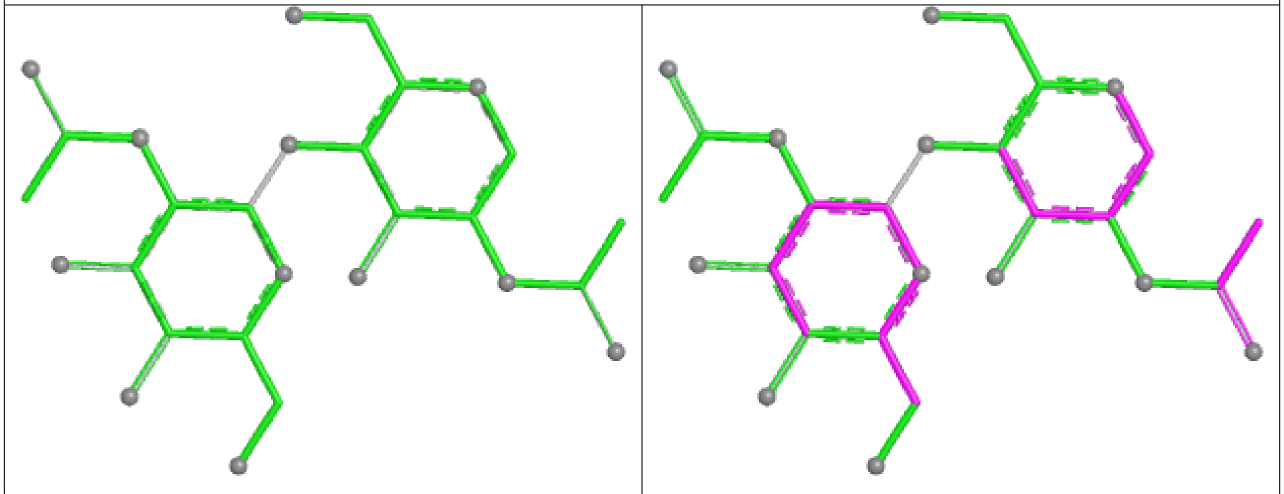
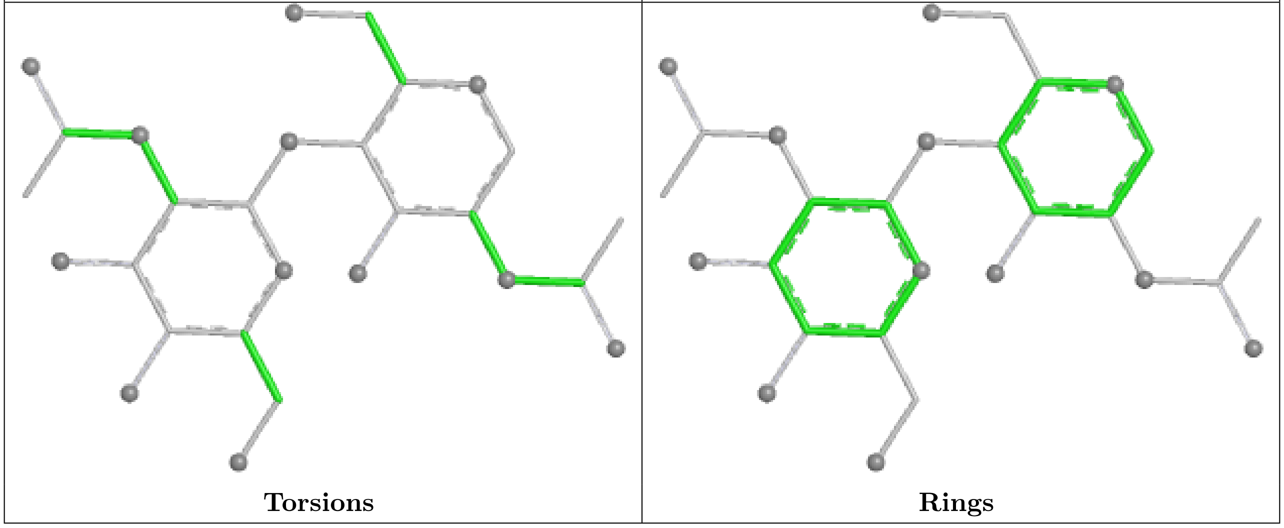


Bond lengths **Bond angles**



Torsions **Rings**

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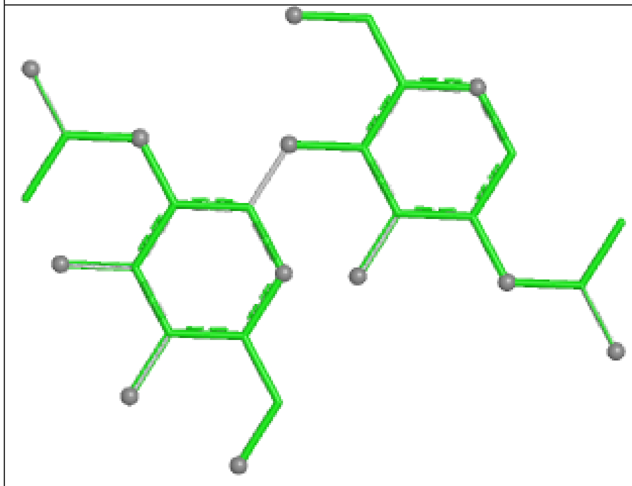
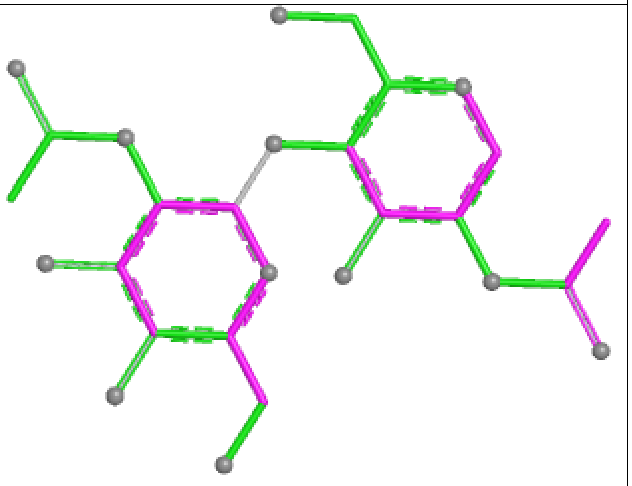
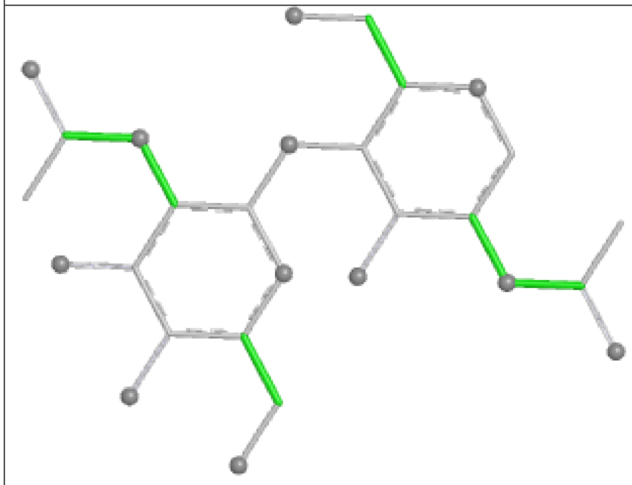
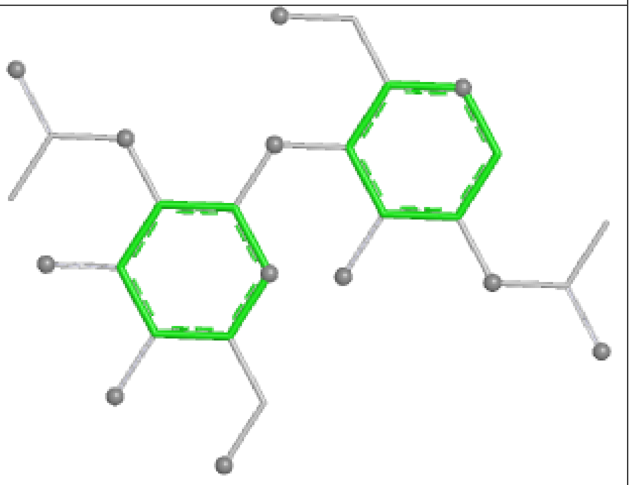
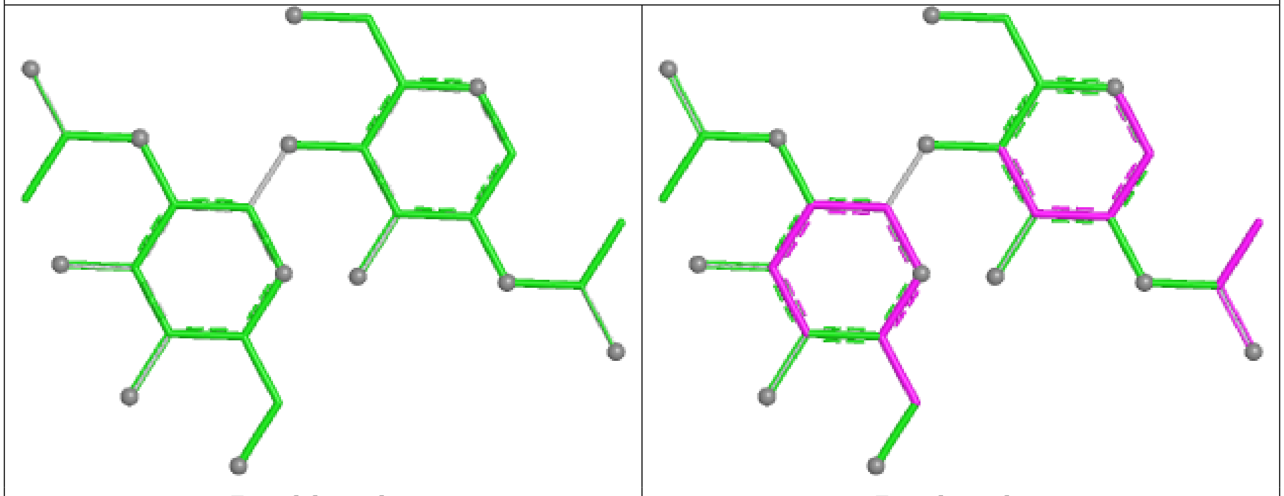
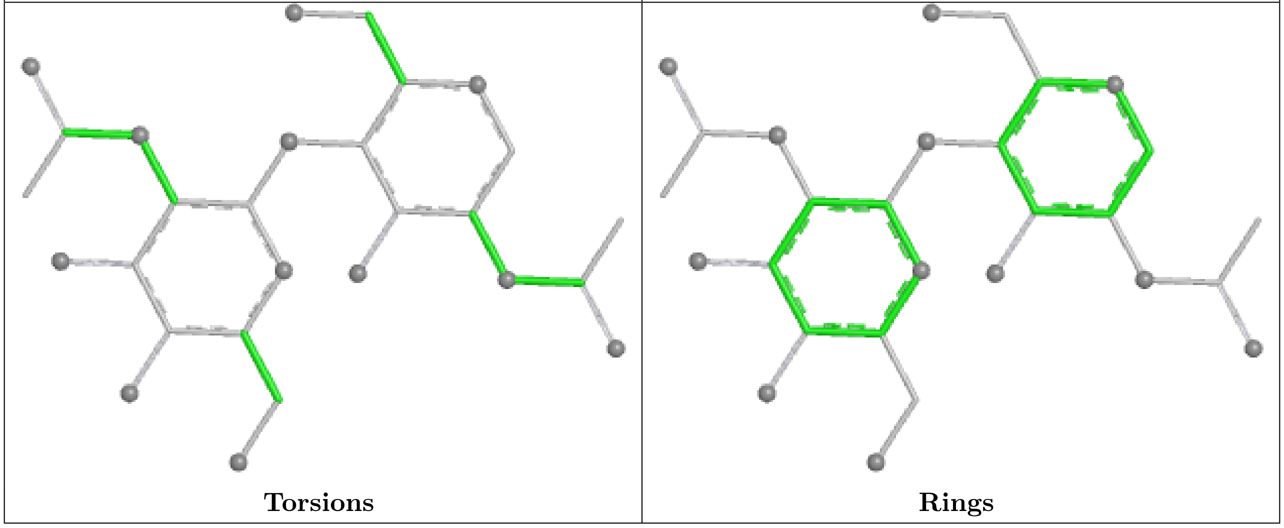
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain 5

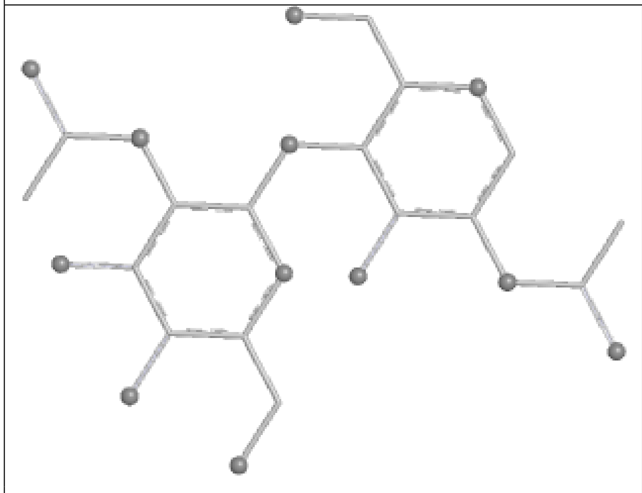


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain AA



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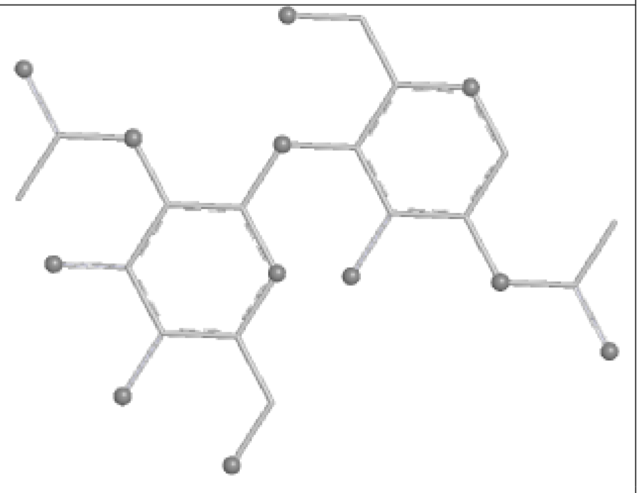

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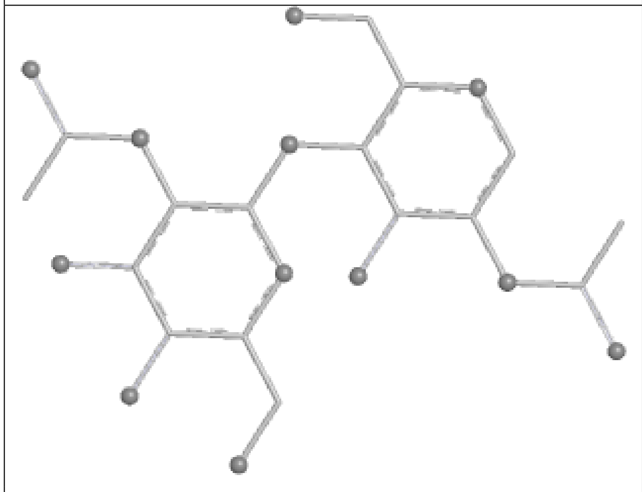

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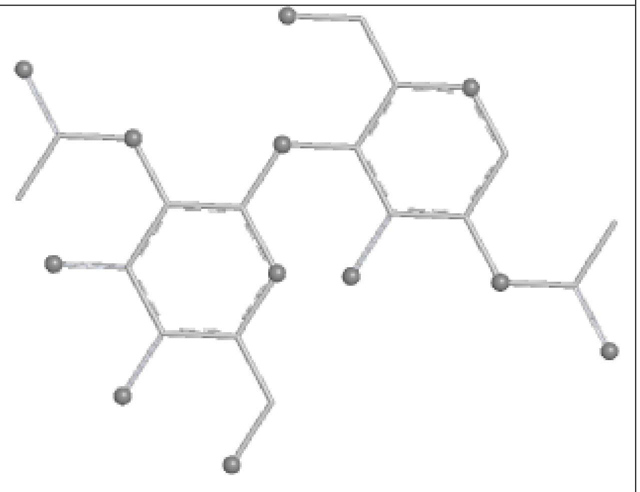
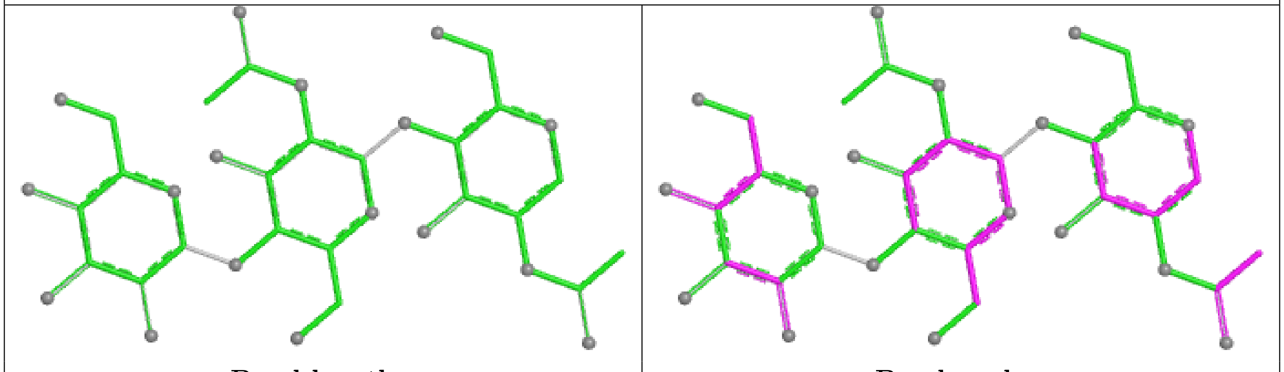


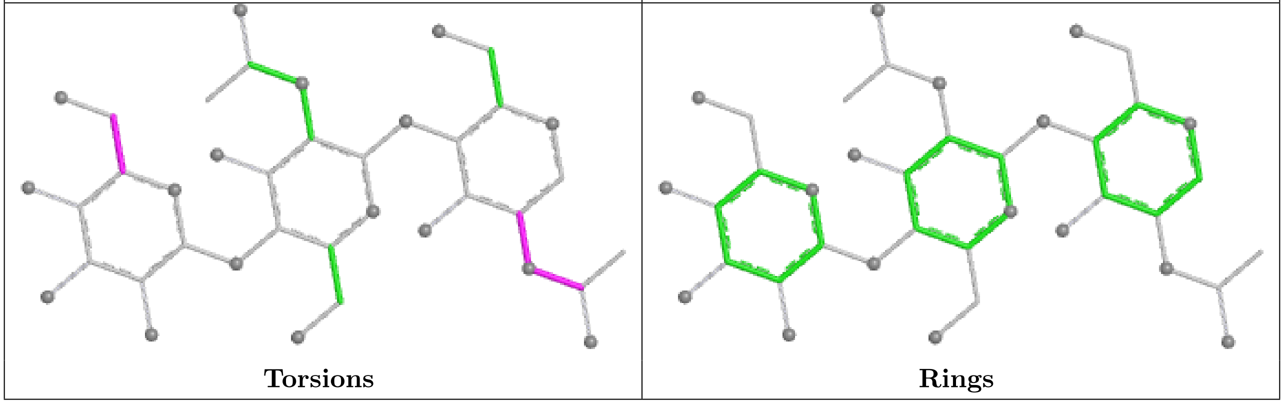
Rings

Oligosaccharide Chain I



Bond lengths

Bond angles



Torsions

Rings

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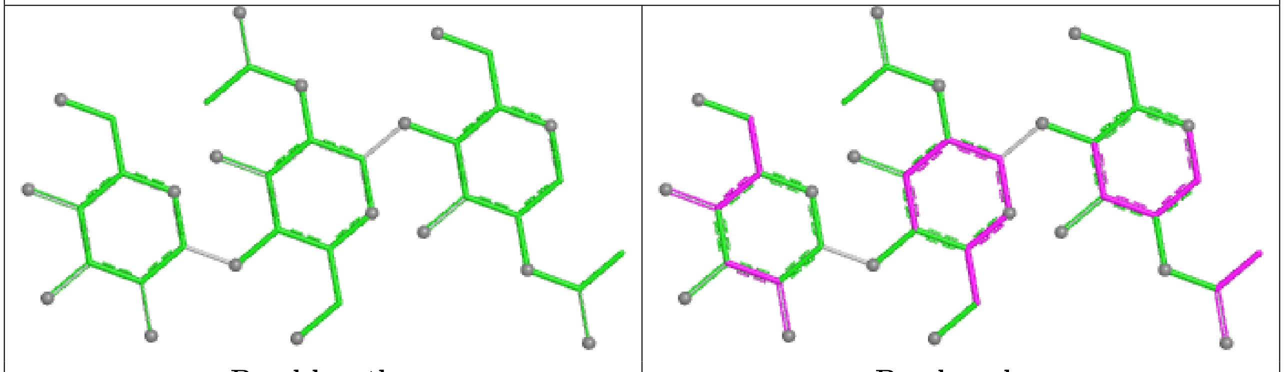
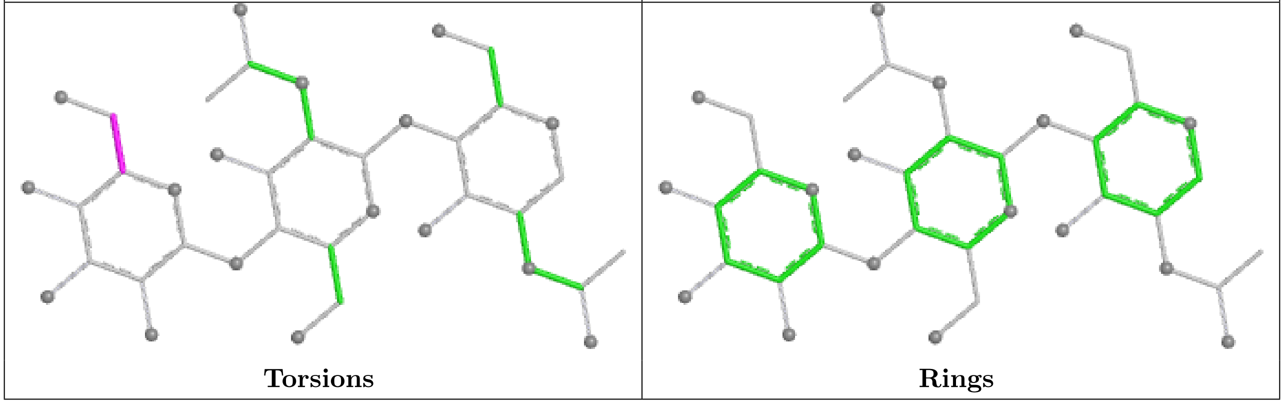


Bond lengths

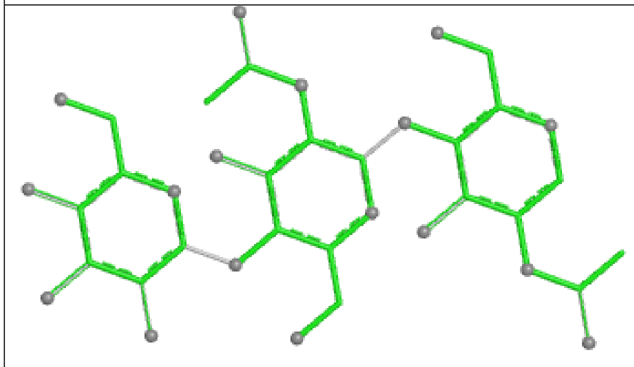
Bond angles



Torsions

Rings

Oligosaccharide Chain K



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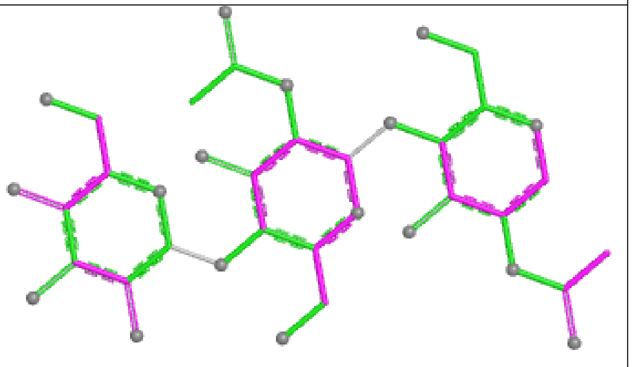

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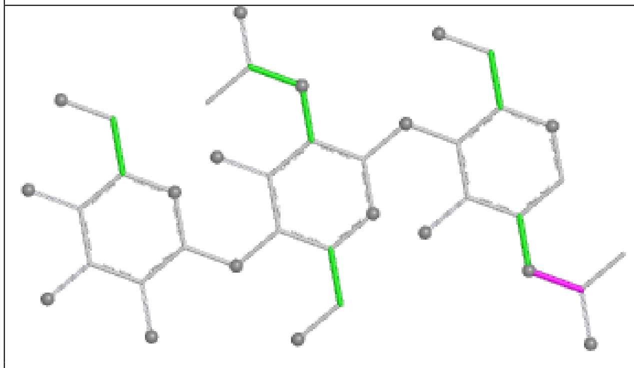

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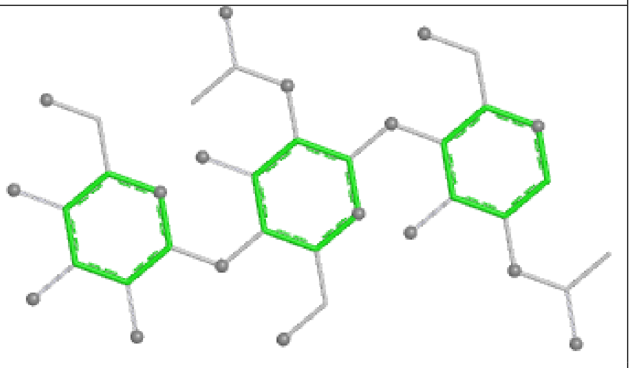
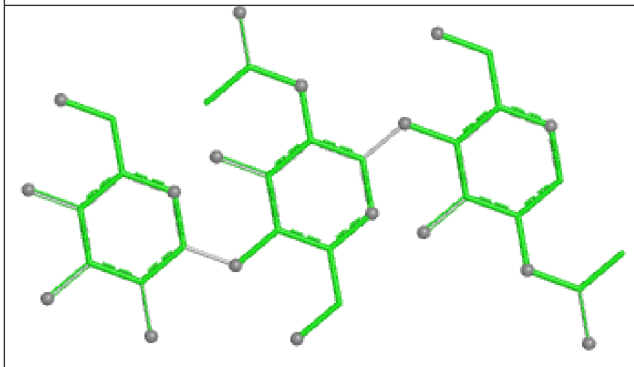


Rings

Oligosaccharide Chain P



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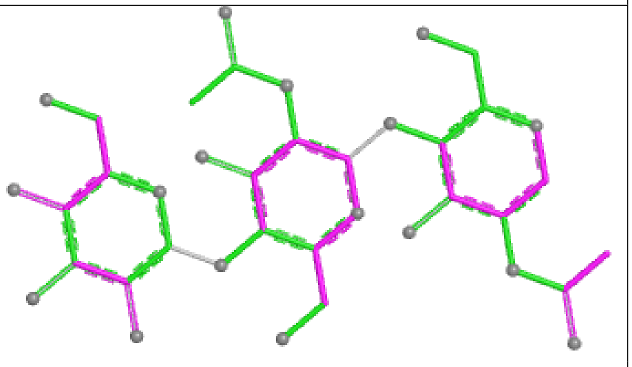

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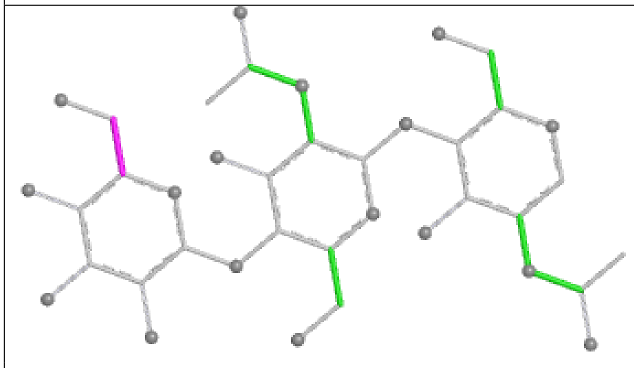

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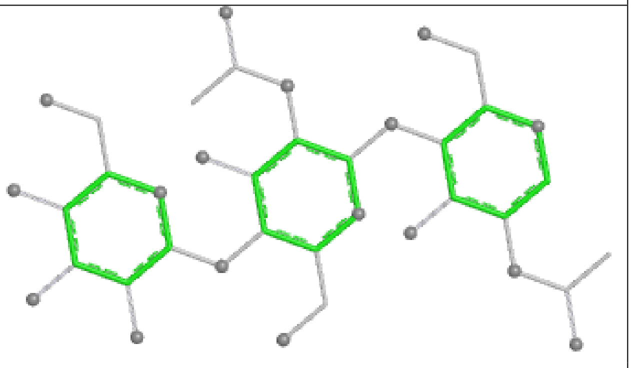
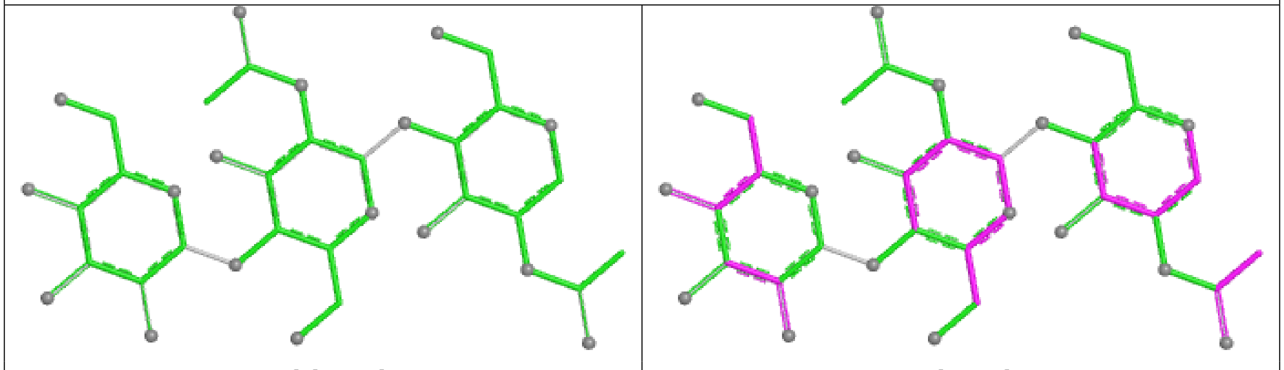
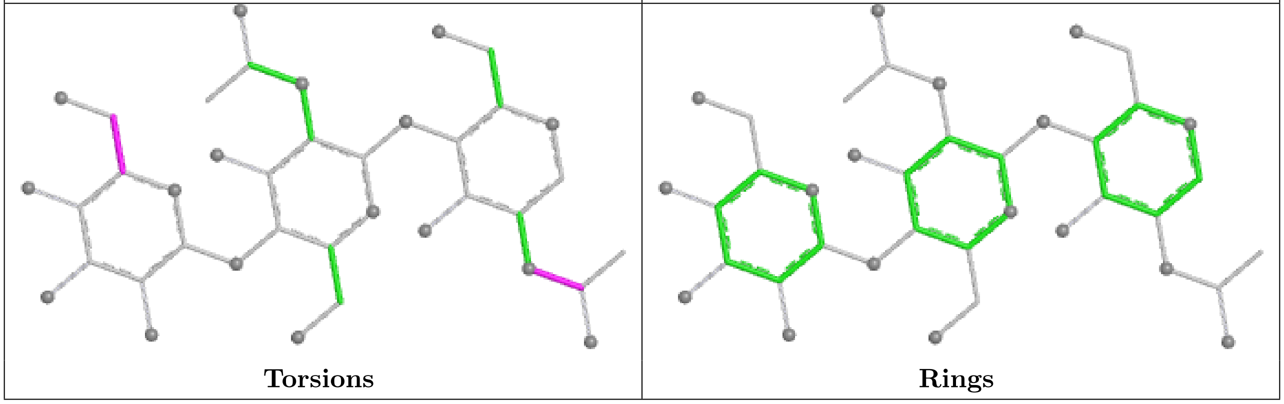


Rings

Oligosaccharide Chain S

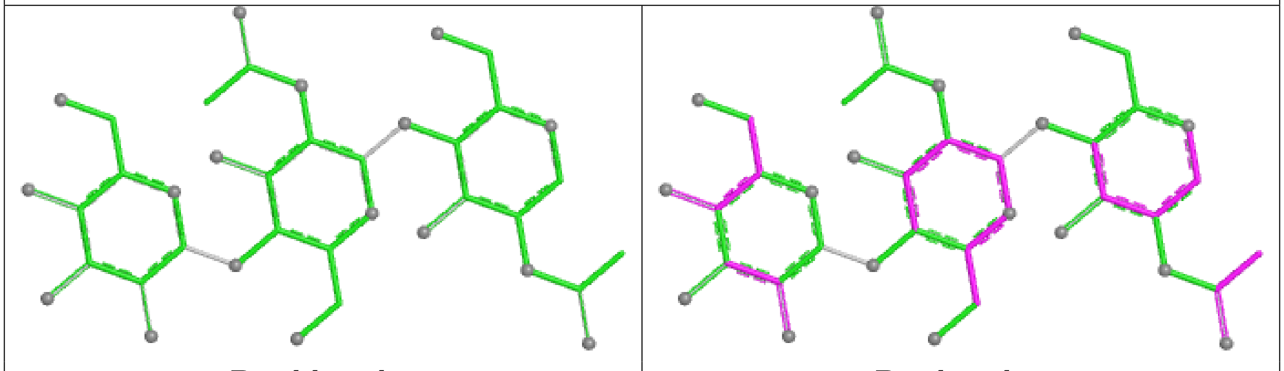


Bond lengths Bond angles

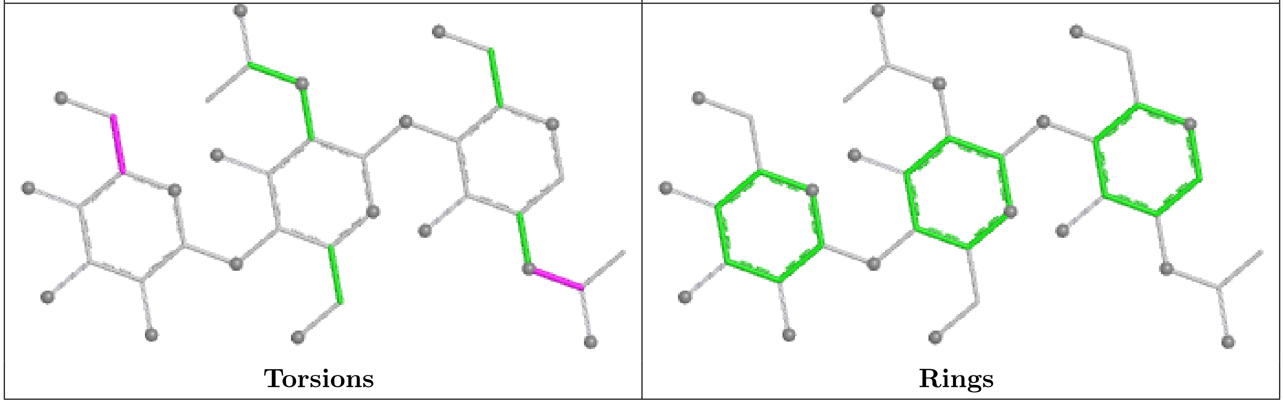


Torsions Rings

Oligosaccharide Chain U



Bond lengths Bond angles



Torsions Rings

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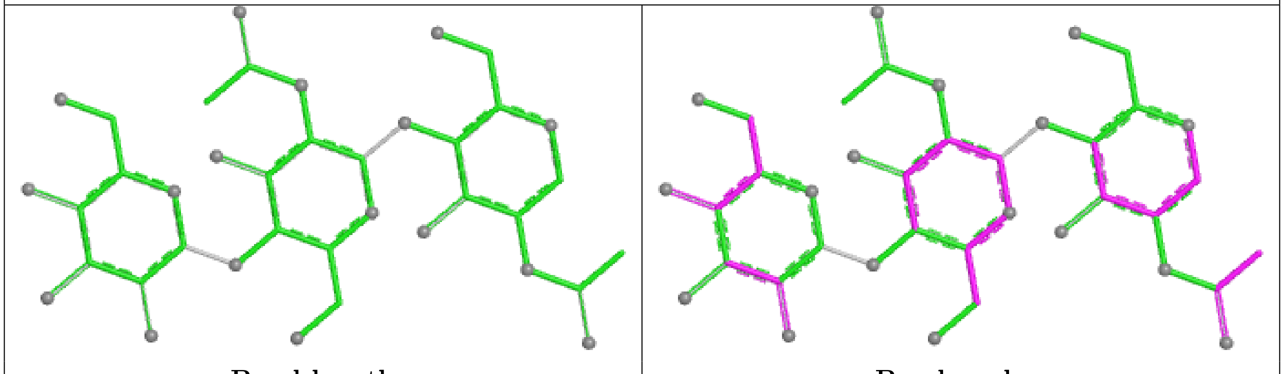
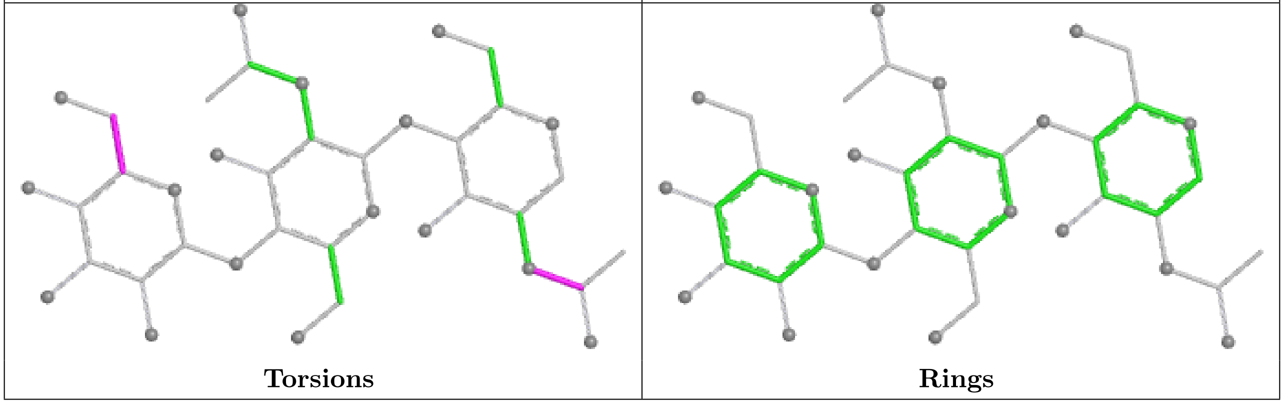


Bond lengths

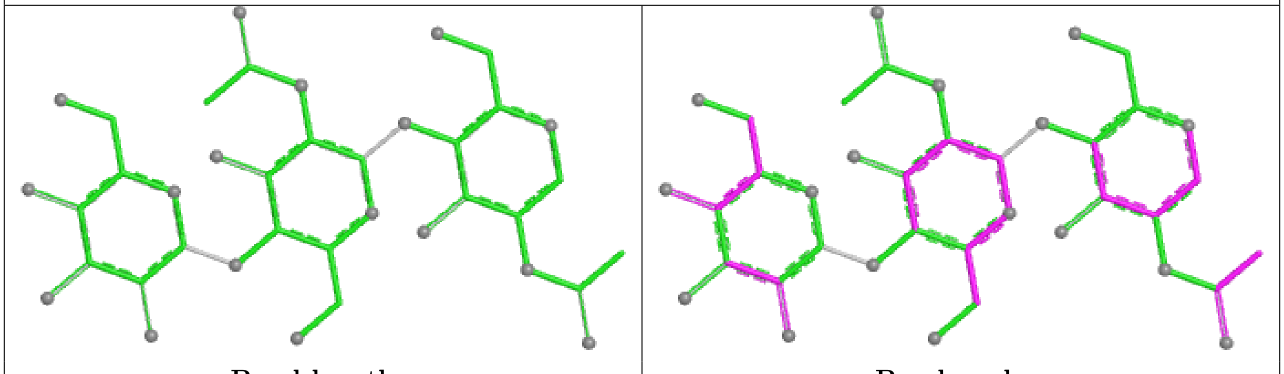
Bond angles



Torsions

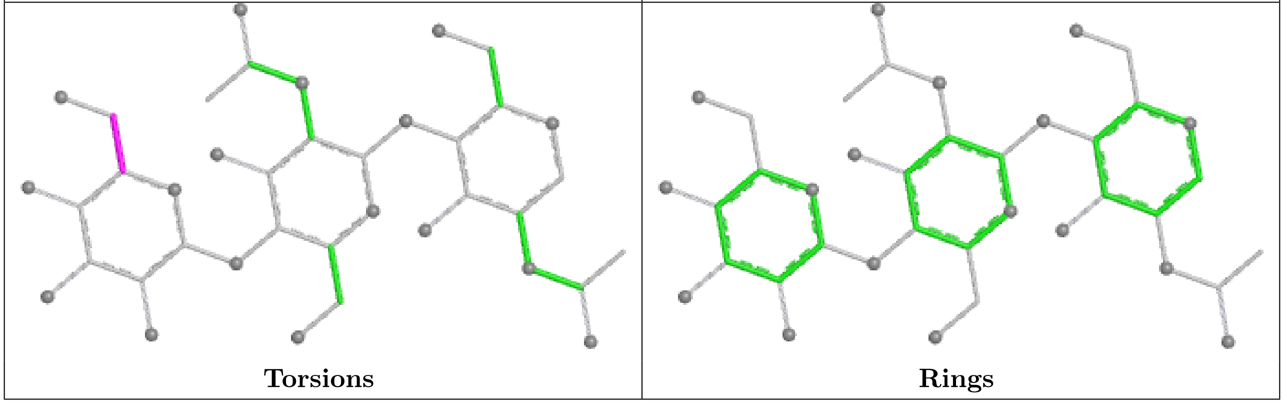
Rings

Oligosaccharide Chain W



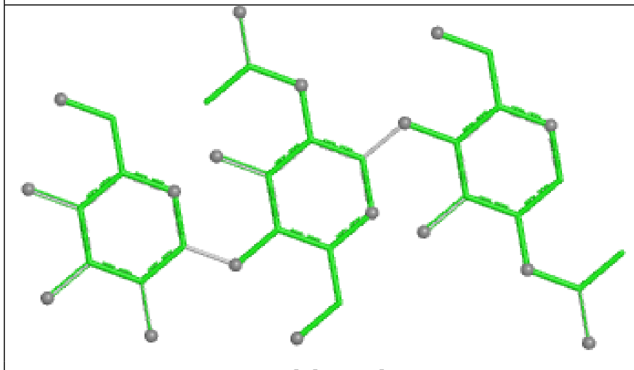
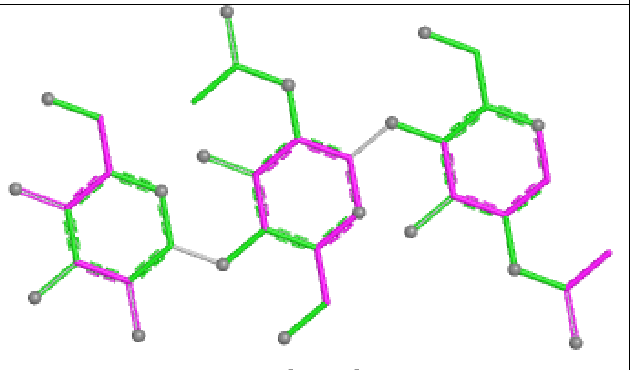
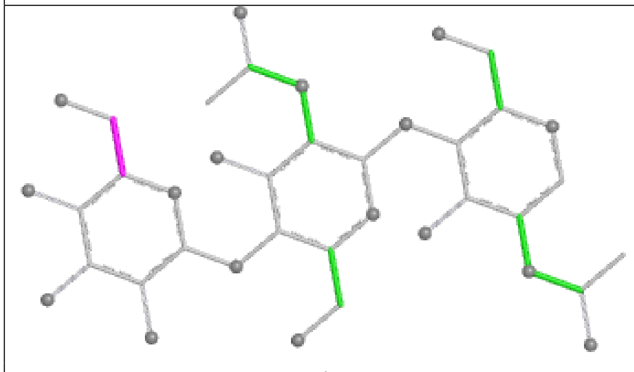
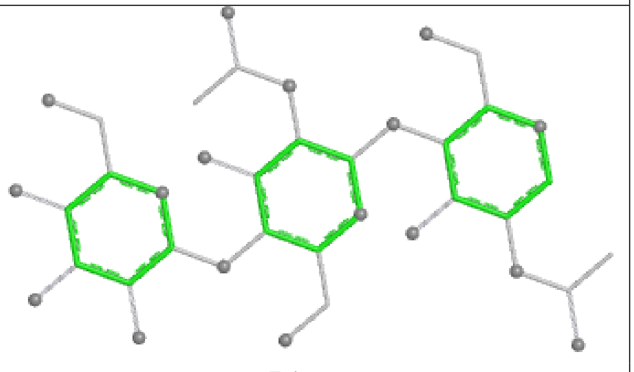
Bond lengths

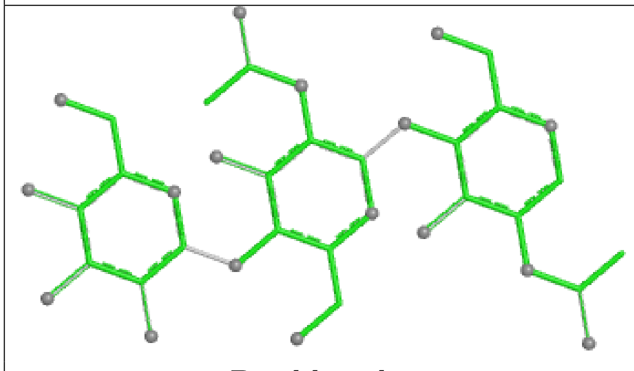
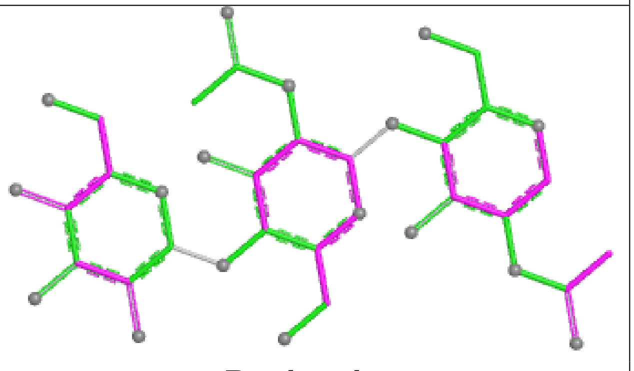
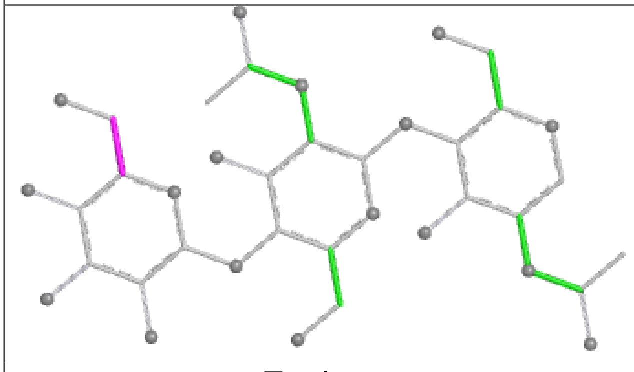
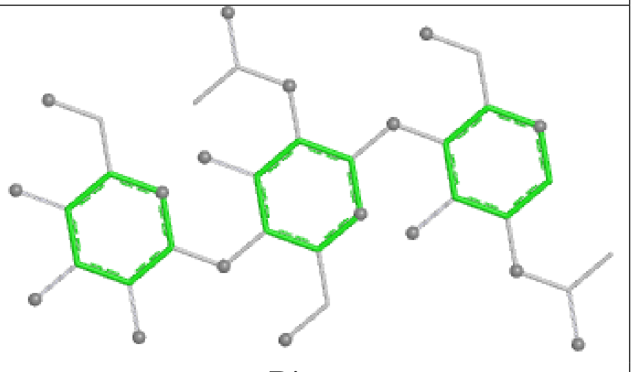
Bond angles



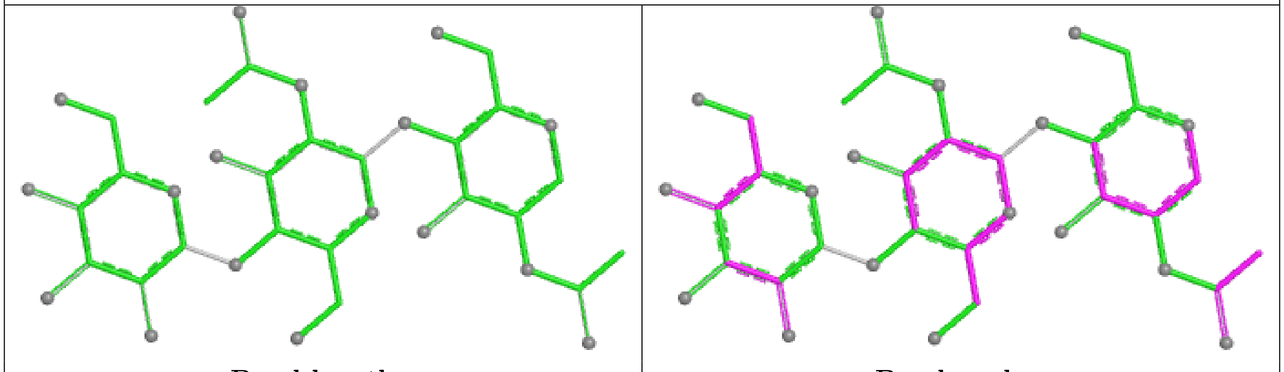
Torsions

Rings

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

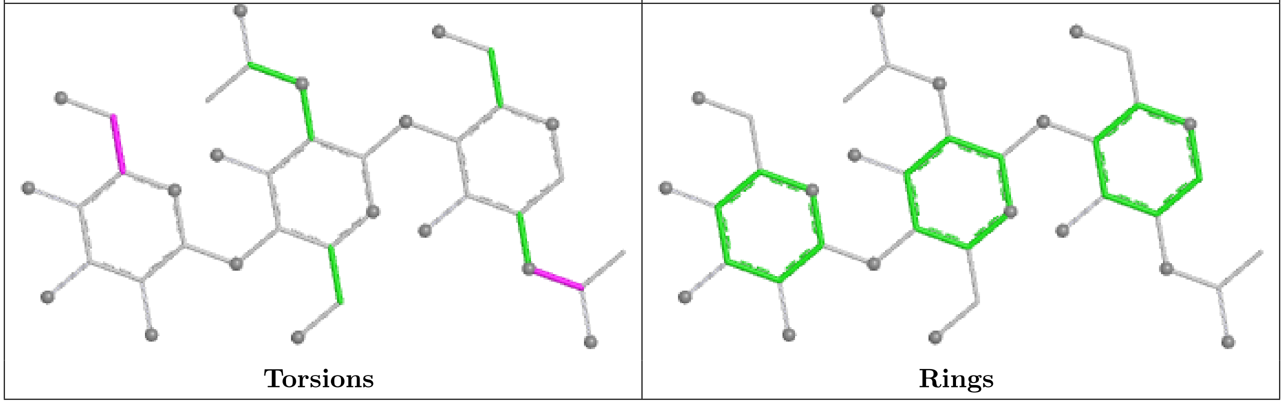
Oligosaccharide Chain d	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain g



Bond lengths

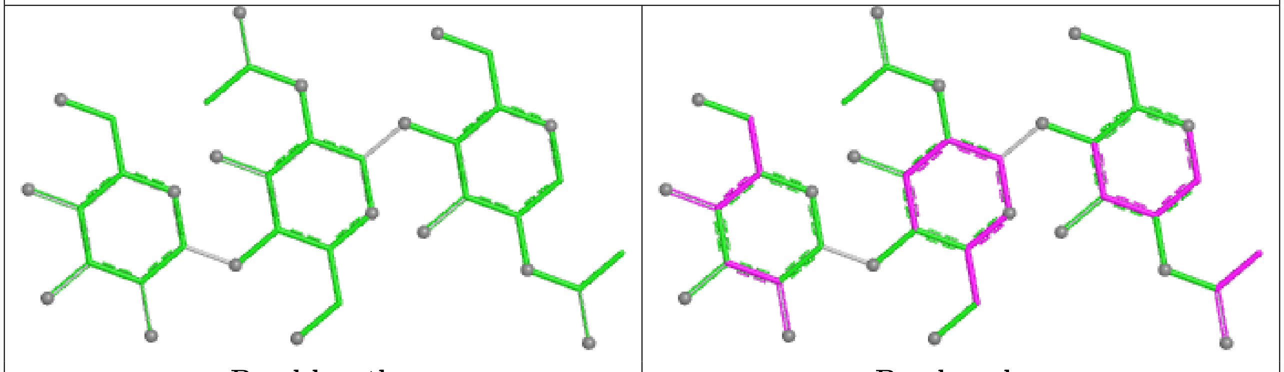
Bond angles



Torsions

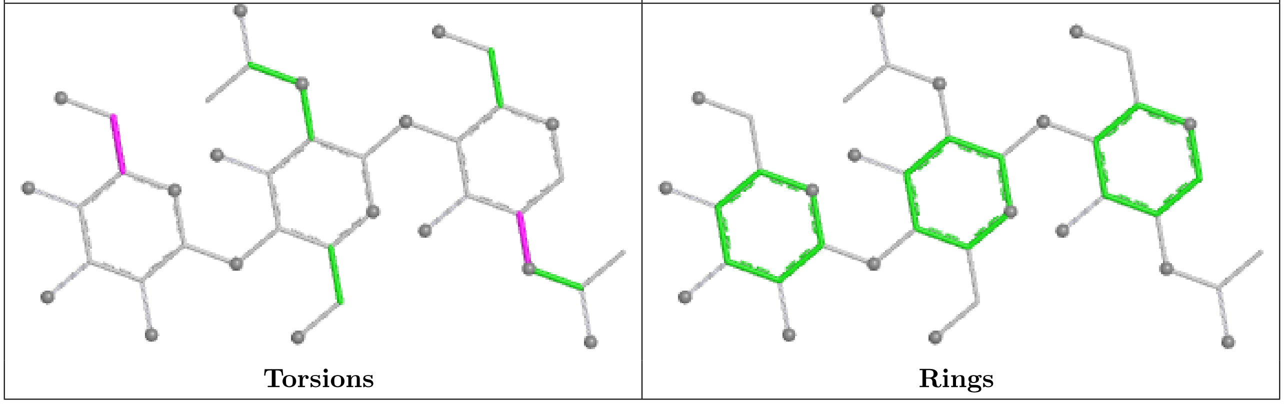
Rings

Oligosaccharide Chain i



Bond lengths

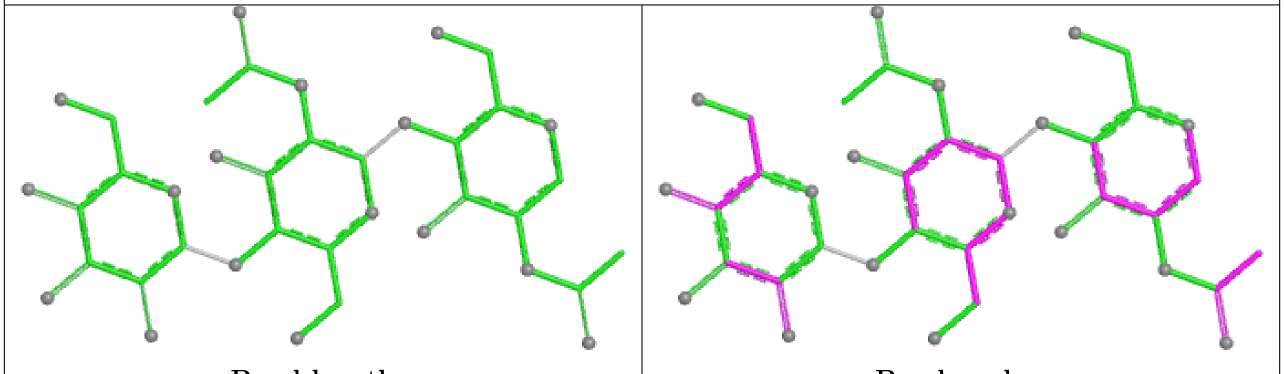
Bond angles



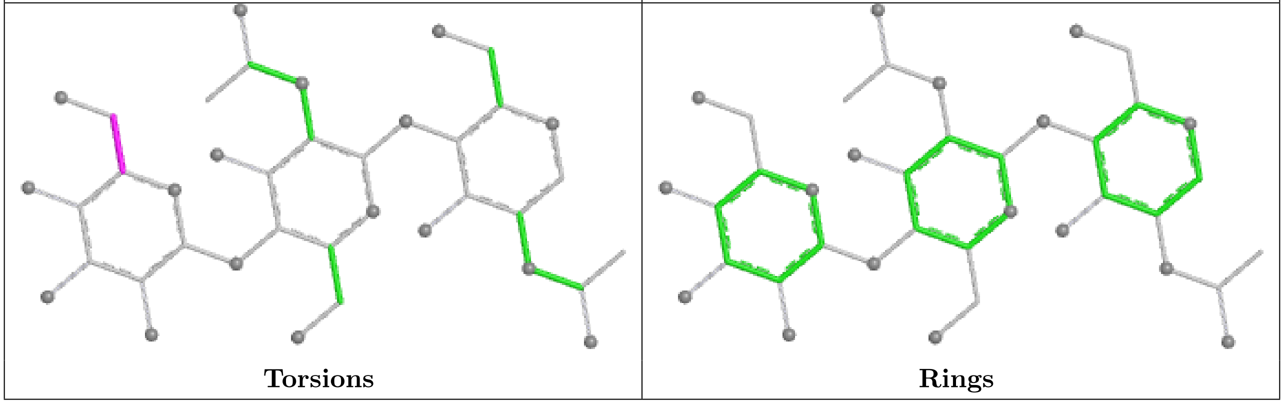
Torsions

Rings

Oligosaccharide Chain j

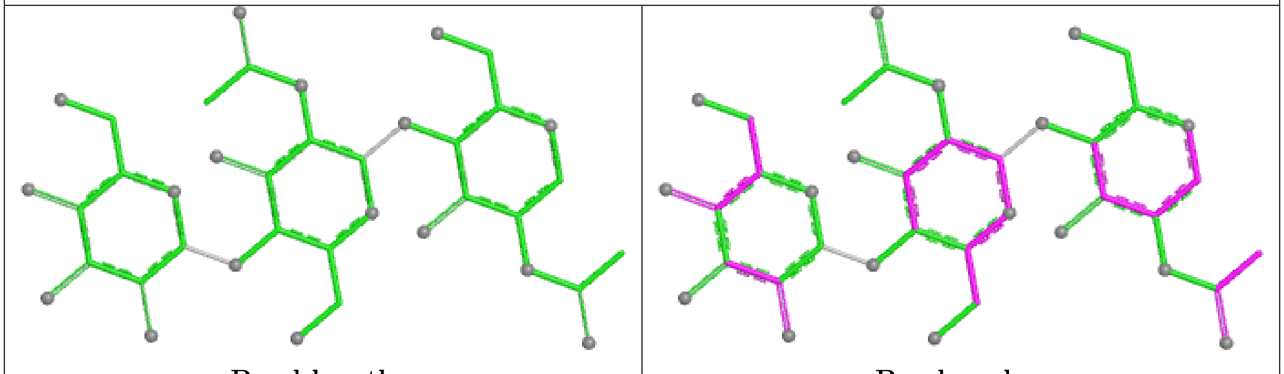


Bond lengths Bond angles

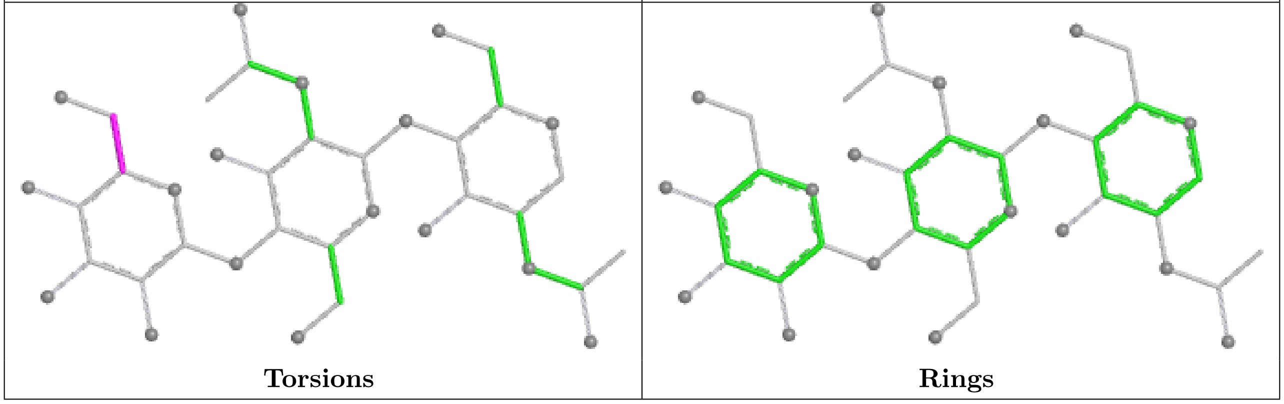


Torsions Rings

Oligosaccharide Chain m

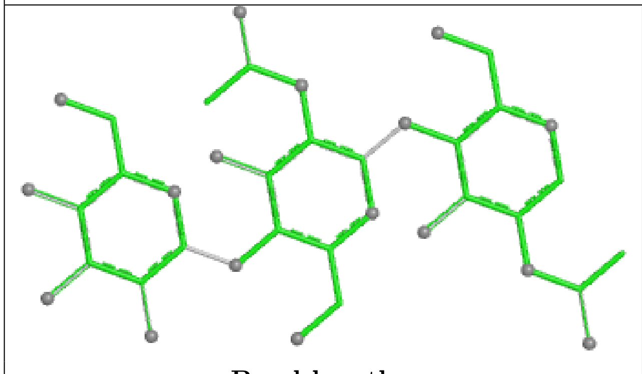


Bond lengths Bond angles

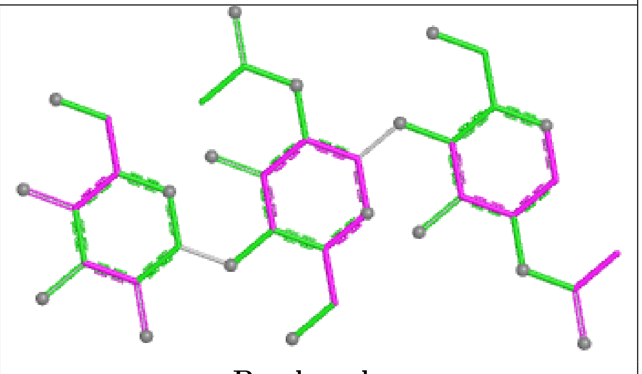


Torsions Rings

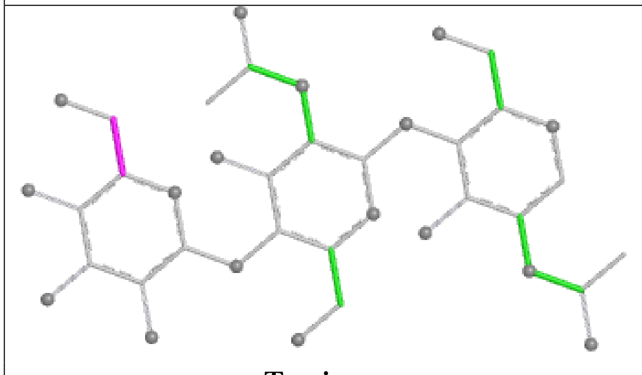
Oligosaccharide Chain n



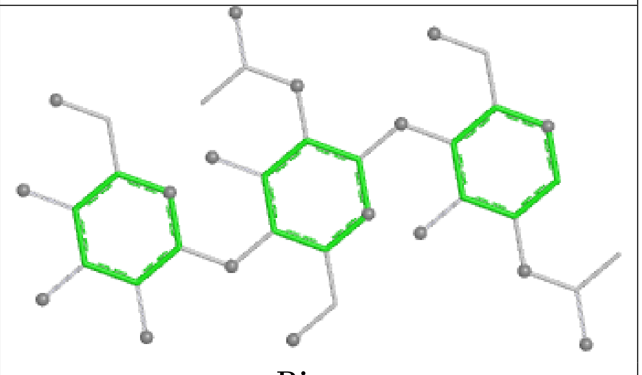
Bond lengths



Bond angles

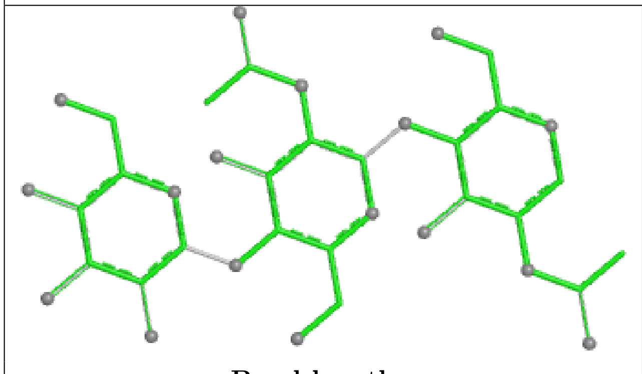


Torsions

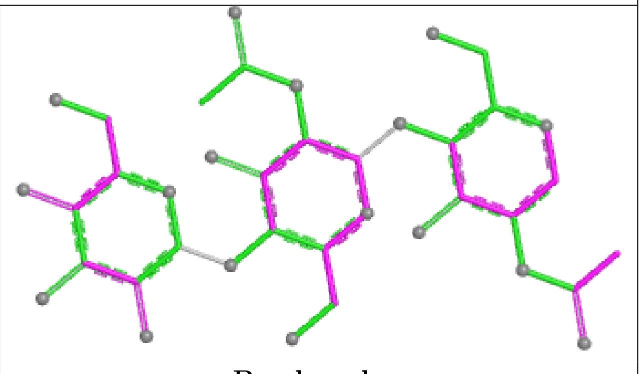


Rings

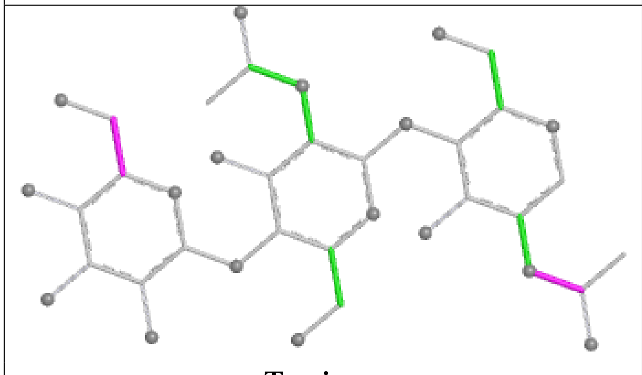
Oligosaccharide Chain t



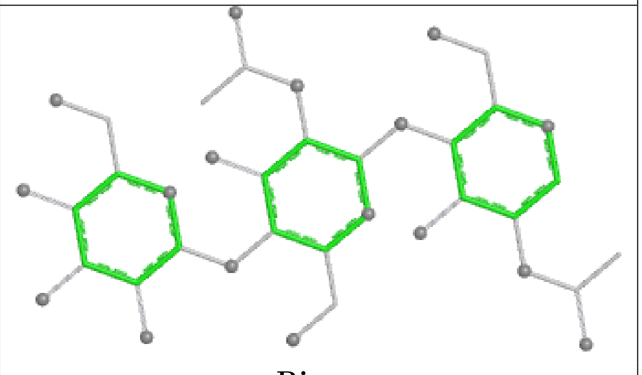
Bond lengths



Bond angles

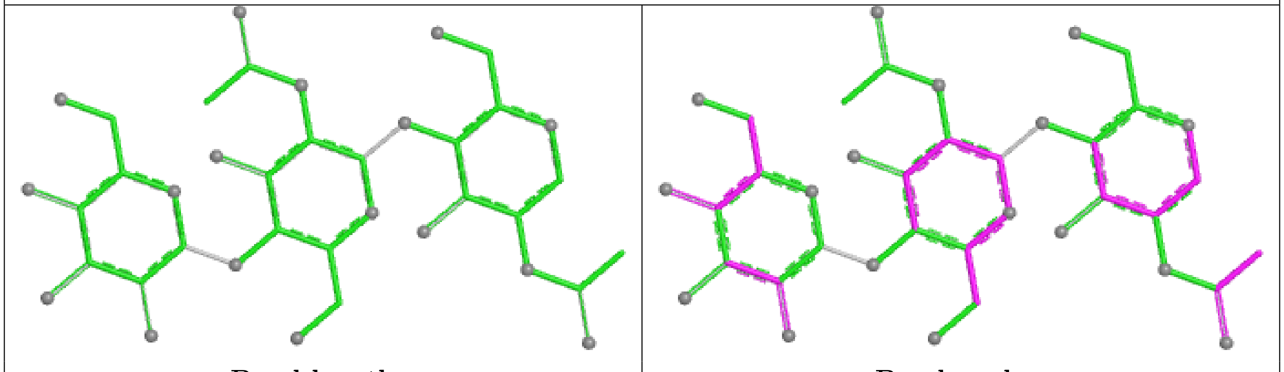


Torsions



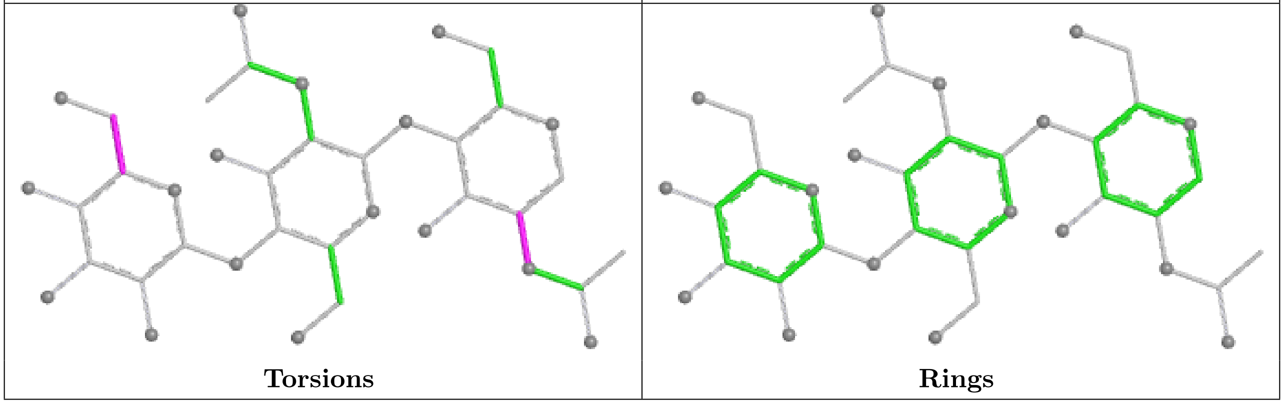
Rings

Oligosaccharide Chain v



Bond lengths

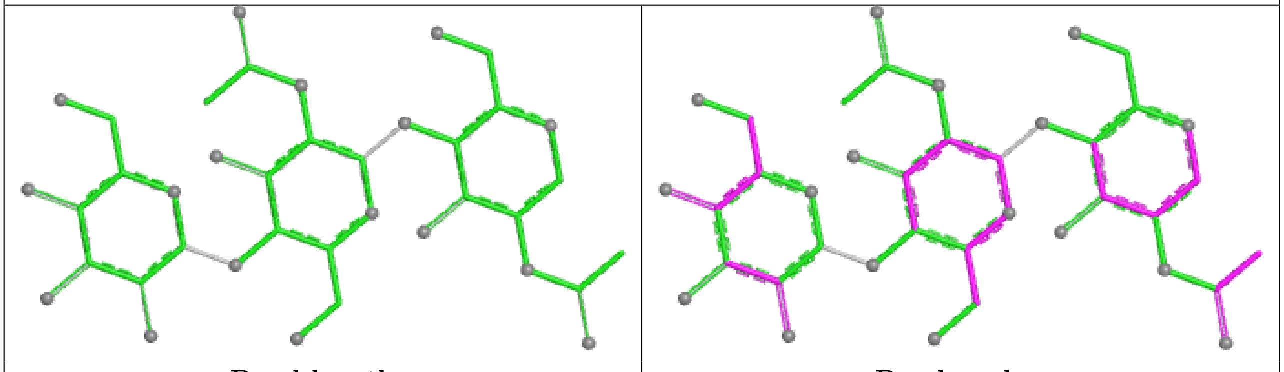
Bond angles



Torsions

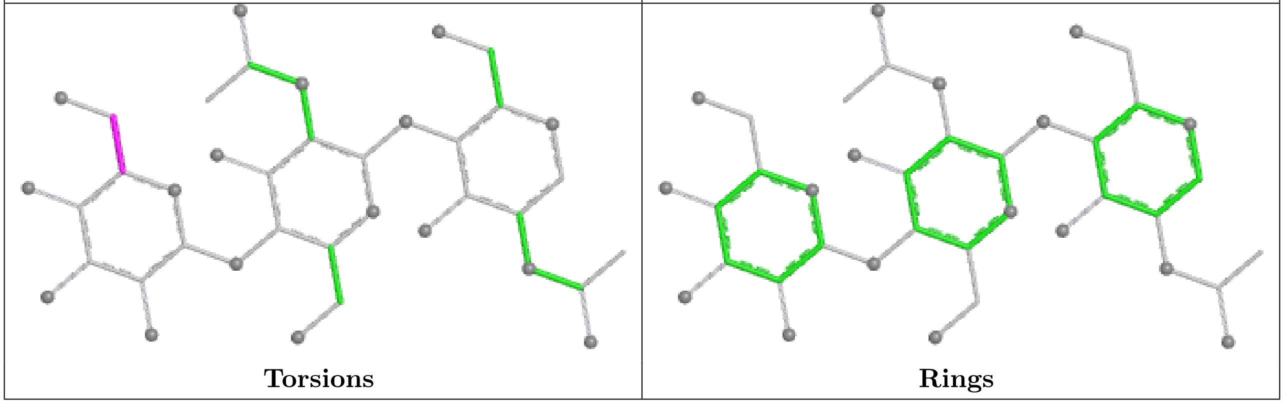
Rings

Oligosaccharide Chain 2



Bond lengths

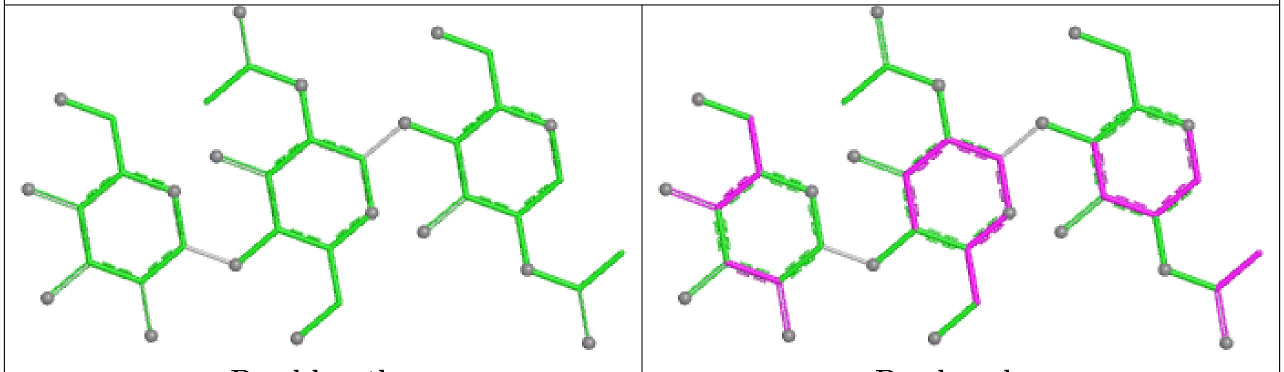
Bond angles



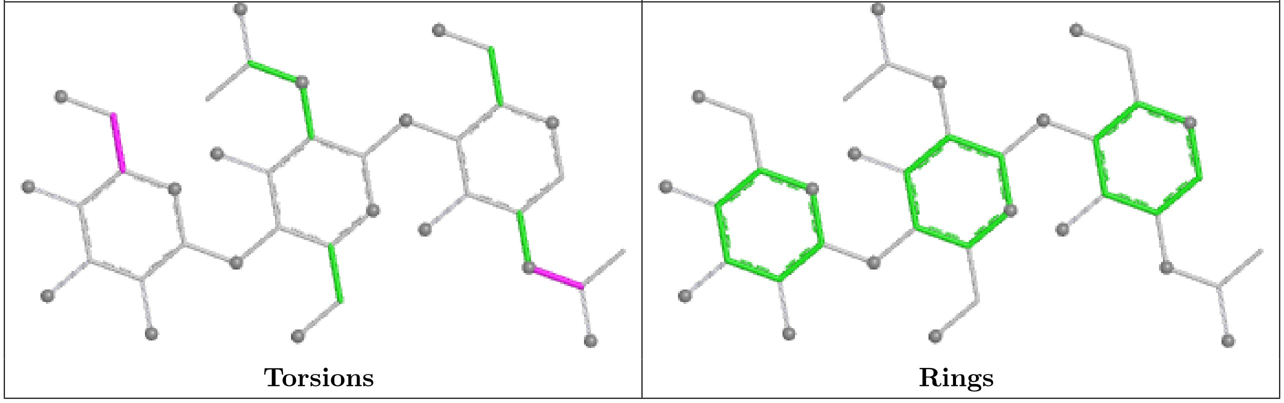
Torsions

Rings

Oligosaccharide Chain 7

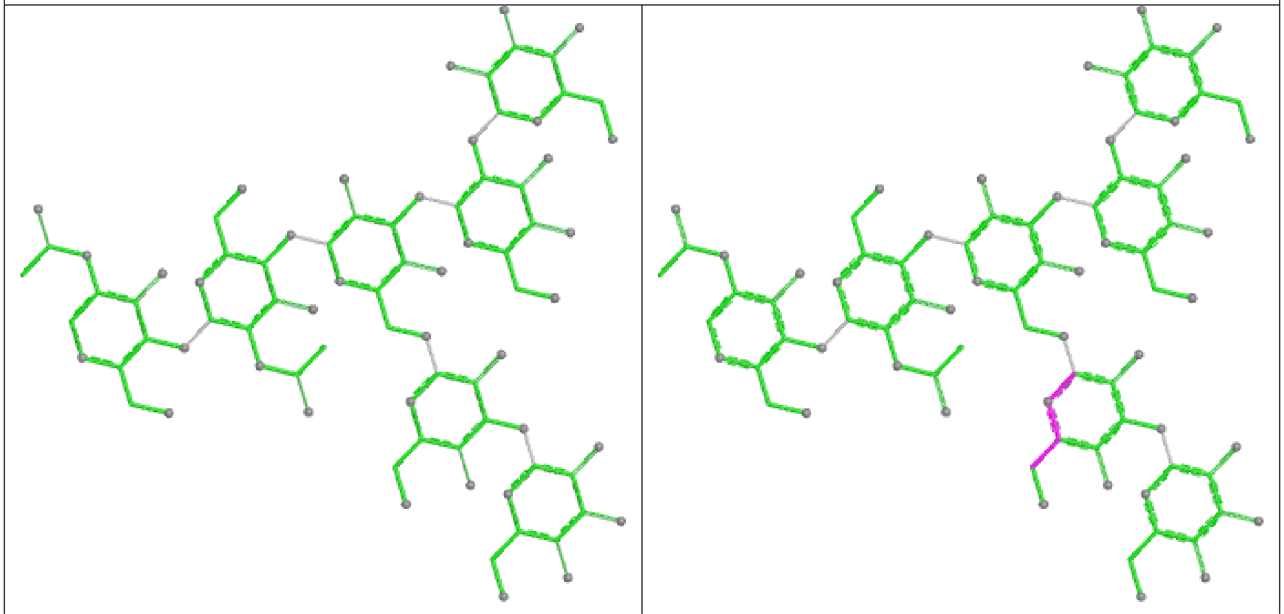


Bond lengths **Bond angles**



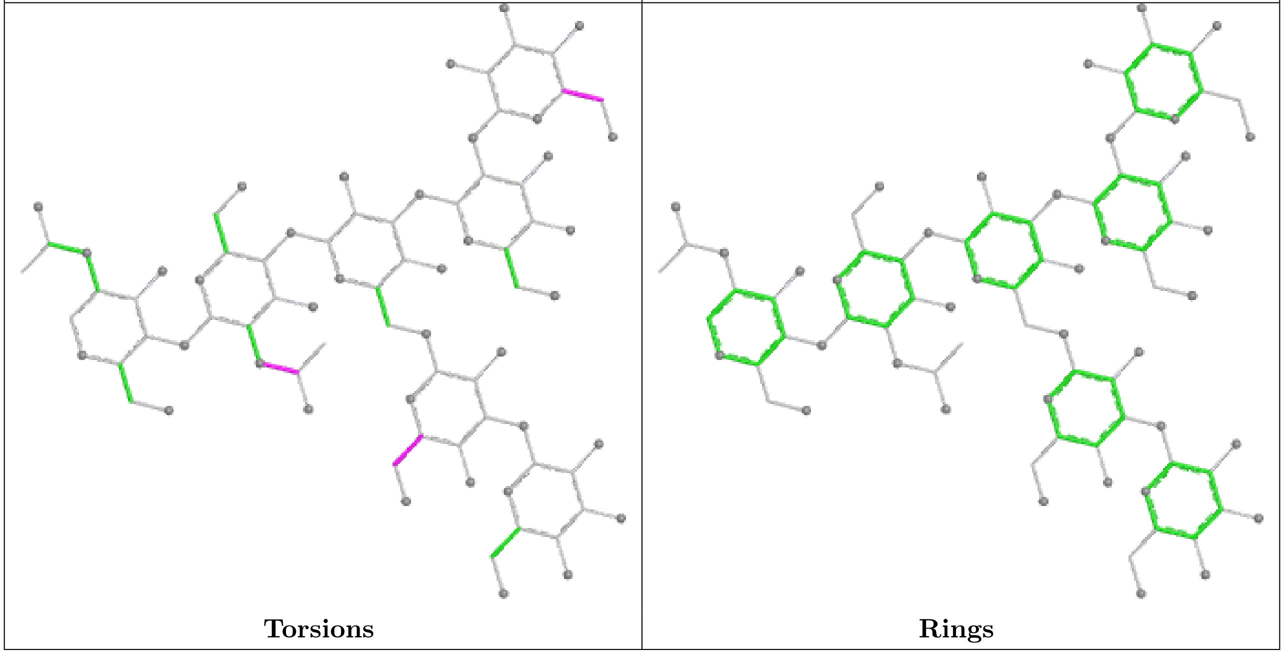
Torsions **Rings**

Oligosaccharide Chain O



Bond lengths

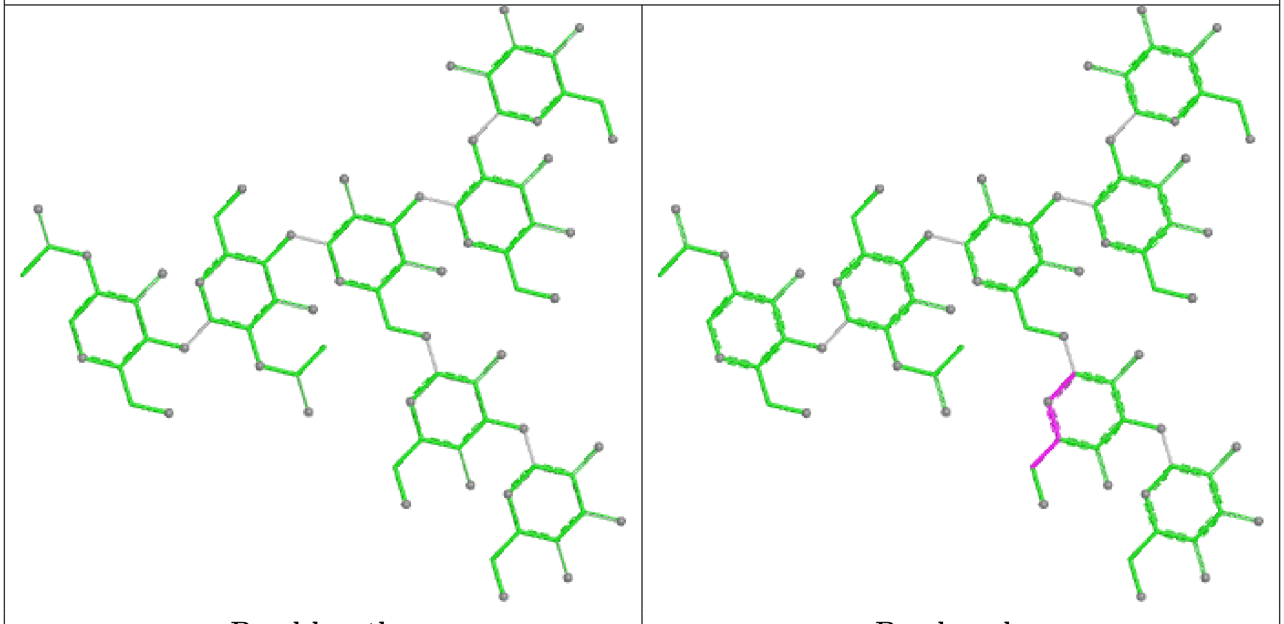
Bond angles



Torsions

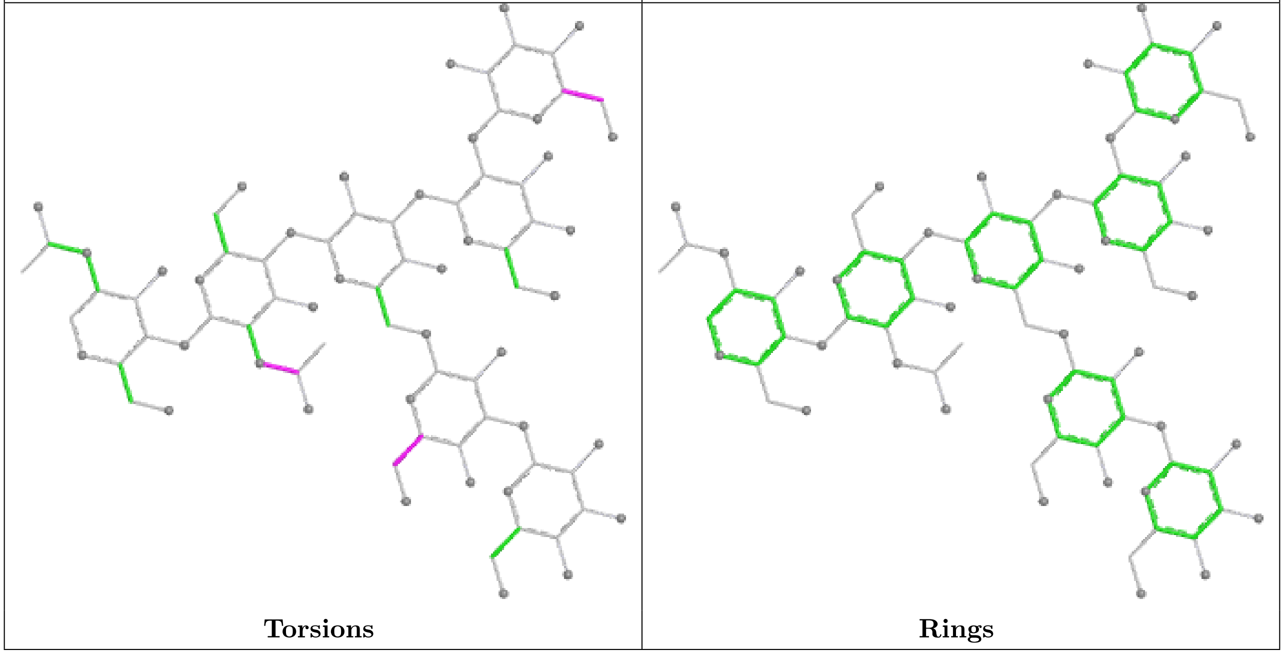
Rings

Oligosaccharide Chain f



Bond lengths

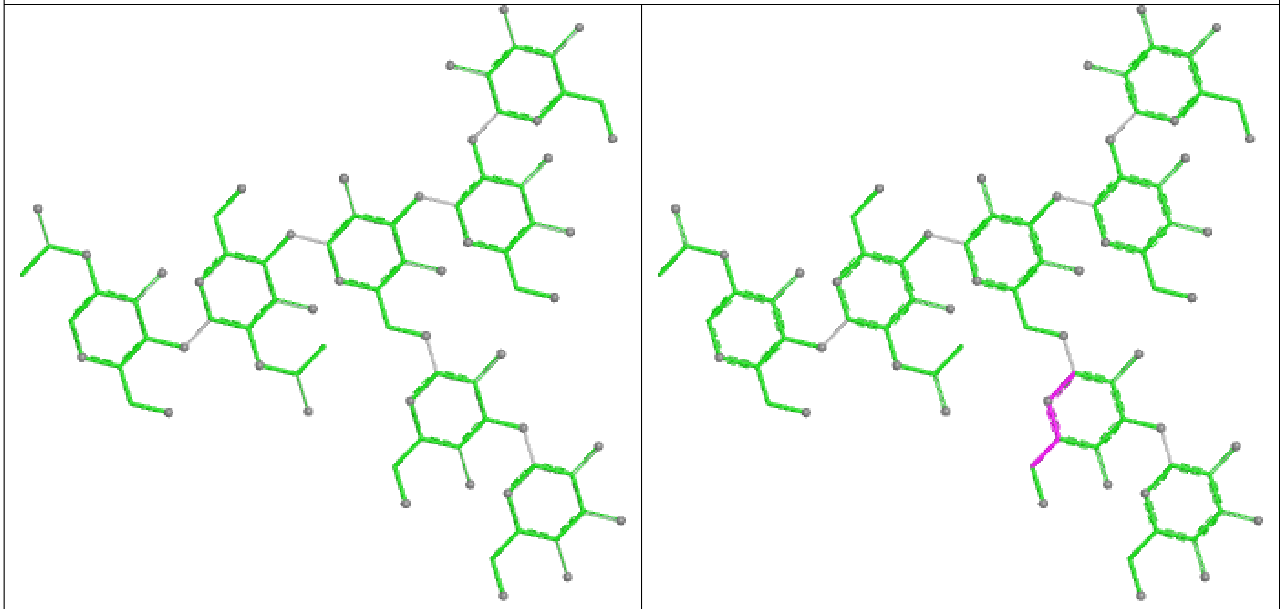
Bond angles



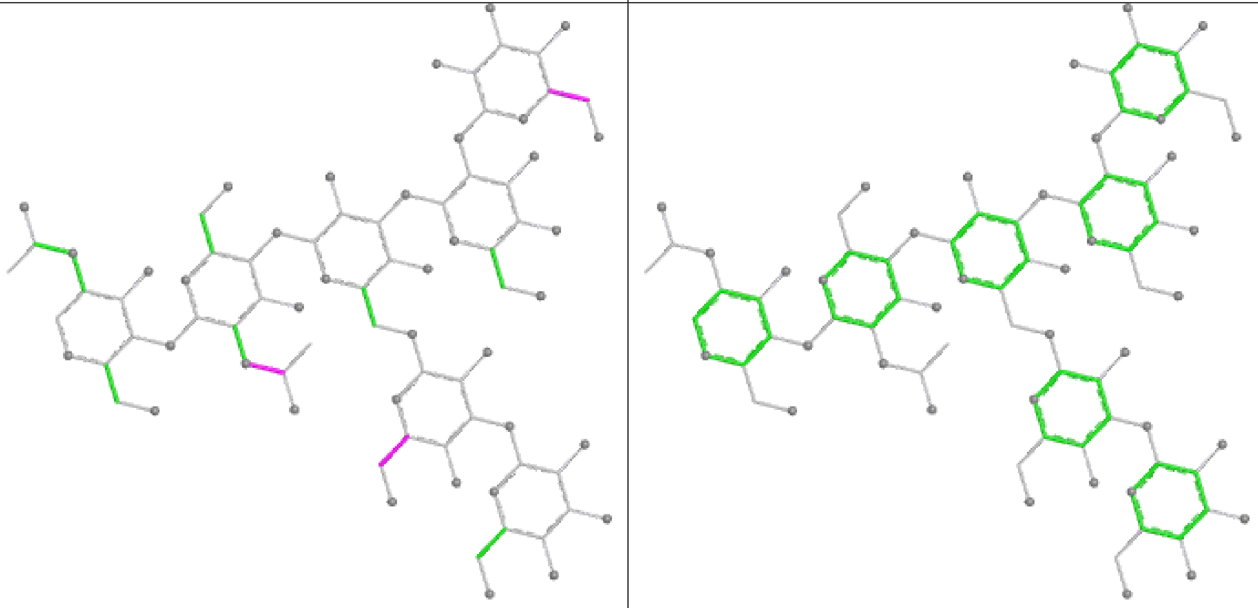
Torsions

Rings

Oligosaccharide Chain y

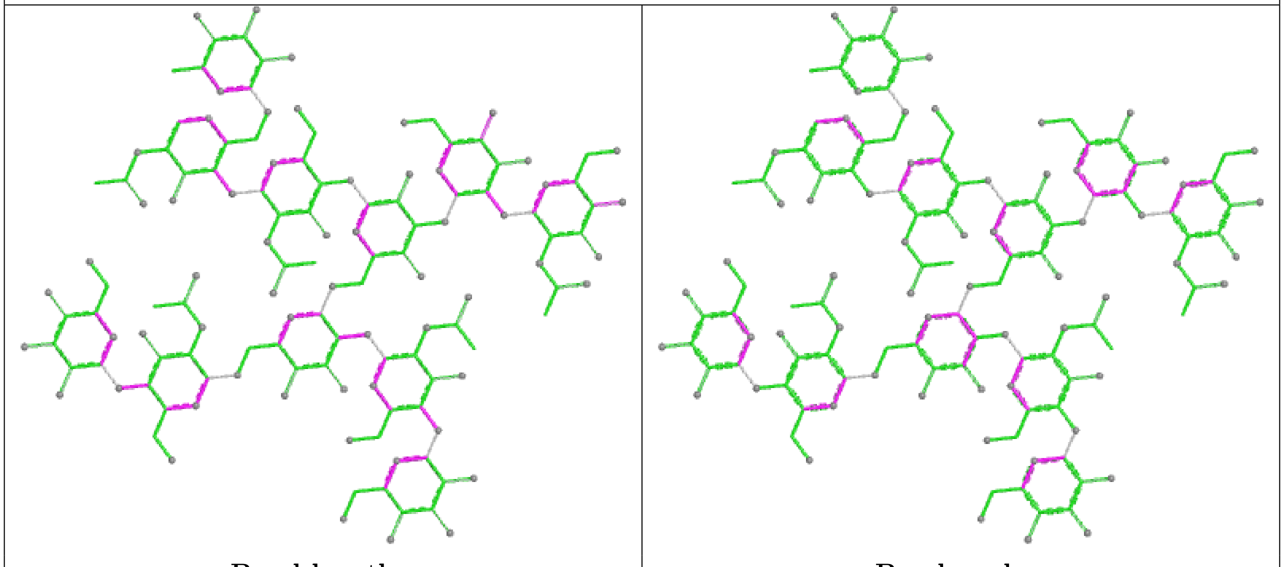


Bond lengths **Bond angles**



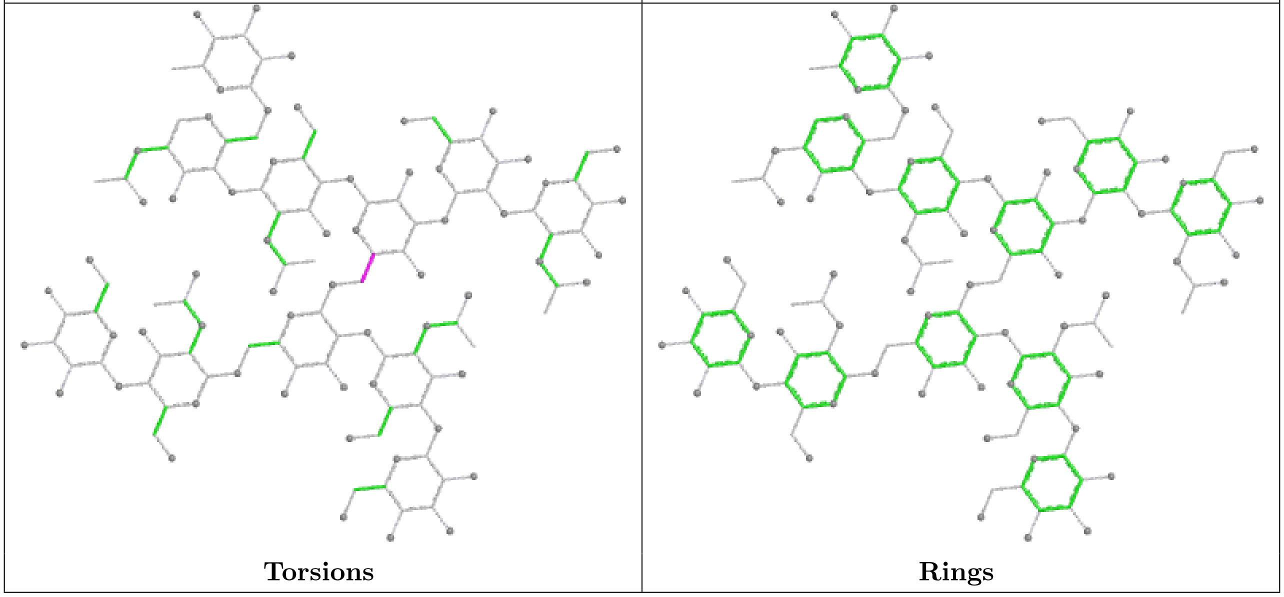
Torsions **Rings**

Oligosaccharide Chain Y



Bond lengths

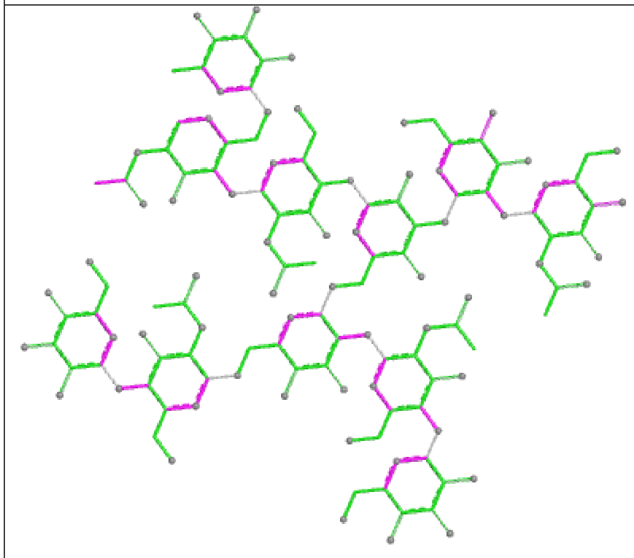
Bond angles



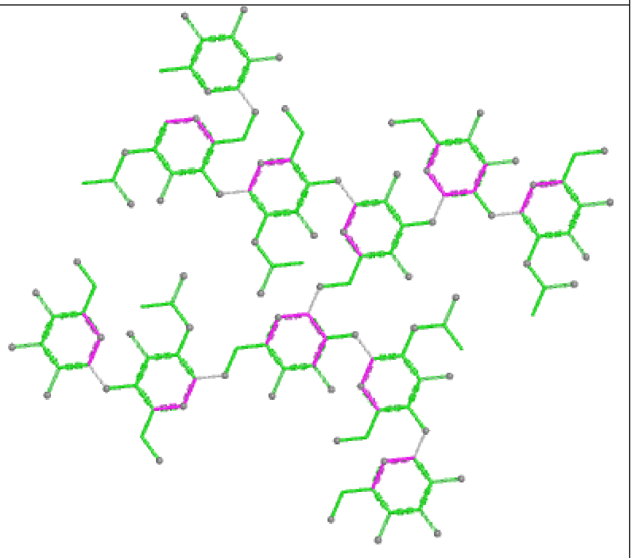
Torsions

Rings

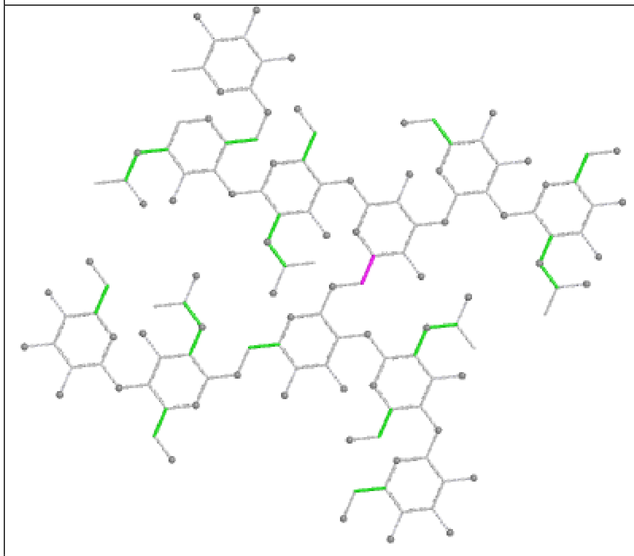
Oligosaccharide Chain 9



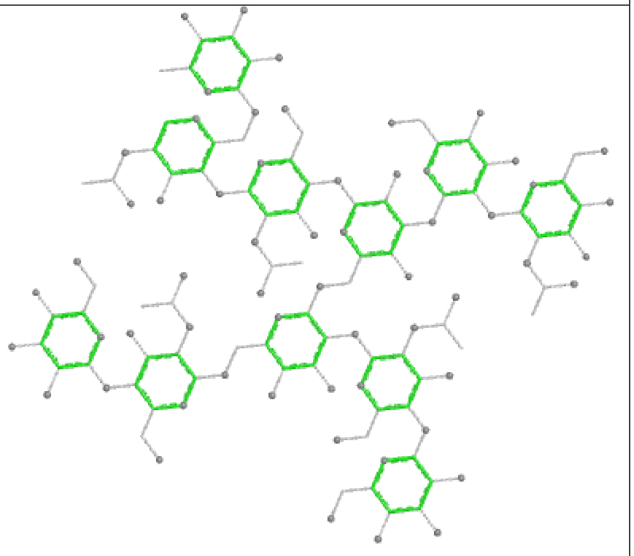
Bond lengths



Bond angles

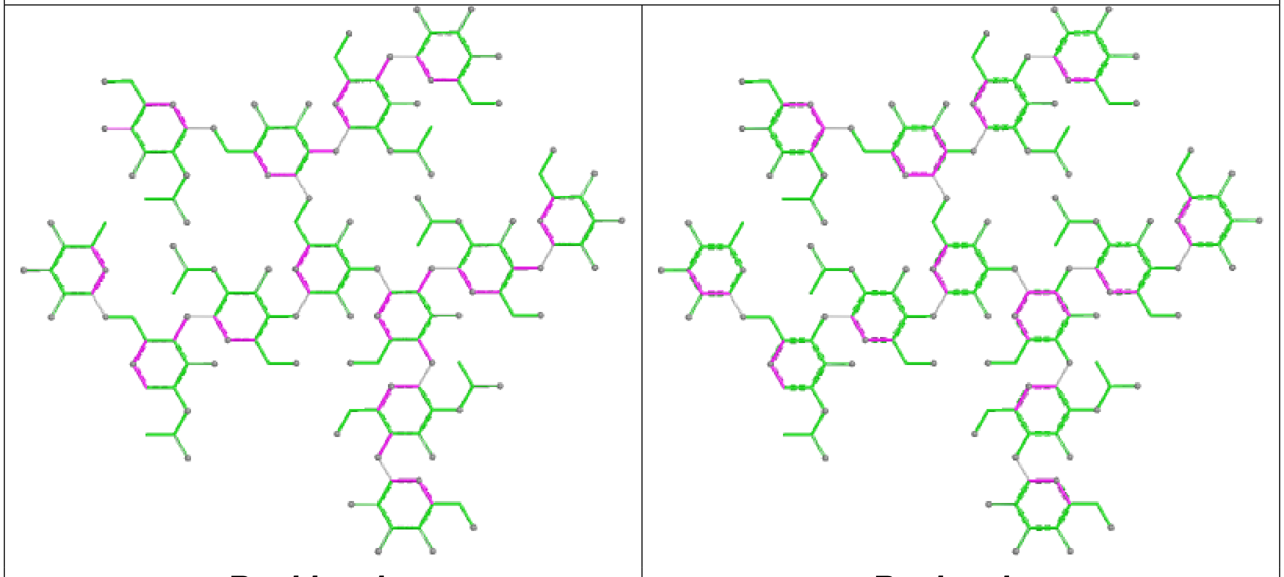


Torsions

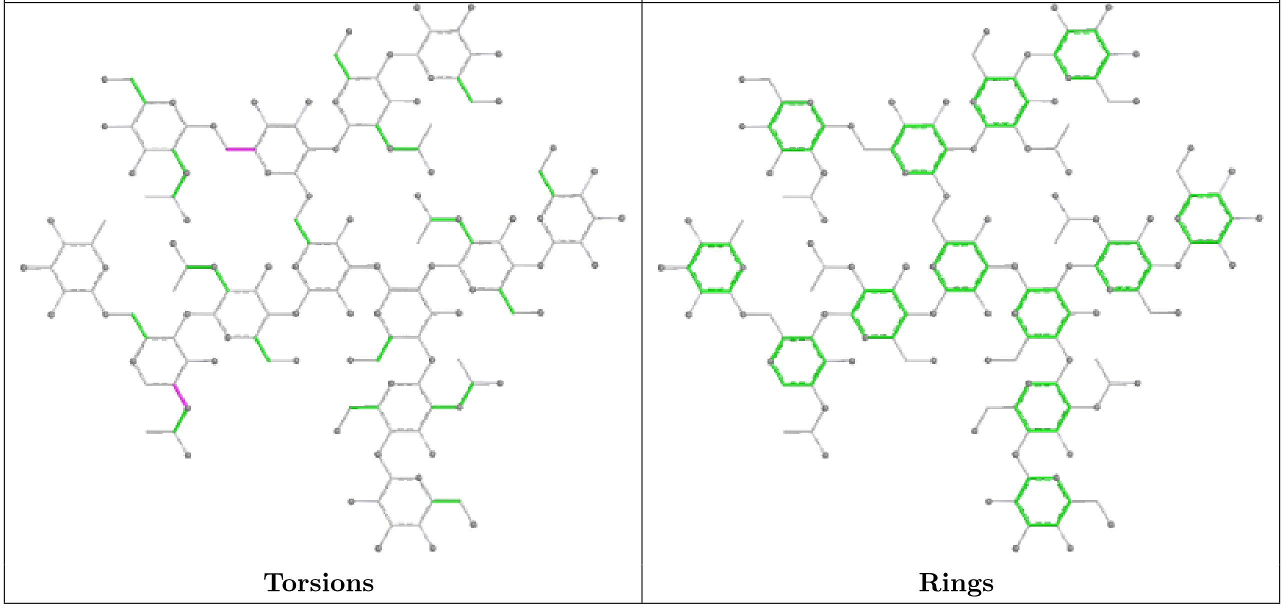


Rings

Oligosaccharide Chain Z

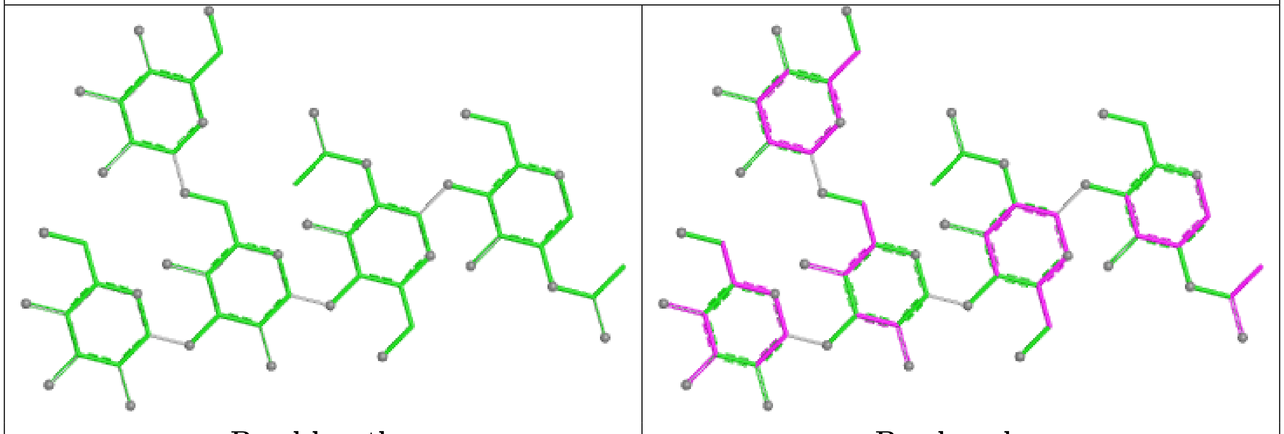


Bond lengths **Bond angles**



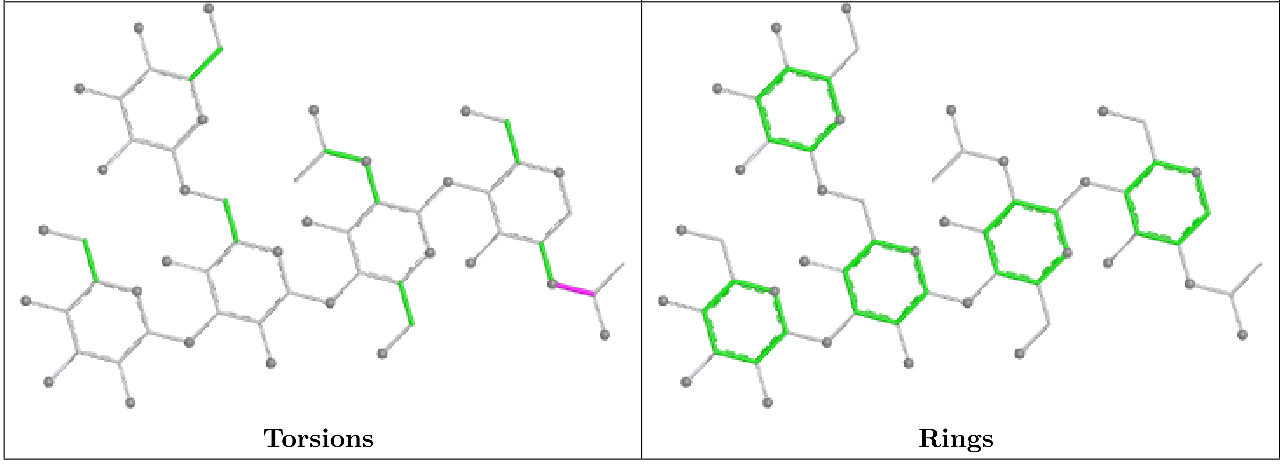
Torsions **Rings**

Oligosaccharide Chain e



Bond lengths

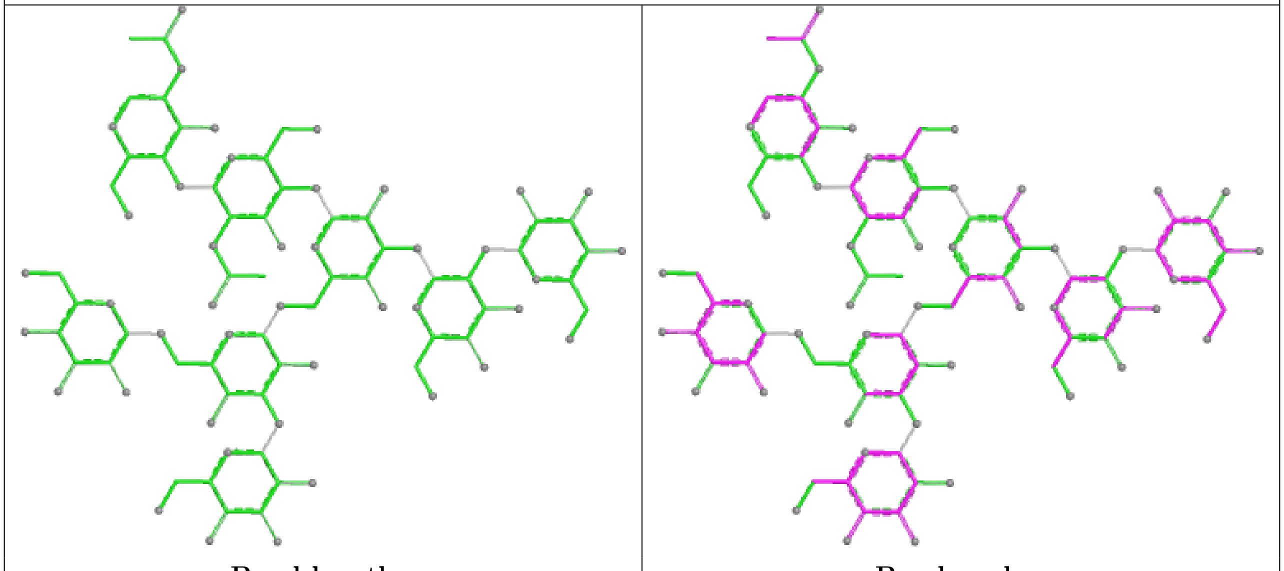
Bond angles



Torsions

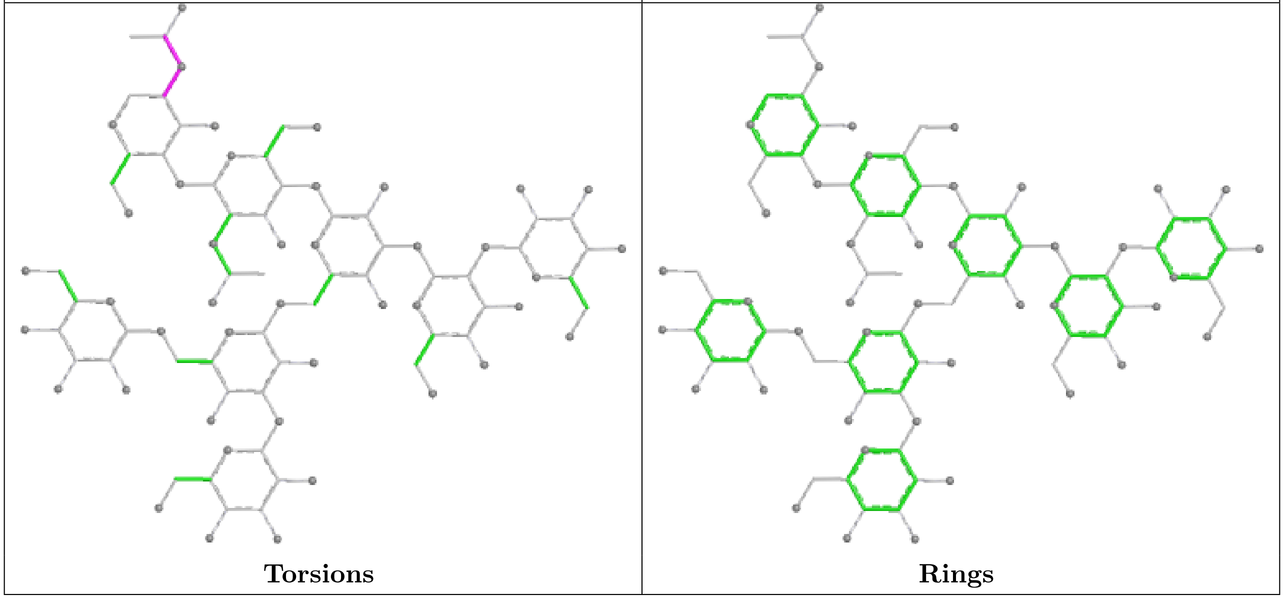
Rings

Oligosaccharide Chain p



Bond lengths

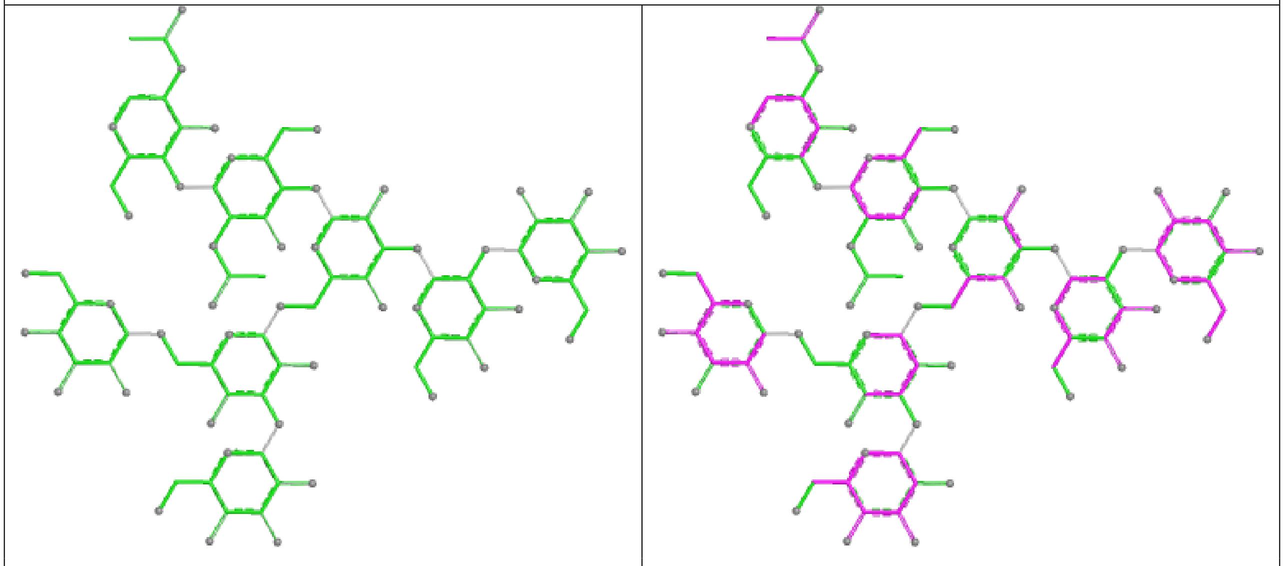
Bond angles



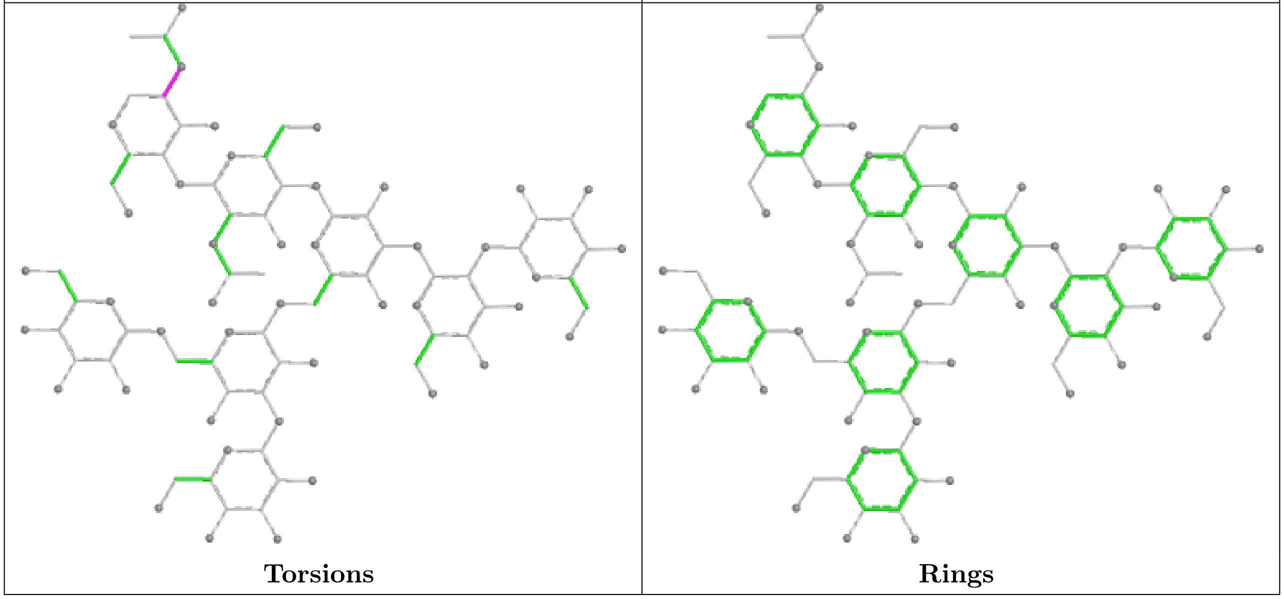
Torsions

Rings

Oligosaccharide Chain 8

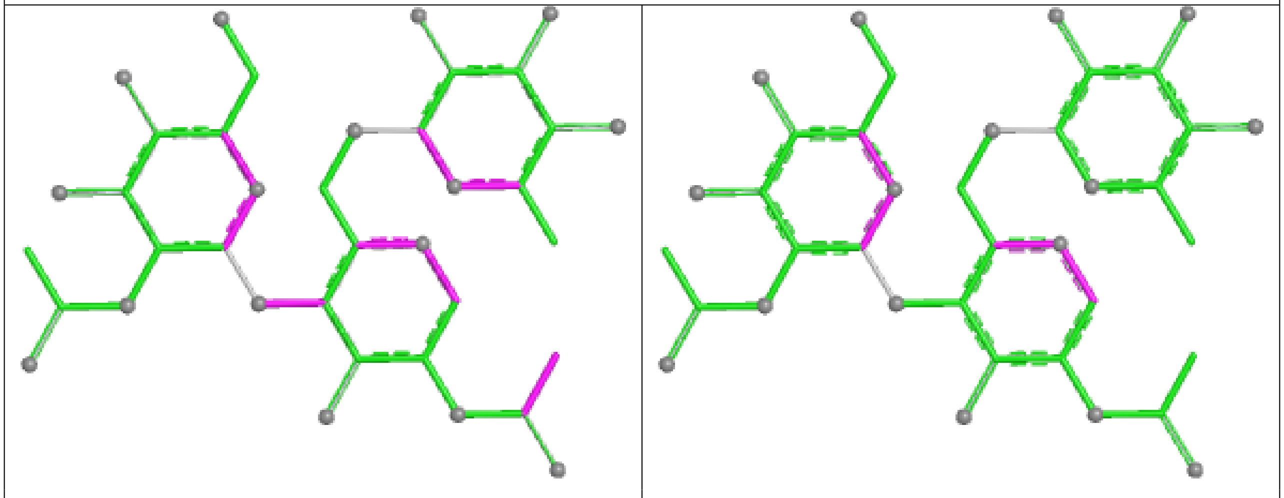


Bond lengths **Bond angles**

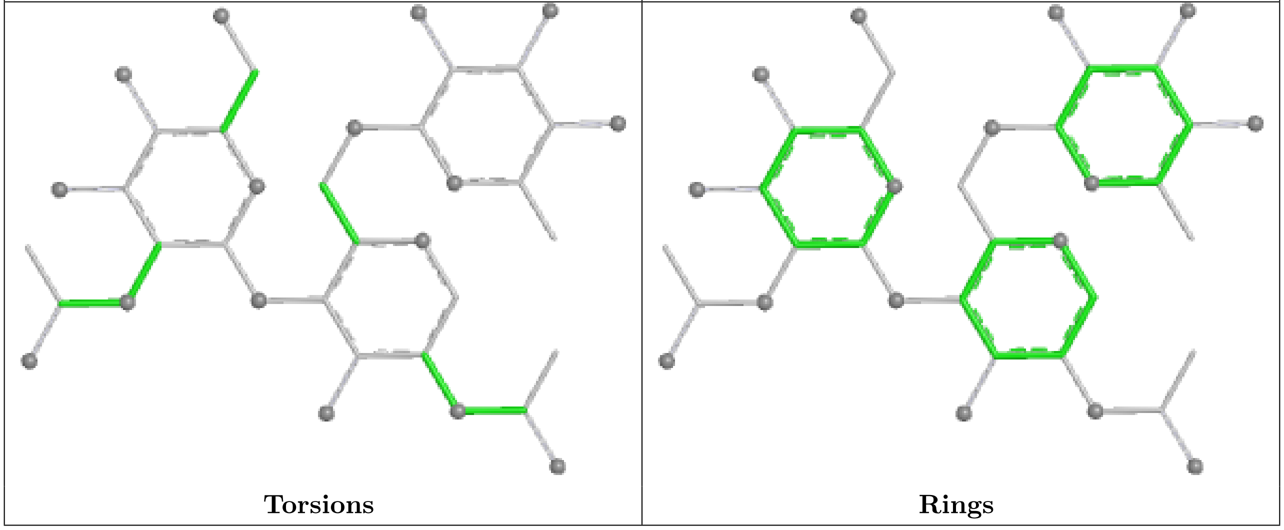


Torsions **Rings**

Oligosaccharide Chain q

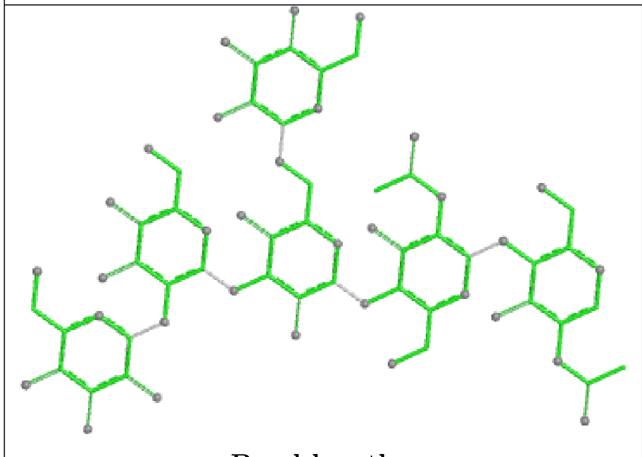


Bond lengths **Bond angles**

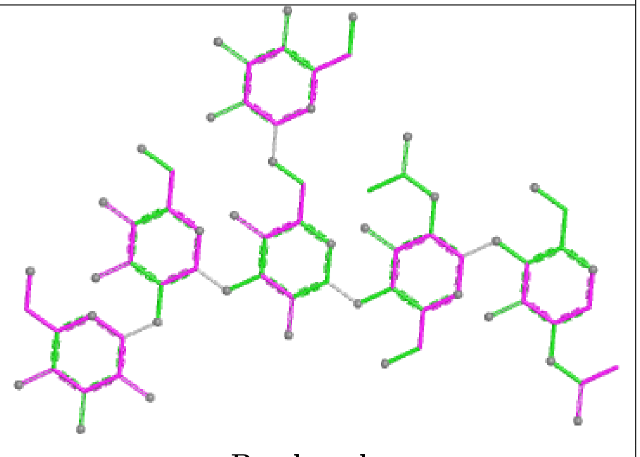


Torsions **Rings**

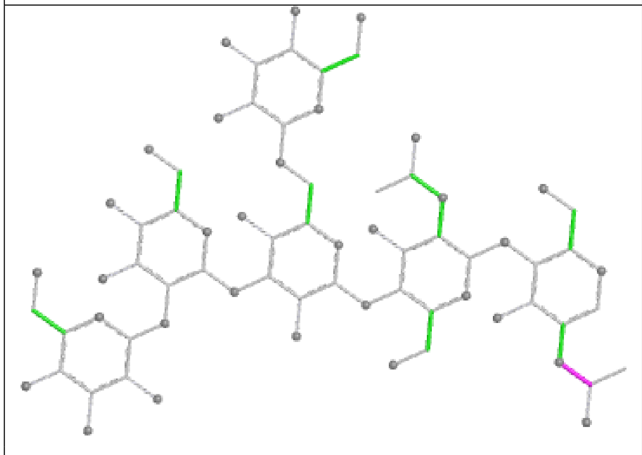
Oligosaccharide Chain x



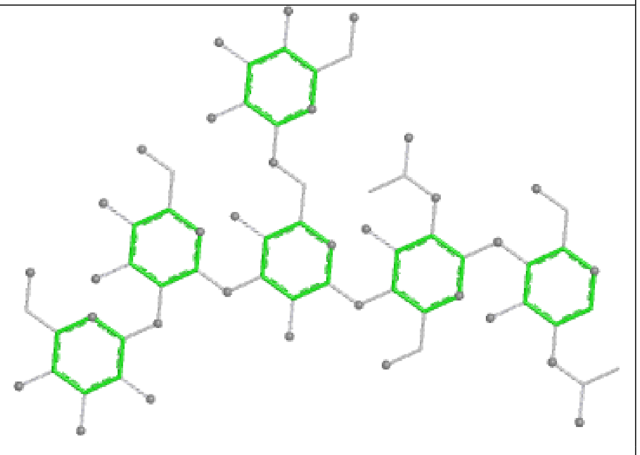
Bond lengths



Bond angles

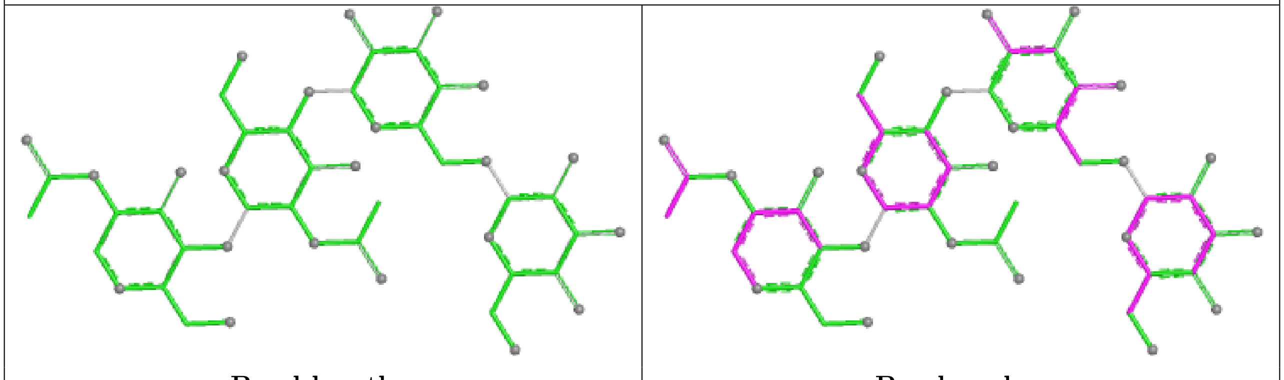


Torsions

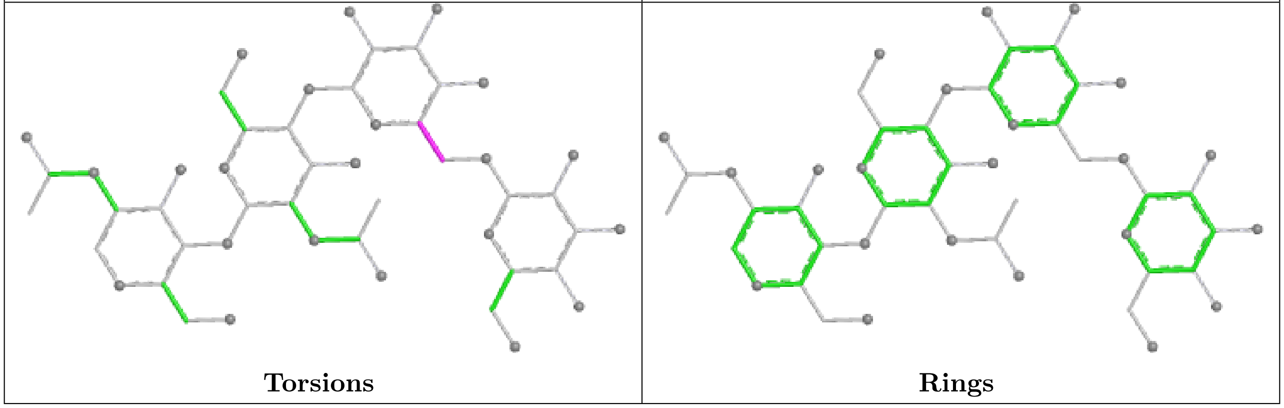


Rings

Oligosaccharide Chain 6

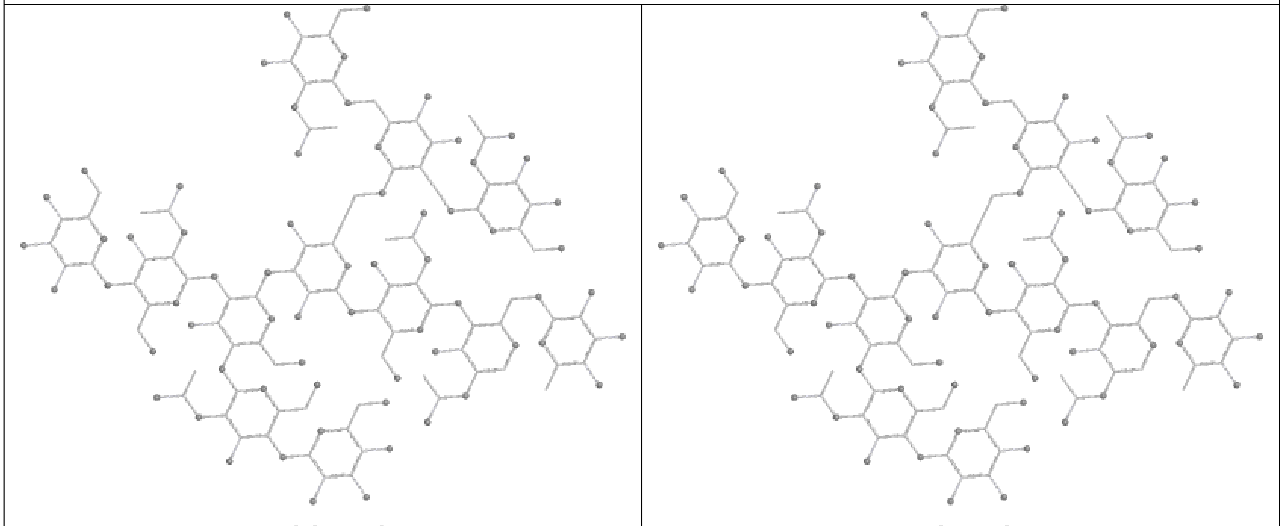


Bond lengths **Bond angles**



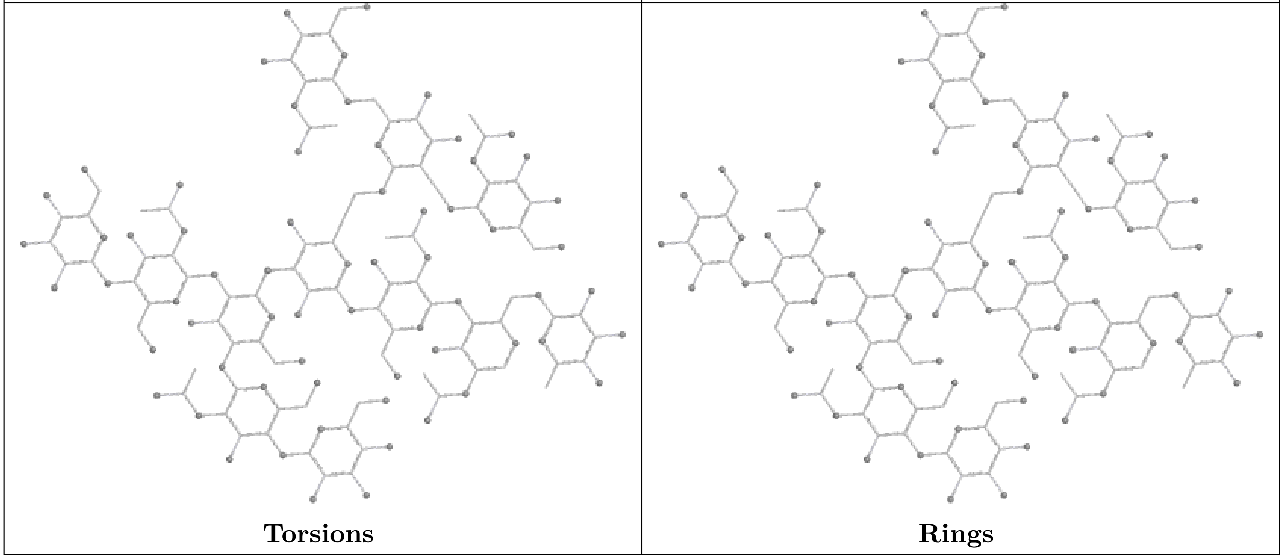
Torsions **Rings**

Oligosaccharide Chain BA



Bond lengths

Bond angles



Torsions

Rings

5.6 Ligand geometry ⓘ

10 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	$\#\|Z\| > 2$
16	NAG	E	1397	1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	NAG	B	1600	2	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
16	NAG	E	1187	1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
16	NAG	A	1135	1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
16	NAG	A	1355	1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
16	NAG	C	1397	1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
16	NAG	B	1625	2	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
16	NAG	F	1600	2	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
16	NAG	D	1600	2	14,14,15	0.52	0	17,19,21	2.25	3 (17%)
16	NAG	A	1397	1	14,14,15	0.50	0	17,19,21	2.23	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
16	NAG	E	1397	1	-	0/6/23/26	0/1/1/1
16	NAG	B	1600	2	-	0/6/23/26	0/1/1/1
16	NAG	E	1187	1	-	0/6/23/26	0/1/1/1
16	NAG	A	1135	1	-	1/6/23/26	0/1/1/1
16	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
16	NAG	C	1397	1	-	0/6/23/26	0/1/1/1
16	NAG	B	1625	2	-	0/6/23/26	0/1/1/1
16	NAG	F	1600	2	-	0/6/23/26	0/1/1/1
16	NAG	D	1600	2	-	1/6/23/26	0/1/1/1
16	NAG	A	1397	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	1600	NAG	O5-C1-C2	-7.39	99.61	111.29
16	C	1397	NAG	O5-C1-C2	-7.38	99.63	111.29
16	F	1600	NAG	O5-C1-C2	-7.38	99.64	111.29
16	A	1355	NAG	O5-C1-C2	-7.38	99.64	111.29
16	A	1135	NAG	O5-C1-C2	-7.37	99.65	111.29
16	B	1600	NAG	O5-C1-C2	-7.36	99.66	111.29
16	B	1625	NAG	O5-C1-C2	-7.34	99.69	111.29
16	E	1397	NAG	O5-C1-C2	-7.34	99.69	111.29
16	E	1187	NAG	O5-C1-C2	-7.34	99.69	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	1397	NAG	O5-C1-C2	-7.33	99.72	111.29
16	D	1600	NAG	O7-C7-C8	-2.83	116.79	122.06
16	A	1397	NAG	O7-C7-C8	-2.81	116.84	122.06
16	C	1397	NAG	O7-C7-C8	-2.81	116.84	122.06
16	E	1397	NAG	O7-C7-C8	-2.80	116.85	122.06
16	B	1600	NAG	O7-C7-C8	-2.79	116.87	122.06
16	E	1187	NAG	O7-C7-C8	-2.78	116.90	122.06
16	F	1600	NAG	O7-C7-C8	-2.77	116.91	122.06
16	B	1625	NAG	O7-C7-C8	-2.76	116.92	122.06
16	A	1135	NAG	O7-C7-C8	-2.76	116.92	122.06
16	A	1355	NAG	O7-C7-C8	-2.75	116.95	122.06
16	D	1600	NAG	C4-C3-C2	-2.72	107.03	111.02
16	A	1355	NAG	C4-C3-C2	-2.68	107.09	111.02
16	A	1135	NAG	C4-C3-C2	-2.67	107.10	111.02
16	B	1600	NAG	C4-C3-C2	-2.67	107.11	111.02
16	F	1600	NAG	C4-C3-C2	-2.67	107.11	111.02
16	B	1625	NAG	C4-C3-C2	-2.66	107.11	111.02
16	E	1187	NAG	C4-C3-C2	-2.66	107.12	111.02
16	C	1397	NAG	C4-C3-C2	-2.66	107.12	111.02
16	A	1397	NAG	C4-C3-C2	-2.63	107.16	111.02
16	E	1397	NAG	C4-C3-C2	-2.62	107.18	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	1135	NAG	O7-C7-N2-C2
16	D	1600	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

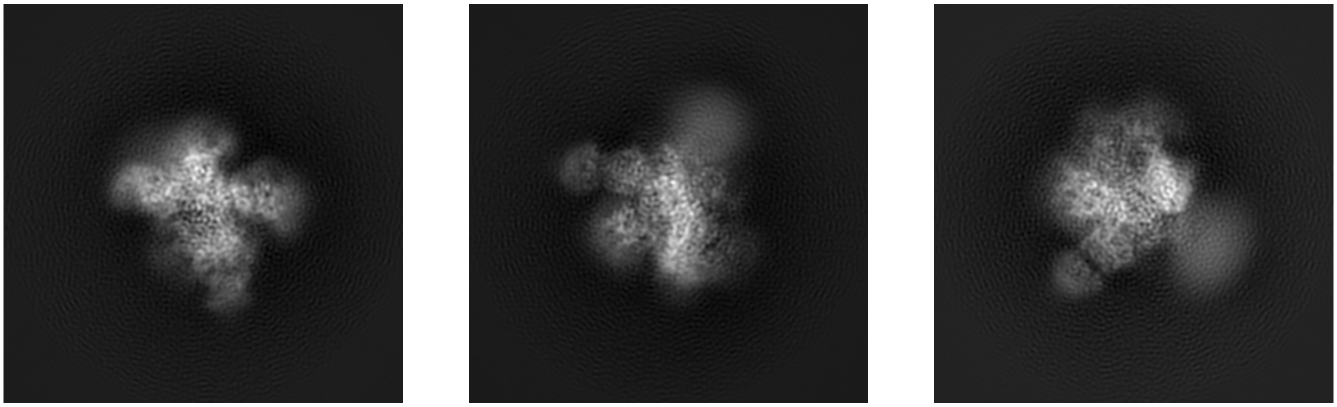
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3308. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

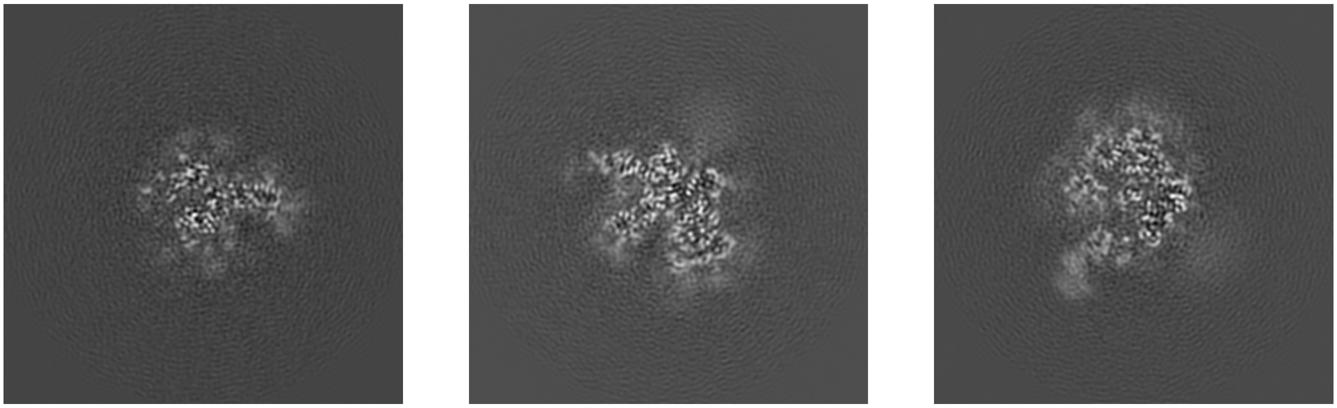
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

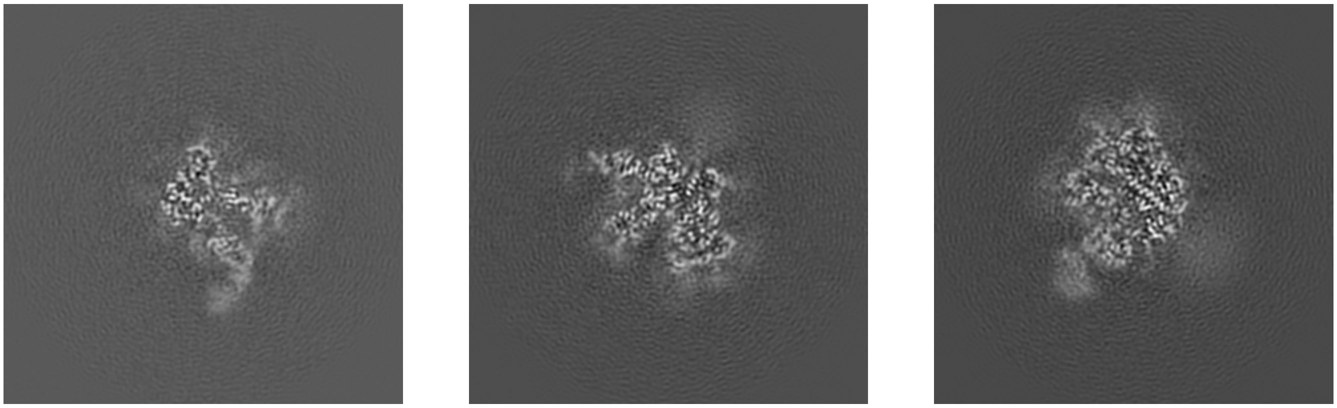
6.2.1 Primary map


X Index: 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

6.3.1 Primary map



X Index: 141 Y Index: 128 Z Index: 132

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

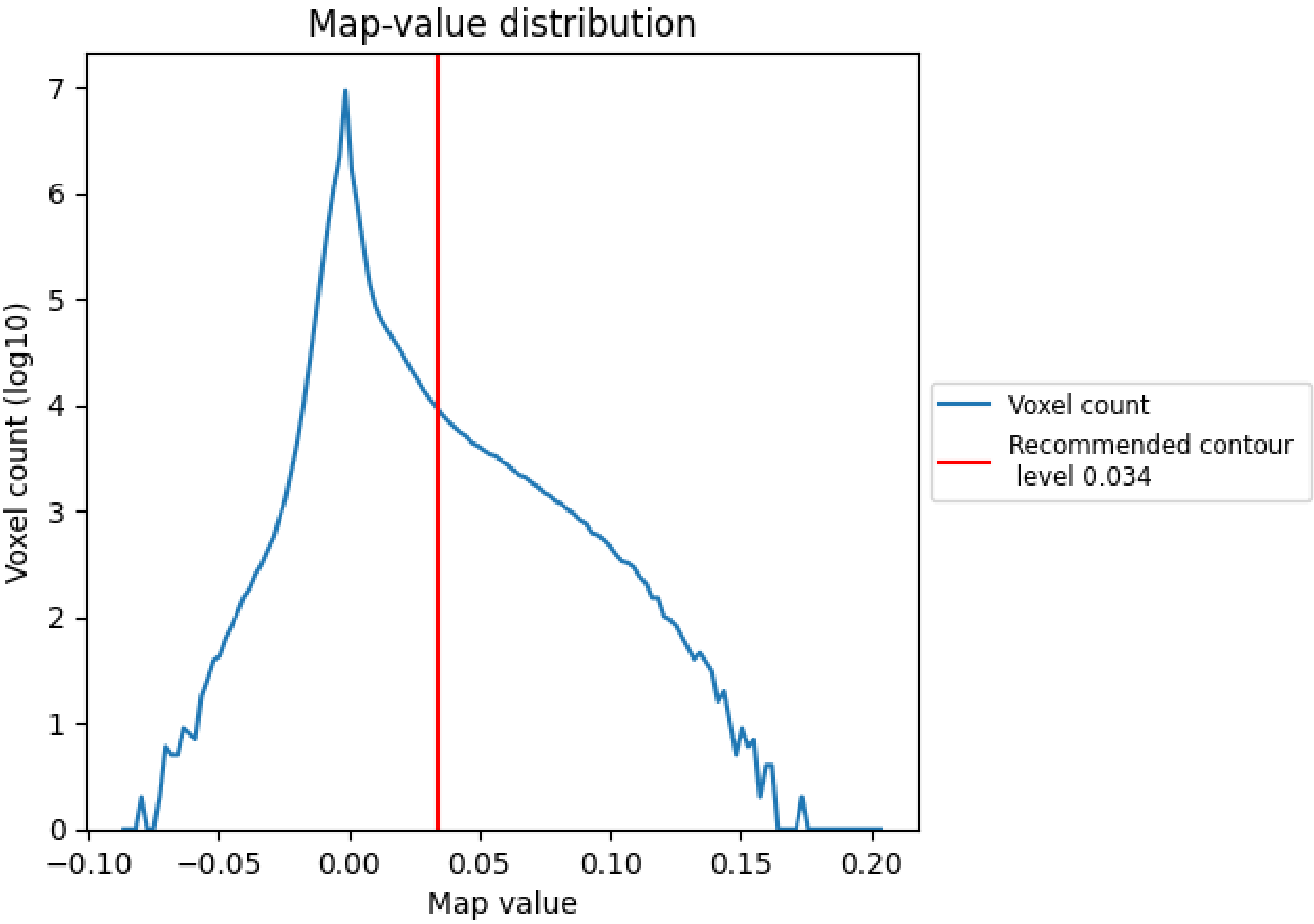
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

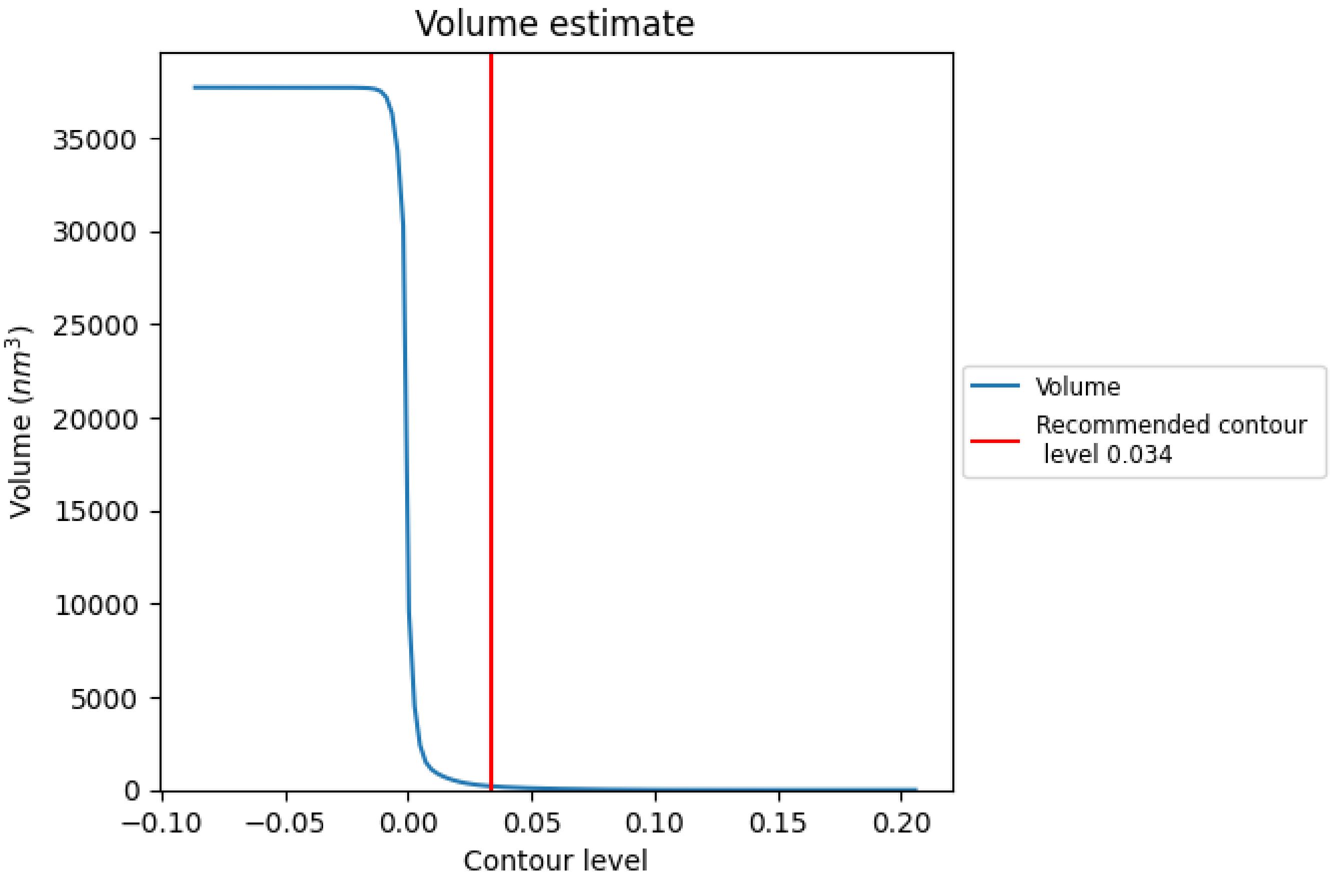
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

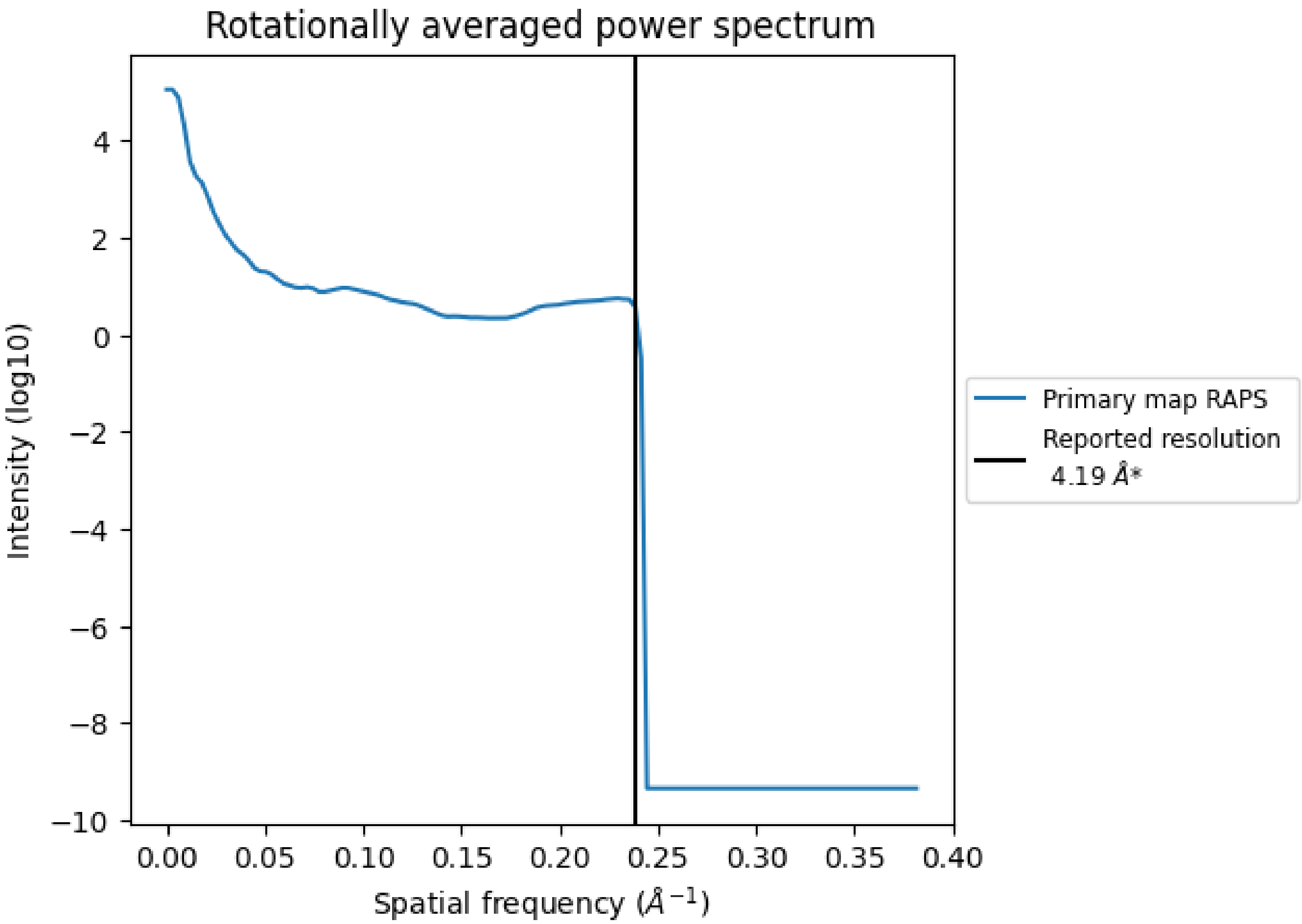
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.239 $Å^{-1}$

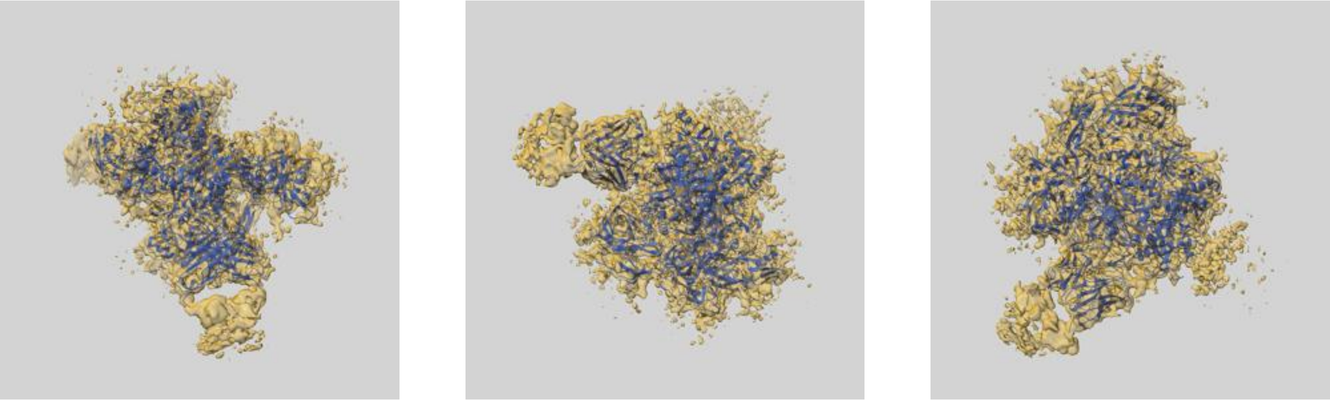
8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3308 and PDB model 5FUU. Per-residue inclusion information can be found in section 3 on page 14.

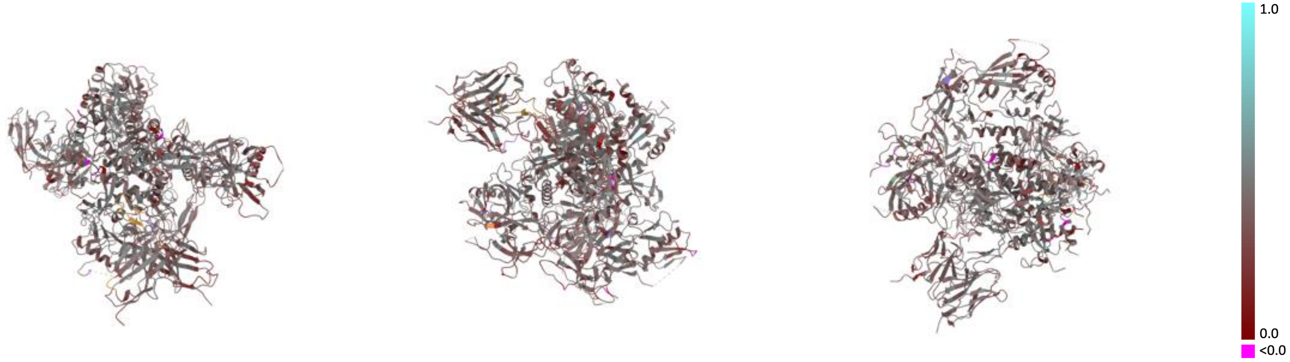
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

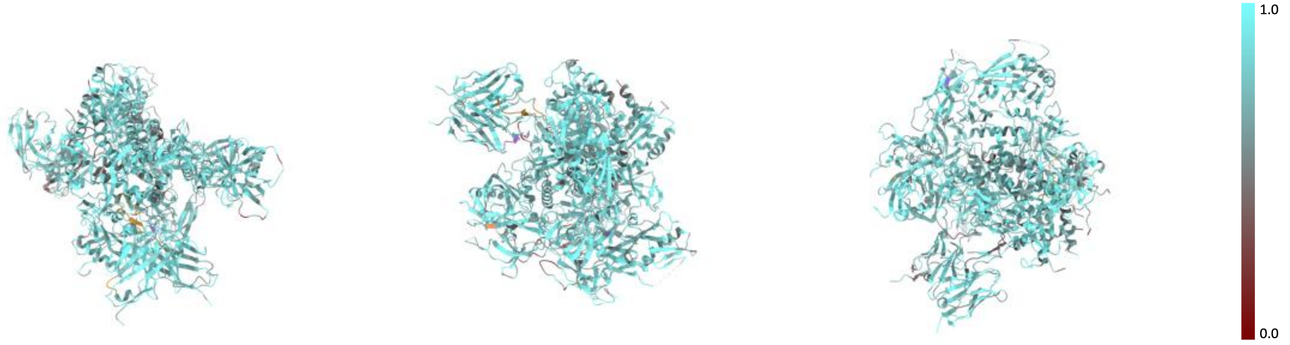
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

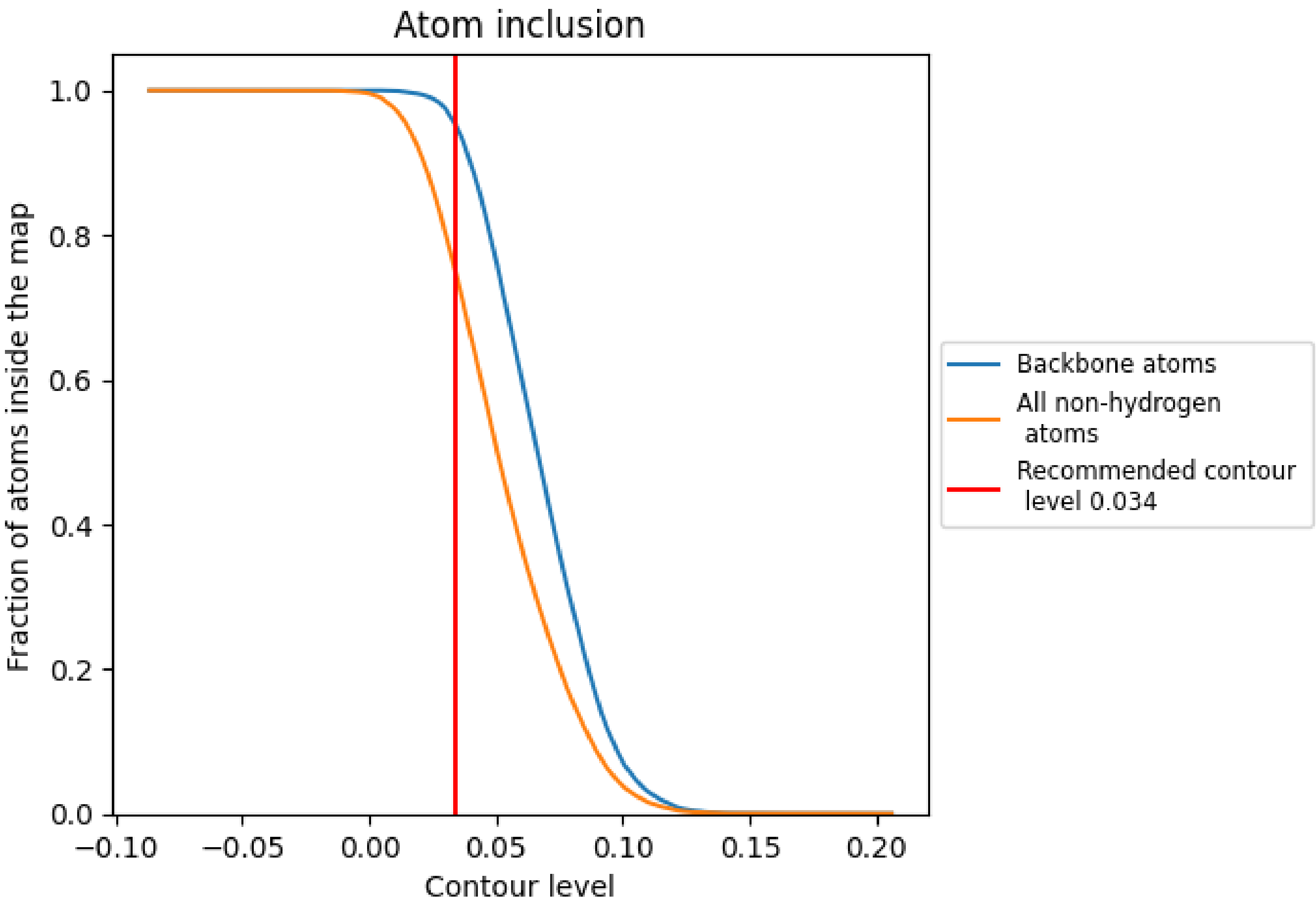
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7508	0.3670
0	0.4643	0.2010
1	0.4643	0.1470
2	0.5897	0.1880
3	0.6071	0.2680
4	0.1786	0.1680
5	0.5714	0.2340
6	0.5600	0.2810
7	0.4872	0.2990
8	0.5319	0.3290
9	0.6889	0.3110
A	0.7775	0.3800
AA	0.3571	0.2390
B	0.7608	0.3620
BA	0.5570	0.2290
C	0.7851	0.3860
D	0.7615	0.3860
E	0.7863	0.3860
F	0.7706	0.3890
G	0.5357	0.2070
H	0.8017	0.3890
I	0.5641	0.2900
J	0.4103	0.3180
K	0.4615	0.2500
L	0.7216	0.3370
M	0.8271	0.3950
N	0.7686	0.3370
O	0.7229	0.3550
P	0.4872	0.2400
Q	0.6071	0.2900
R	0.7143	0.3680
S	0.6154	0.2730
T	0.5714	0.2050
U	0.5128	0.2220
V	0.6667	0.3260

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Chain	Atom inclusion	Q-score
W	0.4872	0.3550
X	0.5357	0.2820
Y	0.6963	0.3470
Z	0.6438	0.3150
a	0.5128	0.2100
b	0.3929	0.2500
c	0.4286	0.1540
d	0.3077	0.1950
e	0.5574	0.3060
f	0.6506	0.3170
g	0.5128	0.2020
h	0.5714	0.3400
i	0.4615	0.3000
j	0.5641	0.2570
k	0.4643	0.3430
l	0.2857	0.2700
m	0.5128	0.2590
n	0.6667	0.3450
o	0.5714	0.2520
p	0.4894	0.3700
q	0.5000	0.2570
r	0.3214	0.2000
s	0.4643	0.3000
t	0.5897	0.2520
u	0.3929	0.3080
v	0.4872	0.2680
w	0.6071	0.3000
x	0.4722	0.2700
y	0.7349	0.3250
z	0.4286	0.2040