wwPDB EM Validation Summary Report ⓘ

Jun 26, 2023 – 04:34 PM EDT

PDB ID	:	7T4G
EMDB ID	:	EMD-25676
Title	:	The Envelope Glycoprotein SIVmac239.K180S SOSIP trimer in complex with 3 copies of the neutralizing antibody K11
Authors	:	Berndsen, Z.T.; Ward, A.B.
Deposited on	:	2021-12-09
Resolution	:	3.70 Å(reported)

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

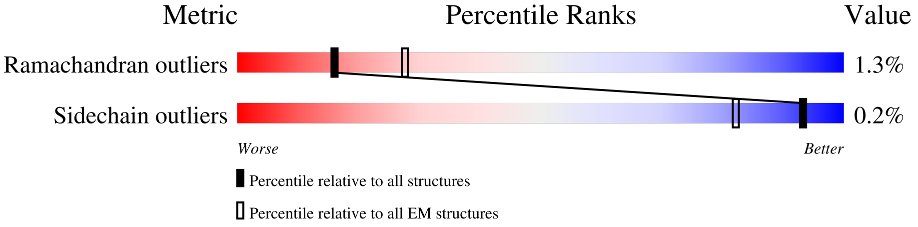
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance ⓘ

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

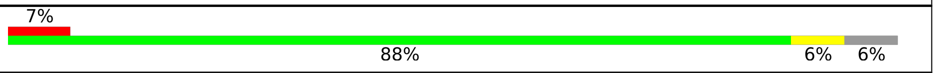
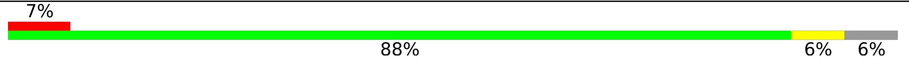
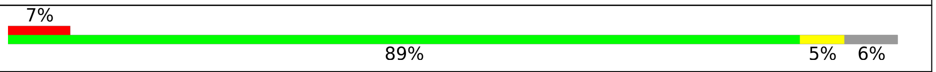
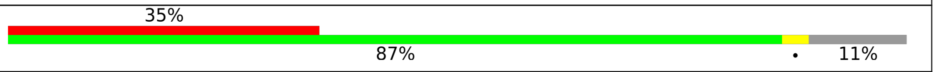
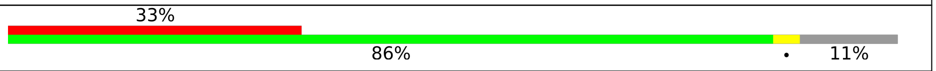
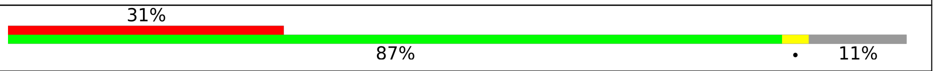
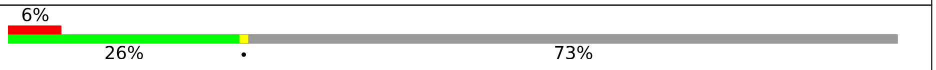
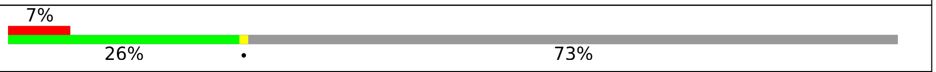
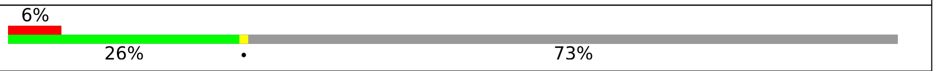
The reported resolution of this entry is 3.70 Å.

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	527	
1	C	527	
1	E	527	
2	B	159	
2	D	159	
2	F	159	
3	G	485	
3	H	485	
3	J	485	

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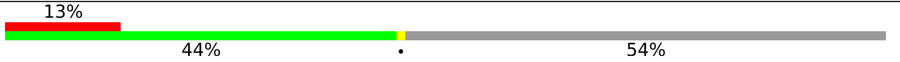
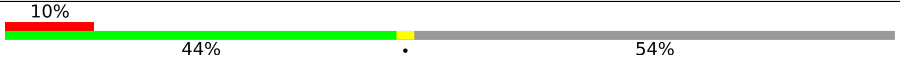
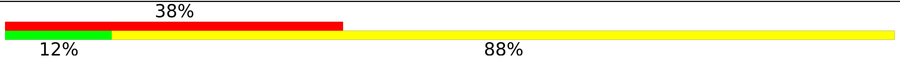
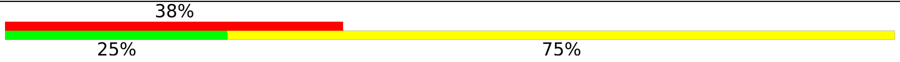
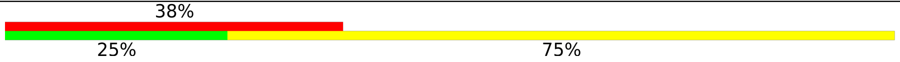
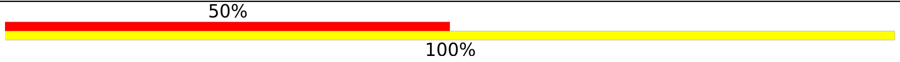
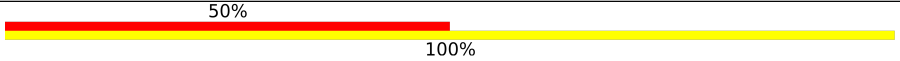
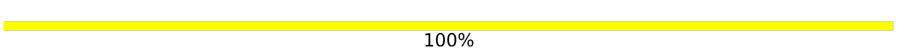
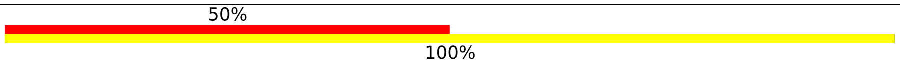
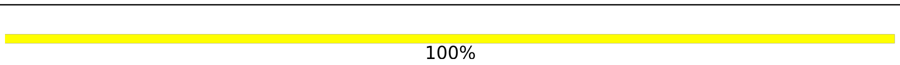
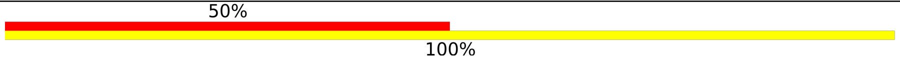
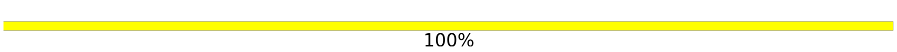
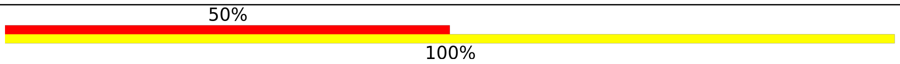
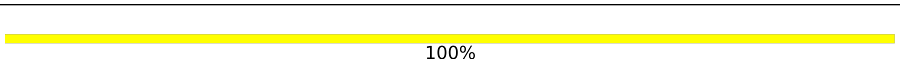
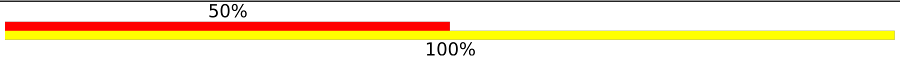
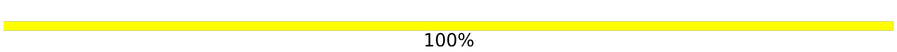
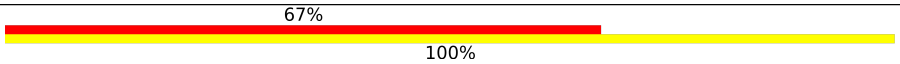
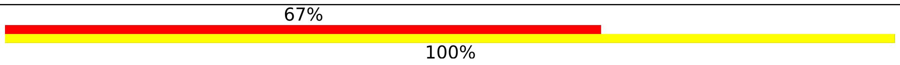
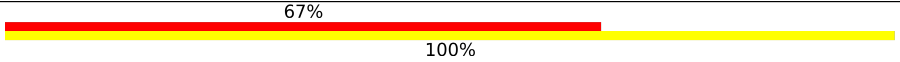
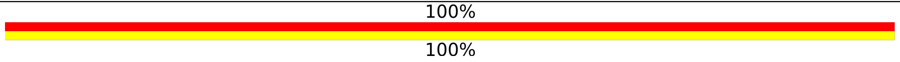
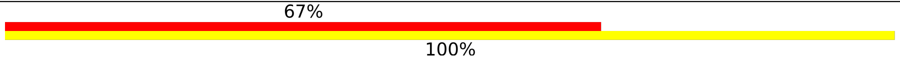
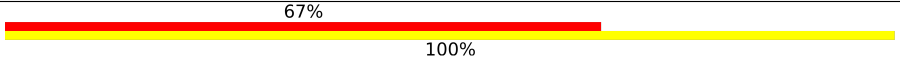
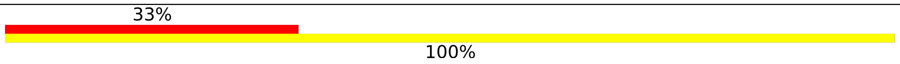
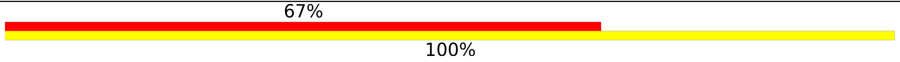
Mol	Chain	Length	Quality of chain
4	I	232	
4	K	232	
4	L	232	
5	M	8	
5	Z	8	
5	m	8	
6	N	2	
6	U	2	
6	X	2	
6	Y	2	
6	a	2	
6	h	2	
6	k	2	
6	l	2	
6	n	2	
6	u	2	
6	x	2	
7	O	3	
7	P	3	
7	Q	3	
7	V	3	
7	b	3	
7	c	3	
7	d	3	
7	i	3	

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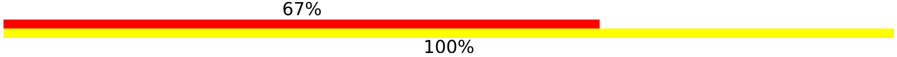
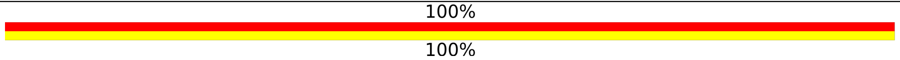
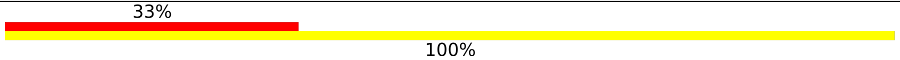
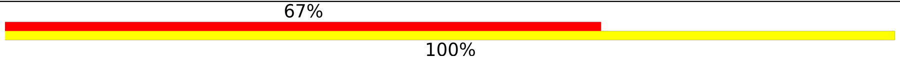
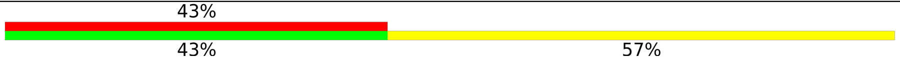
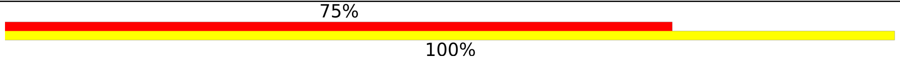
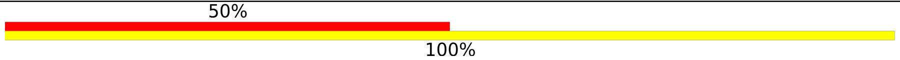
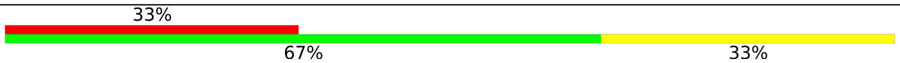
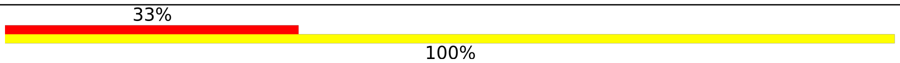
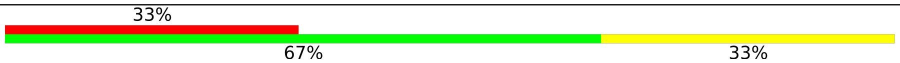
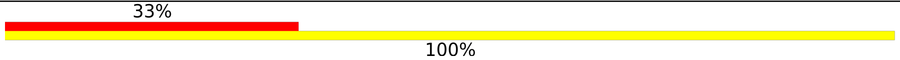
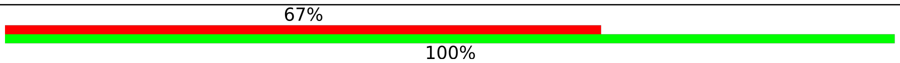
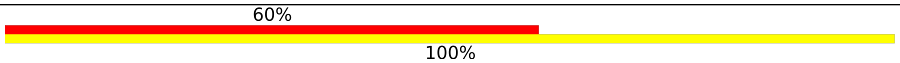
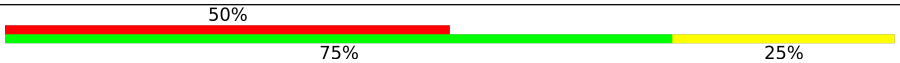
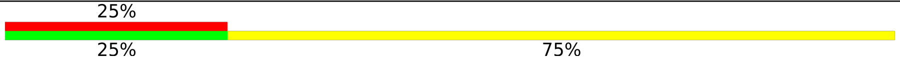
Mol	Chain	Length	Quality of chain
7	o	3	
7	p	3	
7	q	3	
7	v	3	
8	R	7	
8	e	7	
8	r	7	
9	S	4	
9	s	4	
10	T	3	
10	W	3	
10	g	3	
10	j	3	
10	y	3	
11	f	5	
12	t	4	
12	w	4	

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 23045 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	493	3953	2477	688	751	37	0	0
1	C	493	3953	2477	688	751	37	0	0
1	E	493	3953	2477	688	751	37	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	SER	LYS	engineered mutation	UNP A0A5C0E975
A	511	SER	ASP	conflict	UNP A0A5C0E975
A	512	CYS	VAL	conflict	UNP A0A5C0E975
A	523	ARG	ASN	conflict	UNP A0A5C0E975
A	526	ARG	-	expression tag	UNP A0A5C0E975
A	527	ARG	-	expression tag	UNP A0A5C0E975
C	180	SER	LYS	engineered mutation	UNP A0A5C0E975
C	511	SER	ASP	conflict	UNP A0A5C0E975
C	512	CYS	VAL	conflict	UNP A0A5C0E975
C	523	ARG	ASN	conflict	UNP A0A5C0E975
C	526	ARG	-	expression tag	UNP A0A5C0E975
C	527	ARG	-	expression tag	UNP A0A5C0E975
E	180	SER	LYS	engineered mutation	UNP A0A5C0E975
E	511	SER	ASP	conflict	UNP A0A5C0E975
E	512	CYS	VAL	conflict	UNP A0A5C0E975
E	523	ARG	ASN	conflict	UNP A0A5C0E975
E	526	ARG	-	expression tag	UNP A0A5C0E975
E	527	ARG	-	expression tag	UNP A0A5C0E975

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	142	Total 1138	C 724	N 198	O 212	S 4	0	0
2	D	142	Total 1138	C 724	N 198	O 212	S 4	0	0
2	F	142	Total 1138	C 724	N 198	O 212	S 4	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	574	PRO	VAL	conflict	UNP L7XFX7
B	620	CYS	HIS	conflict	UNP L7XFX7
B	676	GLY	-	expression tag	UNP L7XFX7
B	677	SER	-	expression tag	UNP L7XFX7
B	678	GLY	-	expression tag	UNP L7XFX7
B	679	HIS	-	expression tag	UNP L7XFX7
B	680	HIS	-	expression tag	UNP L7XFX7
B	681	HIS	-	expression tag	UNP L7XFX7
B	682	HIS	-	expression tag	UNP L7XFX7
B	683	HIS	-	expression tag	UNP L7XFX7
B	684	HIS	-	expression tag	UNP L7XFX7
B	685	HIS	-	expression tag	UNP L7XFX7
B	686	HIS	-	expression tag	UNP L7XFX7
D	574	PRO	VAL	conflict	UNP L7XFX7
D	620	CYS	HIS	conflict	UNP L7XFX7
D	676	GLY	-	expression tag	UNP L7XFX7
D	677	SER	-	expression tag	UNP L7XFX7
D	678	GLY	-	expression tag	UNP L7XFX7
D	679	HIS	-	expression tag	UNP L7XFX7
D	680	HIS	-	expression tag	UNP L7XFX7
D	681	HIS	-	expression tag	UNP L7XFX7
D	682	HIS	-	expression tag	UNP L7XFX7
D	683	HIS	-	expression tag	UNP L7XFX7
D	684	HIS	-	expression tag	UNP L7XFX7
D	685	HIS	-	expression tag	UNP L7XFX7
D	686	HIS	-	expression tag	UNP L7XFX7
F	574	PRO	VAL	conflict	UNP L7XFX7
F	620	CYS	HIS	conflict	UNP L7XFX7
F	676	GLY	-	expression tag	UNP L7XFX7
F	677	SER	-	expression tag	UNP L7XFX7
F	678	GLY	-	expression tag	UNP L7XFX7
F	679	HIS	-	expression tag	UNP L7XFX7
F	680	HIS	-	expression tag	UNP L7XFX7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	681	HIS	-	expression tag	UNP L7XFX7
F	682	HIS	-	expression tag	UNP L7XFX7
F	683	HIS	-	expression tag	UNP L7XFX7
F	684	HIS	-	expression tag	UNP L7XFX7
F	685	HIS	-	expression tag	UNP L7XFX7
F	686	HIS	-	expression tag	UNP L7XFX7

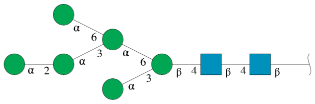
- Molecule 3 is a protein called K11 IgG heavy chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	H	132	Total C N O S 1028 650 173 199 6	0	0
3	G	132	Total C N O S 1028 650 173 199 6	0	0
3	J	132	Total C N O S 1028 650 173 199 6	0	0

- Molecule 4 is a protein called K11 IgG light chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	L	106	Total C N O S 811 512 135 162 2	0	0
4	I	106	Total C N O S 811 512 135 162 2	0	0
4	K	106	Total C N O S 811 512 135 162 2	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
5	M	8	Total C N O 94 52 2 40	0	0
5	Z	8	Total C N O 94 52 2 40	0	0

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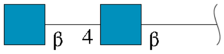
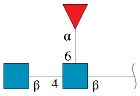
Mol	Chain	Residues	Atoms	AltConf	Trace
5	m	8	Total C N O 94 52 2 40	0	0

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



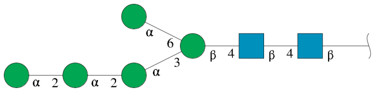
Mol	Chain	Residues	Atoms	AltConf	Trace
6	N	2	Total C N O 28 16 2 10	0	0
6	U	2	Total C N O 28 16 2 10	0	0
6	X	2	Total C N O 28 16 2 10	0	0
6	Y	2	Total C N O 28 16 2 10	0	0
6	a	2	Total C N O 28 16 2 10	0	0
6	h	2	Total C N O 28 16 2 10	0	0
6	k	2	Total C N O 28 16 2 10	0	0
6	l	2	Total C N O 28 16 2 10	0	0
6	n	2	Total C N O 28 16 2 10	0	0
6	u	2	Total C N O 28 16 2 10	0	0
6	x	2	Total C N O 28 16 2 10	0	0

- Molecule 7 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.



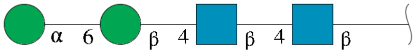
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total 38	C 22	N 2	O 14	0	0
7	P	3	Total 38	C 22	N 2	O 14	0	0
7	Q	3	Total 38	C 22	N 2	O 14	0	0
7	V	3	Total 38	C 22	N 2	O 14	0	0
7	b	3	Total 38	C 22	N 2	O 14	0	0
7	c	3	Total 38	C 22	N 2	O 14	0	0
7	d	3	Total 38	C 22	N 2	O 14	0	0
7	i	3	Total 38	C 22	N 2	O 14	0	0
7	o	3	Total 38	C 22	N 2	O 14	0	0
7	p	3	Total 38	C 22	N 2	O 14	0	0
7	q	3	Total 38	C 22	N 2	O 14	0	0
7	v	3	Total 38	C 22	N 2	O 14	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



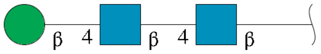
Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	7	Total 83	C 46	N 2	O 35	0	0
8	e	7	Total 83	C 46	N 2	O 35	0	0
8	r	7	Total 83	C 46	N 2	O 35	0	0

- Molecule 9 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-gluco pyranose.



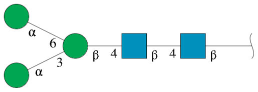
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	S	4	50	28	2	20	0	0
9	s	4	50	28	2	20	0	0

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



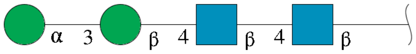
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	T	3	39	22	2	15	0	0
10	W	3	39	22	2	15	0	0
10	g	3	39	22	2	15	0	0
10	j	3	39	22	2	15	0	0
10	y	3	39	22	2	15	0	0

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



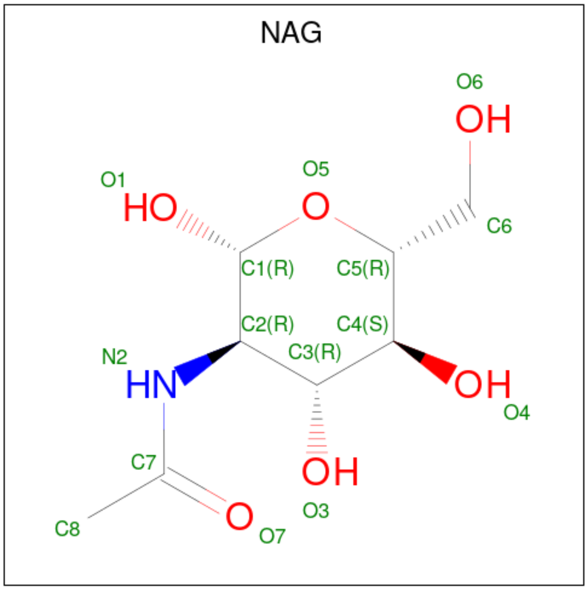
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	f	5	61	34	2	25	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
12	t	4	Total C N O 50 28 2 20	0	0
12	w	4	Total C N O 50 28 2 20	0	0

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



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

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

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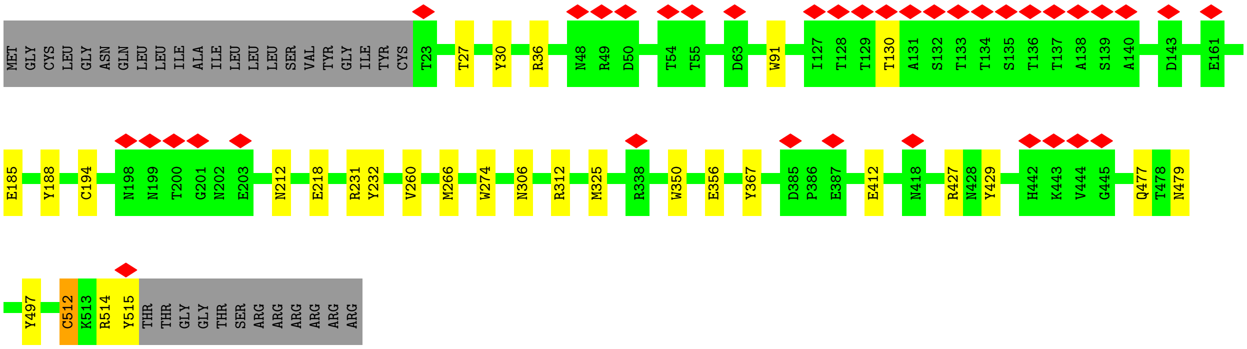
Mol	Chain	Residues	Atoms	AltConf
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	E	1	Total C N O 14 8 1 5	0
13	F	1	Total C N O 14 8 1 5	0
13	F	1	Total C N O 14 8 1 5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

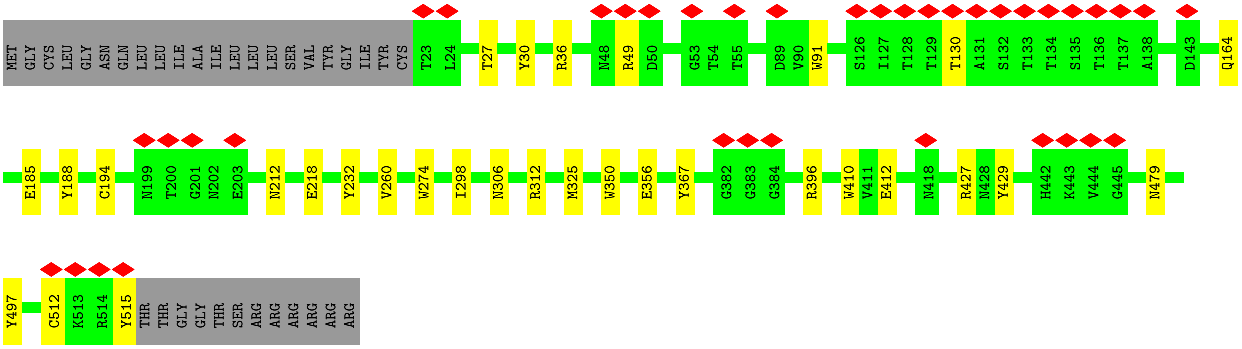
- Molecule 1: Envelope glycoprotein gp120

Chain A:



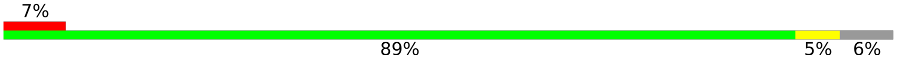
- Molecule 1: Envelope glycoprotein gp120

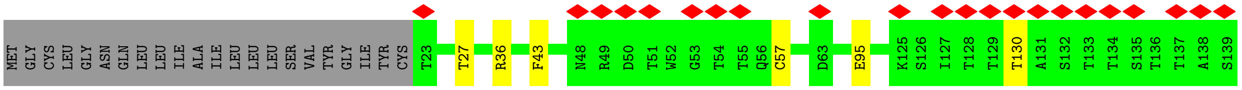
Chain C:

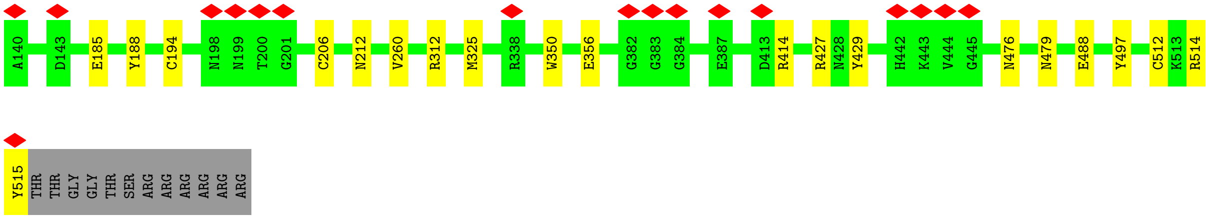


- Molecule 1: Envelope glycoprotein gp120

Chain E:

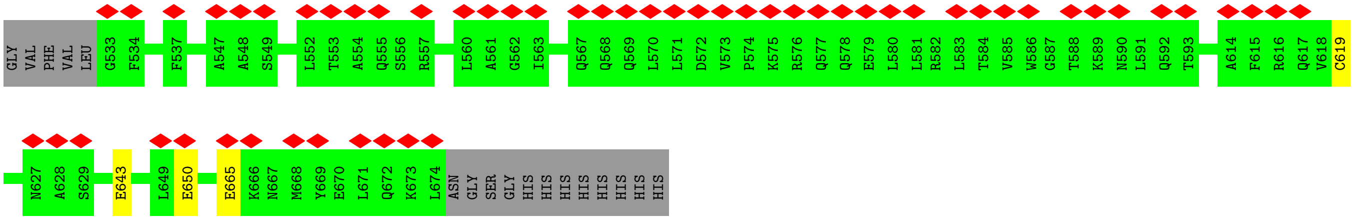






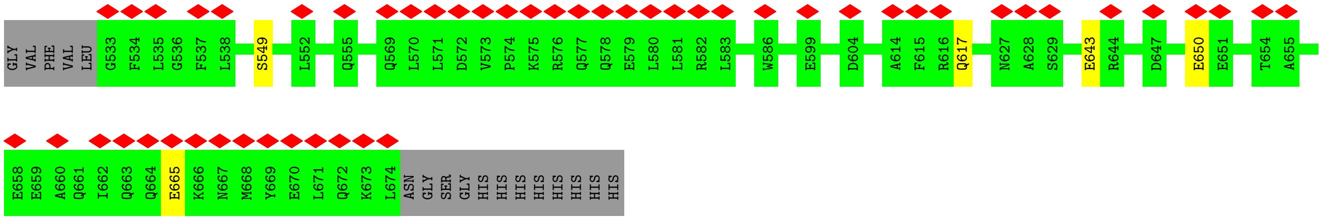
- Molecule 2: Envelope glycoprotein gp41

Chain B:



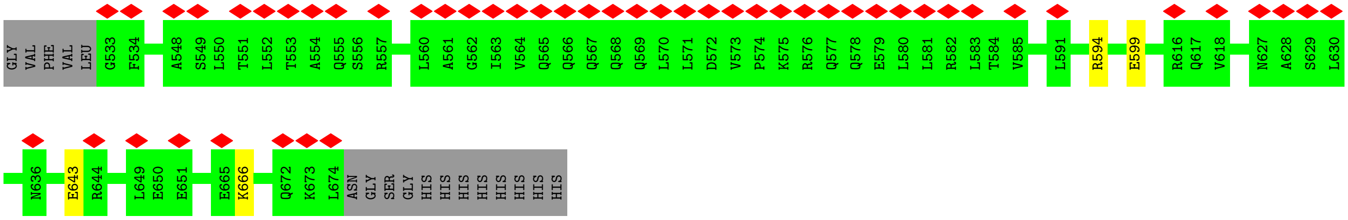
- Molecule 2: Envelope glycoprotein gp41

Chain D:



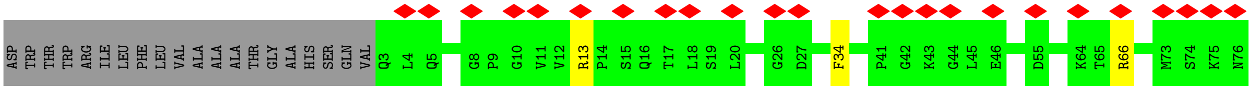
- Molecule 2: Envelope glycoprotein gp41

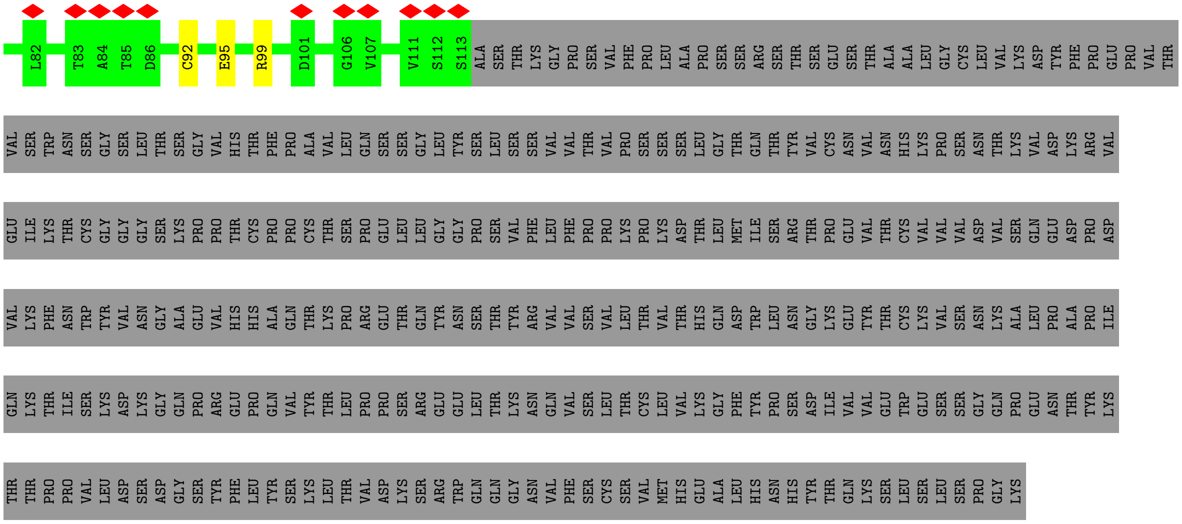
Chain F:



- Molecule 3: K11 IgG heavy chain

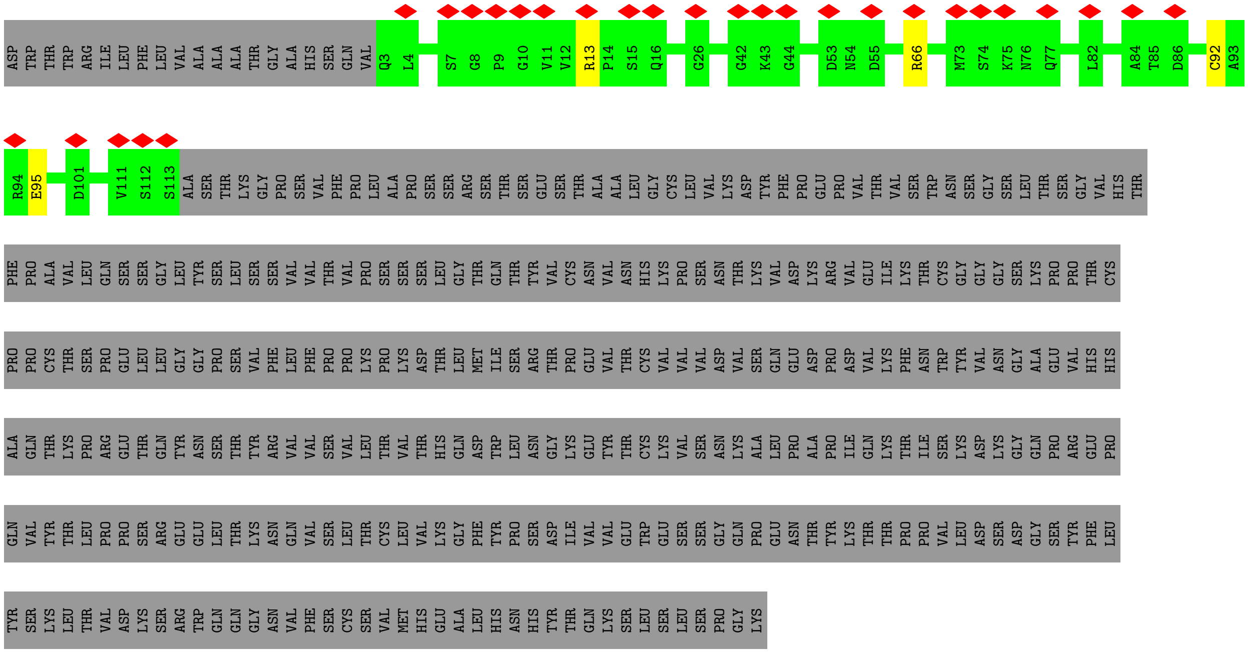
Chain H:





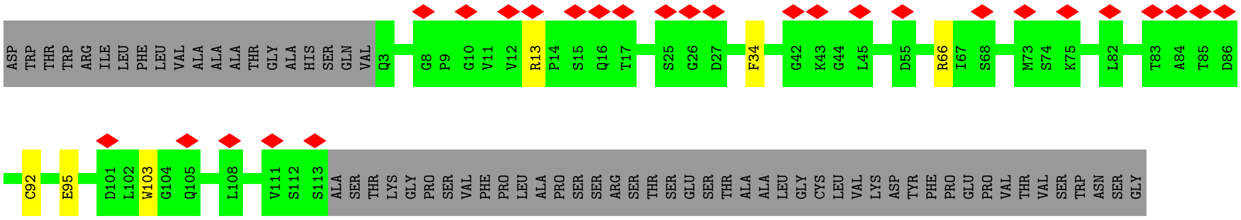
- Molecule 3: K11 IgG heavy chain

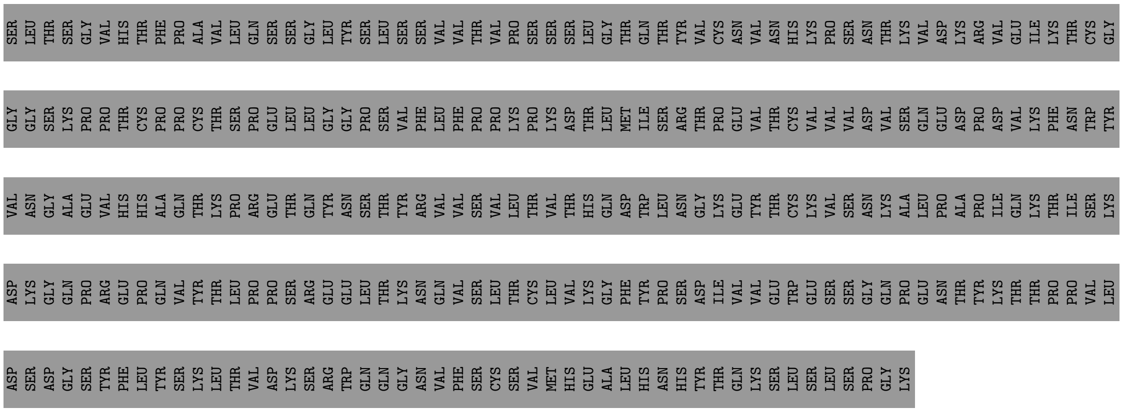
Chain G:



- Molecule 3: K11 IgG heavy chain

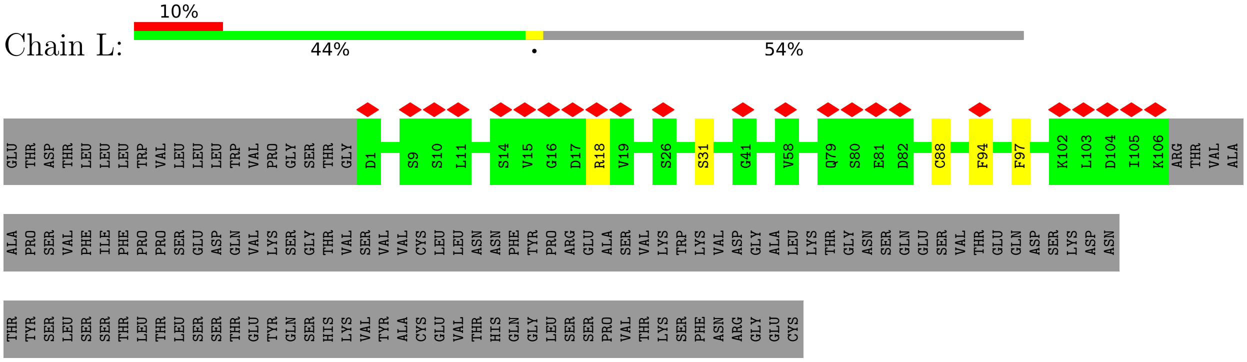
Chain J:





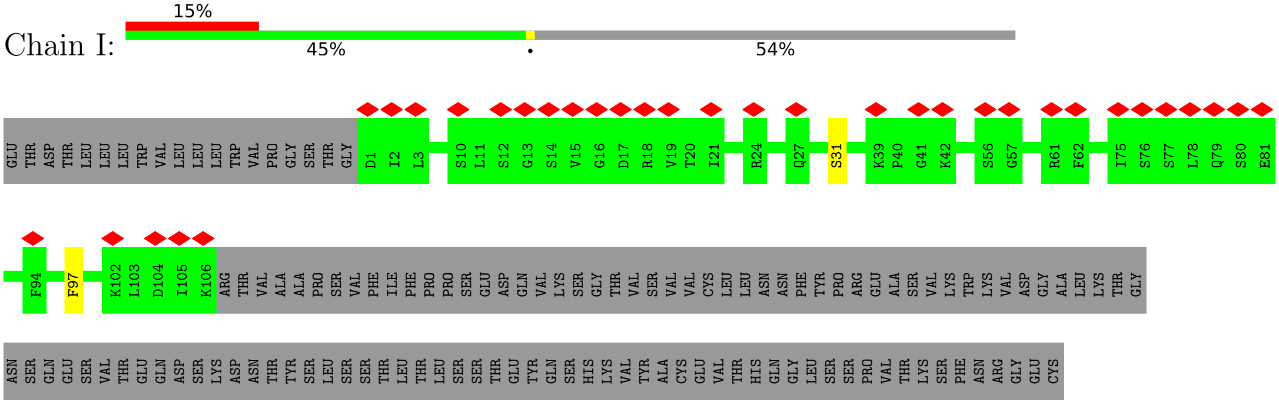
- Molecule 4: K11 IgG light chain

Chain L:



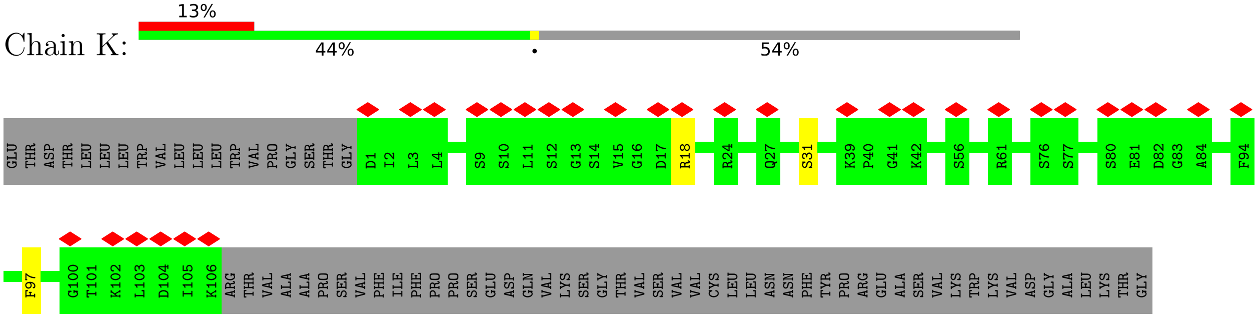
- Molecule 4: K11 IgG light chain

Chain I:



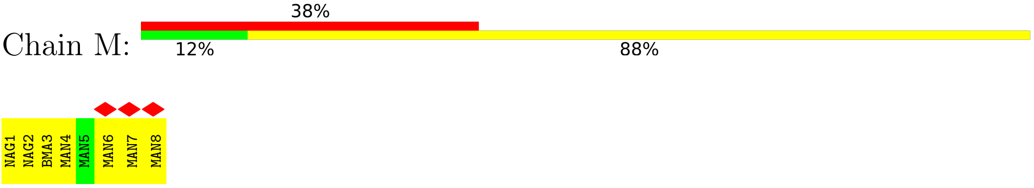
- Molecule 4: K11 IgG light chain

Chain K:



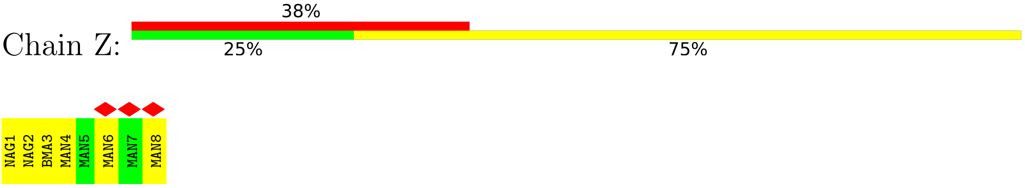
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



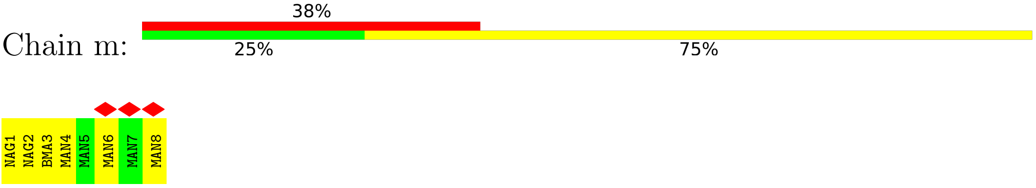
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



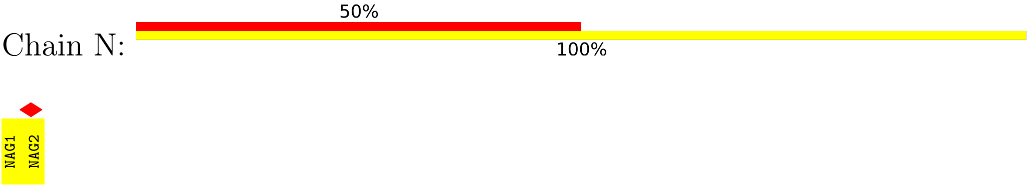
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



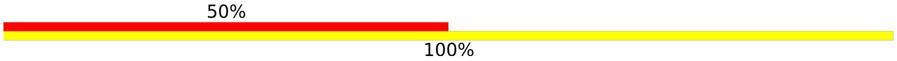
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



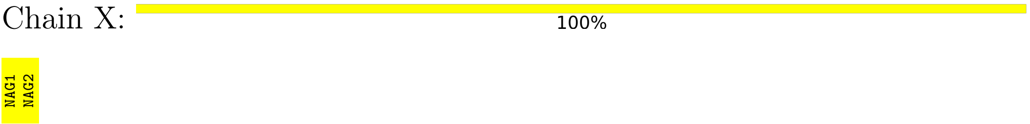
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



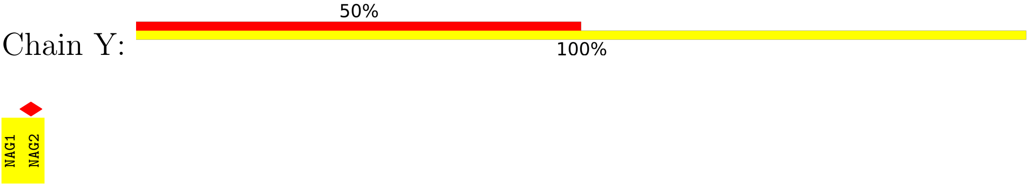
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



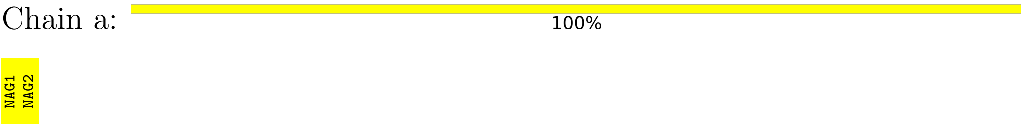
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



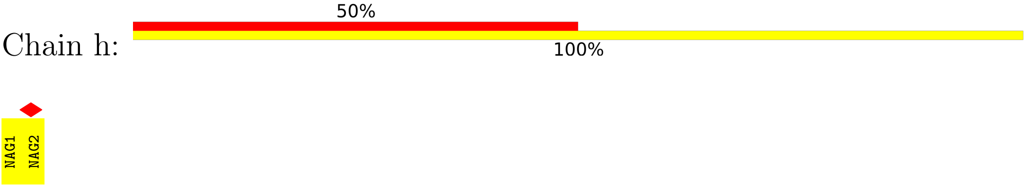
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



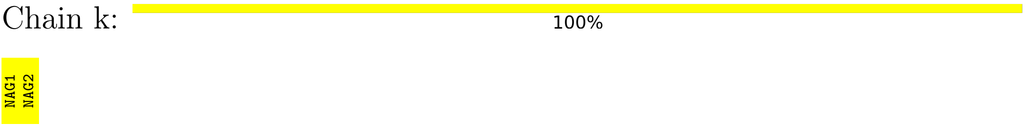
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



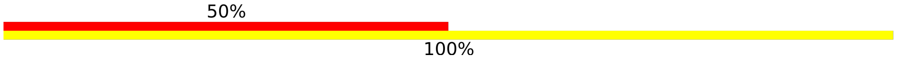
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



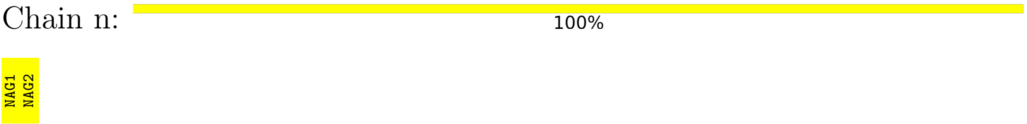
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



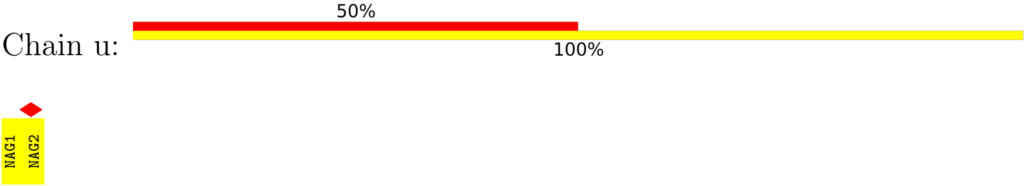
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



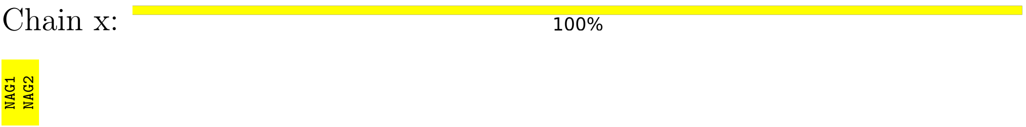
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



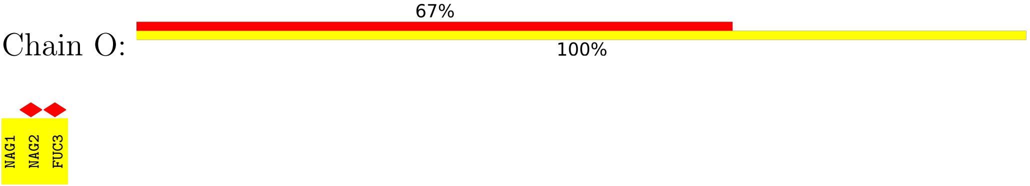
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



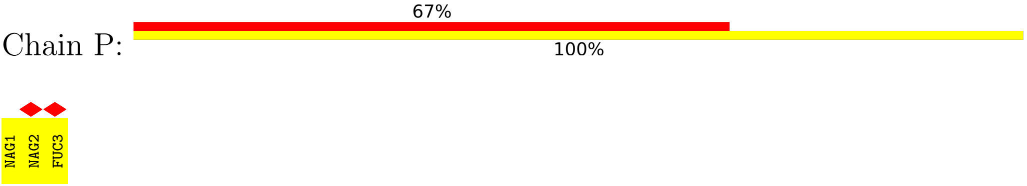
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



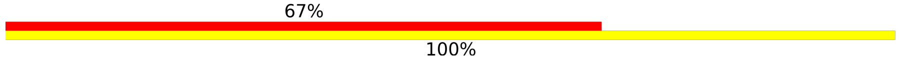
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



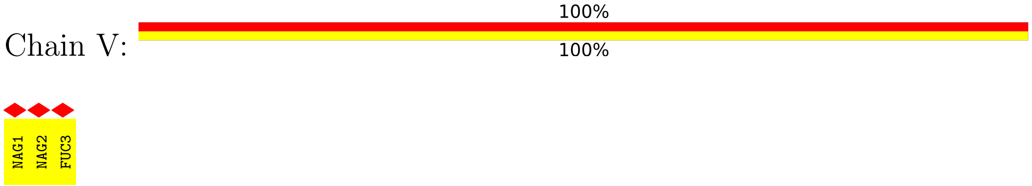
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



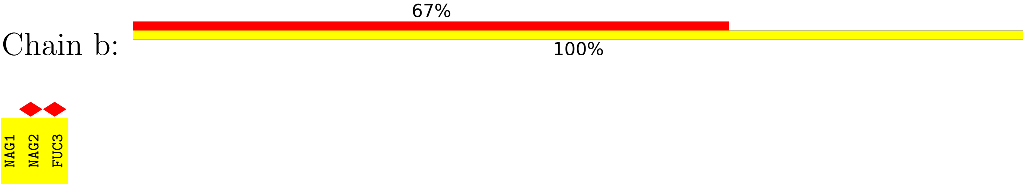
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



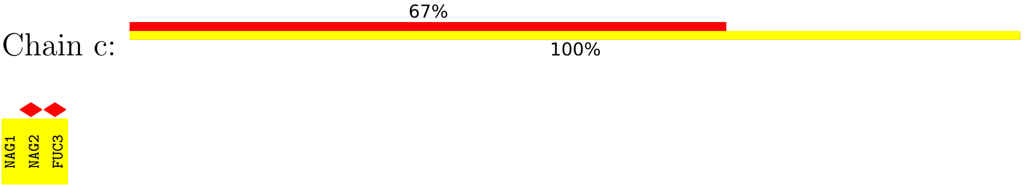
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



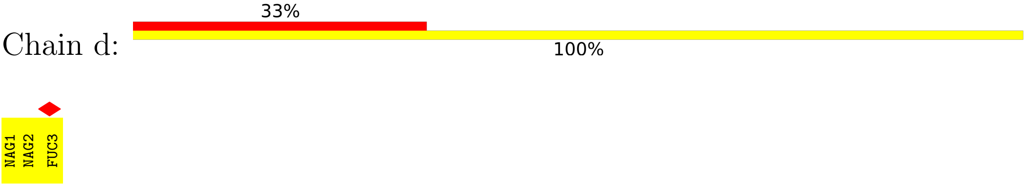
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



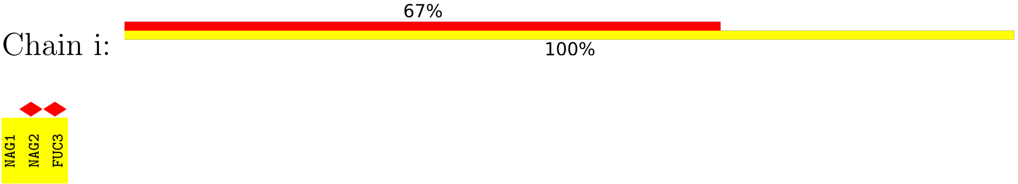
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



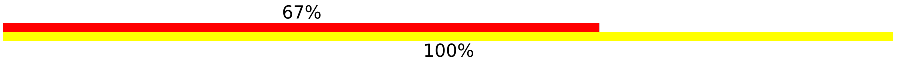
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



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

Chain o:

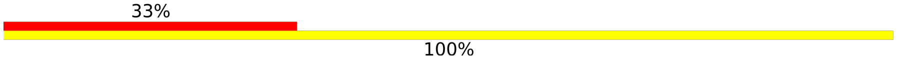


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

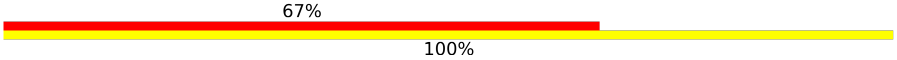
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



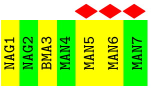
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



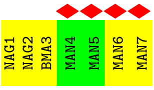
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



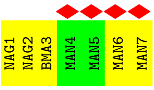
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



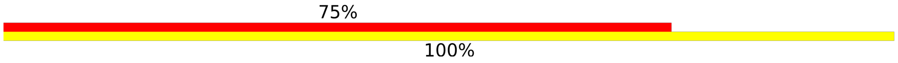
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

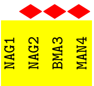
Chain r:



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

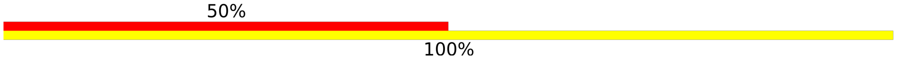
Chain S:





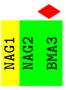
- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



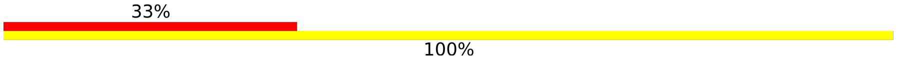
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



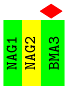
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



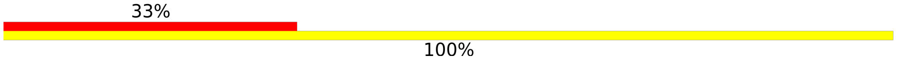
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



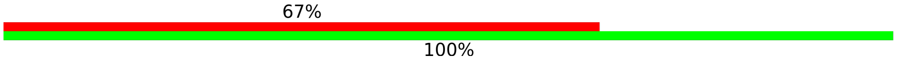
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



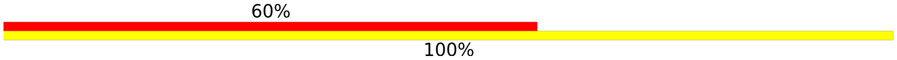
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

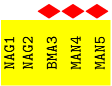
Chain y:



- Molecule 11: 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

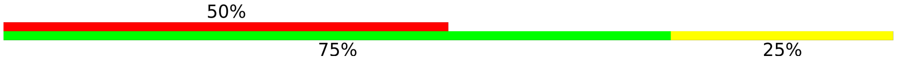
Chain f:

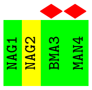




- Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

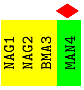
Chain t:





- Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.812	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.12	20/4050 (0.5%)	0.95	11/5506 (0.2%)
1	C	1.13	21/4050 (0.5%)	0.95	7/5506 (0.1%)
1	E	1.11	20/4050 (0.5%)	0.94	6/5506 (0.1%)
2	B	1.08	4/1159 (0.3%)	0.85	0/1574
2	D	1.03	5/1159 (0.4%)	0.81	0/1574
2	F	1.03	2/1159 (0.2%)	0.84	1/1574 (0.1%)
3	G	1.03	2/1055 (0.2%)	0.97	3/1438 (0.2%)
3	H	1.09	3/1055 (0.3%)	0.98	4/1438 (0.3%)
3	J	1.12	4/1055 (0.4%)	0.98	3/1438 (0.2%)
4	I	0.94	0/829	0.91	0/1124
4	K	0.93	0/829	0.96	1/1124 (0.1%)
4	L	0.95	1/829 (0.1%)	0.97	1/1124 (0.1%)
All	All	1.08	82/21279 (0.4%)	0.93	37/28926 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	92	CYS	CB-SG	-9.69	1.65	1.82
3	H	92	CYS	CB-SG	-8.77	1.67	1.82
3	J	92	CYS	CB-SG	-8.19	1.68	1.82
1	A	515	TYR	CG-CD1	8.17	1.49	1.39
1	C	515	TYR	CE1-CZ	8.01	1.49	1.38

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	427	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	E	427	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	C	312	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	C	427	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	312	ARG	NE-CZ-NH2	-9.97	115.31	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	491/527 (93%)	469 (96%)	13 (3%)	9 (2%)	8	41
1	C	491/527 (93%)	467 (95%)	15 (3%)	9 (2%)	8	41
1	E	491/527 (93%)	467 (95%)	17 (4%)	7 (1%)	11	45
2	B	140/159 (88%)	132 (94%)	7 (5%)	1 (1%)	22	59
2	D	140/159 (88%)	132 (94%)	6 (4%)	2 (1%)	11	45
2	F	140/159 (88%)	134 (96%)	6 (4%)	0	100	100
3	G	130/485 (27%)	129 (99%)	1 (1%)	0	100	100
3	H	130/485 (27%)	129 (99%)	1 (1%)	0	100	100
3	J	130/485 (27%)	130 (100%)	0	0	100	100
4	I	104/232 (45%)	99 (95%)	3 (3%)	2 (2%)	8	40
4	K	104/232 (45%)	99 (95%)	3 (3%)	2 (2%)	8	40
4	L	104/232 (45%)	99 (95%)	2 (2%)	3 (3%)	4	32
All	All	2595/4209 (62%)	2486 (96%)	74 (3%)	35 (1%)	16	47

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	MET
1	A	479	ASN
1	C	325	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	479	ASN
1	E	325	MET

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	443/471 (94%)	442 (100%)	1 (0%)	93	97
1	C	443/471 (94%)	441 (100%)	2 (0%)	88	94
1	E	443/471 (94%)	442 (100%)	1 (0%)	93	97
2	B	120/135 (89%)	120 (100%)	0	100	100
2	D	120/135 (89%)	120 (100%)	0	100	100
2	F	120/135 (89%)	119 (99%)	1 (1%)	81	89
3	G	116/436 (27%)	116 (100%)	0	100	100
3	H	116/436 (27%)	116 (100%)	0	100	100
3	J	116/436 (27%)	116 (100%)	0	100	100
4	I	91/205 (44%)	91 (100%)	0	100	100
4	K	91/205 (44%)	91 (100%)	0	100	100
4	L	91/205 (44%)	91 (100%)	0	100	100
All	All	2310/3741 (62%)	2305 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	C	298	ILE
1	C	306	ASN
1	E	476	ASN
2	F	666	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	HIS
1	C	270	GLN
1	E	291	HIS
1	E	433	HIS

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 ⓘ

139 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	M	1	1,5	14,14,15	2.02	4 (28%)	17,19,21	0.98	1 (5%)
5	NAG	M	2	5	14,14,15	1.78	6 (42%)	17,19,21	1.29	1 (5%)
5	BMA	M	3	5	11,11,12	1.42	3 (27%)	15,15,17	0.59	0
5	MAN	M	4	5	11,11,12	1.40	2 (18%)	15,15,17	0.87	0
5	MAN	M	5	5	11,11,12	0.63	0	15,15,17	0.77	0
5	MAN	M	6	5	11,11,12	1.96	6 (54%)	15,15,17	0.70	0
5	MAN	M	7	5	11,11,12	0.86	1 (9%)	15,15,17	0.84	0
5	MAN	M	8	5	11,11,12	1.96	6 (54%)	15,15,17	0.69	0
6	NAG	N	1	6,1	14,14,15	2.01	5 (35%)	17,19,21	1.26	2 (11%)
6	NAG	N	2	6	14,14,15	1.99	5 (35%)	17,19,21	0.84	1 (5%)
7	NAG	O	1	7,1	14,14,15	1.42	2 (14%)	17,19,21	0.96	2 (11%)
7	NAG	O	2	7	14,14,15	1.92	5 (35%)	17,19,21	0.92	1 (5%)
7	FUC	O	3	7	10,10,11	1.93	5 (50%)	14,14,16	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	P	1	7,1	14,14,15	1.46	2 (14%)	17,19,21	1.02	1 (5%)
7	NAG	P	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.79	0
7	FUC	P	3	7	10,10,11	1.96	5 (50%)	14,14,16	0.69	0
7	NAG	Q	1	7,1	14,14,15	1.45	2 (14%)	17,19,21	1.12	1 (5%)
7	NAG	Q	2	7	14,14,15	2.03	4 (28%)	17,19,21	0.83	0
7	FUC	Q	3	7	10,10,11	1.82	5 (50%)	14,14,16	0.70	0
8	NAG	R	1	8,1	14,14,15	0.55	0	17,19,21	1.48	1 (5%)
8	NAG	R	2	8	14,14,15	0.42	0	17,19,21	0.64	0
8	BMA	R	3	8	11,11,12	0.36	0	15,15,17	1.27	2 (13%)
8	MAN	R	4	8	11,11,12	0.33	0	15,15,17	0.84	0
8	MAN	R	5	8	11,11,12	0.23	0	15,15,17	1.08	1 (6%)
8	MAN	R	6	8	11,11,12	0.20	0	15,15,17	0.76	1 (6%)
8	MAN	R	7	8	11,11,12	0.22	0	15,15,17	0.71	0
9	NAG	S	1	9,1	14,14,15	2.01	4 (28%)	17,19,21	0.98	1 (5%)
9	NAG	S	2	9	14,14,15	1.99	6 (42%)	17,19,21	0.90	1 (5%)
9	BMA	S	3	9	11,11,12	1.48	3 (27%)	15,15,17	0.61	0
9	MAN	S	4	9	11,11,12	1.98	5 (45%)	15,15,17	0.72	0
10	NAG	T	1	1,10	14,14,15	0.56	0	17,19,21	1.39	4 (23%)
10	NAG	T	2	10	14,14,15	0.44	0	17,19,21	0.83	0
10	BMA	T	3	10	11,11,12	0.21	0	15,15,17	0.63	0
6	NAG	U	1	6,1	14,14,15	2.16	6 (42%)	17,19,21	1.00	1 (5%)
6	NAG	U	2	6	14,14,15	1.95	5 (35%)	17,19,21	0.85	1 (5%)
7	NAG	V	1	7,1	14,14,15	1.47	2 (14%)	17,19,21	0.91	1 (5%)
7	NAG	V	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.96	2 (11%)
7	FUC	V	3	7	10,10,11	2.06	6 (60%)	14,14,16	0.63	0
10	NAG	W	1	1,10	14,14,15	1.91	3 (21%)	17,19,21	1.25	2 (11%)
10	NAG	W	2	10	14,14,15	2.01	6 (42%)	17,19,21	0.99	1 (5%)
10	BMA	W	3	10	11,11,12	2.02	6 (54%)	15,15,17	0.68	0
6	NAG	X	1	6,1	14,14,15	2.03	7 (50%)	17,19,21	1.61	3 (17%)
6	NAG	X	2	6	14,14,15	1.90	6 (42%)	17,19,21	0.93	1 (5%)
6	NAG	Y	1	6,1	14,14,15	2.03	6 (42%)	17,19,21	1.07	1 (5%)
6	NAG	Y	2	6	14,14,15	1.98	5 (35%)	17,19,21	0.86	1 (5%)
5	NAG	Z	1	1,5	14,14,15	2.01	5 (35%)	17,19,21	0.97	1 (5%)
5	NAG	Z	2	5	14,14,15	1.86	6 (42%)	17,19,21	1.31	2 (11%)
5	BMA	Z	3	5	11,11,12	1.41	3 (27%)	15,15,17	0.59	0
5	MAN	Z	4	5	11,11,12	1.41	2 (18%)	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	Z	5	5	11,11,12	0.69	0	15,15,17	0.82	0
5	MAN	Z	6	5	11,11,12	1.98	6 (54%)	15,15,17	0.68	0
5	MAN	Z	7	5	11,11,12	0.78	0	15,15,17	0.88	0
5	MAN	Z	8	5	11,11,12	2.01	6 (54%)	15,15,17	0.68	0
6	NAG	a	1	6,1	14,14,15	2.05	6 (42%)	17,19,21	1.09	2 (11%)
6	NAG	a	2	6	14,14,15	1.94	5 (35%)	17,19,21	0.83	0
7	NAG	b	1	7,1	14,14,15	1.45	2 (14%)	17,19,21	0.95	1 (5%)
7	NAG	b	2	7	14,14,15	1.93	6 (42%)	17,19,21	0.93	1 (5%)
7	FUC	b	3	7	10,10,11	1.94	5 (50%)	14,14,16	0.64	0
7	NAG	c	1	7,1	14,14,15	1.43	2 (14%)	17,19,21	1.00	1 (5%)
7	NAG	c	2	7	14,14,15	2.06	7 (50%)	17,19,21	0.82	1 (5%)
7	FUC	c	3	7	10,10,11	1.93	5 (50%)	14,14,16	0.67	0
7	NAG	d	1	7,1	14,14,15	1.44	2 (14%)	17,19,21	1.07	1 (5%)
7	NAG	d	2	7	14,14,15	2.01	5 (35%)	17,19,21	0.86	1 (5%)
7	FUC	d	3	7	10,10,11	1.85	5 (50%)	14,14,16	0.71	0
8	NAG	e	1	8,1	14,14,15	1.85	4 (28%)	17,19,21	1.18	1 (5%)
8	NAG	e	2	8	14,14,15	1.87	5 (35%)	17,19,21	0.85	1 (5%)
8	BMA	e	3	8	11,11,12	1.36	3 (27%)	15,15,17	0.68	0
8	MAN	e	4	8	11,11,12	0.69	0	15,15,17	0.72	0
8	MAN	e	5	8	11,11,12	0.67	0	15,15,17	0.90	0
8	MAN	e	6	8	11,11,12	2.13	5 (45%)	15,15,17	0.72	0
8	MAN	e	7	8	11,11,12	1.93	5 (45%)	15,15,17	0.74	0
11	NAG	f	1	1,11	14,14,15	1.99	4 (28%)	17,19,21	0.97	0
11	NAG	f	2	11	14,14,15	1.93	5 (35%)	17,19,21	0.89	1 (5%)
11	BMA	f	3	11	11,11,12	1.47	3 (27%)	15,15,17	0.61	0
11	MAN	f	4	11	11,11,12	1.98	5 (45%)	15,15,17	0.72	0
11	MAN	f	5	11	11,11,12	1.99	5 (45%)	15,15,17	0.73	0
10	NAG	g	1	1,10	14,14,15	0.50	0	17,19,21	0.79	0
10	NAG	g	2	10	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
10	BMA	g	3	10	11,11,12	0.23	0	15,15,17	0.71	0
6	NAG	h	1	6,1	14,14,15	2.17	6 (42%)	17,19,21	0.96	1 (5%)
6	NAG	h	2	6	14,14,15	1.96	6 (42%)	17,19,21	0.84	1 (5%)
7	NAG	i	1	7,1	14,14,15	1.62	2 (14%)	17,19,21	1.16	2 (11%)
7	NAG	i	2	7	14,14,15	2.10	6 (42%)	17,19,21	1.05	2 (11%)
7	FUC	i	3	7	10,10,11	2.00	5 (50%)	14,14,16	0.59	0
10	NAG	j	1	1,10	14,14,15	1.91	4 (28%)	17,19,21	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
10	NAG	j	2	10	14,14,15	1.98	6 (42%)	17,19,21	1.03	1 (5%)
10	BMA	j	3	10	11,11,12	2.03	6 (54%)	15,15,17	0.74	0
6	NAG	k	1	6,1	14,14,15	2.08	7 (50%)	17,19,21	1.64	3 (17%)
6	NAG	k	2	6	14,14,15	1.91	6 (42%)	17,19,21	0.93	1 (5%)
6	NAG	l	1	6,1	14,14,15	1.97	6 (42%)	17,19,21	1.04	1 (5%)
6	NAG	l	2	6	14,14,15	1.91	4 (28%)	17,19,21	0.87	1 (5%)
5	NAG	m	1	1,5	14,14,15	2.09	5 (35%)	17,19,21	1.05	1 (5%)
5	NAG	m	2	5	14,14,15	1.87	6 (42%)	17,19,21	1.29	2 (11%)
5	BMA	m	3	5	11,11,12	1.39	3 (27%)	15,15,17	0.61	0
5	MAN	m	4	5	11,11,12	1.38	2 (18%)	15,15,17	0.85	1 (6%)
5	MAN	m	5	5	11,11,12	0.67	0	15,15,17	0.78	0
5	MAN	m	6	5	11,11,12	1.93	6 (54%)	15,15,17	0.69	0
5	MAN	m	7	5	11,11,12	0.80	0	15,15,17	0.92	0
5	MAN	m	8	5	11,11,12	1.97	5 (45%)	15,15,17	0.67	0
6	NAG	n	1	6,1	14,14,15	1.97	6 (42%)	17,19,21	1.10	1 (5%)
6	NAG	n	2	6	14,14,15	1.94	4 (28%)	17,19,21	0.82	1 (5%)
7	NAG	o	1	7,1	14,14,15	1.43	2 (14%)	17,19,21	0.96	1 (5%)
7	NAG	o	2	7	14,14,15	1.89	5 (35%)	17,19,21	0.90	0
7	FUC	o	3	7	10,10,11	1.95	5 (50%)	14,14,16	0.65	0
7	NAG	p	1	7,1	14,14,15	1.51	2 (14%)	17,19,21	1.06	1 (5%)
7	NAG	p	2	7	14,14,15	2.09	7 (50%)	17,19,21	0.88	1 (5%)
7	FUC	p	3	7	10,10,11	1.99	5 (50%)	14,14,16	0.63	0
7	NAG	q	1	7,1	14,14,15	1.51	2 (14%)	17,19,21	1.08	1 (5%)
7	NAG	q	2	7	14,14,15	1.96	5 (35%)	17,19,21	0.88	1 (5%)
7	FUC	q	3	7	10,10,11	1.83	5 (50%)	14,14,16	0.71	0
8	NAG	r	1	8,1	14,14,15	1.80	3 (21%)	17,19,21	1.15	1 (5%)
8	NAG	r	2	8	14,14,15	1.83	5 (35%)	17,19,21	0.77	0
8	BMA	r	3	8	11,11,12	1.39	3 (27%)	15,15,17	0.73	0
8	MAN	r	4	8	11,11,12	0.65	0	15,15,17	0.70	0
8	MAN	r	5	8	11,11,12	0.66	0	15,15,17	0.84	0
8	MAN	r	6	8	11,11,12	2.07	5 (45%)	15,15,17	0.76	0
8	MAN	r	7	8	11,11,12	1.91	5 (45%)	15,15,17	0.72	0
9	NAG	s	1	9,1	14,14,15	1.94	4 (28%)	17,19,21	0.92	1 (5%)
9	NAG	s	2	9	14,14,15	1.93	6 (42%)	17,19,21	0.92	1 (5%)
9	BMA	s	3	9	11,11,12	1.47	3 (27%)	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
9	MAN	s	4	9	11,11,12	1.97	5 (45%)	15,15,17	0.74	0
12	NAG	t	1	1,12	14,14,15	0.53	0	17,19,21	0.93	0
12	NAG	t	2	12	14,14,15	0.38	0	17,19,21	0.97	1 (5%)
12	BMA	t	3	12	11,11,12	0.25	0	15,15,17	0.85	0
12	MAN	t	4	12	11,11,12	0.22	0	15,15,17	0.66	0
6	NAG	u	1	6,1	14,14,15	2.19	7 (50%)	17,19,21	1.09	2 (11%)
6	NAG	u	2	6	14,14,15	1.94	5 (35%)	17,19,21	0.83	0
7	NAG	v	1	7,1	14,14,15	1.58	2 (14%)	17,19,21	1.12	1 (5%)
7	NAG	v	2	7	14,14,15	2.02	6 (42%)	17,19,21	1.03	2 (11%)
7	FUC	v	3	7	10,10,11	2.03	6 (60%)	14,14,16	0.60	0
12	NAG	w	1	1,12	14,14,15	0.60	0	17,19,21	1.15	3 (17%)
12	NAG	w	2	12	14,14,15	0.47	0	17,19,21	0.93	1 (5%)
12	BMA	w	3	12	11,11,12	0.42	0	15,15,17	1.07	1 (6%)
12	MAN	w	4	12	11,11,12	0.22	0	15,15,17	0.64	0
6	NAG	x	1	6,1	14,14,15	2.03	7 (50%)	17,19,21	1.63	3 (17%)
6	NAG	x	2	6	14,14,15	1.93	6 (42%)	17,19,21	0.95	1 (5%)
10	NAG	y	1	1,10	14,14,15	0.33	0	17,19,21	0.52	0
10	NAG	y	2	10	14,14,15	0.35	0	17,19,21	0.64	0
10	BMA	y	3	10	11,11,12	0.22	0	15,15,17	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	1/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	1/2/19/22	0/1/1/1
5	MAN	M	8	5	-	0/2/19/22	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
7	NAG	O	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	FUC	O	3	7	-	-	0/1/1/1
7	NAG	P	1	7,1	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	b	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	FUC	b	3	7	-	-	0/1/1/1
7	NAG	c	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	FUC	c	3	7	-	-	0/1/1/1
7	NAG	d	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	FUC	d	3	7	-	-	0/1/1/1
8	NAG	e	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	0/2/19/22	0/1/1/1
8	MAN	e	4	8	-	1/2/19/22	0/1/1/1
8	MAN	e	5	8	-	2/2/19/22	0/1/1/1
8	MAN	e	6	8	-	1/2/19/22	0/1/1/1
8	MAN	e	7	8	-	0/2/19/22	0/1/1/1
11	NAG	f	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	f	2	11	-	0/6/23/26	0/1/1/1
11	BMA	f	3	11	-	0/2/19/22	0/1/1/1
11	MAN	f	4	11	-	0/2/19/22	0/1/1/1
11	MAN	f	5	11	-	0/2/19/22	0/1/1/1
10	NAG	g	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	0/2/19/22	0/1/1/1
6	NAG	h	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
7	NAG	i	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	FUC	i	3	7	-	-	0/1/1/1
10	NAG	j	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	j	2	10	-	0/6/23/26	0/1/1/1
10	BMA	j	3	10	-	0/2/19/22	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	NAG	l	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	l	2	6	-	0/6/23/26	0/1/1/1
5	NAG	m	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	m	2	5	-	0/6/23/26	0/1/1/1
5	BMA	m	3	5	-	0/2/19/22	0/1/1/1
5	MAN	m	4	5	-	2/2/19/22	0/1/1/1
5	MAN	m	5	5	-	1/2/19/22	0/1/1/1
5	MAN	m	6	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	m	7	5	-	1/2/19/22	0/1/1/1
5	MAN	m	8	5	-	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
7	NAG	o	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	o	2	7	-	0/6/23/26	0/1/1/1
7	FUC	o	3	7	-	-	0/1/1/1
7	NAG	p	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	p	2	7	-	0/6/23/26	0/1/1/1
7	FUC	p	3	7	-	-	0/1/1/1
7	NAG	q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	q	2	7	-	1/6/23/26	0/1/1/1
7	FUC	q	3	7	-	-	0/1/1/1
8	NAG	r	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	r	2	8	-	0/6/23/26	0/1/1/1
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
8	MAN	r	4	8	-	1/2/19/22	0/1/1/1
8	MAN	r	5	8	-	2/2/19/22	0/1/1/1
8	MAN	r	6	8	-	2/2/19/22	0/1/1/1
8	MAN	r	7	8	-	0/2/19/22	0/1/1/1
9	NAG	s	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1
9	BMA	s	3	9	-	0/2/19/22	0/1/1/1
9	MAN	s	4	9	-	0/2/19/22	0/1/1/1
12	NAG	t	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	t	2	12	-	2/6/23/26	0/1/1/1
12	BMA	t	3	12	-	0/2/19/22	0/1/1/1
12	MAN	t	4	12	-	1/2/19/22	0/1/1/1
6	NAG	u	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	u	2	6	-	0/6/23/26	0/1/1/1
7	NAG	v	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
7	FUC	v	3	7	-	-	0/1/1/1
12	NAG	w	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	w	2	12	-	0/6/23/26	0/1/1/1
12	BMA	w	3	12	-	0/2/19/22	0/1/1/1
12	MAN	w	4	12	-	0/2/19/22	0/1/1/1
6	NAG	x	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	x	2	6	-	0/6/23/26	0/1/1/1
10	NAG	y	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	y	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1

The worst 5 of 495 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	u	1	NAG	C1-C2	5.36	1.60	1.52
6	h	1	NAG	C1-C2	5.36	1.60	1.52
6	U	1	NAG	C1-C2	5.22	1.60	1.52
10	W	1	NAG	C1-C2	5.18	1.60	1.52
7	p	2	NAG	C1-C2	5.12	1.60	1.52

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	1	NAG	C1-O5-C5	4.65	118.49	112.19
6	X	1	NAG	C2-N2-C7	4.47	129.26	122.90
6	x	1	NAG	C2-N2-C7	4.44	129.23	122.90
6	k	1	NAG	C2-N2-C7	4.41	129.18	122.90
5	m	2	NAG	C8-C7-N2	3.44	121.92	116.10

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

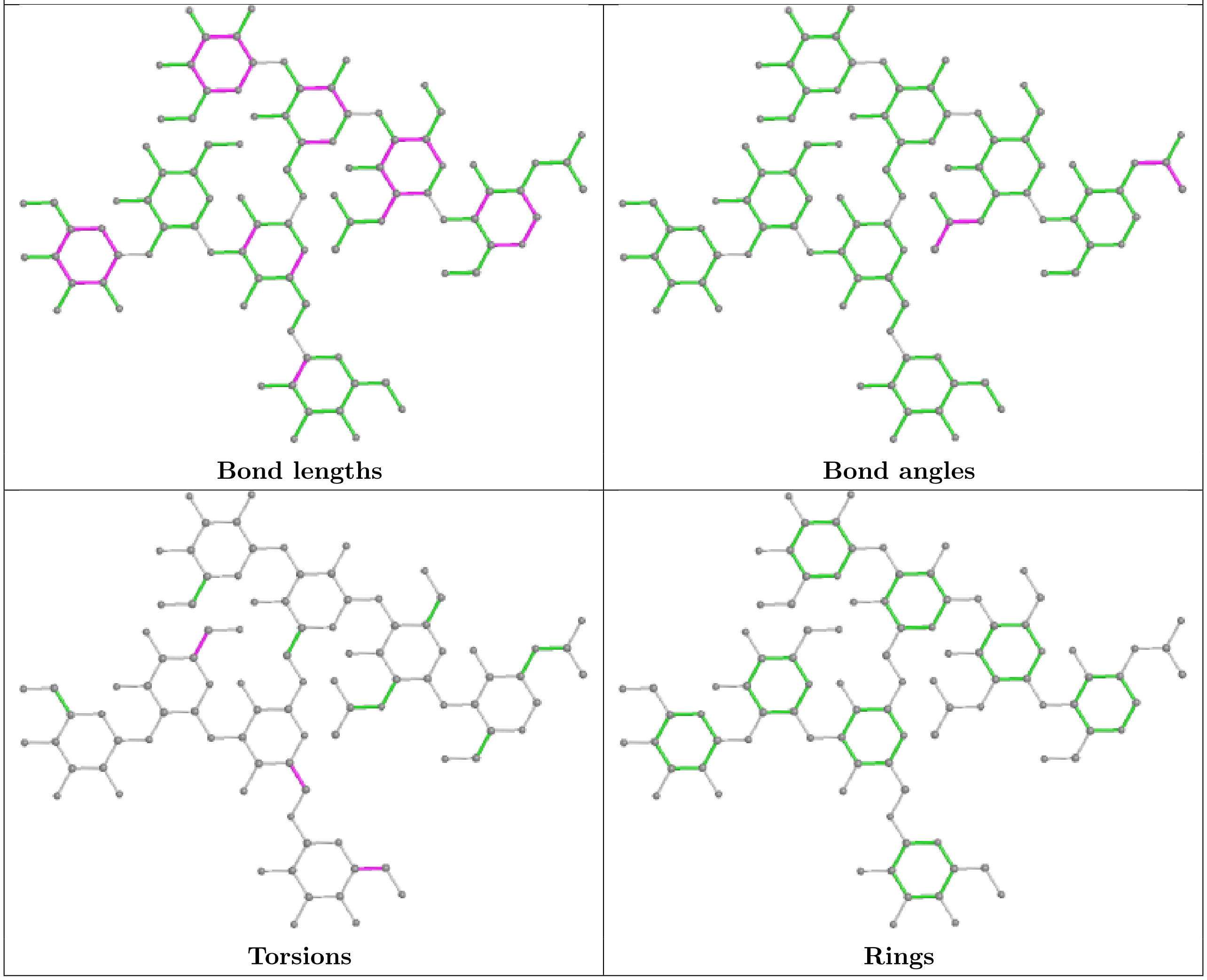
Mol	Chain	Res	Type	Atoms
6	X	1	NAG	C3-C2-N2-C7
6	k	1	NAG	C3-C2-N2-C7
6	x	1	NAG	C3-C2-N2-C7
5	Z	4	MAN	O5-C5-C6-O6
12	t	2	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain M



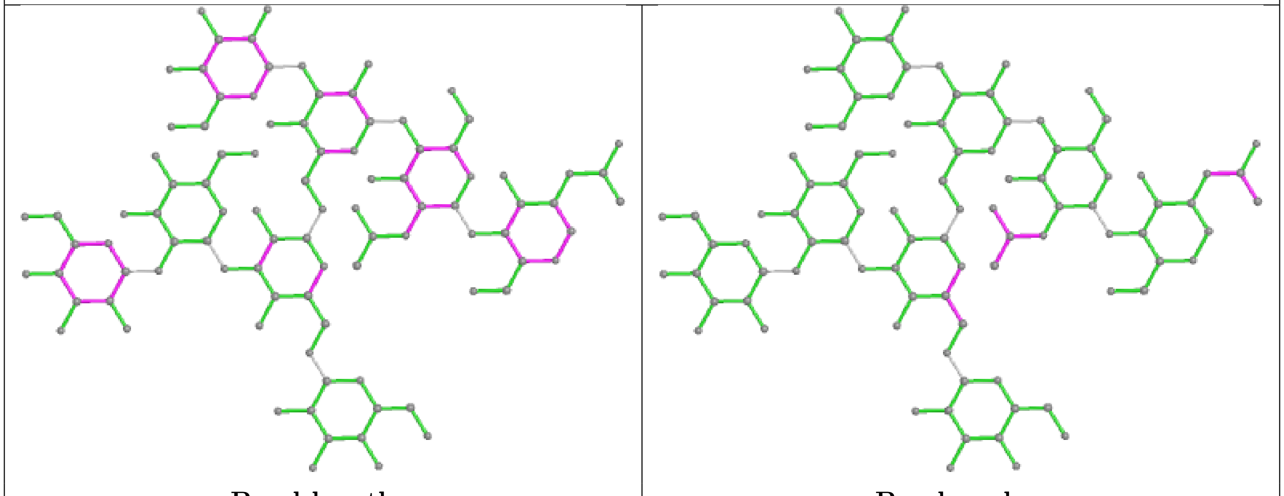
Bond lengths

Bond angles

Torsions

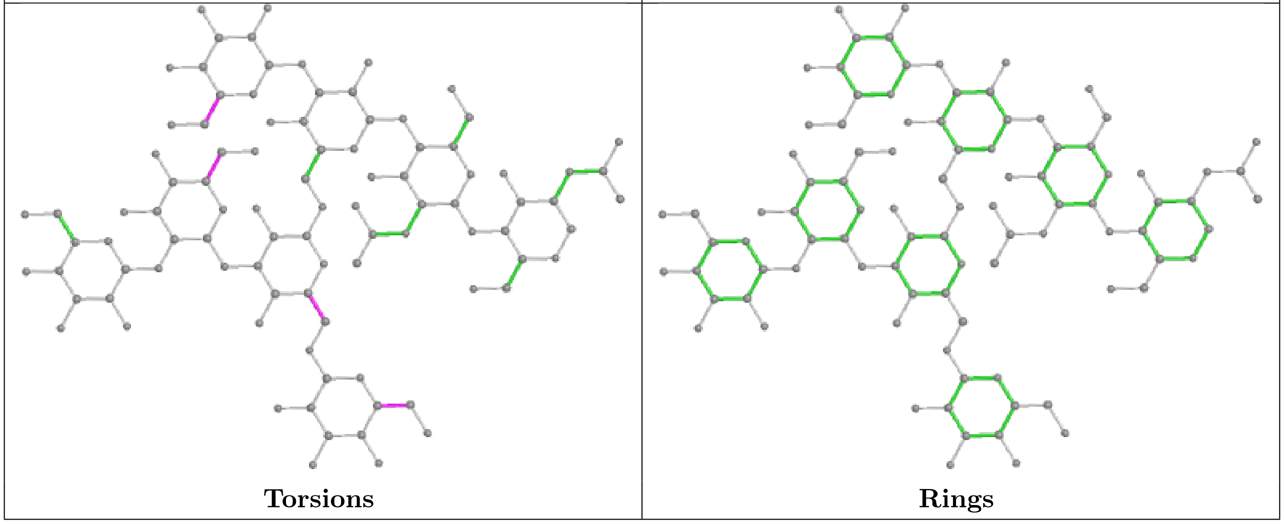
Rings

Oligosaccharide Chain Z



Bond lengths

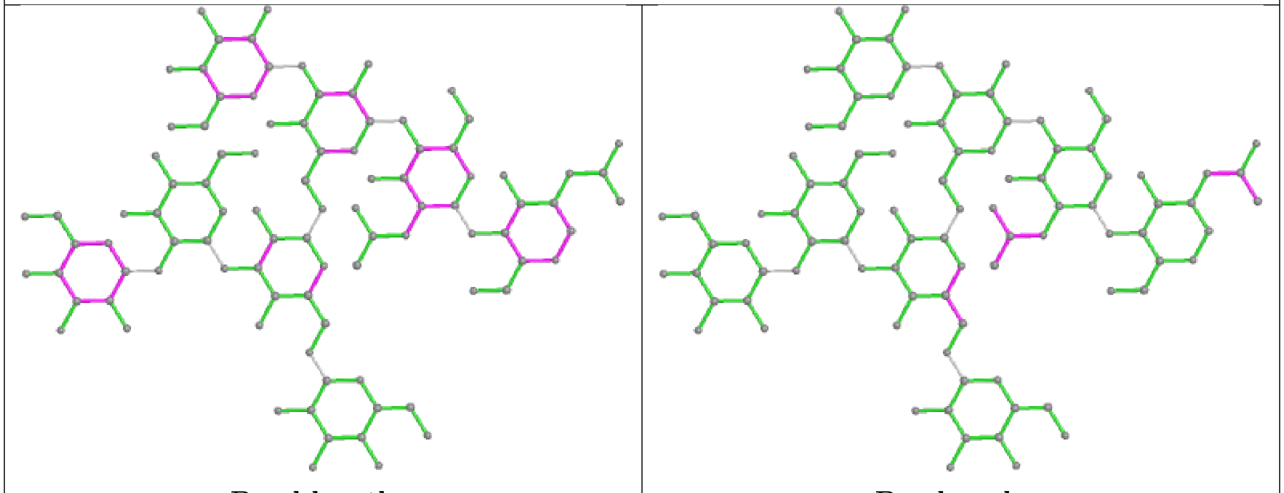
Bond angles



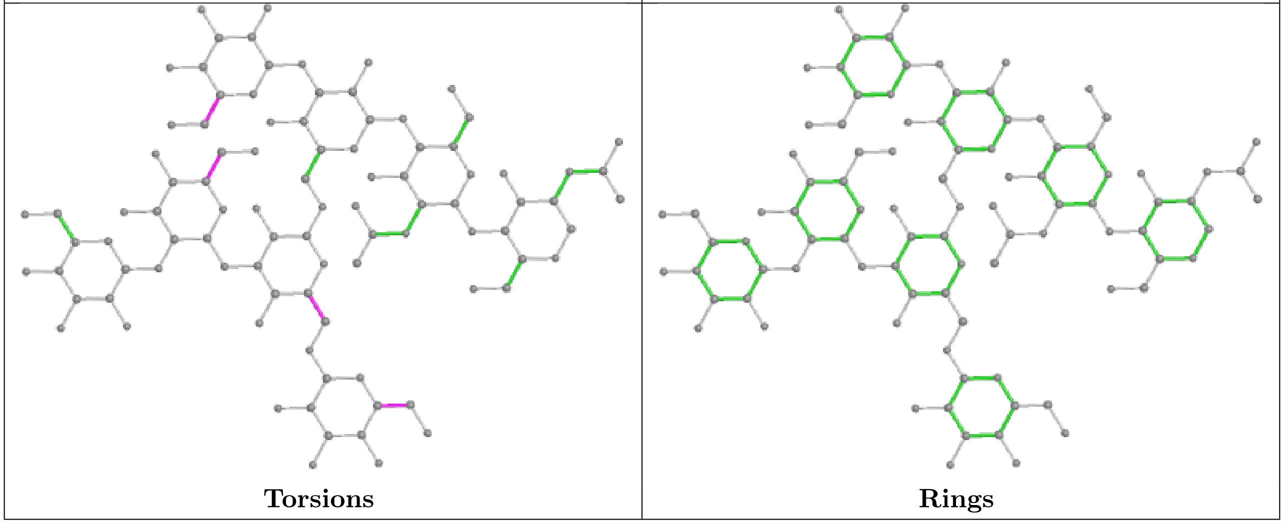
Torsions

Rings

Oligosaccharide Chain m

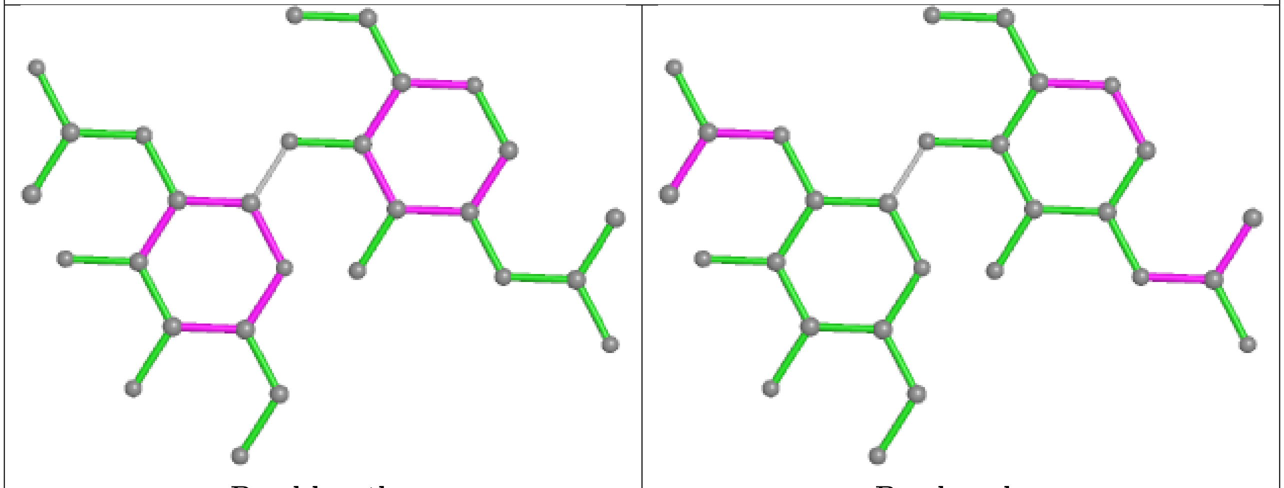


Bond lengths **Bond angles**



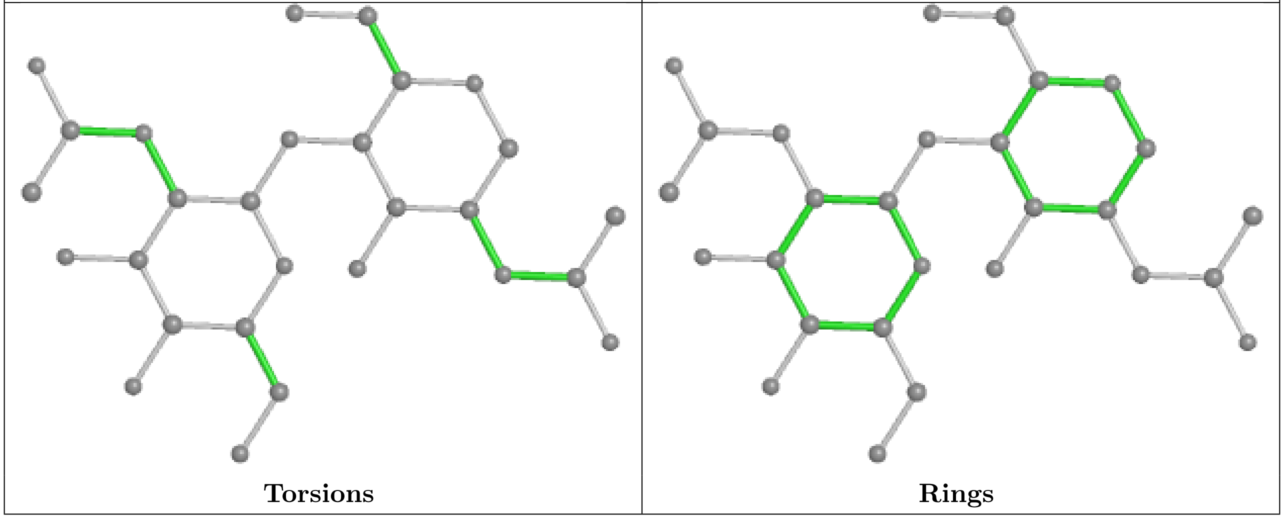
Torsions **Rings**

Oligosaccharide Chain N



Bond lengths

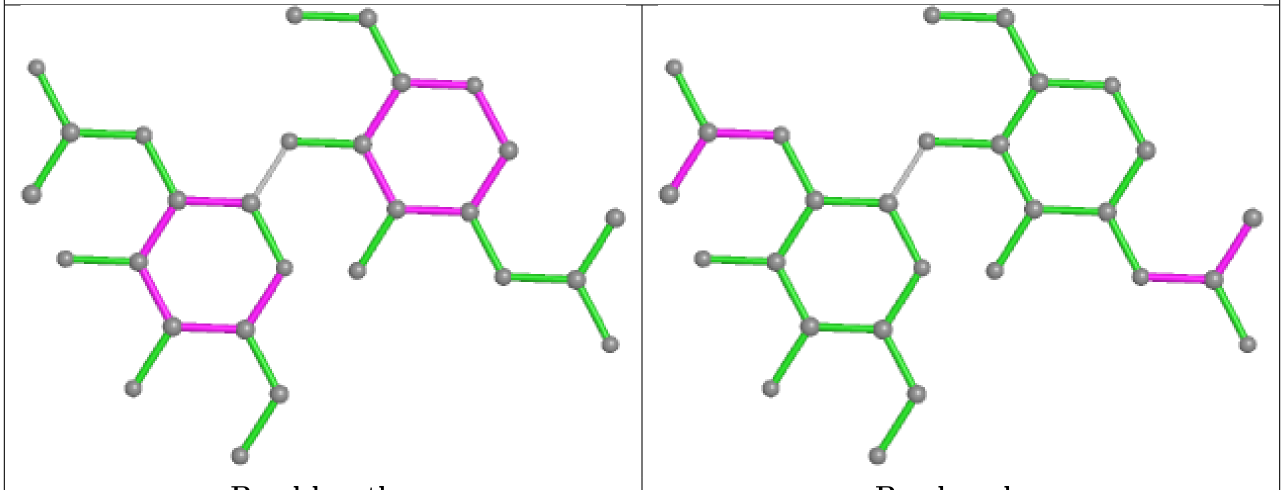
Bond angles



Torsions

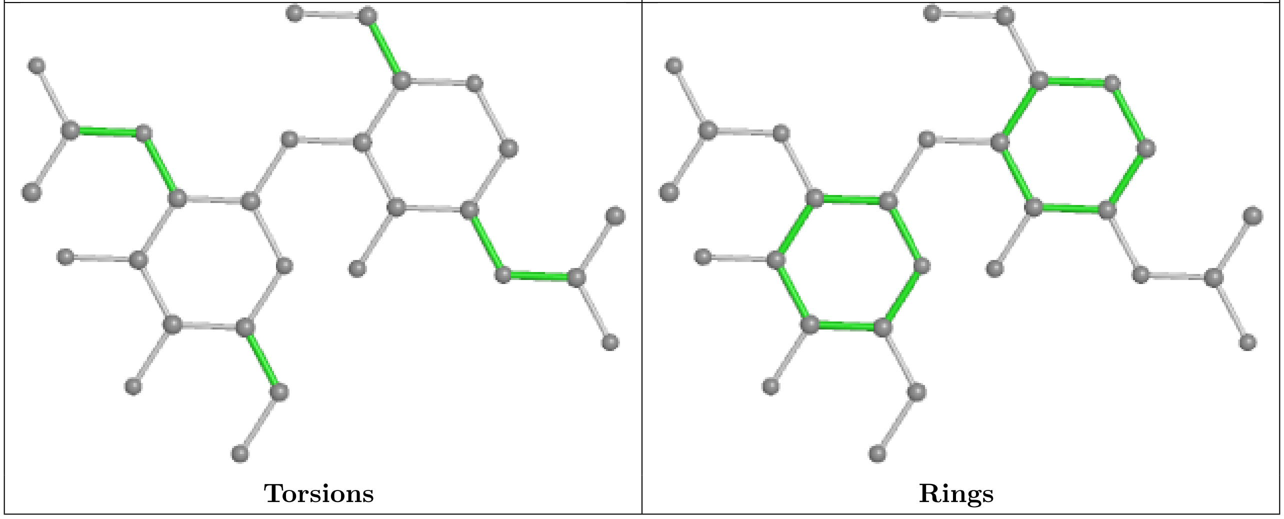
Rings

Oligosaccharide Chain U



Bond lengths

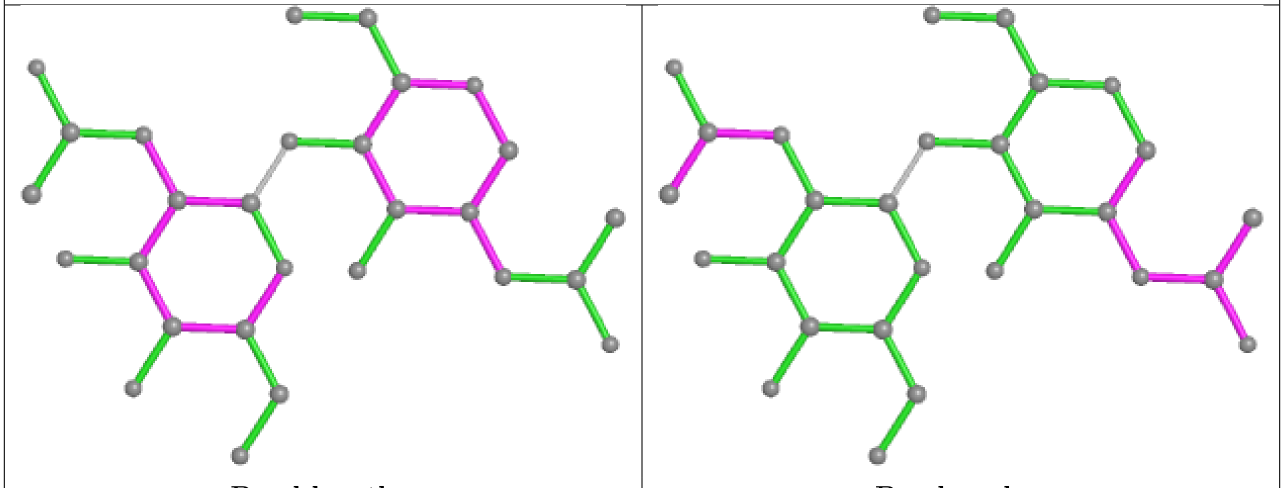
Bond angles



Torsions

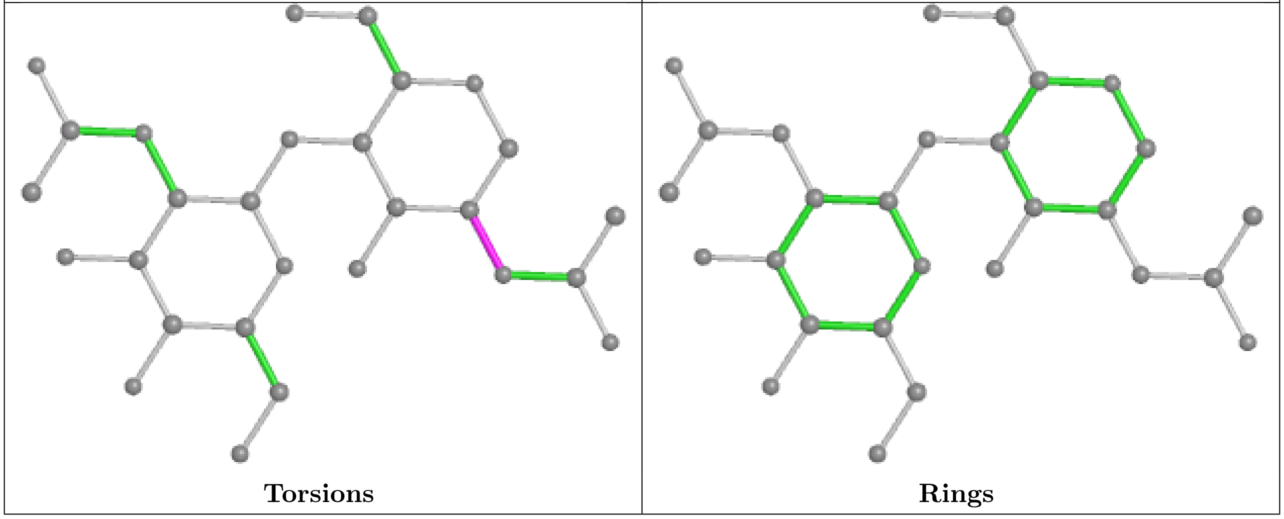
Rings

Oligosaccharide Chain X



Bond lengths

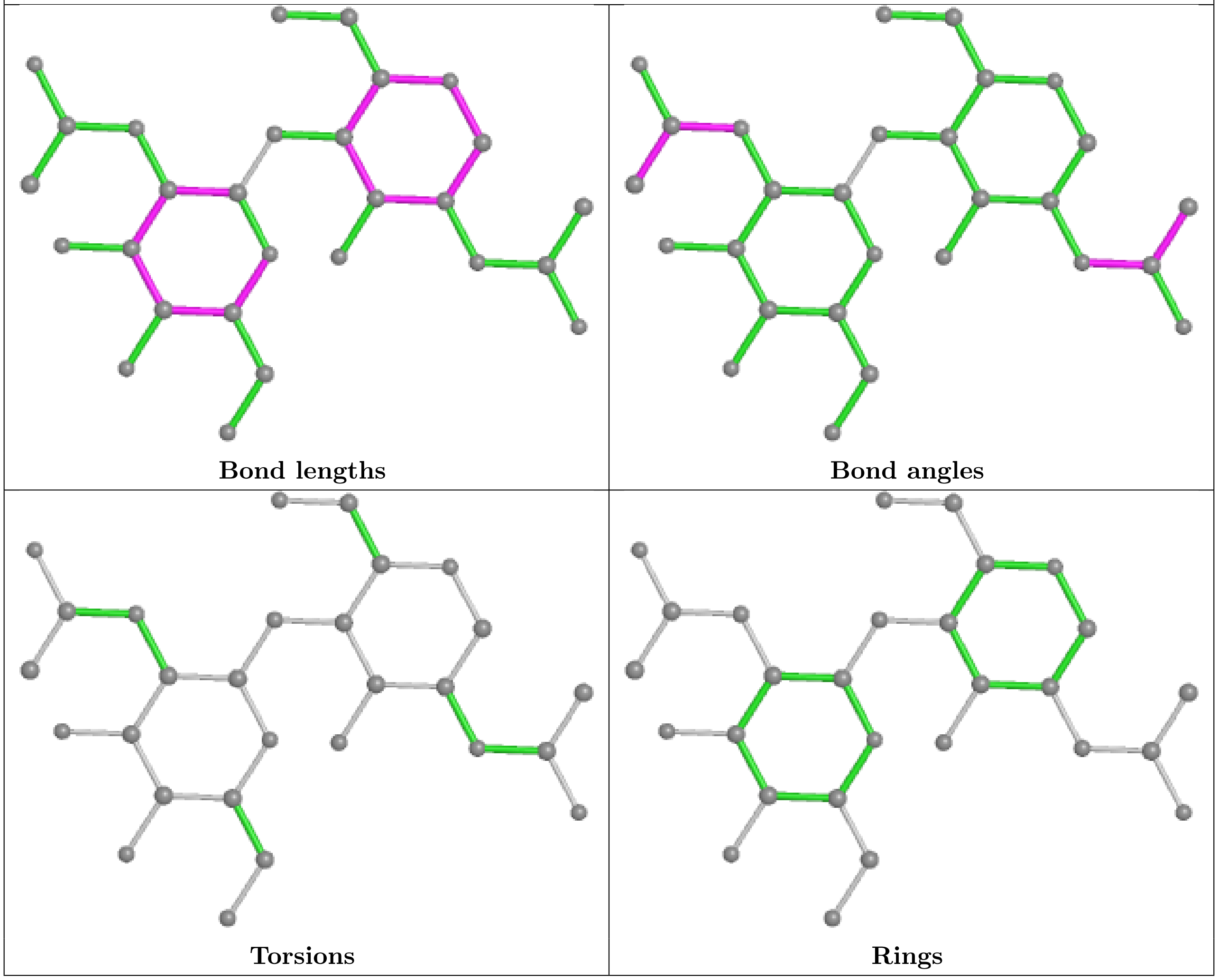
Bond angles



Torsions

Rings

Oligosaccharide Chain Y



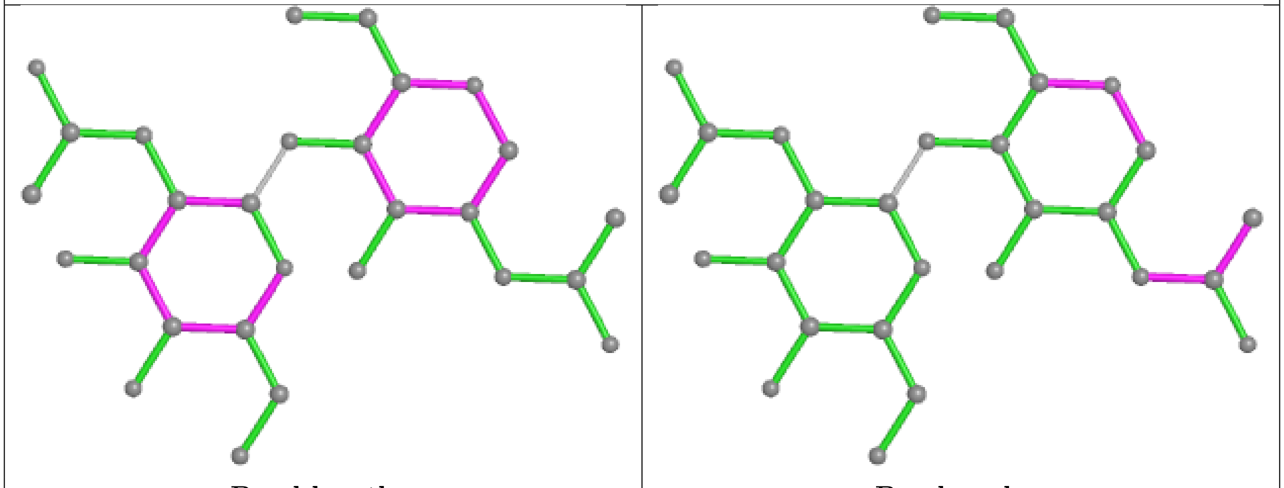
Bond lengths

Bond angles

Torsions

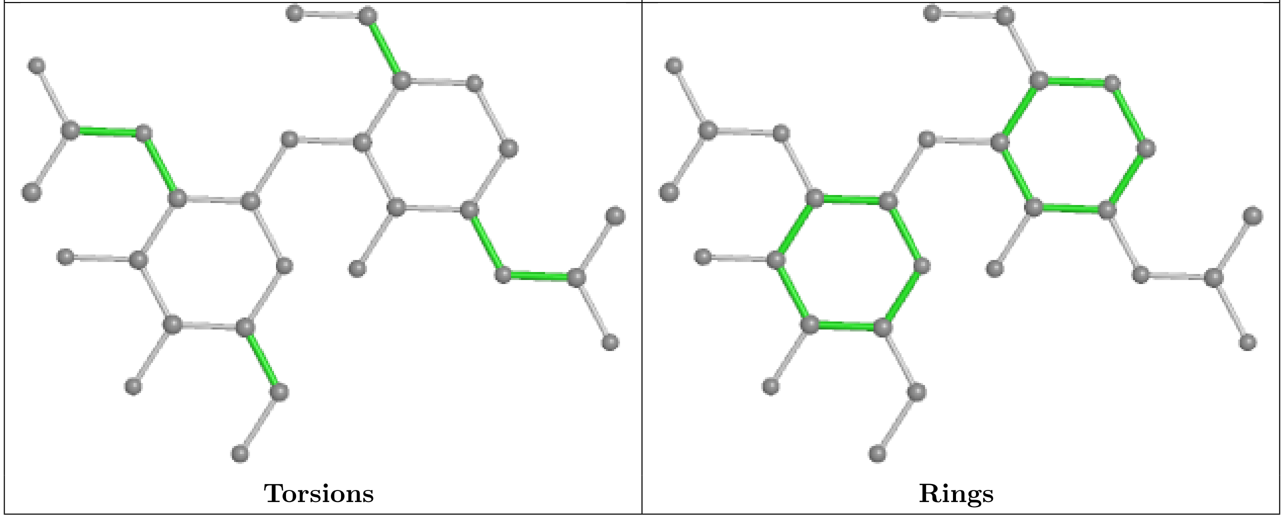
Rings

Oligosaccharide Chain a



Bond lengths

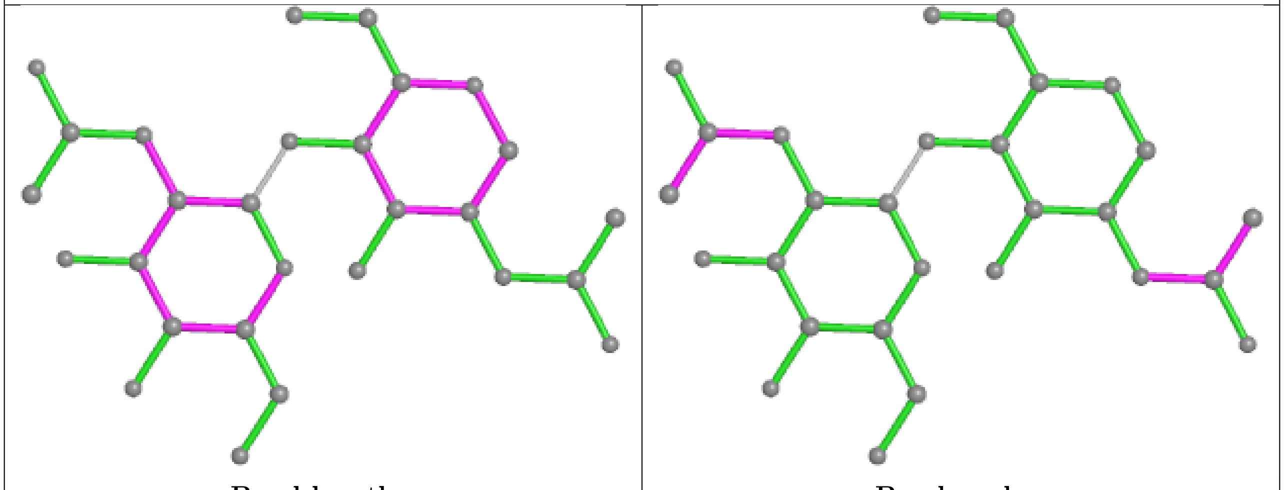
Bond angles



Torsions

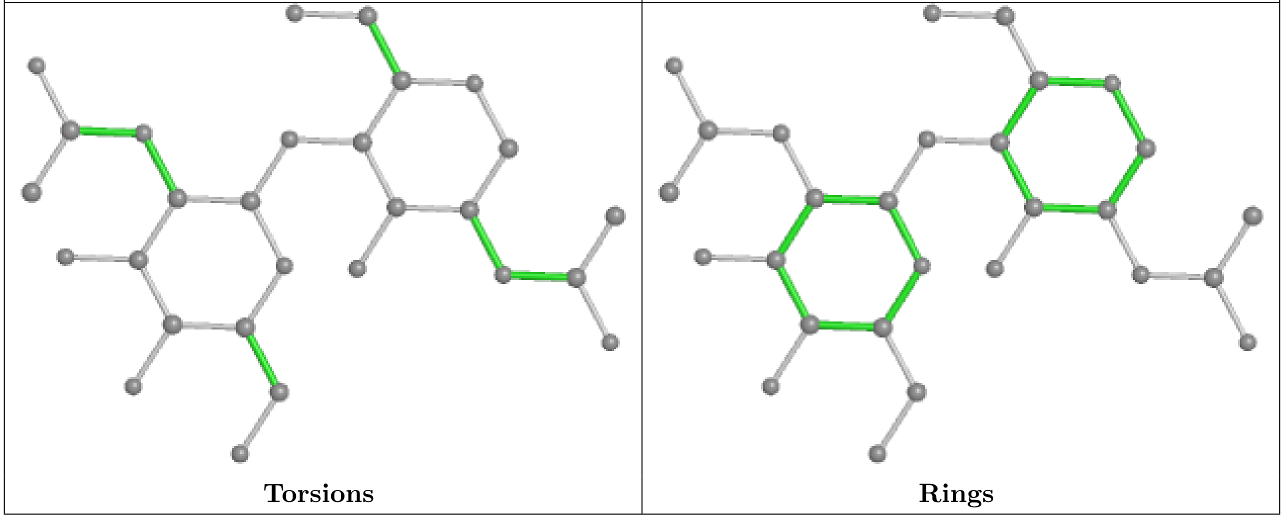
Rings

Oligosaccharide Chain h



Bond lengths

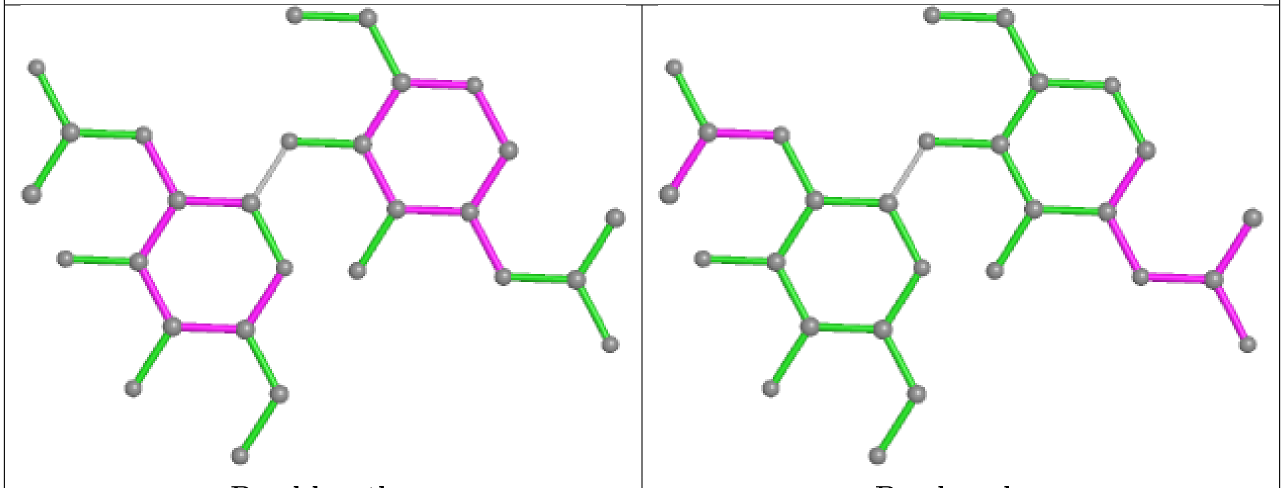
Bond angles



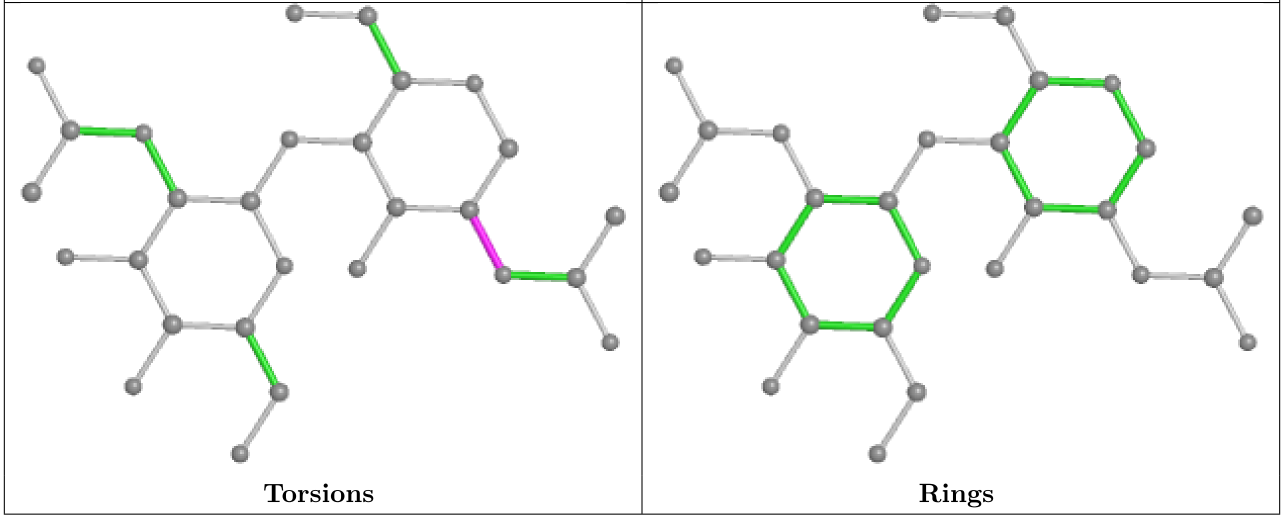
Torsions

Rings

Oligosaccharide Chain k

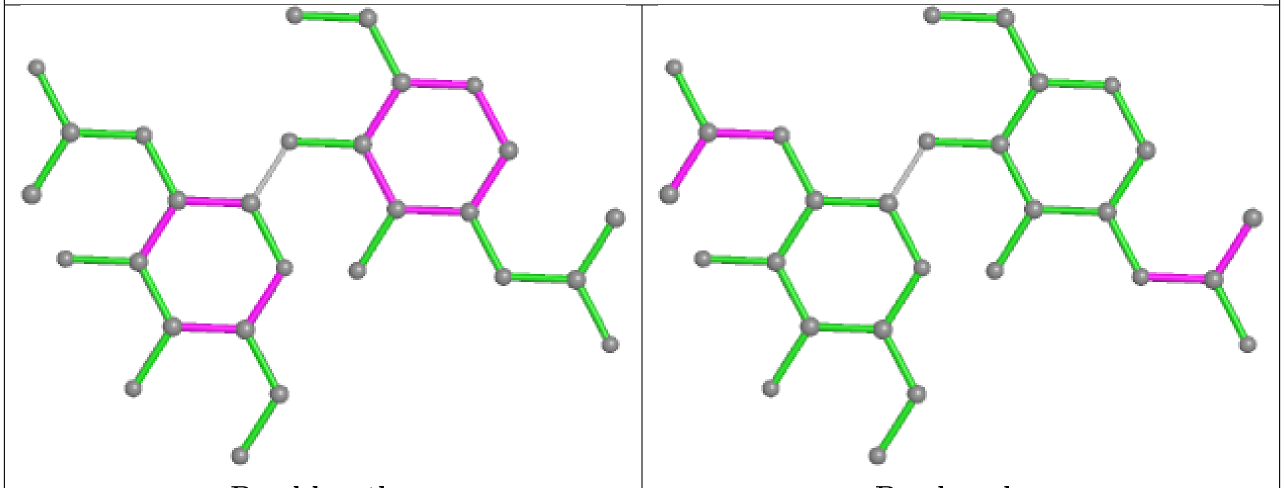


Bond lengths Bond angles



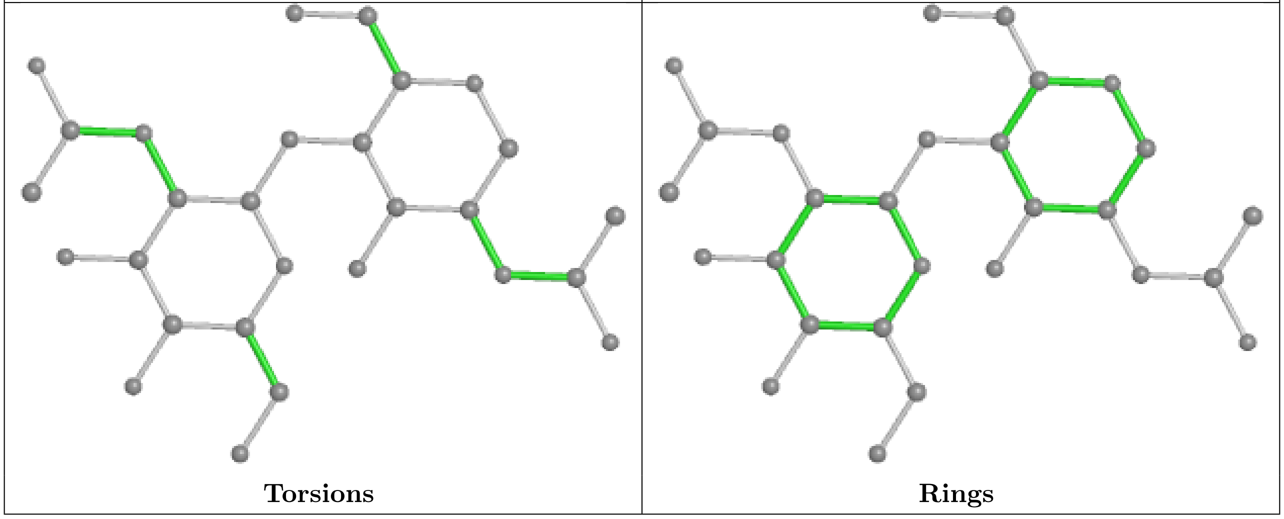
Torsions Rings

Oligosaccharide Chain l



Bond lengths

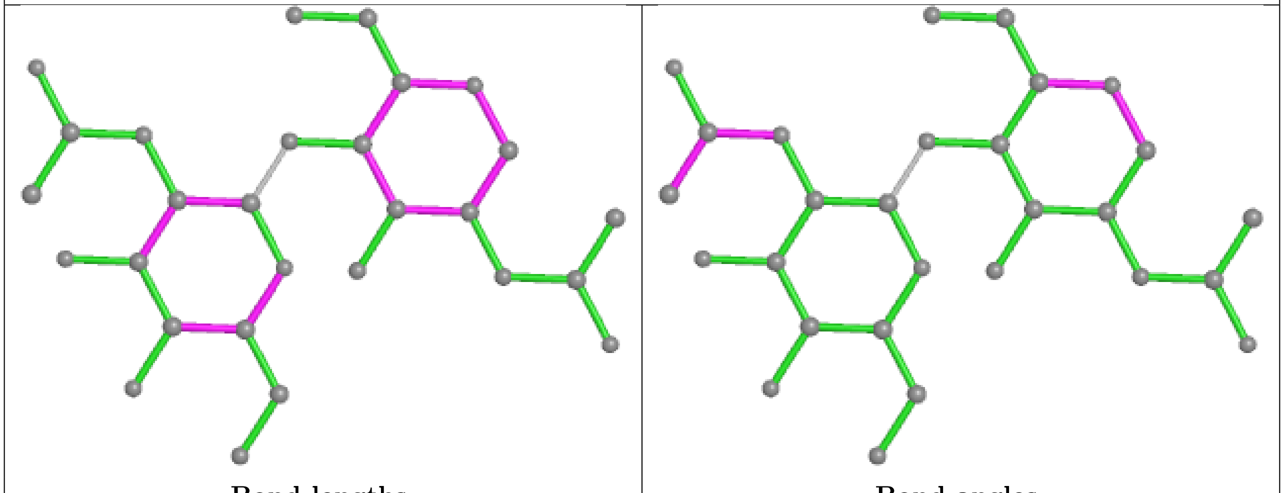
Bond angles



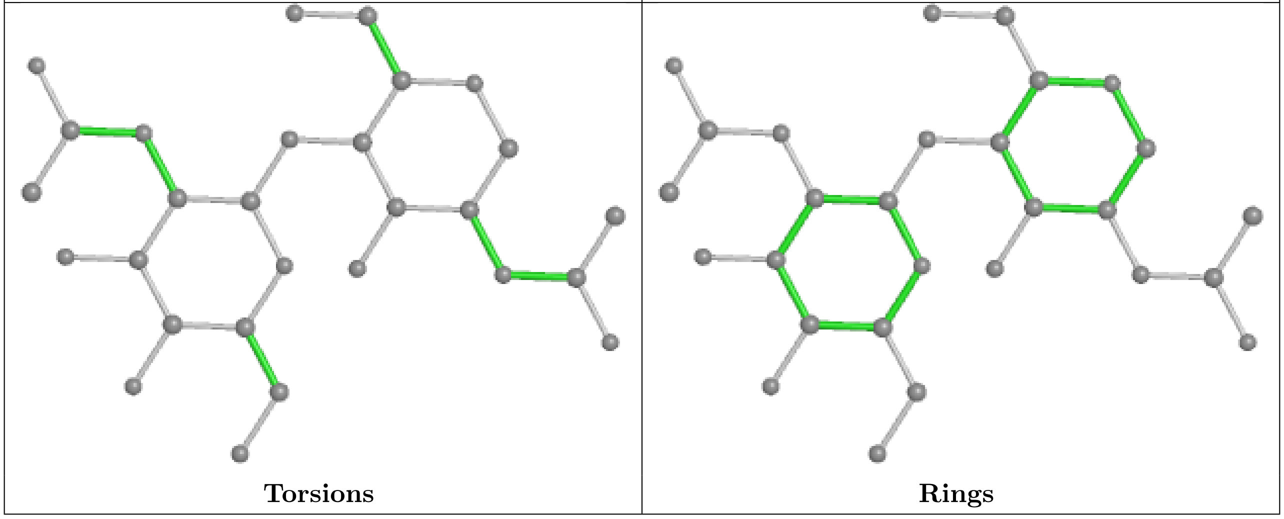
Torsions

Rings

Oligosaccharide Chain n

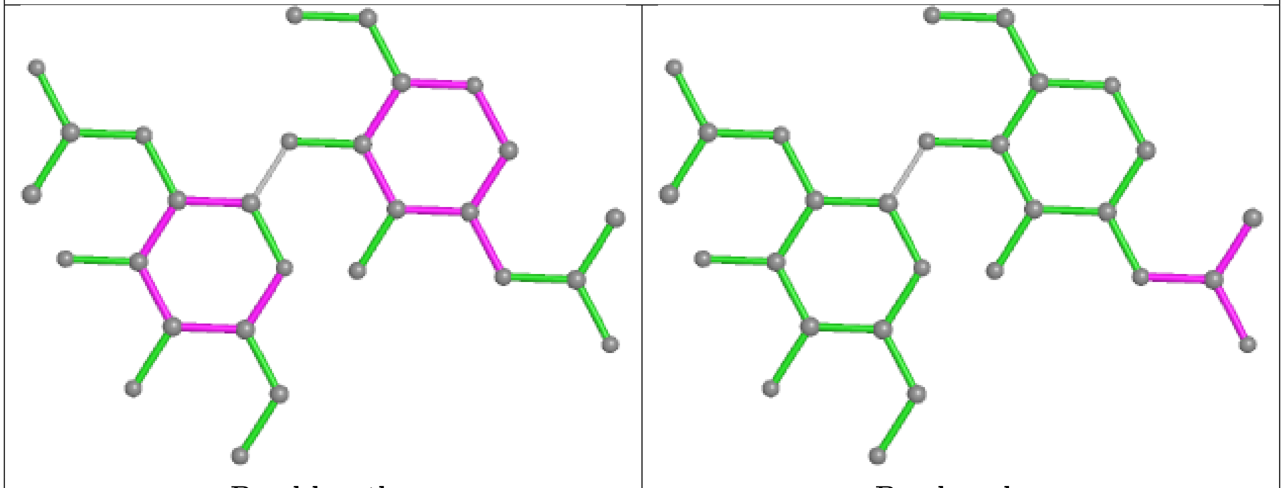


Bond lengths **Bond angles**



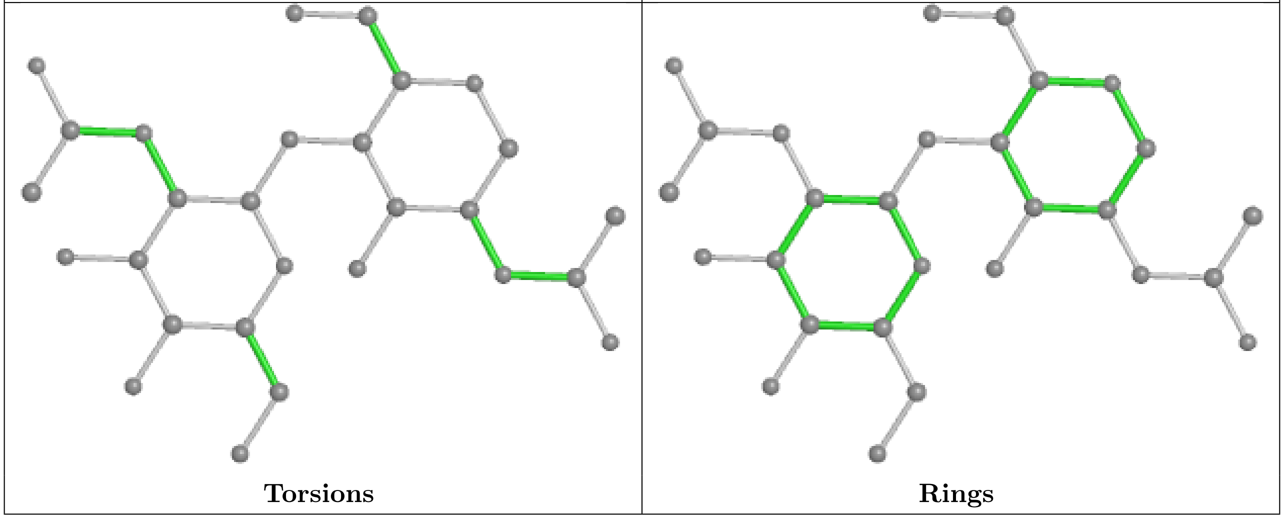
Torsions **Rings**

Oligosaccharide Chain u



Bond lengths

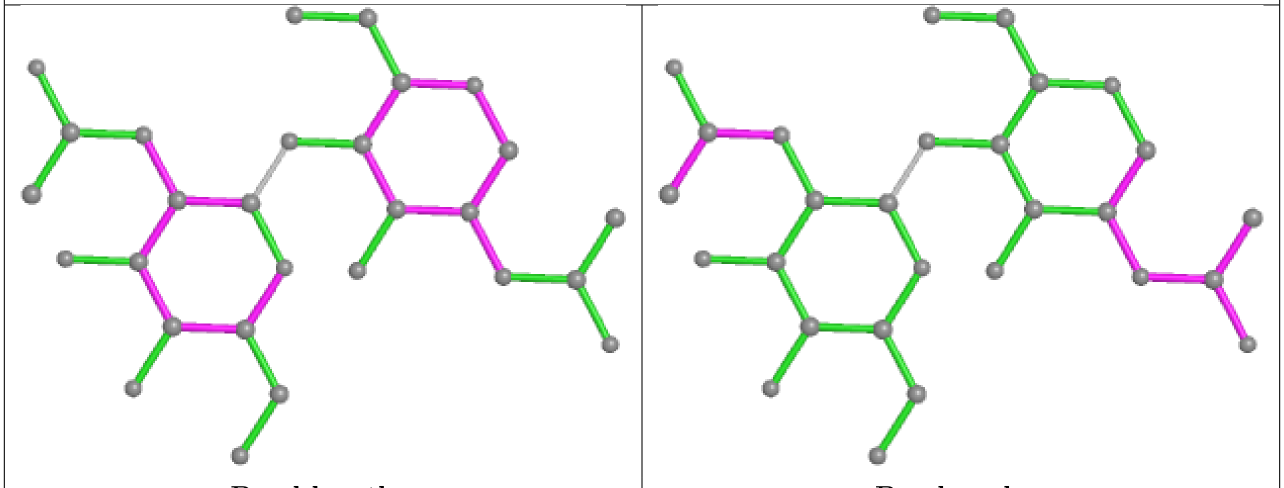
Bond angles



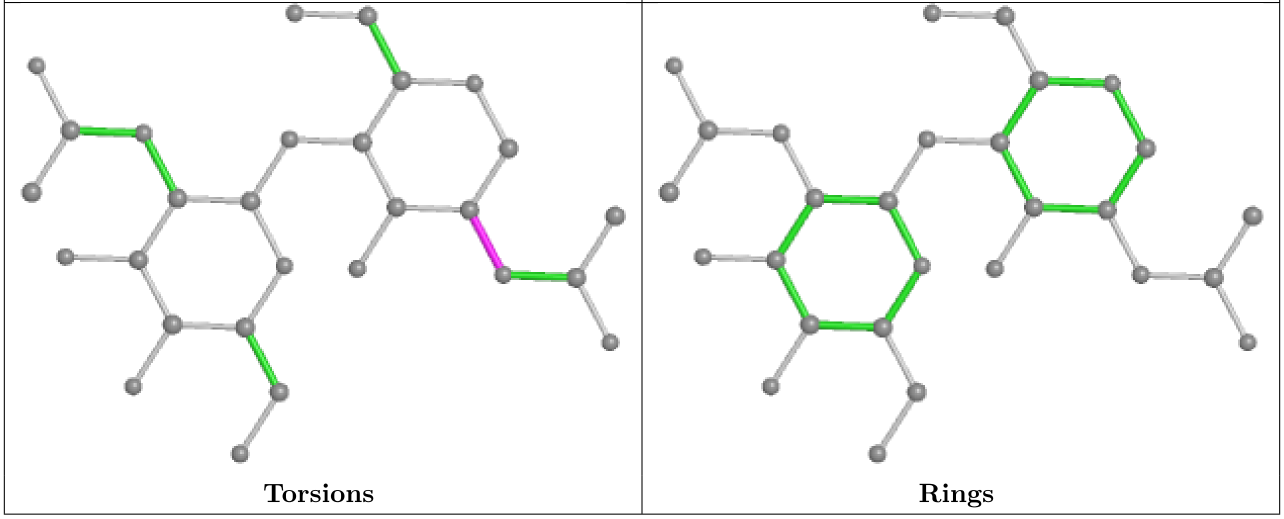
Torsions

Rings

Oligosaccharide Chain x

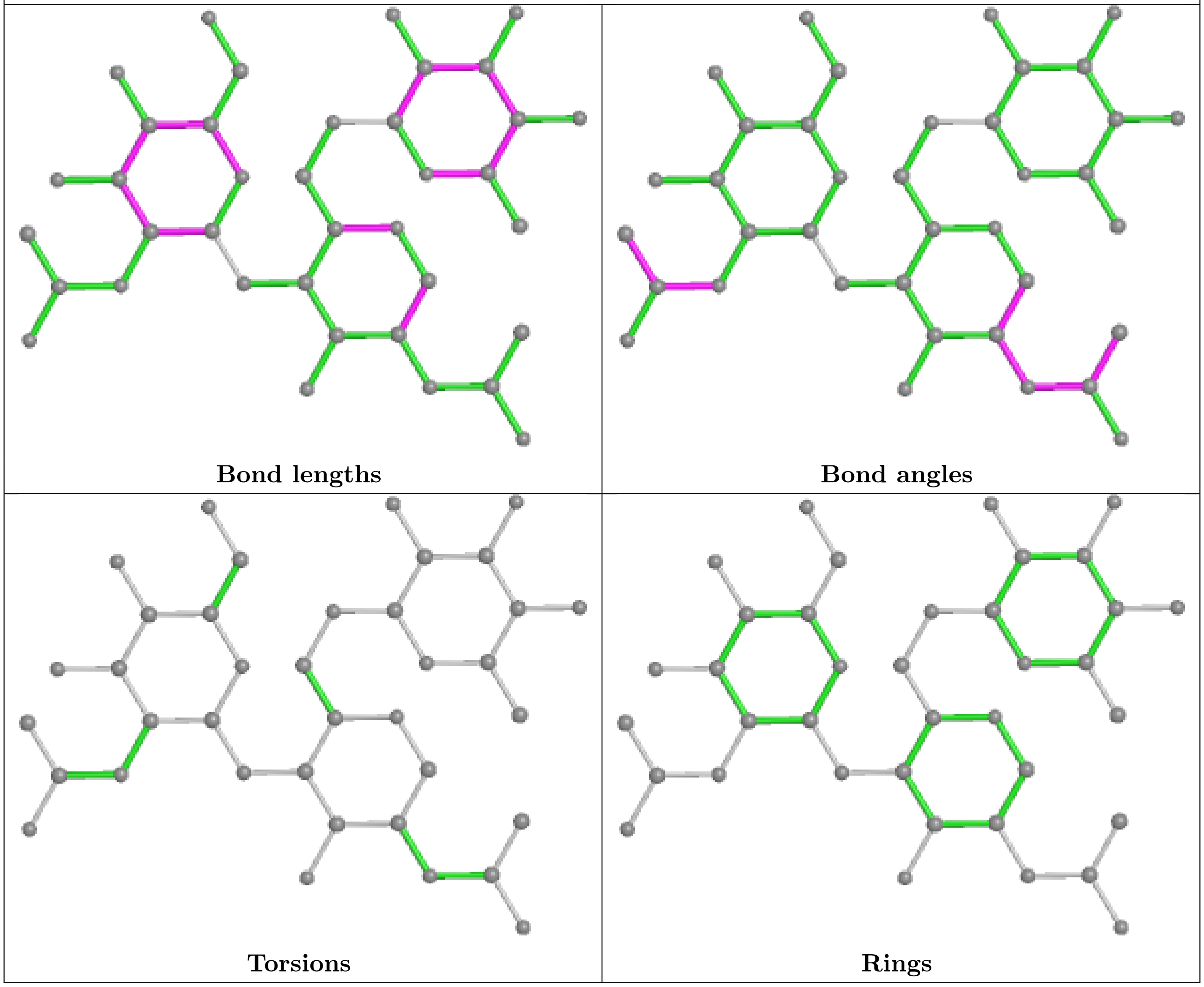


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain O



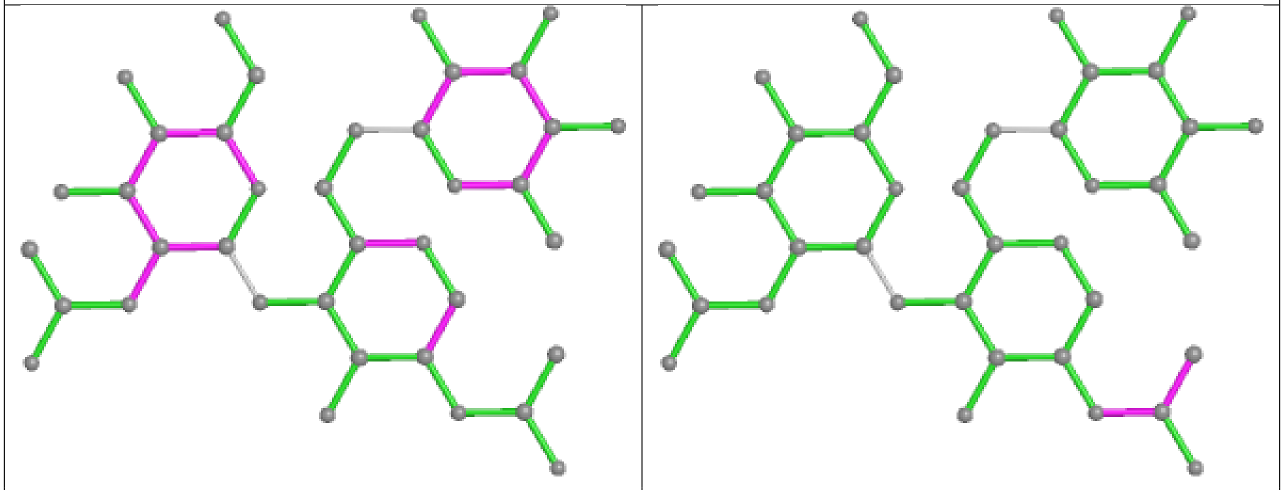
Bond lengths

Bond angles

Torsions

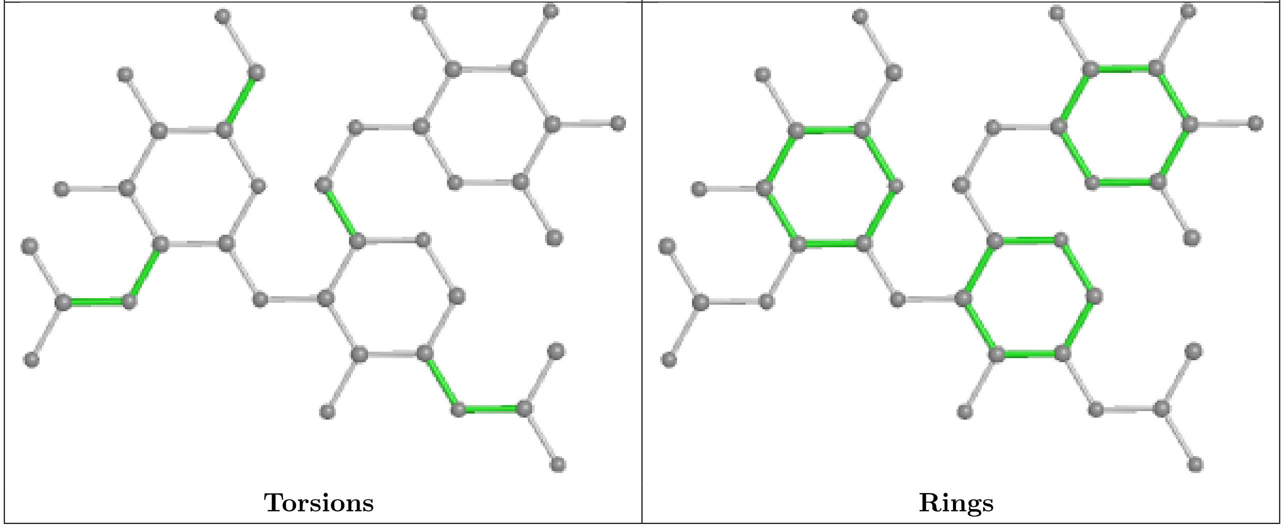
Rings

Oligosaccharide Chain P



Bond lengths

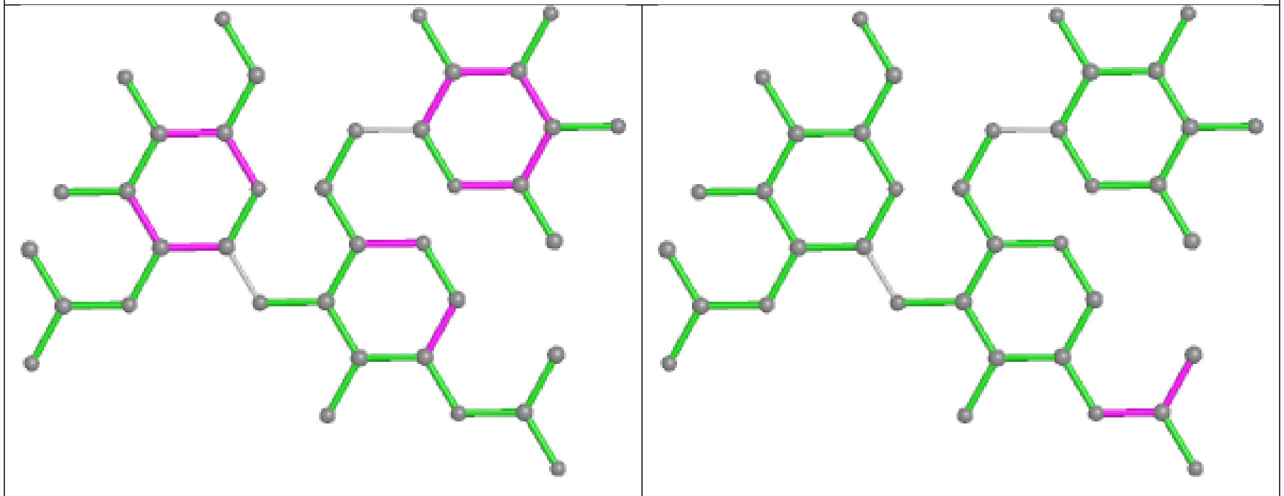
Bond angles



Torsions

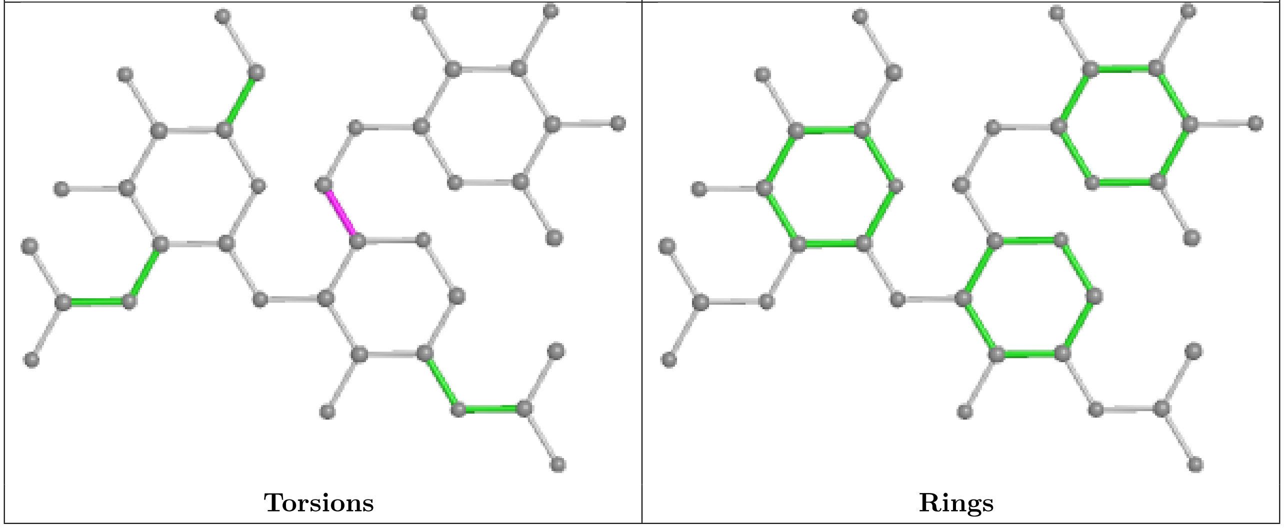
Rings

Oligosaccharide Chain Q



Bond lengths

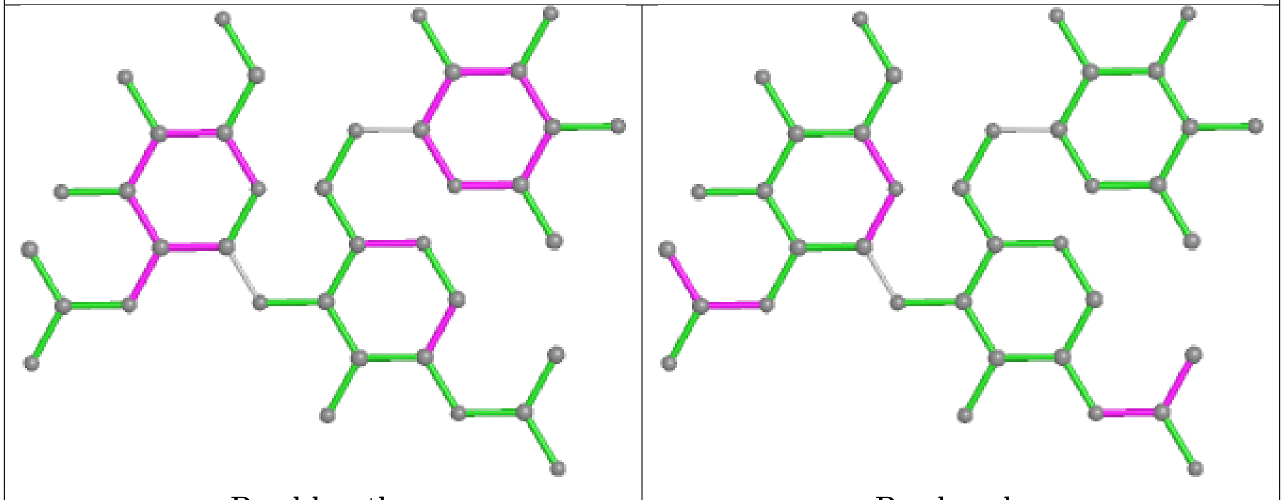
Bond angles



Torsions

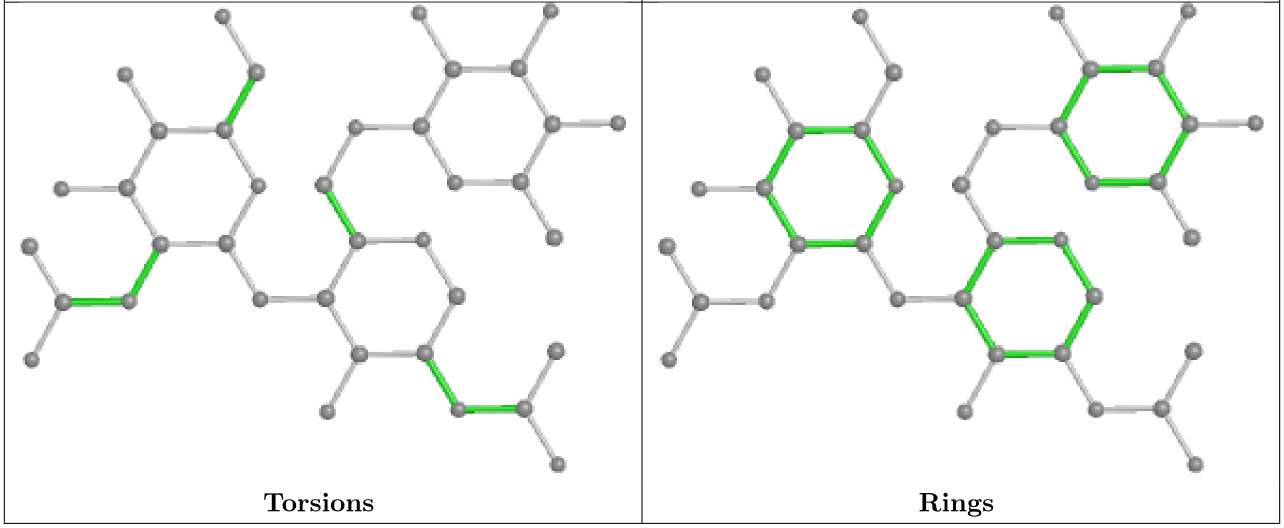
Rings

Oligosaccharide Chain V



Bond lengths

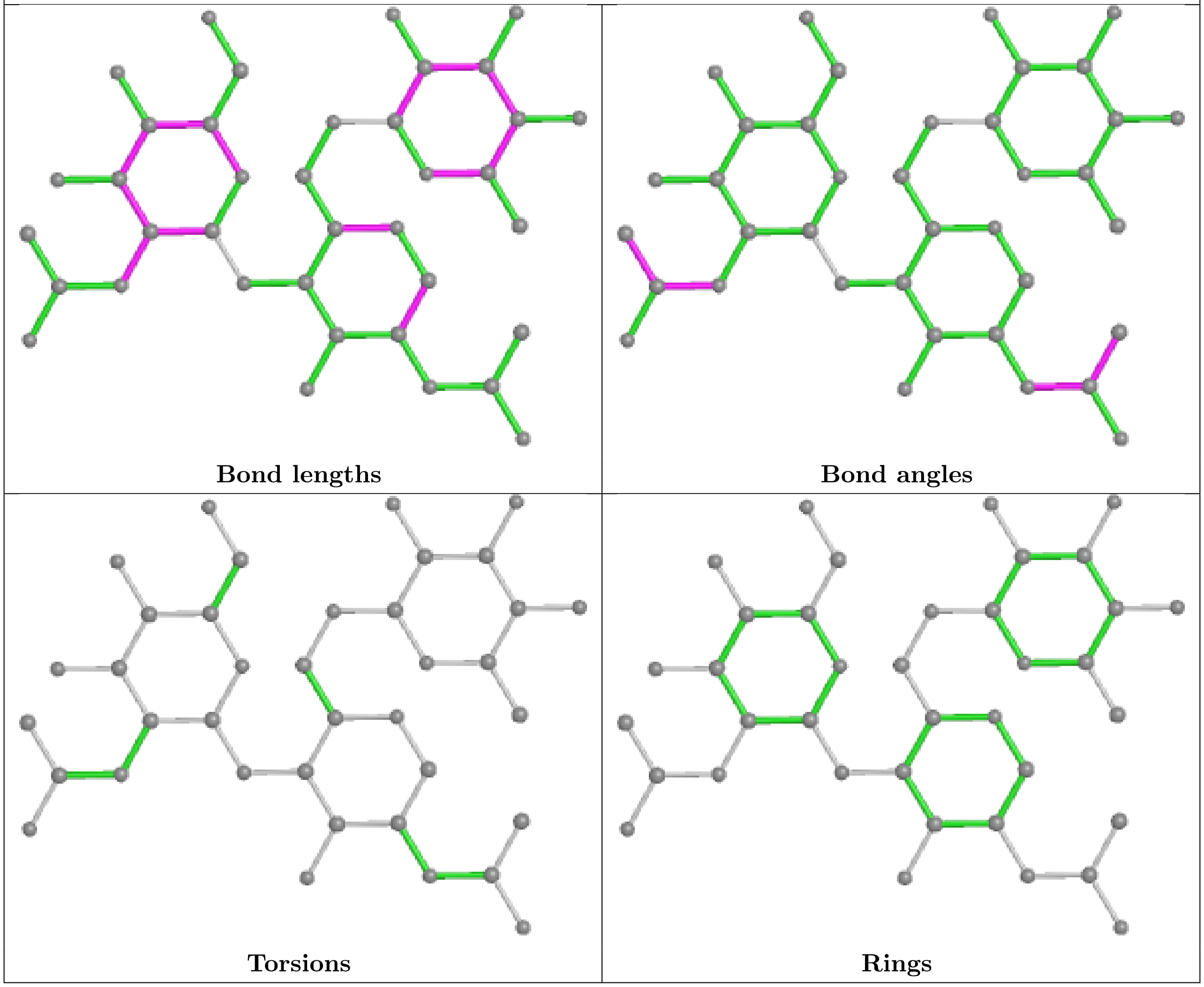
Bond angles



Torsions

Rings

Oligosaccharide Chain b



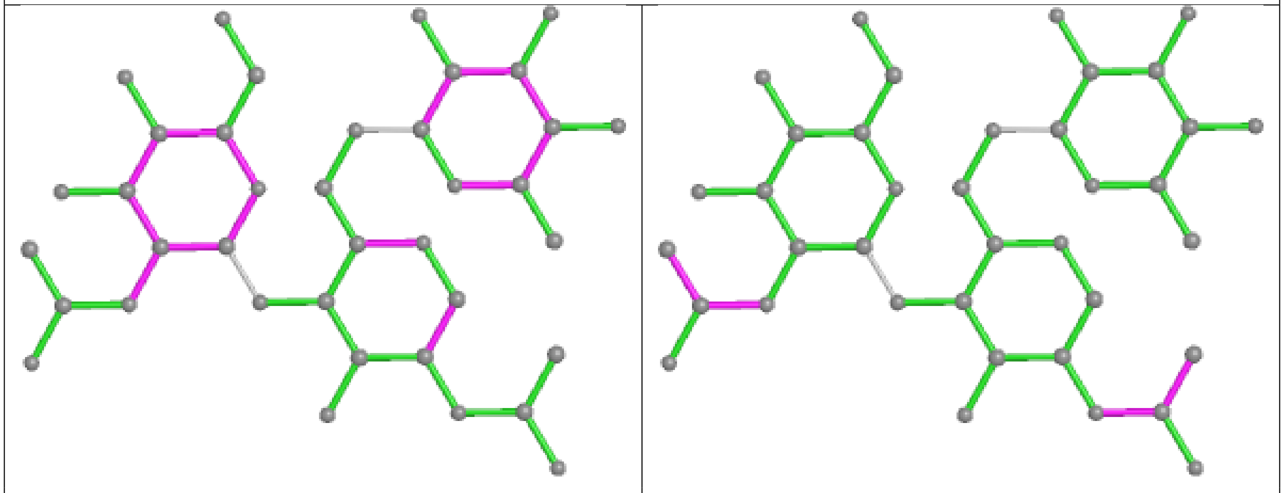
Bond lengths

Bond angles

Torsions

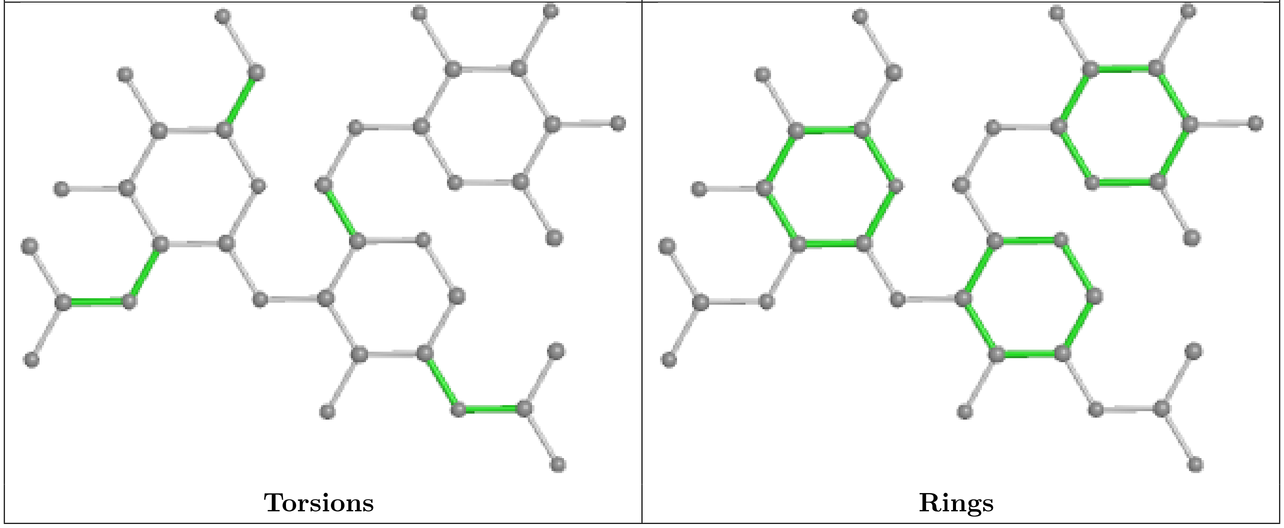
Rings

Oligosaccharide Chain c



Bond lengths

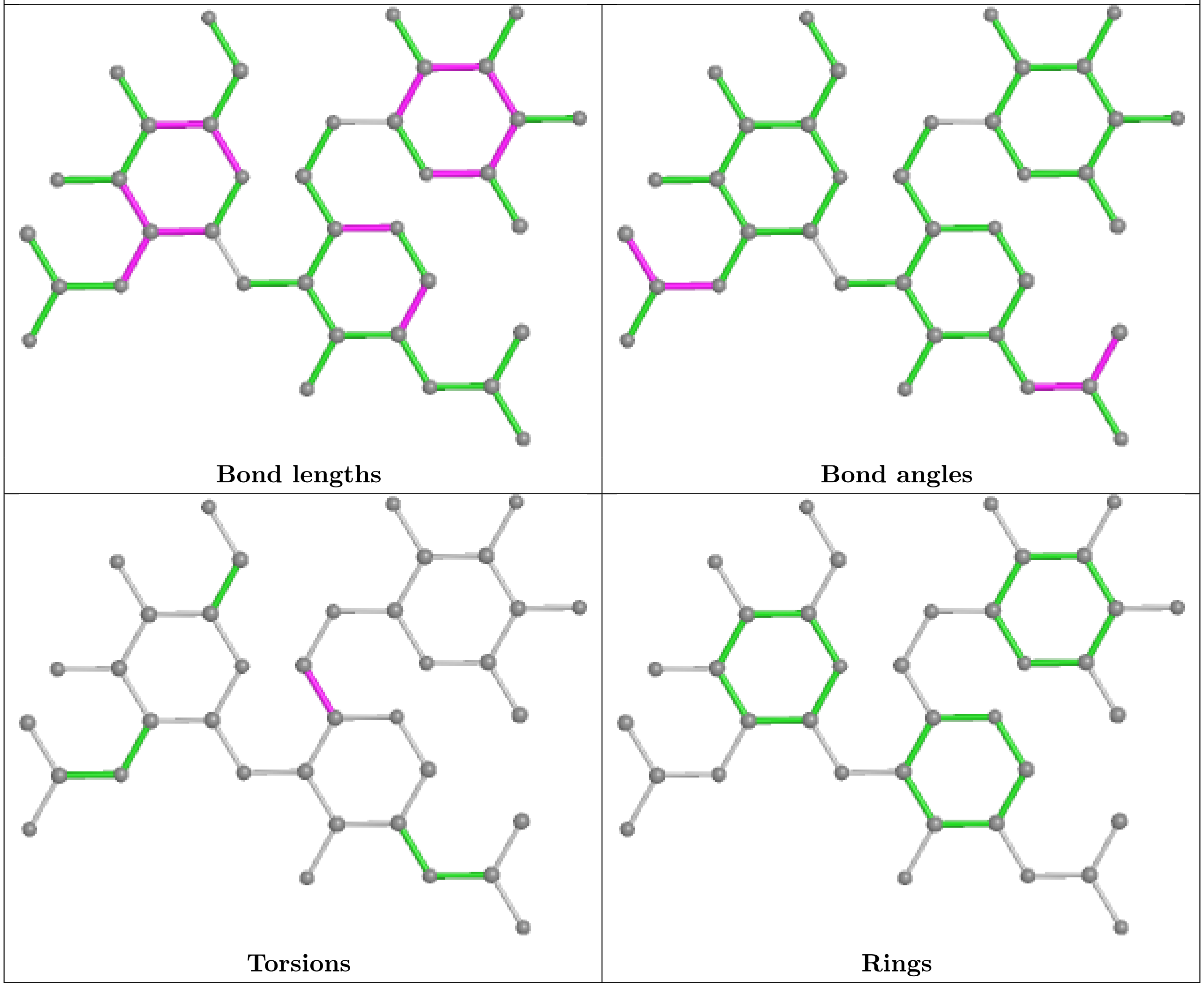
Bond angles



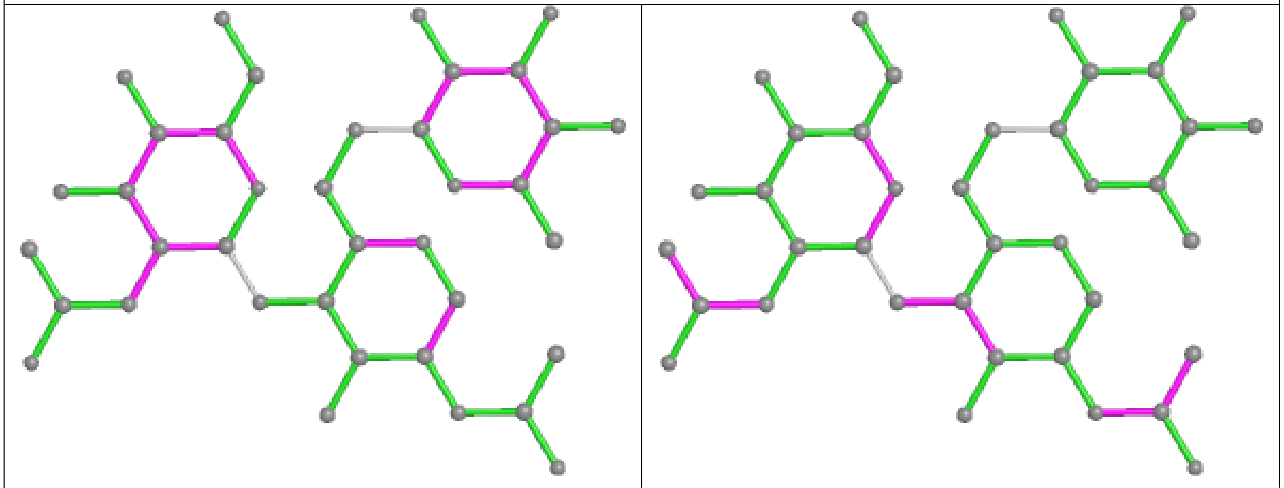
Torsions

Rings

Oligosaccharide Chain d

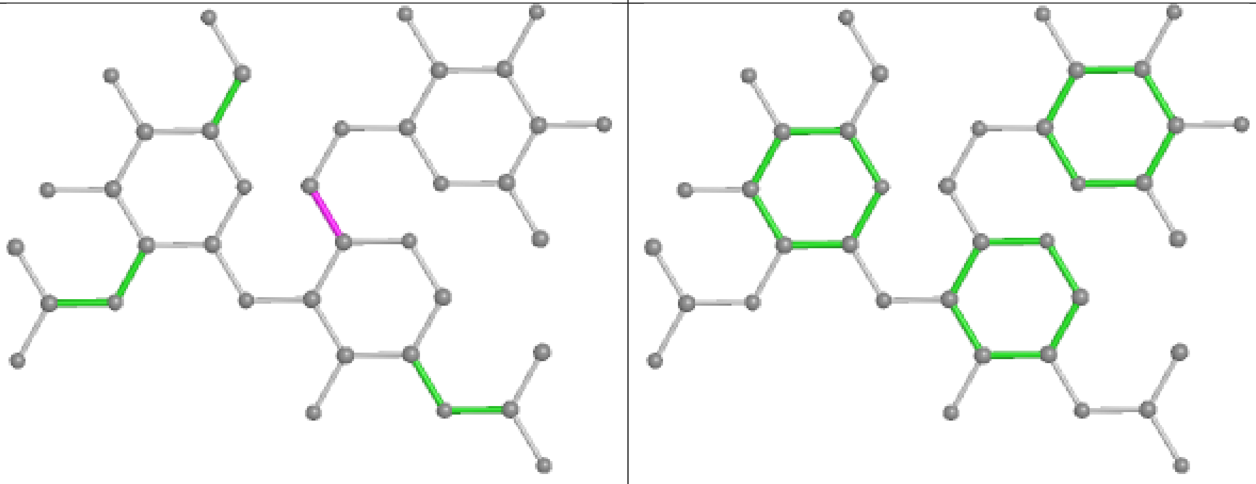


Oligosaccharide Chain i



Bond lengths

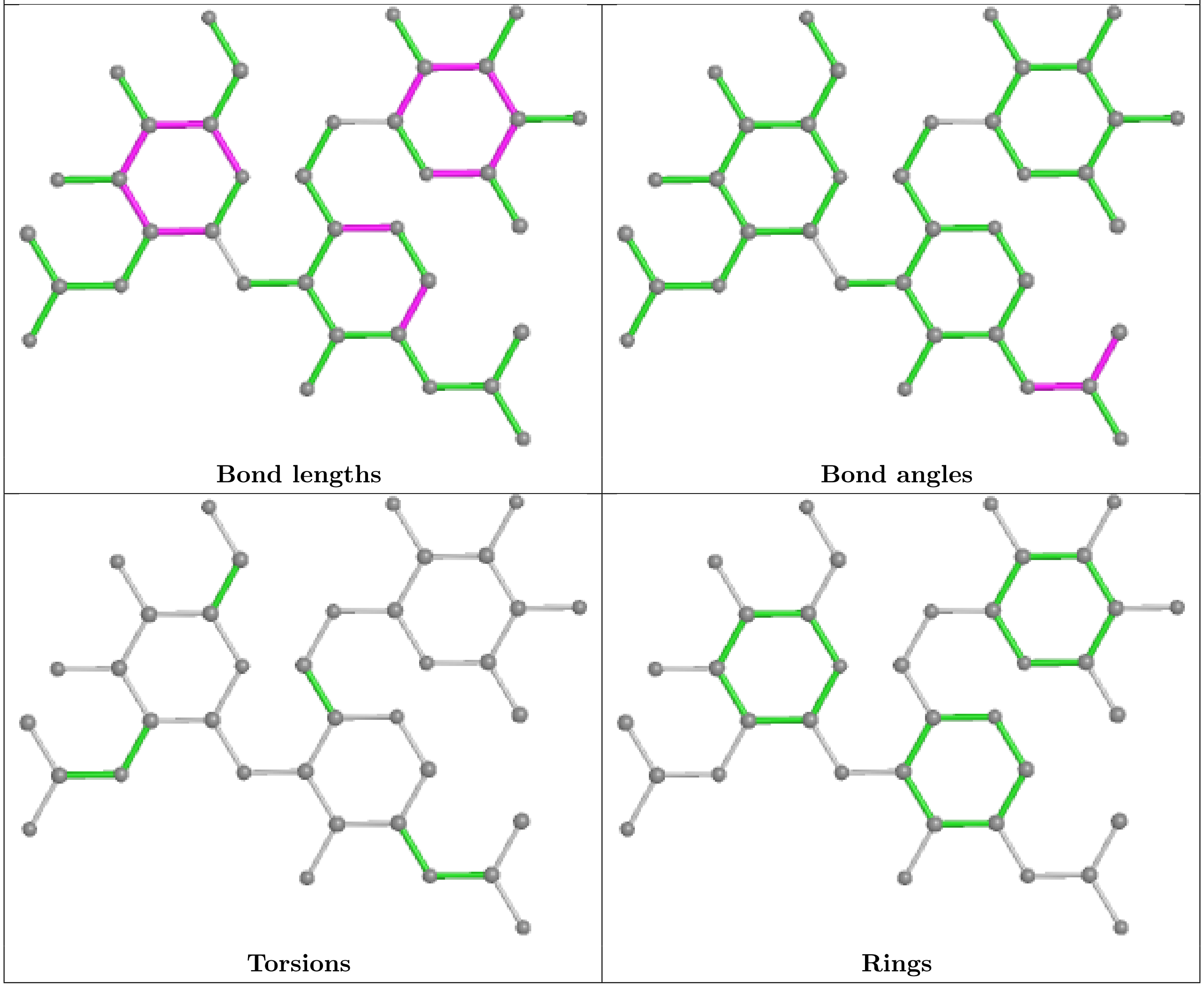
Bond angles



Torsions

Rings

Oligosaccharide Chain o



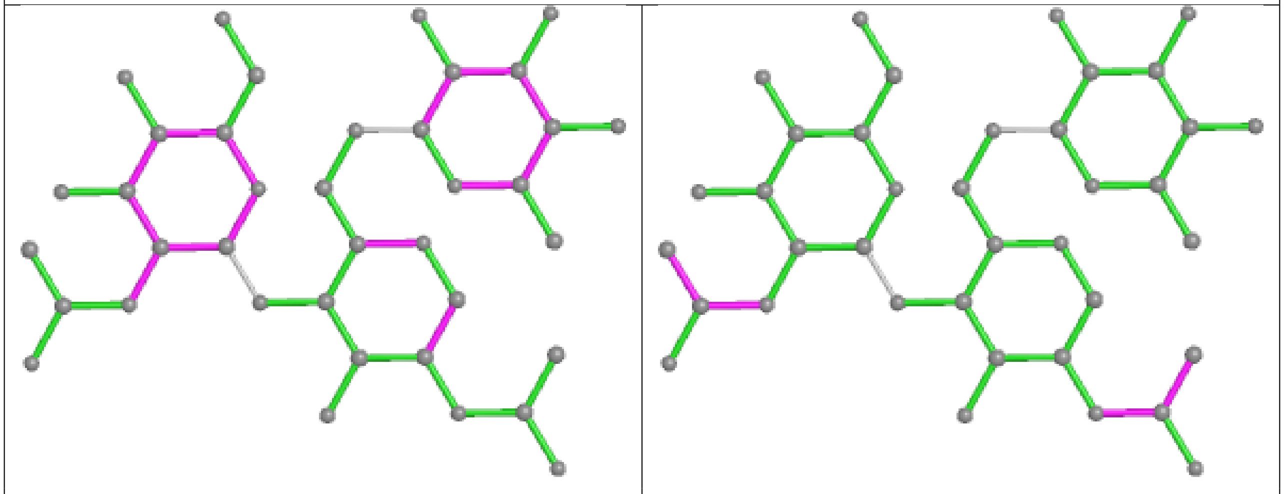
Bond lengths

Bond angles

Torsions

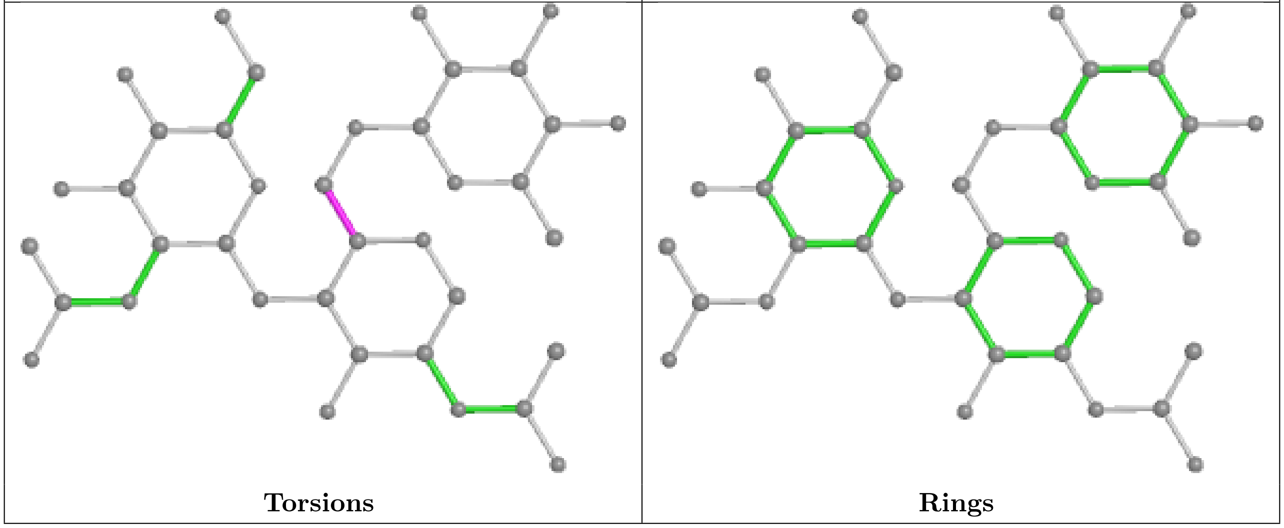
Rings

Oligosaccharide Chain p



Bond lengths

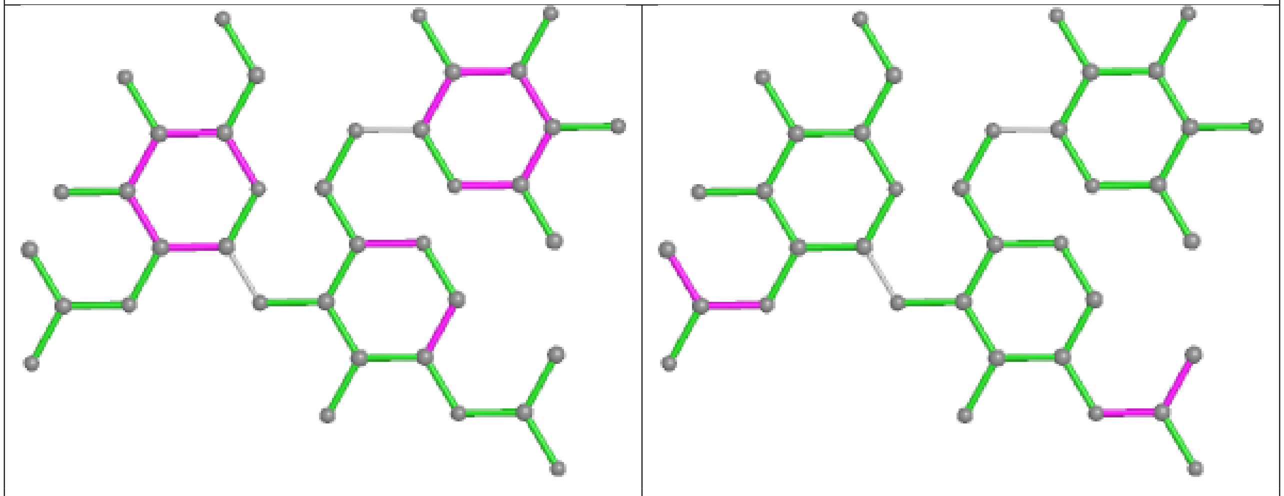
Bond angles



Torsions

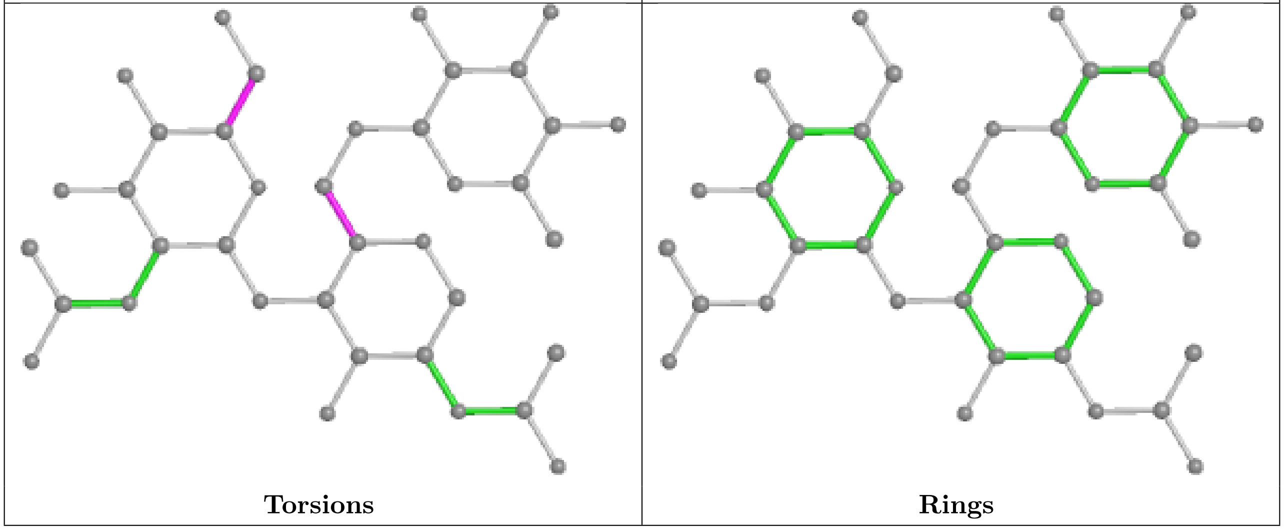
Rings

Oligosaccharide Chain q



Bond lengths

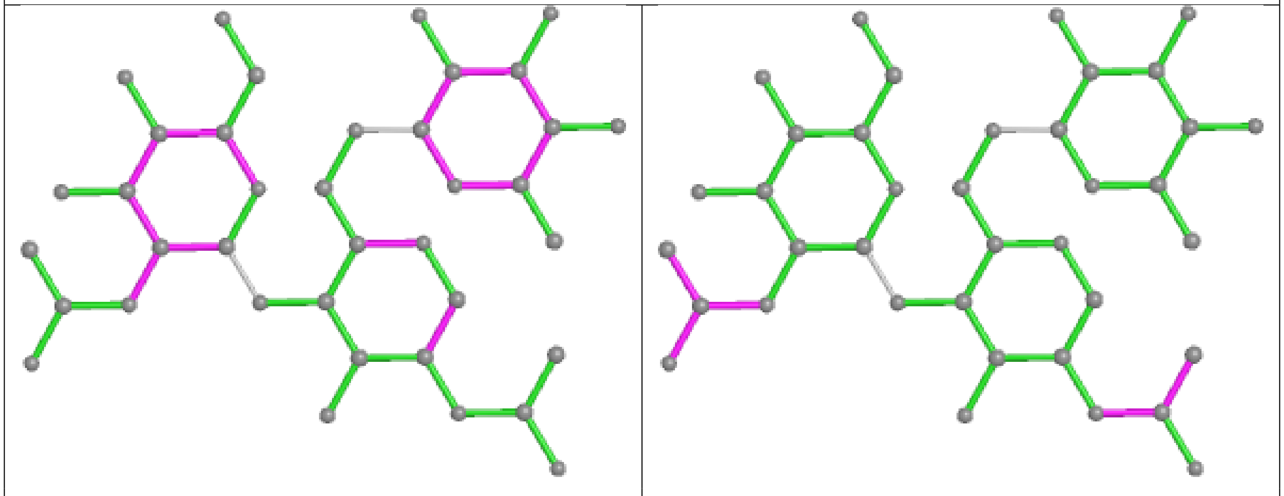
Bond angles



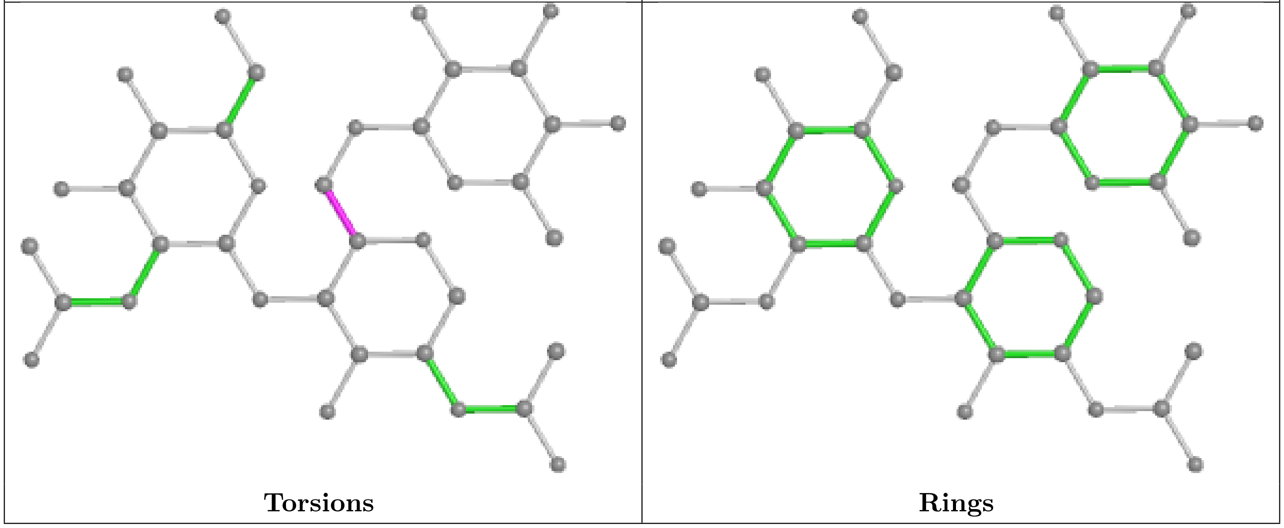
Torsions

Rings

Oligosaccharide Chain v

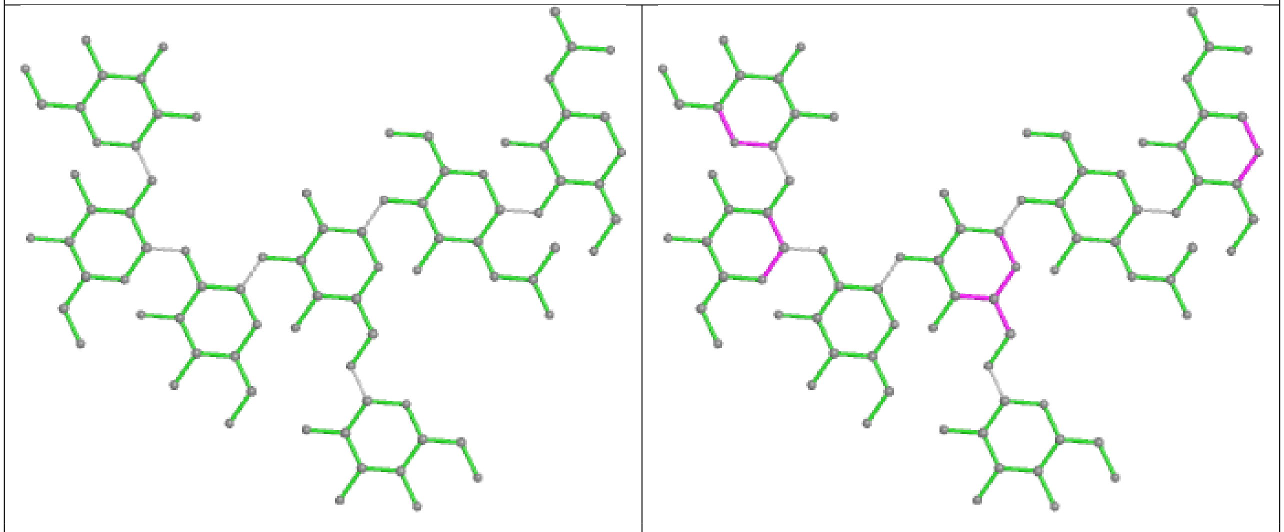


Bond lengths **Bond angles**



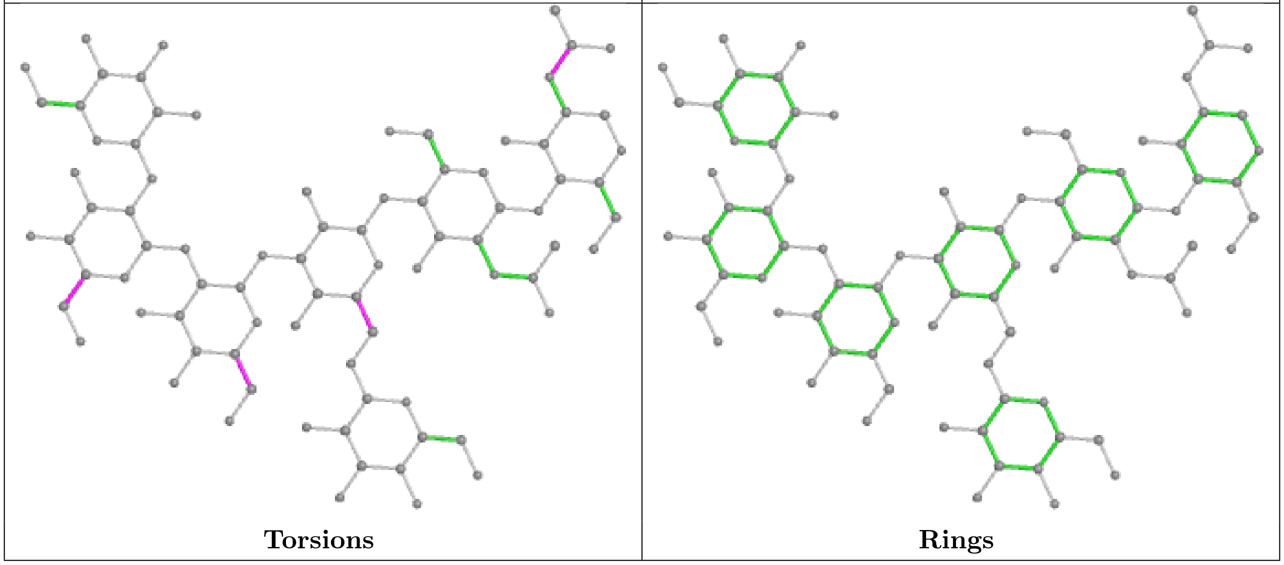
Torsions **Rings**

Oligosaccharide Chain R



Bond lengths

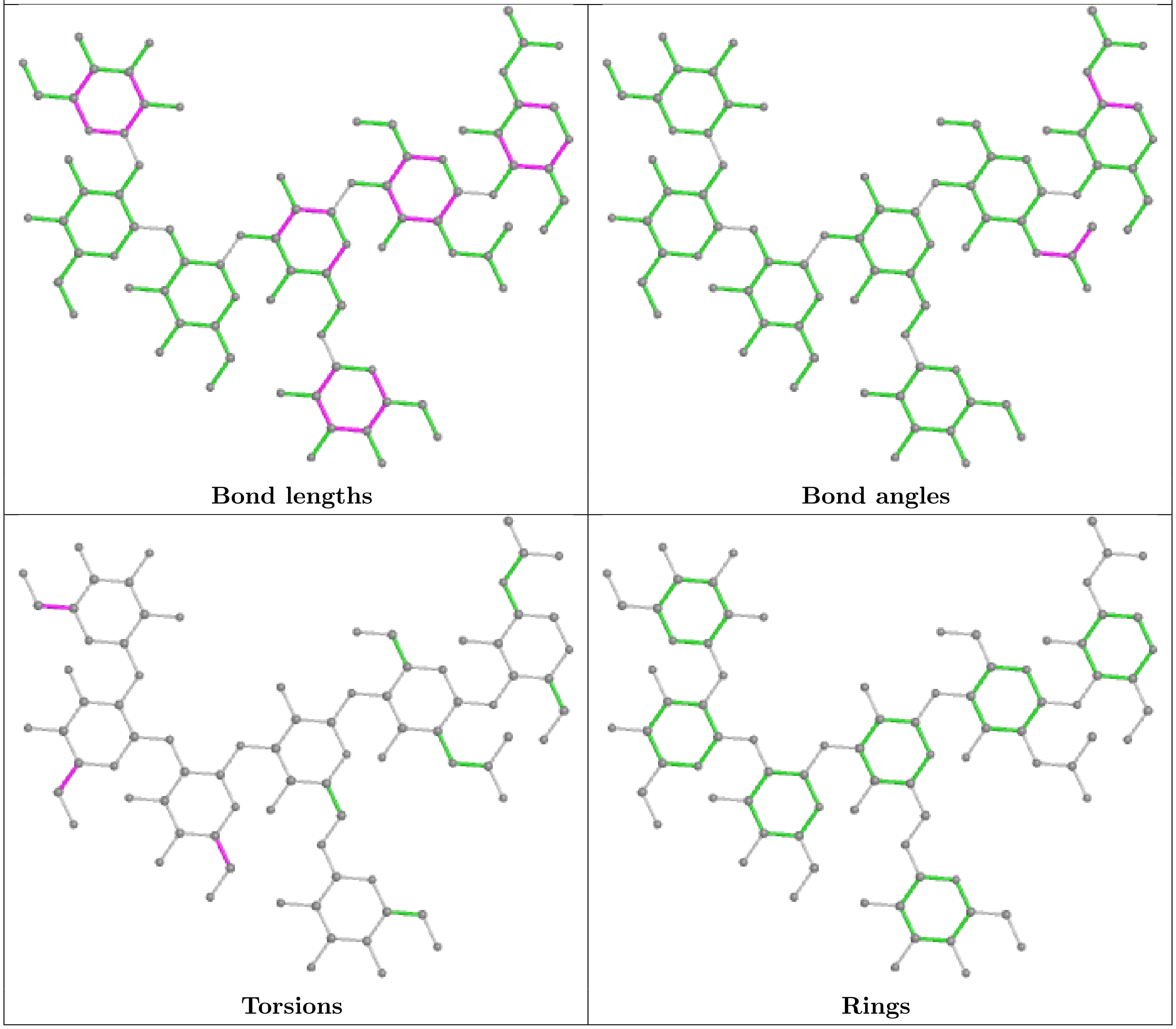
Bond angles



Torsions

Rings

Oligosaccharide Chain e



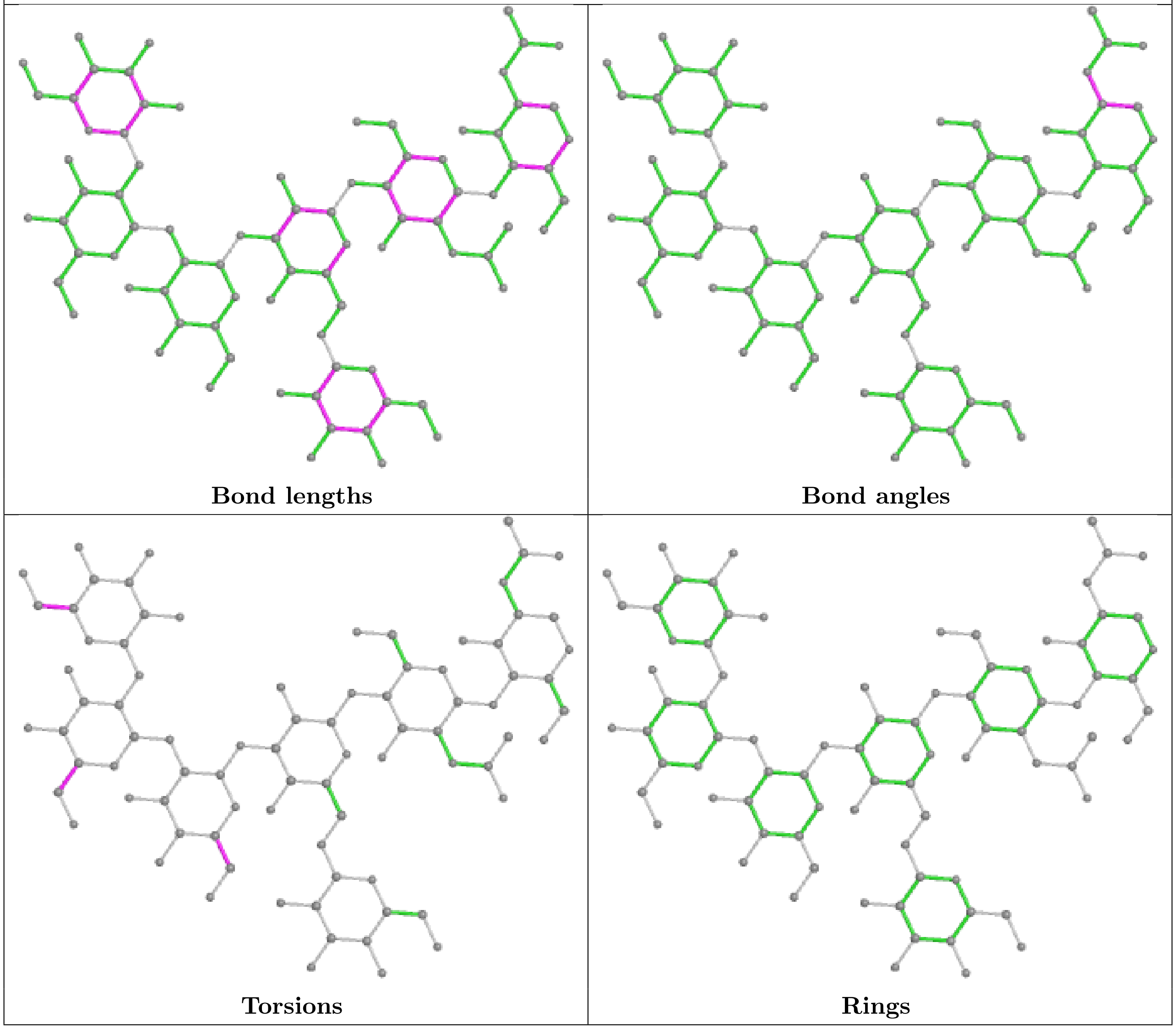
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain r



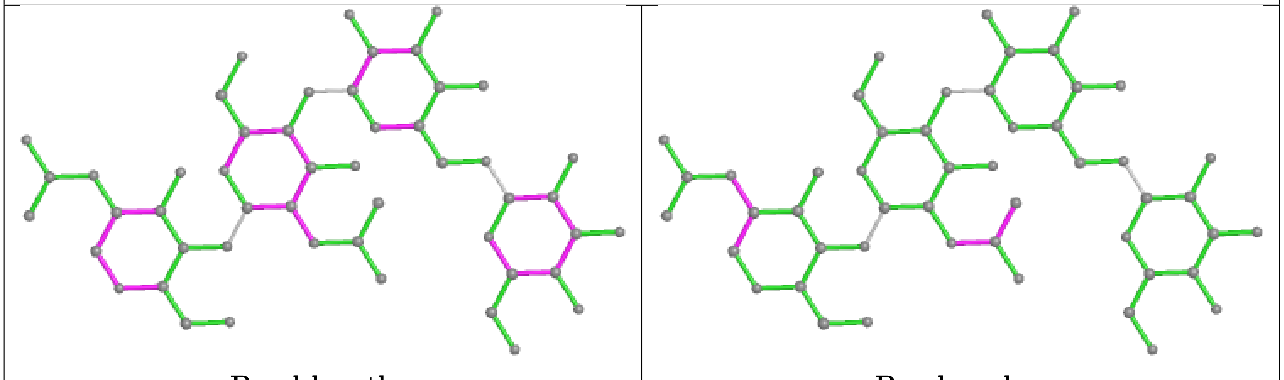
Bond lengths

Bond angles

Torsions

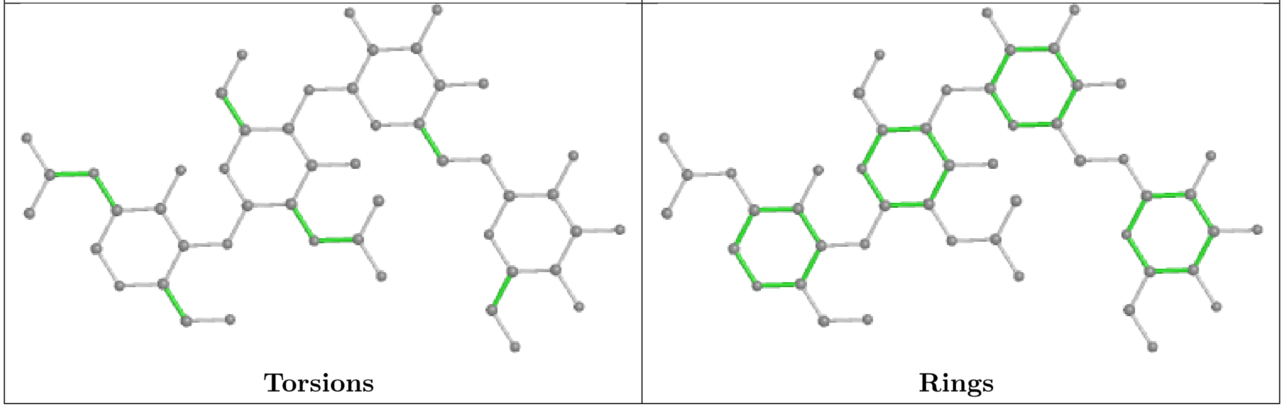
Rings

Oligosaccharide Chain S



Bond lengths

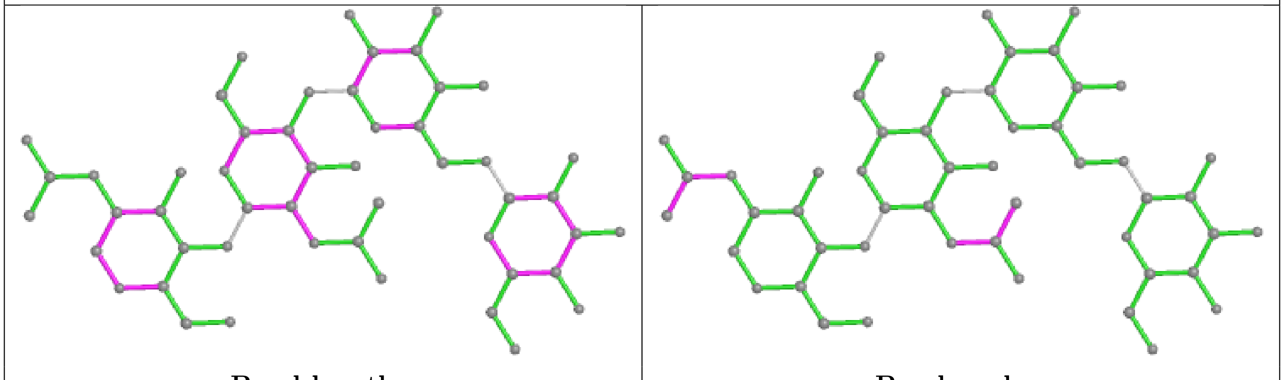
Bond angles



Torsions

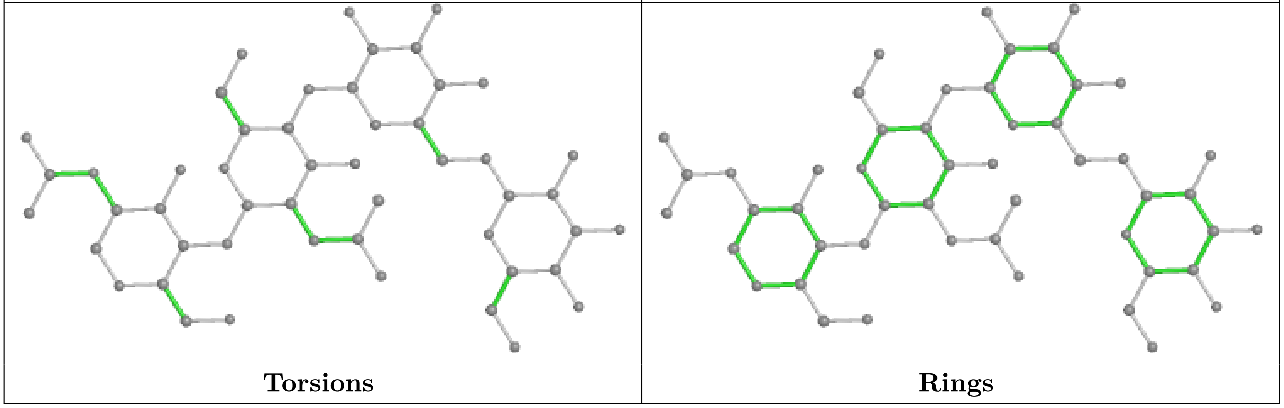
Rings

Oligosaccharide Chain s



Bond lengths

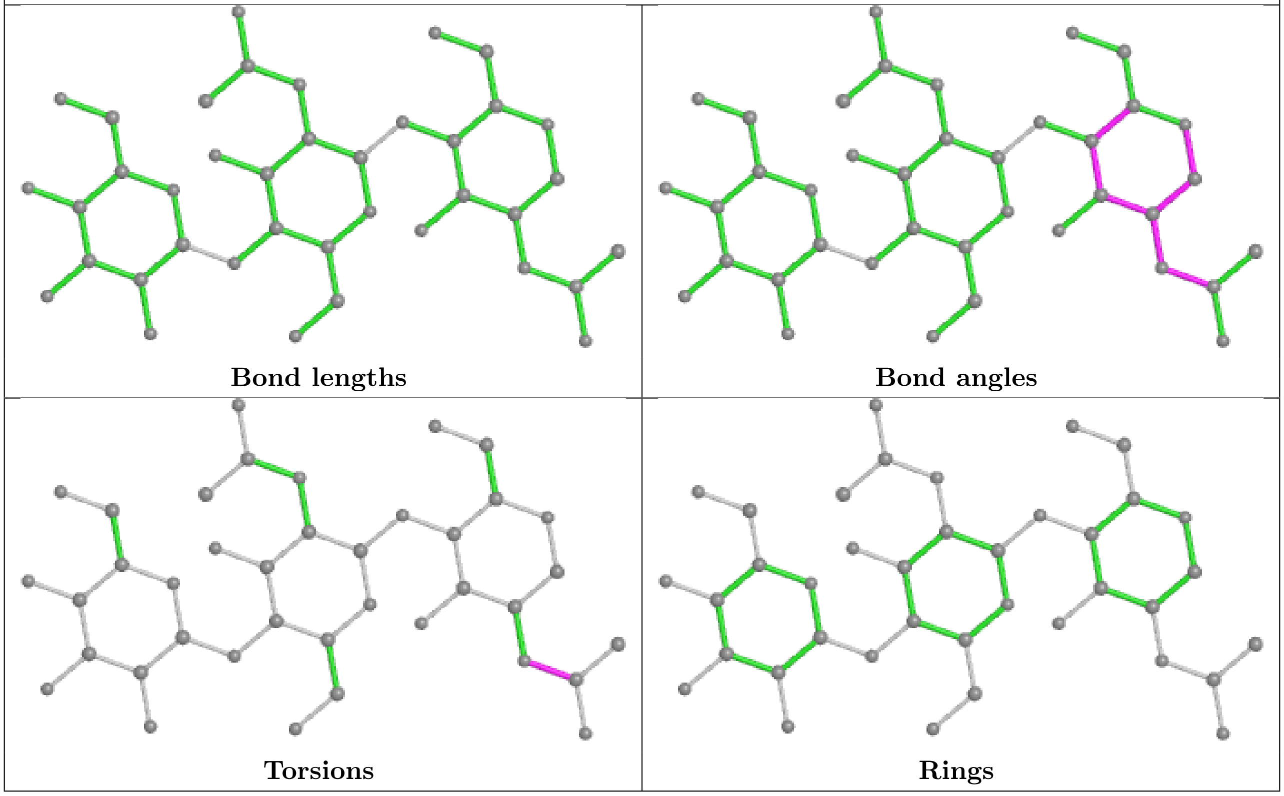
Bond angles



Torsions

Rings

Oligosaccharide Chain T



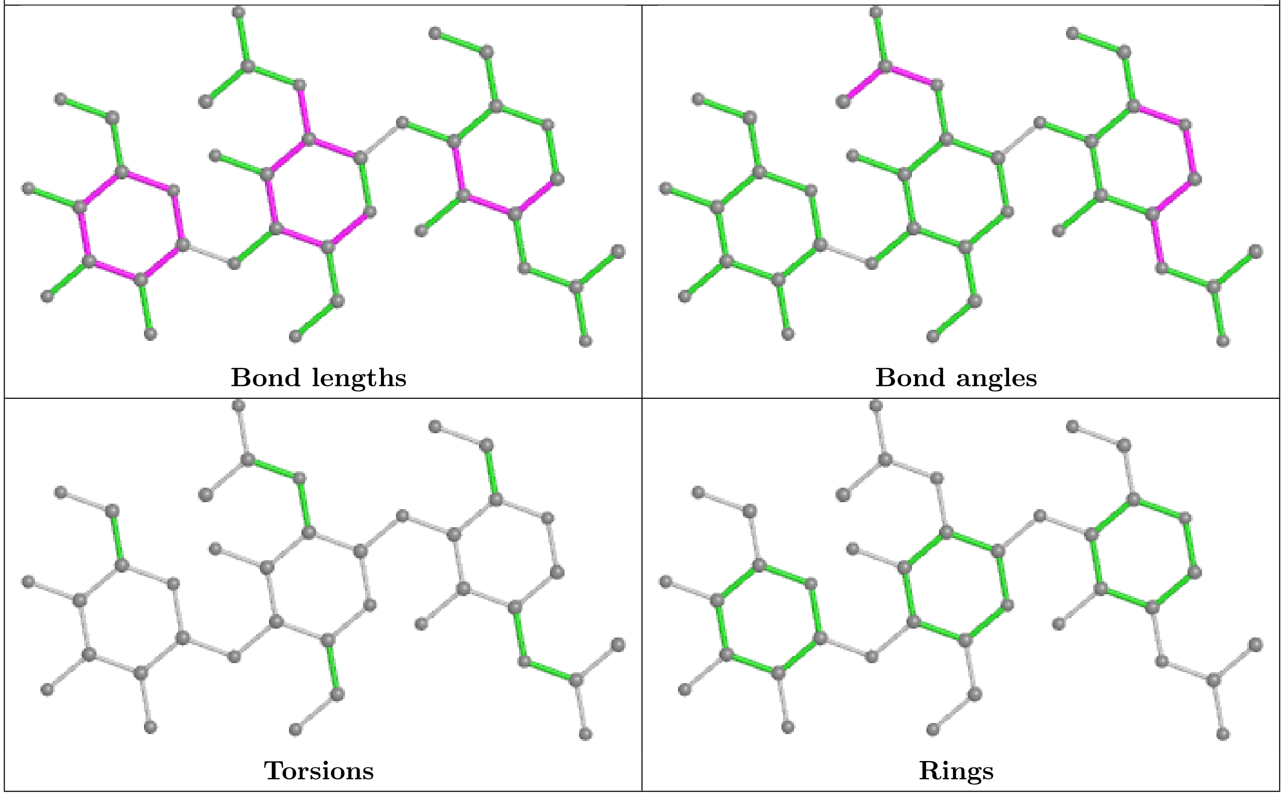
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain W



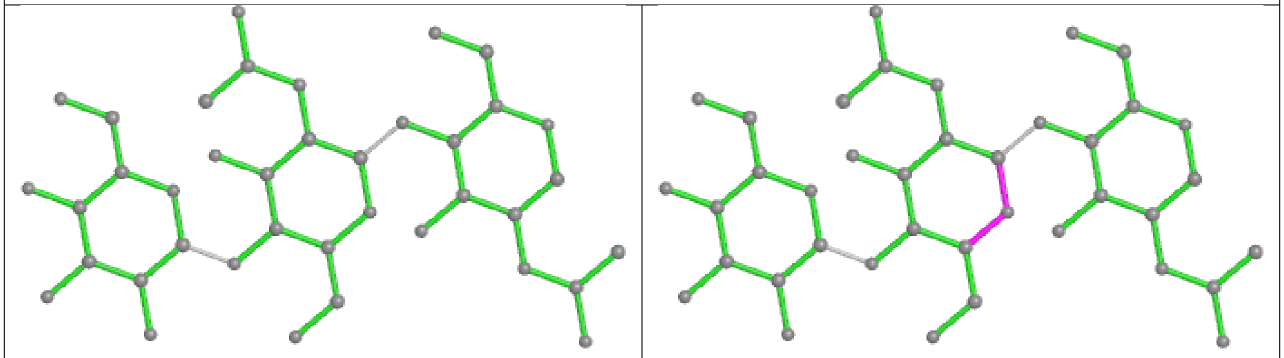
Bond lengths

Bond angles

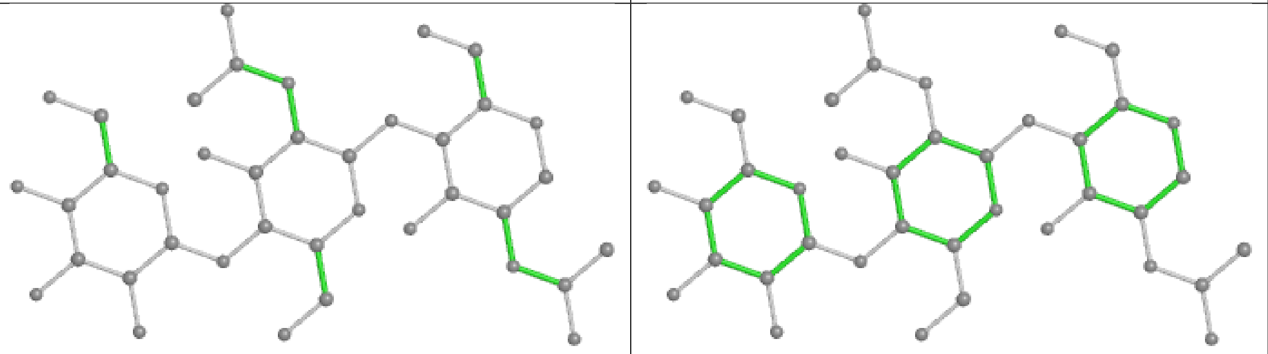
Torsions

Rings

Oligosaccharide Chain g

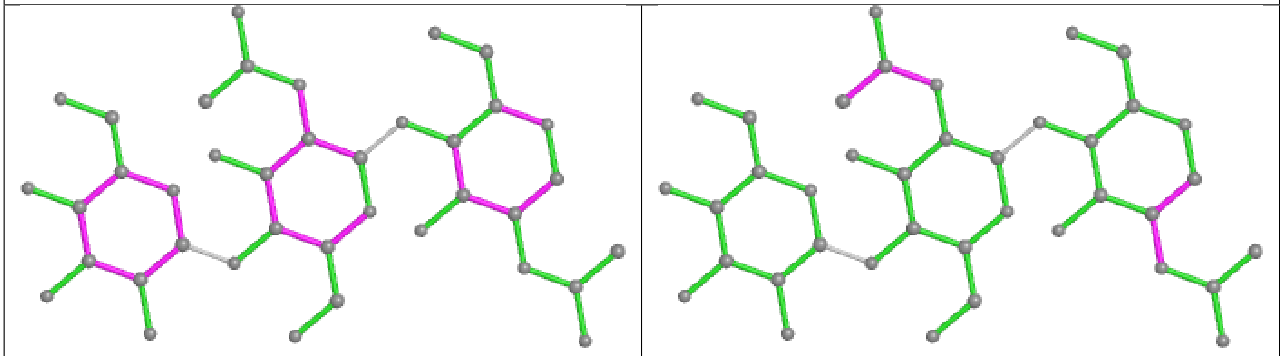


Bond lengths **Bond angles**

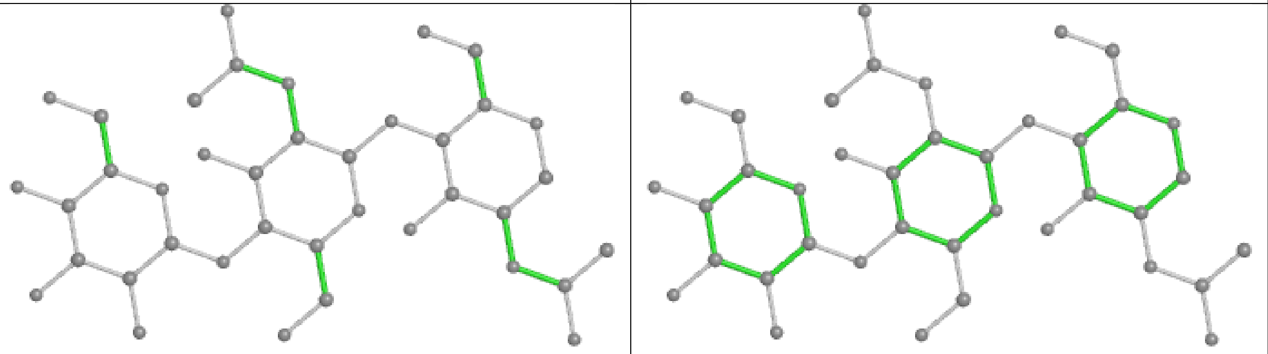


Torsions **Rings**

Oligosaccharide Chain j

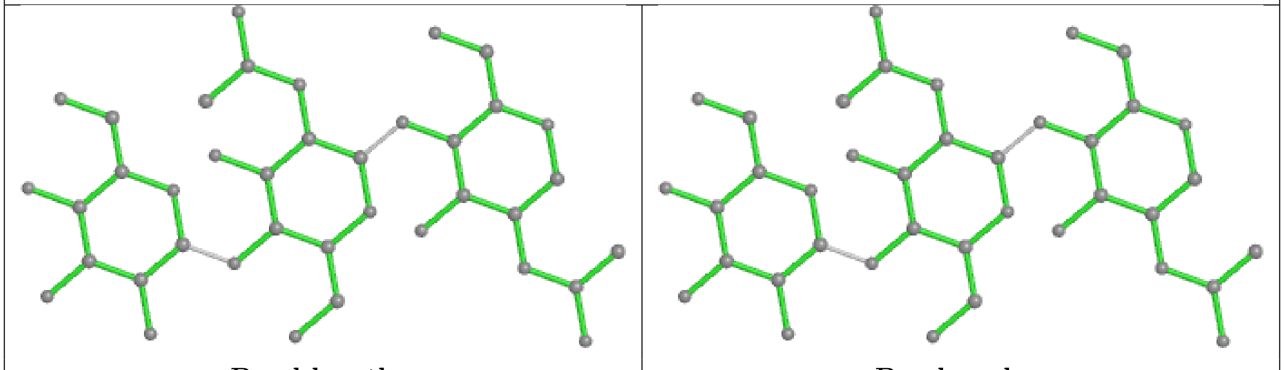


Bond lengths **Bond angles**



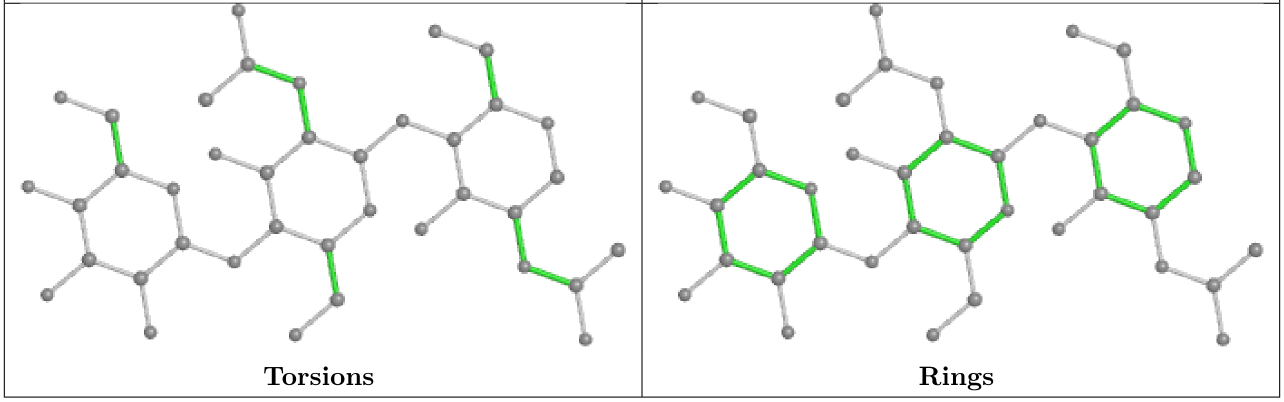
Torsions **Rings**

Oligosaccharide Chain y



Bond lengths

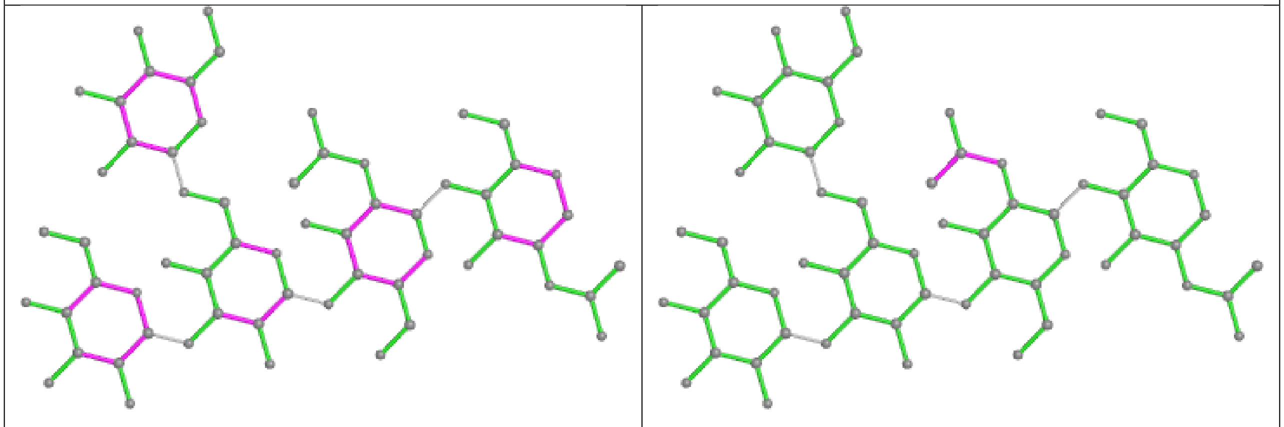
Bond angles



Torsions

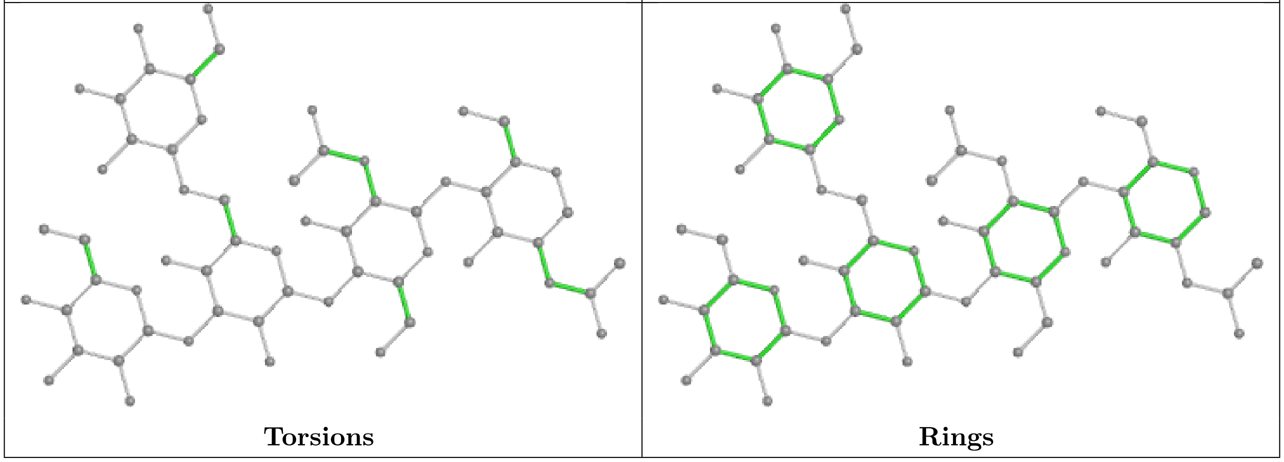
Rings

Oligosaccharide Chain f



Bond lengths

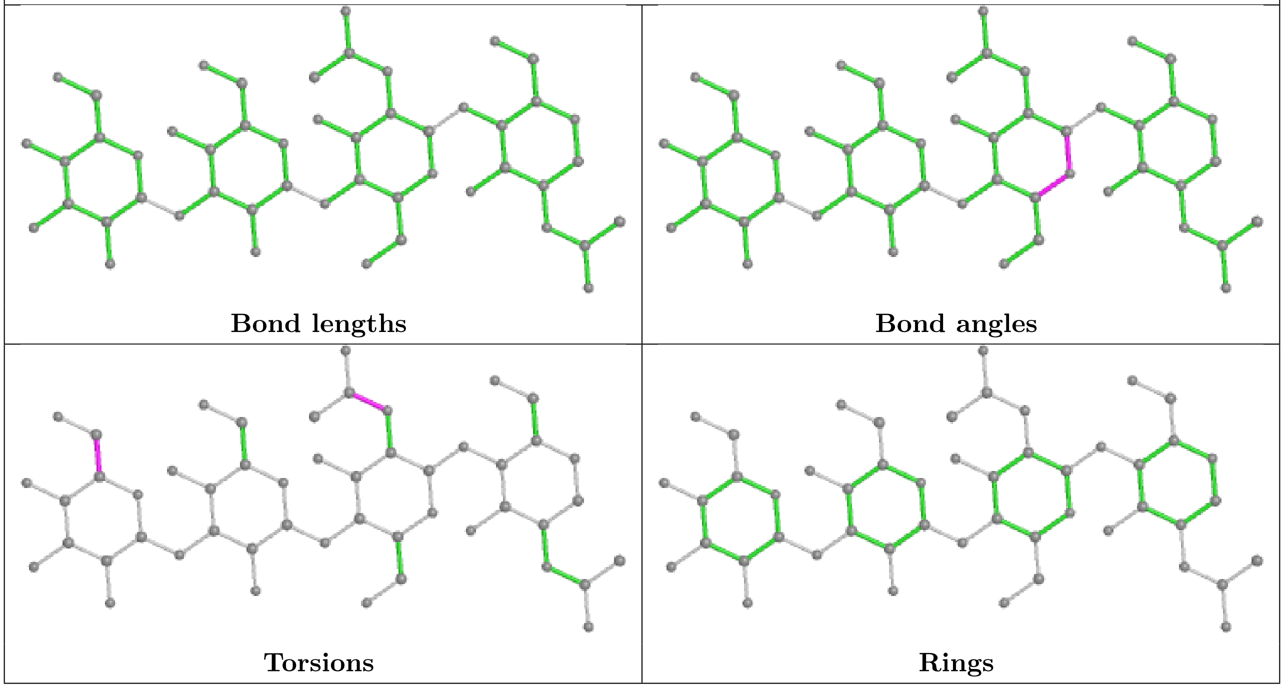
Bond angles



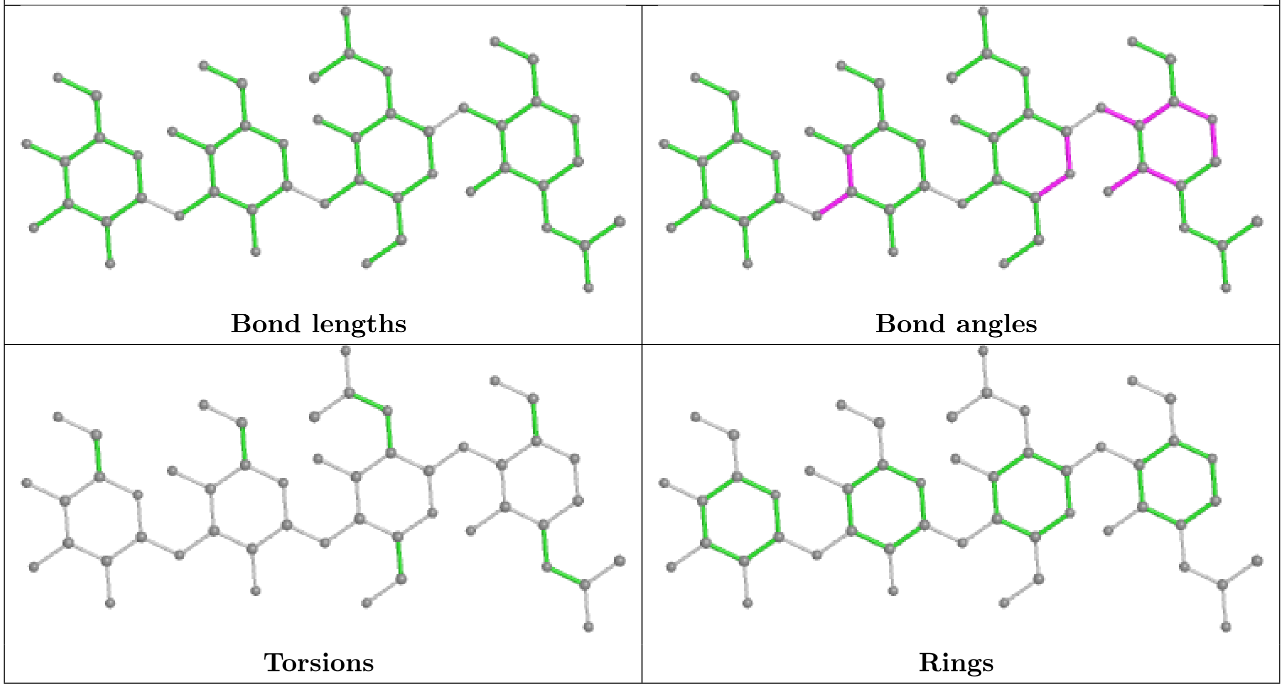
Torsions

Rings

Oligosaccharide Chain t



Oligosaccharide Chain w



5.6 Ligand geometry ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	C	603	1	14,14,15	2.09	5 (35%)	17,19,21	1.08	2 (11%)
13	NAG	C	601	1	14,14,15	2.19	6 (42%)	17,19,21	0.93	1 (5%)
13	NAG	E	602	1	14,14,15	0.28	0	17,19,21	0.74	1 (5%)
13	NAG	A	609	1	14,14,15	2.21	6 (42%)	17,19,21	0.97	1 (5%)
13	NAG	A	607	1	14,14,15	2.07	5 (35%)	17,19,21	1.13	2 (11%)
13	NAG	C	609	1	14,14,15	2.23	7 (50%)	17,19,21	0.93	1 (5%)
13	NAG	A	605	1	14,14,15	2.21	7 (50%)	17,19,21	1.03	2 (11%)
13	NAG	B	702	2	14,14,15	2.05	6 (42%)	17,19,21	1.11	3 (17%)
13	NAG	C	605	1	14,14,15	2.19	7 (50%)	17,19,21	1.04	2 (11%)
13	NAG	E	609	1	14,14,15	2.19	5 (35%)	17,19,21	0.95	0
13	NAG	E	603	1	14,14,15	2.14	5 (35%)	17,19,21	1.07	2 (11%)
13	NAG	E	605	1	14,14,15	2.22	7 (50%)	17,19,21	1.03	2 (11%)
13	NAG	B	703	2	14,14,15	2.14	6 (42%)	17,19,21	1.04	2 (11%)
13	NAG	C	602	1	14,14,15	2.13	5 (35%)	17,19,21	0.94	1 (5%)
13	NAG	E	604	1	14,14,15	2.14	5 (35%)	17,19,21	1.02	1 (5%)
13	NAG	D	701	2	14,14,15	2.06	6 (42%)	17,19,21	1.03	1 (5%)
13	NAG	E	606	1	14,14,15	2.13	6 (42%)	17,19,21	0.95	1 (5%)
13	NAG	A	608	1	14,14,15	1.99	5 (35%)	17,19,21	1.07	2 (11%)
13	NAG	F	701	2	14,14,15	2.01	6 (42%)	17,19,21	1.93	2 (11%)
13	NAG	A	603	1	14,14,15	2.08	5 (35%)	17,19,21	1.09	2 (11%)
13	NAG	D	702	2	14,14,15	2.00	6 (42%)	17,19,21	1.03	2 (11%)
13	NAG	C	606	1	14,14,15	2.17	6 (42%)	17,19,21	0.96	1 (5%)
13	NAG	A	604	1	14,14,15	2.12	5 (35%)	17,19,21	1.05	1 (5%)
13	NAG	A	606	1	14,14,15	2.19	6 (42%)	17,19,21	0.93	1 (5%)
13	NAG	C	607	1	14,14,15	2.09	5 (35%)	17,19,21	1.15	3 (17%)
13	NAG	E	601	1	14,14,15	2.24	7 (50%)	17,19,21	0.96	1 (5%)
13	NAG	F	703	2	14,14,15	2.24	7 (50%)	17,19,21	1.07	2 (11%)
13	NAG	F	702	2	14,14,15	2.26	5 (35%)	17,19,21	1.07	1 (5%)
13	NAG	E	607	1	14,14,15	2.07	6 (42%)	17,19,21	1.13	2 (11%)
13	NAG	D	703	2	14,14,15	2.22	7 (50%)	17,19,21	0.97	1 (5%)
13	NAG	A	602	1	14,14,15	2.14	5 (35%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	NAG	C	608	1	14,14,15	2.02	5 (35%)	17,19,21	1.12	2 (11%)
13	NAG	B	701	2	14,14,15	2.03	6 (42%)	17,19,21	1.15	2 (11%)
13	NAG	A	601	1	14,14,15	2.24	7 (50%)	17,19,21	1.03	2 (11%)
13	NAG	C	604	1	14,14,15	2.13	5 (35%)	17,19,21	0.94	0
13	NAG	E	608	1	14,14,15	2.00	5 (35%)	17,19,21	1.06	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	C	603	1	-	0/6/23/26	0/1/1/1
13	NAG	C	601	1	-	0/6/23/26	0/1/1/1
13	NAG	E	602	1	-	0/6/23/26	0/1/1/1
13	NAG	A	609	1	-	0/6/23/26	0/1/1/1
13	NAG	A	607	1	-	0/6/23/26	0/1/1/1
13	NAG	C	609	1	-	0/6/23/26	0/1/1/1
13	NAG	A	605	1	-	0/6/23/26	0/1/1/1
13	NAG	B	702	2	-	0/6/23/26	0/1/1/1
13	NAG	C	605	1	-	0/6/23/26	0/1/1/1
13	NAG	E	609	1	-	0/6/23/26	0/1/1/1
13	NAG	E	603	1	-	0/6/23/26	0/1/1/1
13	NAG	E	605	1	-	0/6/23/26	0/1/1/1
13	NAG	B	703	2	-	0/6/23/26	0/1/1/1
13	NAG	C	602	1	-	0/6/23/26	0/1/1/1
13	NAG	E	604	1	-	0/6/23/26	0/1/1/1
13	NAG	D	701	2	-	0/6/23/26	0/1/1/1
13	NAG	E	606	1	-	0/6/23/26	0/1/1/1
13	NAG	A	608	1	-	2/6/23/26	0/1/1/1
13	NAG	F	701	2	-	3/6/23/26	0/1/1/1
13	NAG	A	603	1	-	0/6/23/26	0/1/1/1
13	NAG	D	702	2	-	0/6/23/26	0/1/1/1
13	NAG	C	606	1	-	0/6/23/26	0/1/1/1
13	NAG	A	604	1	-	0/6/23/26	0/1/1/1
13	NAG	A	606	1	-	0/6/23/26	0/1/1/1
13	NAG	C	607	1	-	0/6/23/26	0/1/1/1
13	NAG	E	601	1	-	0/6/23/26	0/1/1/1
13	NAG	F	703	2	-	0/6/23/26	0/1/1/1
13	NAG	F	702	2	-	0/6/23/26	0/1/1/1
13	NAG	E	607	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	D	703	2	-	0/6/23/26	0/1/1/1
13	NAG	A	602	1	-	1/6/23/26	0/1/1/1
13	NAG	C	608	1	-	2/6/23/26	0/1/1/1
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
13	NAG	A	601	1	-	0/6/23/26	0/1/1/1
13	NAG	C	604	1	-	0/6/23/26	0/1/1/1
13	NAG	E	608	1	-	1/6/23/26	0/1/1/1

The worst 5 of 203 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	702	NAG	C1-C2	6.17	1.61	1.52
13	E	609	NAG	C1-C2	5.66	1.60	1.52
13	E	603	NAG	C1-C2	5.64	1.60	1.52
13	C	609	NAG	C1-C2	5.63	1.60	1.52
13	A	601	NAG	C1-C2	5.60	1.60	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	701	NAG	C8-C7-N2	5.63	125.63	116.10
13	F	701	NAG	O7-C7-N2	-3.73	115.09	121.95
13	B	701	NAG	C8-C7-N2	2.95	121.10	116.10
13	C	607	NAG	C8-C7-N2	2.92	121.05	116.10
13	A	607	NAG	C8-C7-N2	2.76	120.77	116.10

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	608	NAG	O5-C5-C6-O6
13	F	701	NAG	C8-C7-N2-C2
13	F	701	NAG	O7-C7-N2-C2
13	C	608	NAG	C4-C5-C6-O6
13	F	701	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

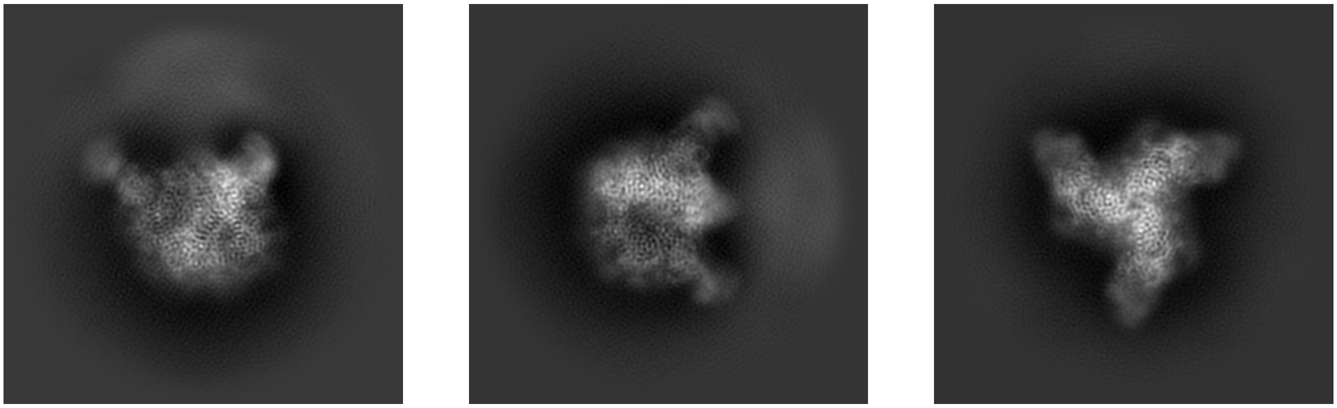
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25676. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

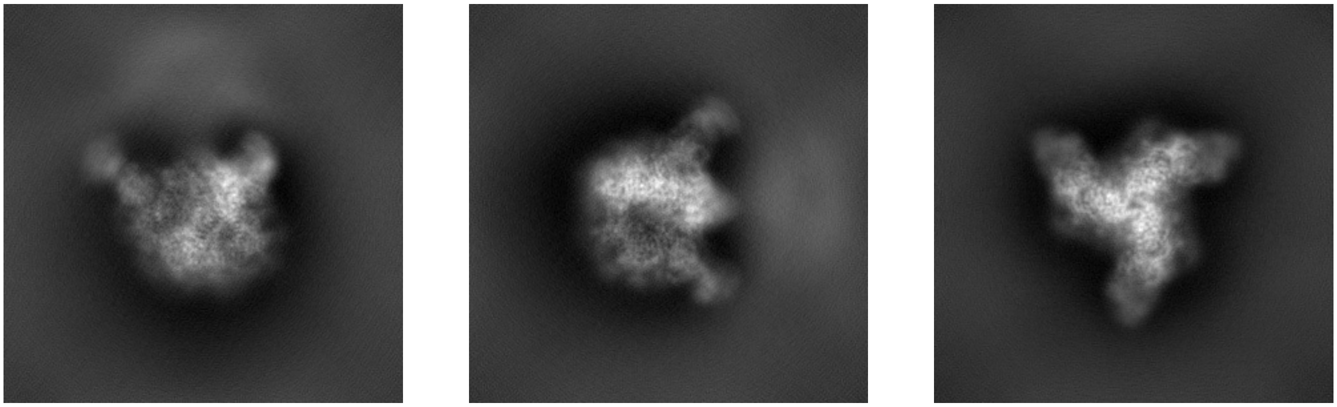
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

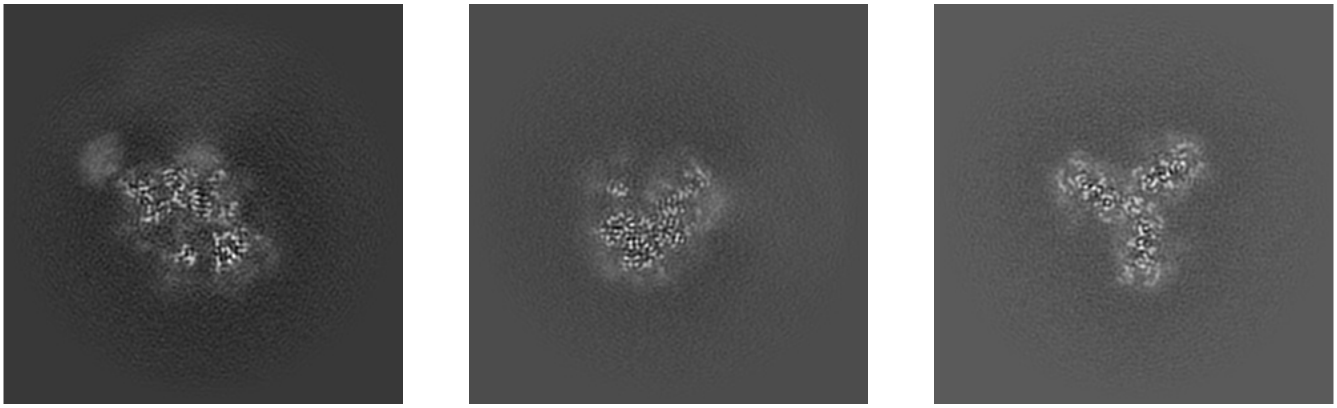


X Y Z

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

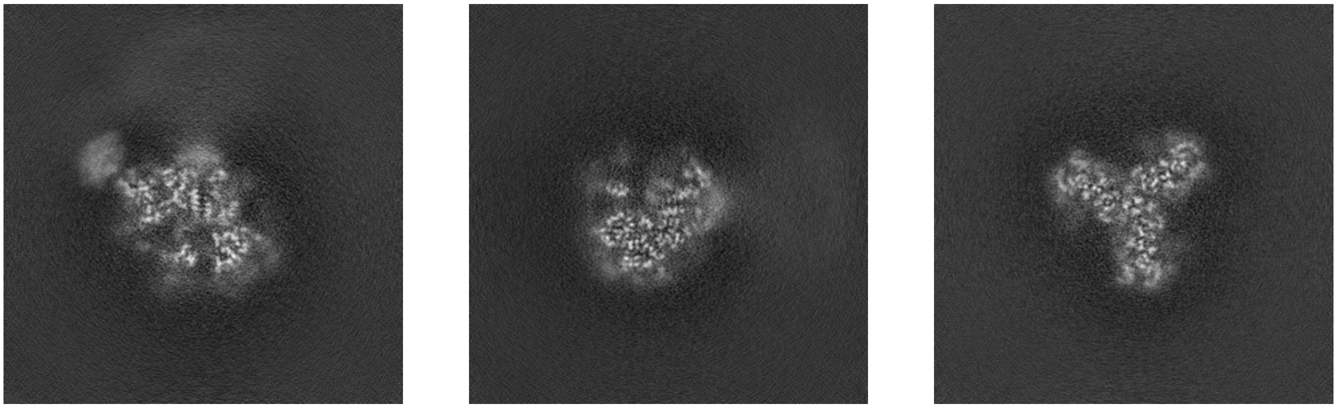
6.2 Central slices ⓘ

6.2.1 Primary map



X Index: 150 Y Index: 150 Z Index: 150

6.2.2 Raw map

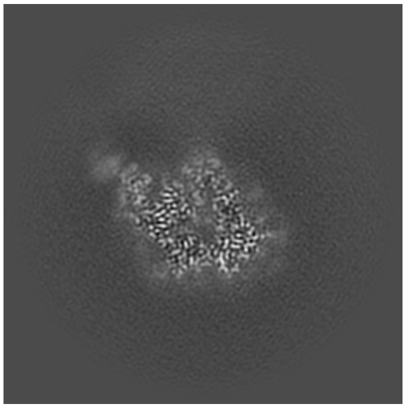


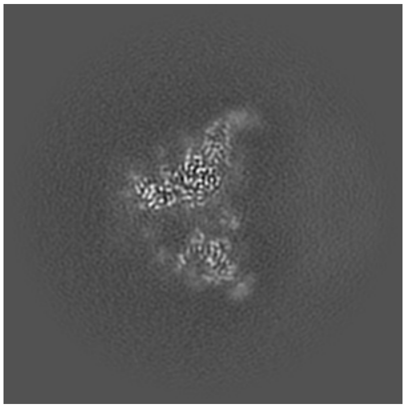
X Index: 150 Y Index: 150 Z Index: 150

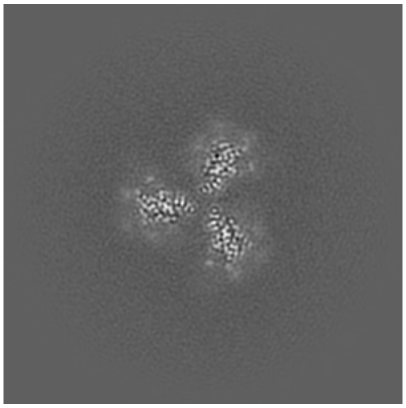
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

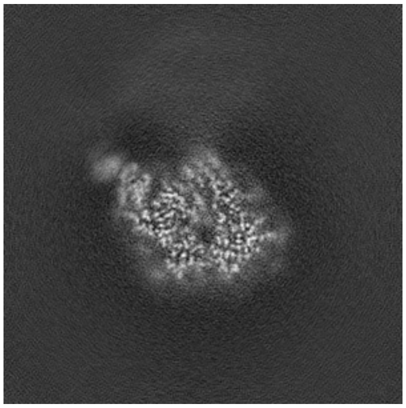
6.3.1 Primary map

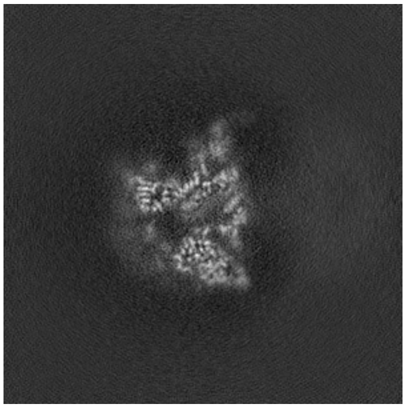

X Index: 161

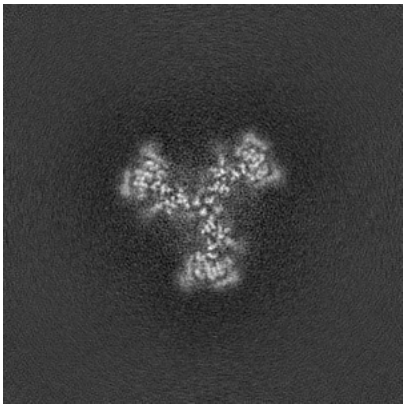

Y Index: 172


Z Index: 122

6.3.2 Raw map


X Index: 162

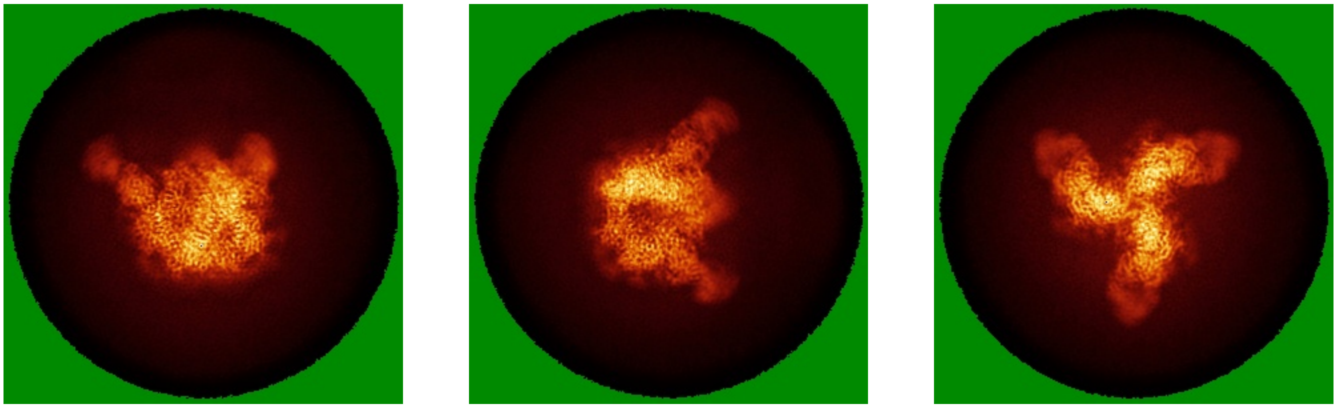

Y Index: 164


Z Index: 155

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

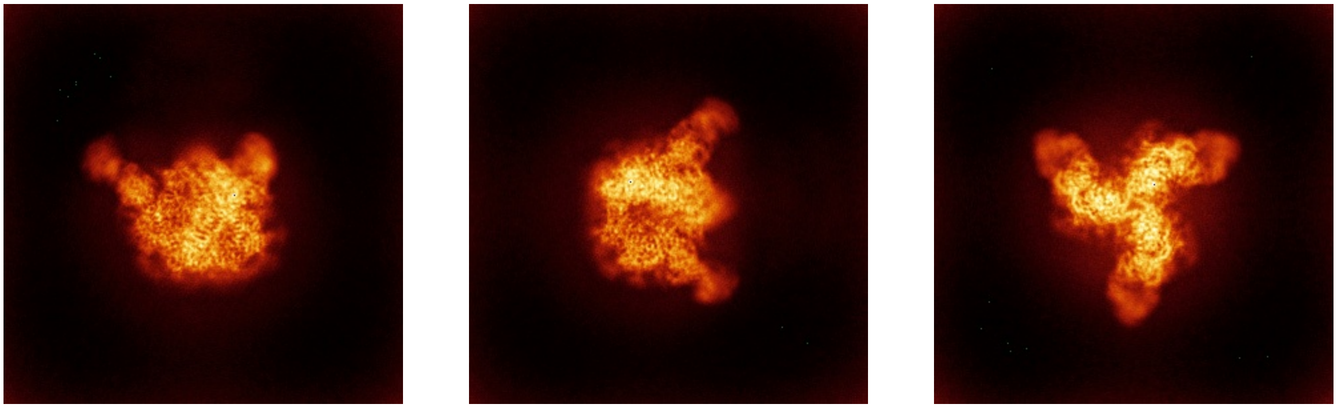
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

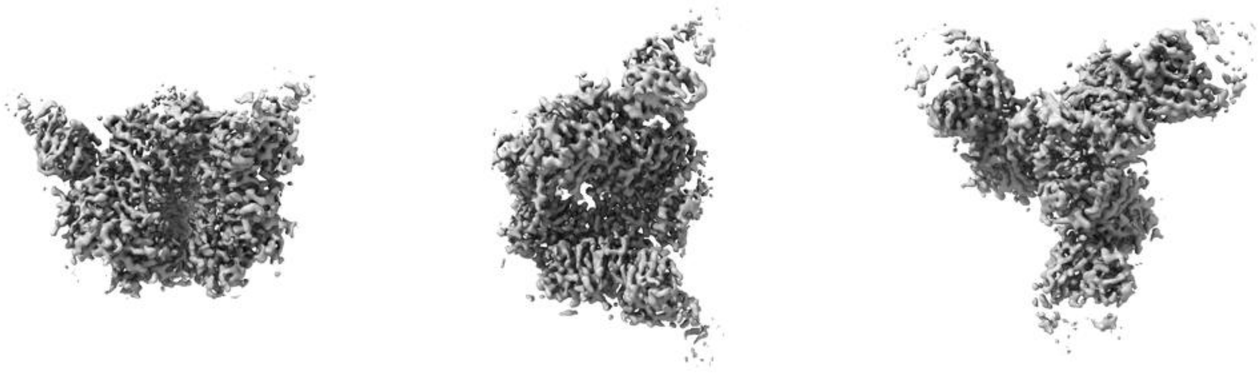


X Y Z

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

6.5 Orthogonal surface views

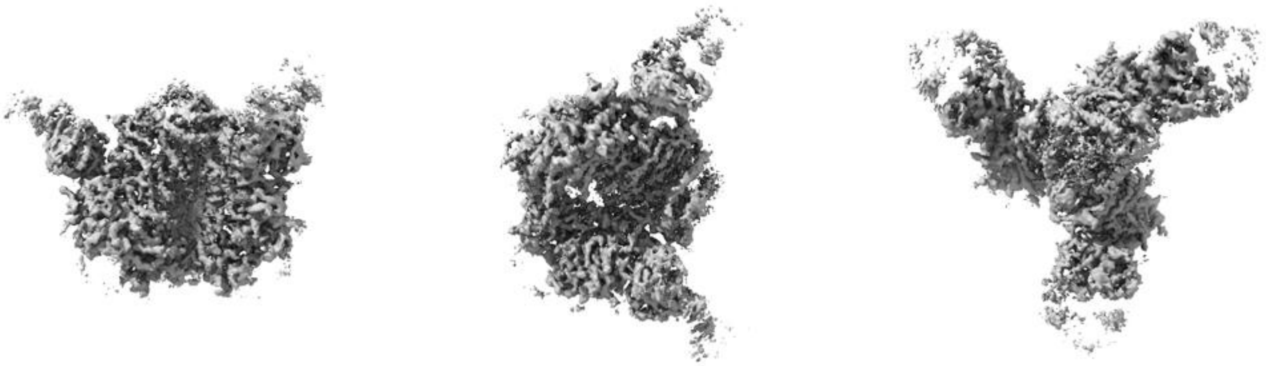
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

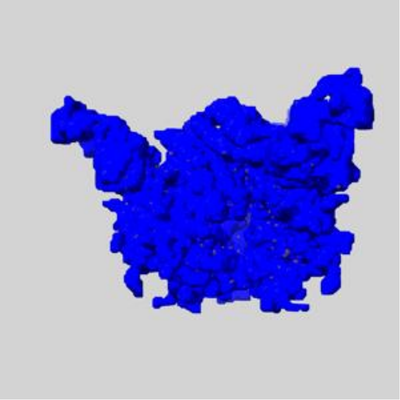
6.6 Mask visualisation ⓘ

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

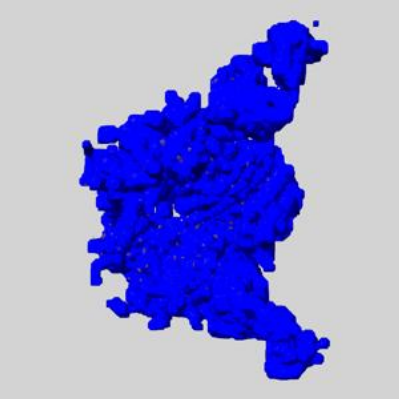
A mask typically either:

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

6.6.1 emd_25676_msk_1.map ⓘ



X



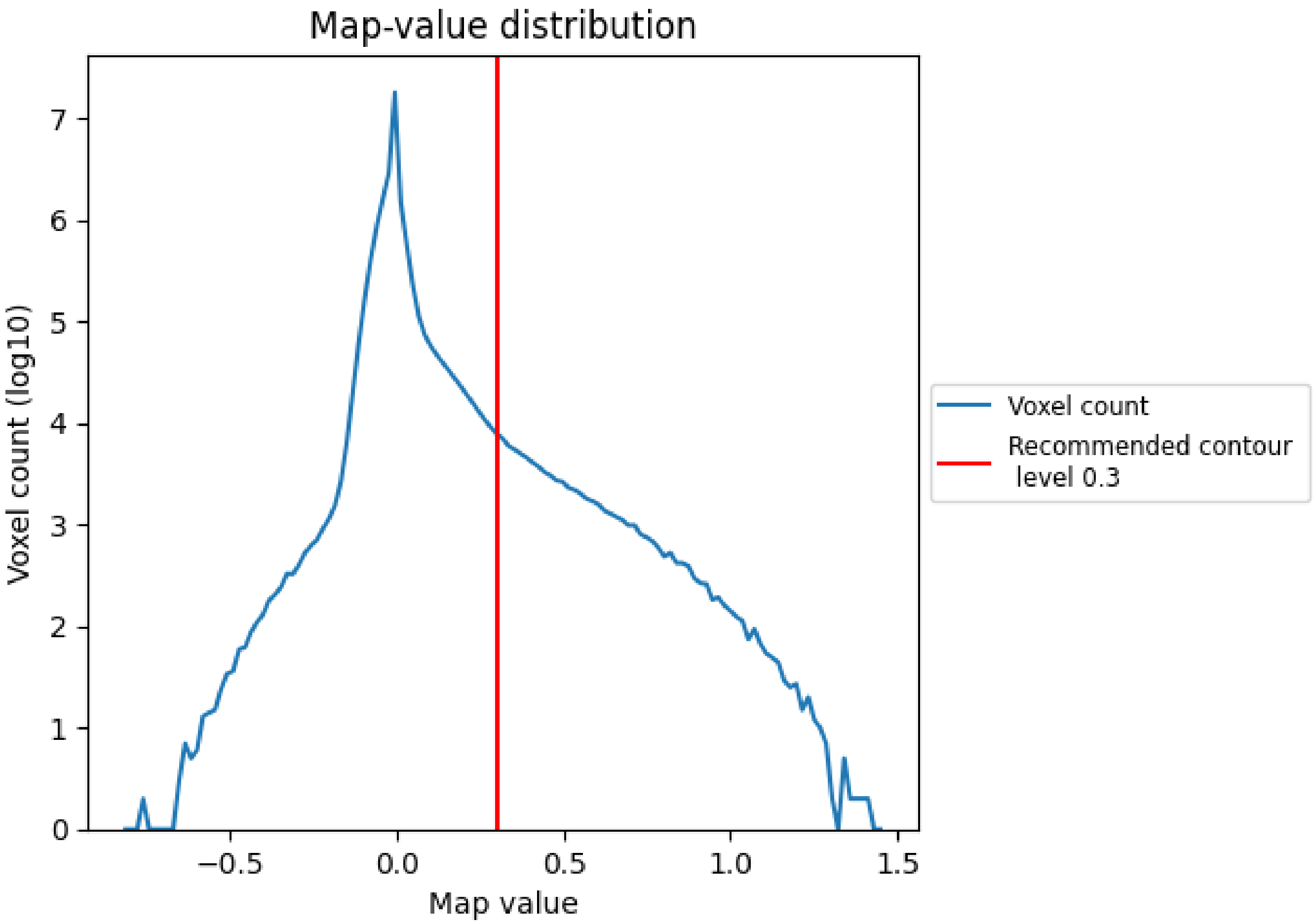
Y

Z

7 Map analysis ⓘ

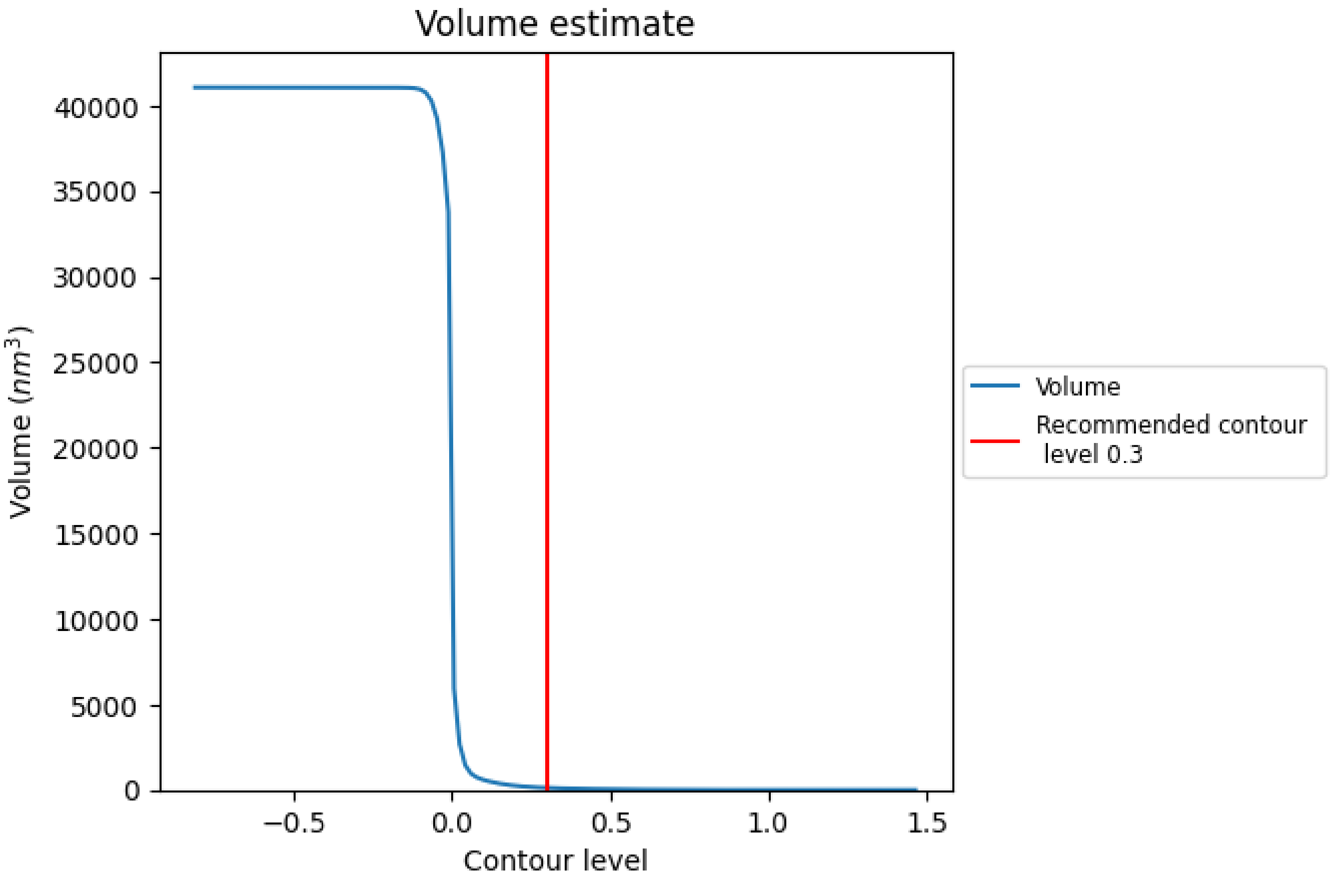
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

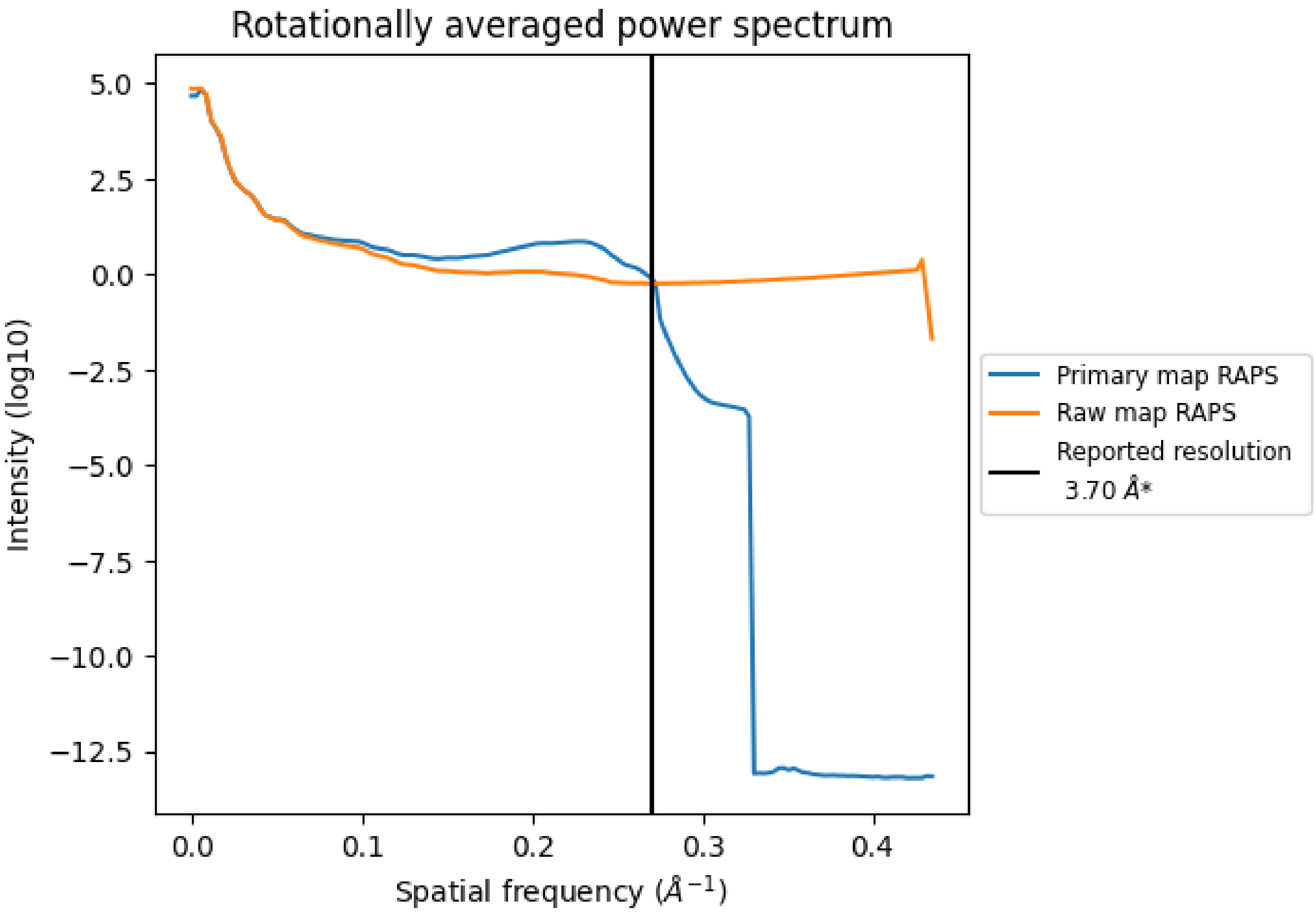
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 112 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 ⓘ

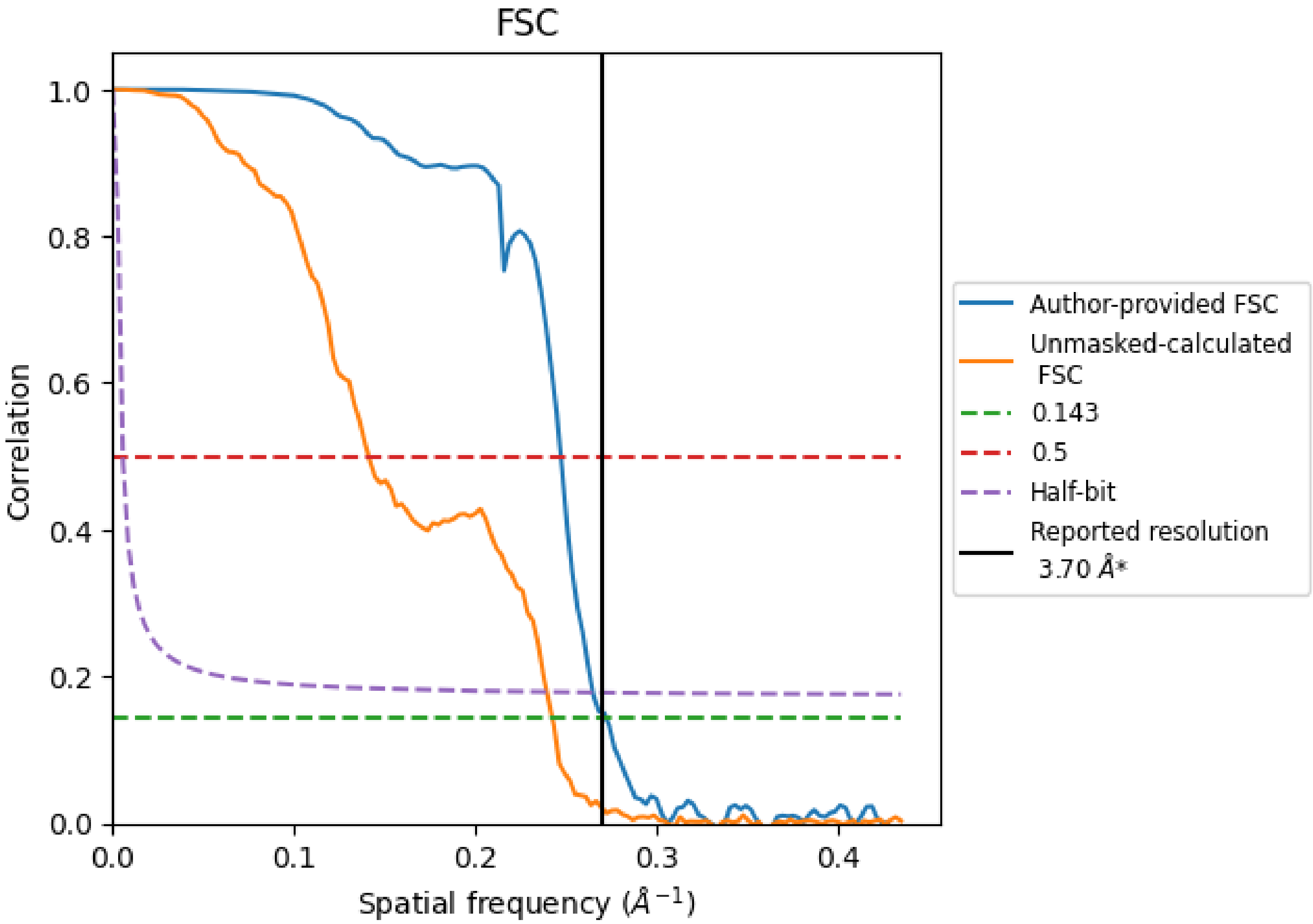


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates ⓘ

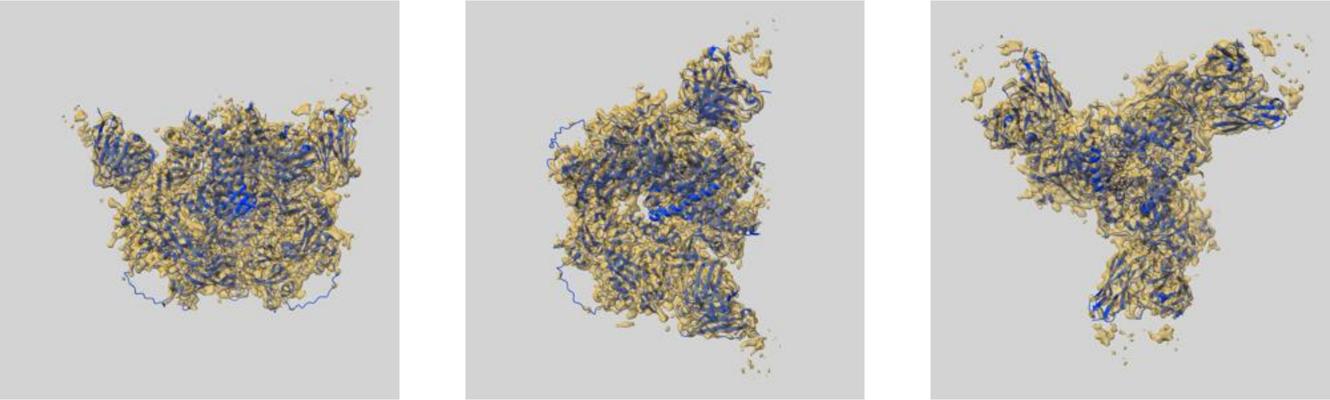
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.04	3.78
Unmasked-calculated*	4.12	7.08	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.7 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-25676 and PDB model 7T4G. Per-residue inclusion information can be found in section 3 on page 14.

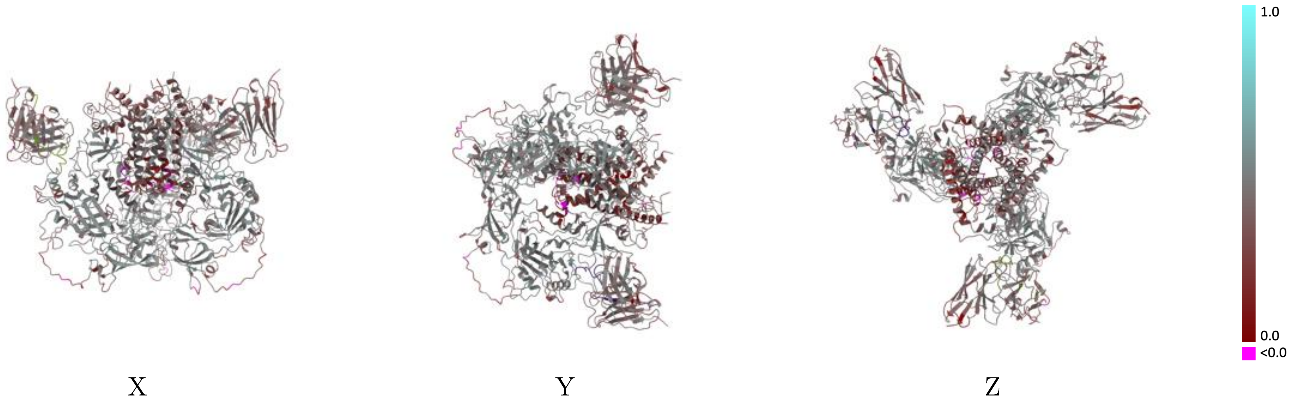
9.1 Map-model overlay ⓘ



X Y Z

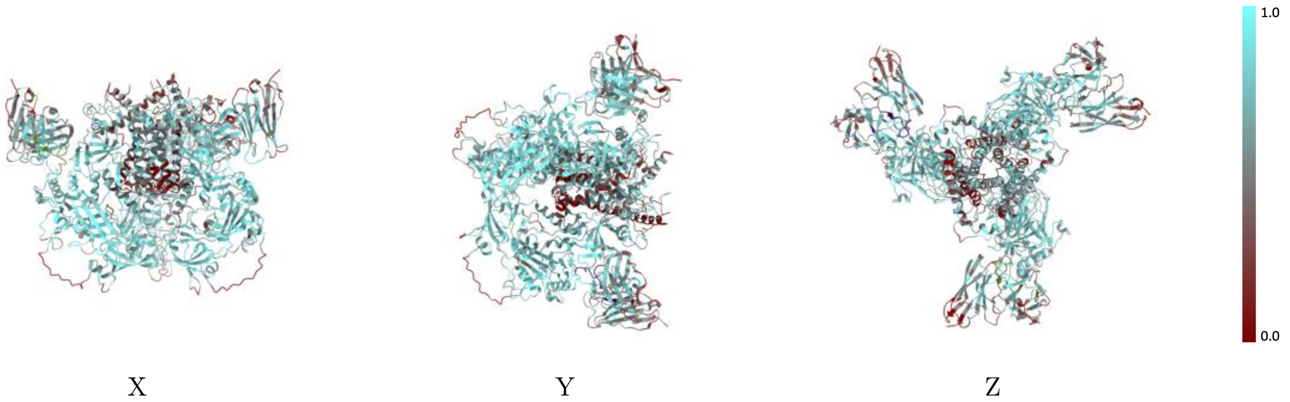
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



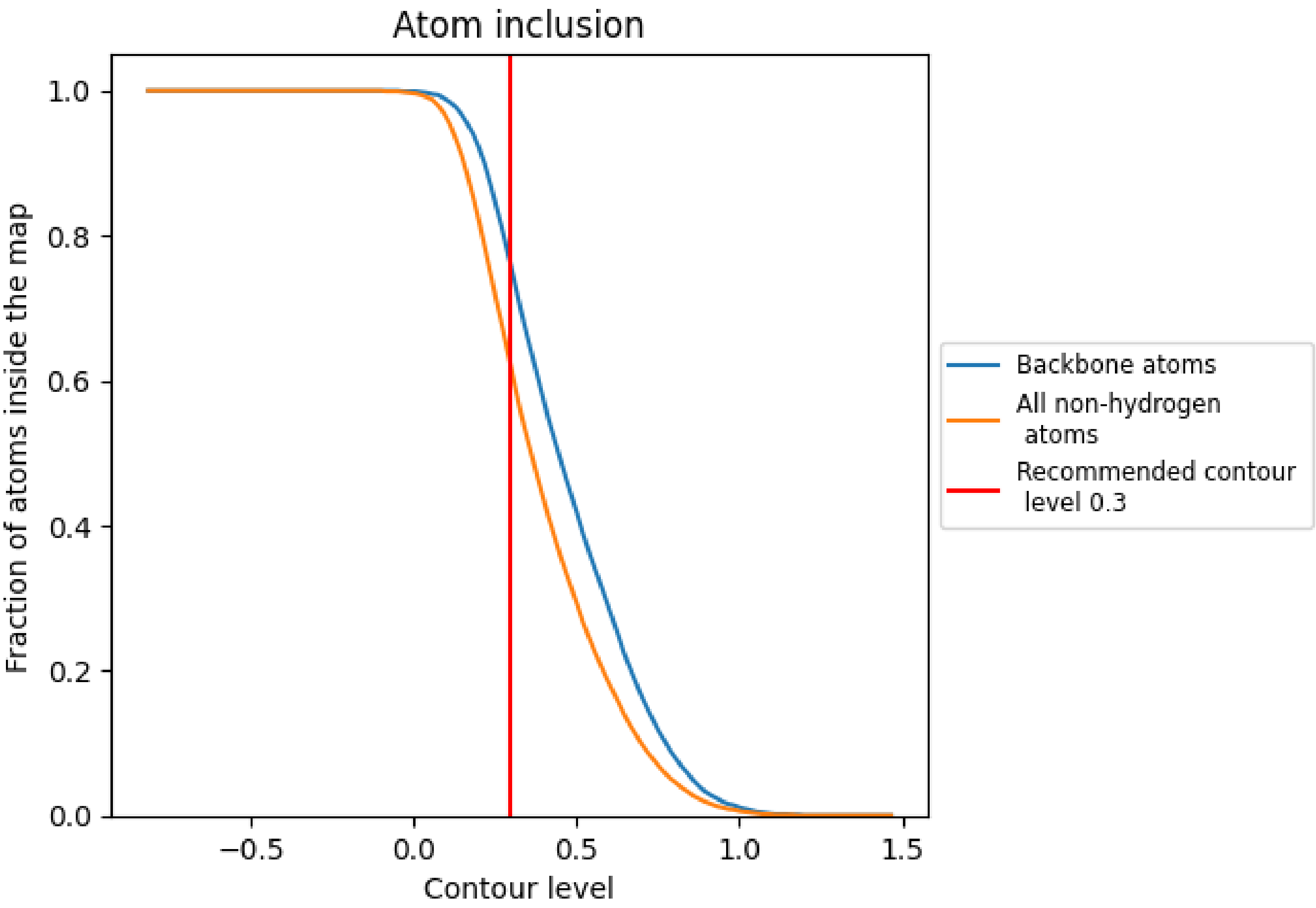
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 62% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.4060
A	0.7180	0.4460
B	0.4420	0.2990
C	0.7050	0.4420
D	0.4530	0.3100
E	0.7120	0.4400
F	0.4470	0.3130
G	0.5950	0.3990
H	0.6210	0.4050
I	0.5250	0.3880
J	0.6220	0.4080
K	0.5590	0.4000
L	0.5800	0.3960
M	0.4890	0.3920
N	0.5360	0.4390
O	0.3160	0.3420
P	0.2370	0.2890
Q	0.4740	0.3490
R	0.4460	0.4030
S	0.3400	0.3660
T	0.5130	0.4680
U	0.3930	0.3210
V	0.1050	0.2320
W	0.4870	0.3940
X	0.6070	0.4130
Y	0.5000	0.3890
Z	0.5110	0.4240
a	0.5360	0.3450
b	0.2890	0.3540
c	0.3680	0.3340
d	0.5260	0.3900
e	0.4460	0.3480
f	0.2950	0.3390
g	0.5130	0.4450
h	0.2500	0.2450

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Chain	Atom inclusion	Q-score
i	0.1580	0.2910
j	0.5640	0.3260
k	0.6070	0.4470
l	0.5360	0.3150
m	0.5320	0.4110
n	0.6070	0.3640
o	0.2630	0.3340
p	0.1580	0.3730
q	0.5000	0.3630
r	0.4220	0.3970
s	0.3800	0.3840
t	0.4000	0.4060
u	0.3210	0.2530
v	0.2100	0.2190
w	0.5000	0.4390
x	0.6790	0.4290
y	0.4100	0.3970