



## wwPDB EM Validation Summary Report ⓘ

May 21, 2026 – 02:41 PM EDT

PDB ID : 9Q3S / pdb\_00009q3s  
EMDB ID : EMD-72206  
Title : Cryo-EM structure of PGT121 Fab and Rhesus macaque Ab4 Fab in complex with HIV-1 Env trimer BG505 SOSIP.664  
Authors : Chandravanshi, M.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2025-08-19  
Resolution : 3.01 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

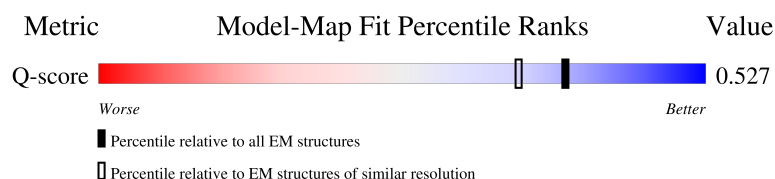
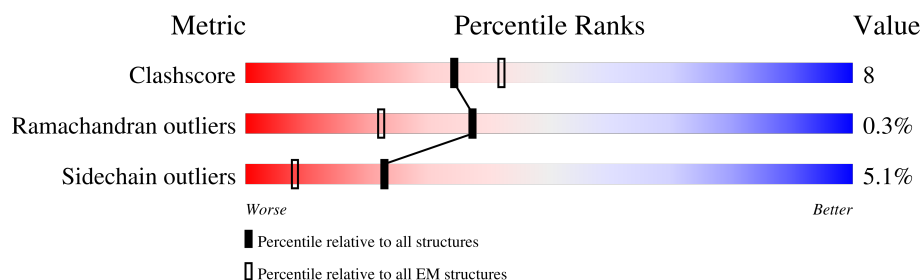
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.01 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.





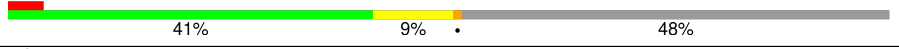

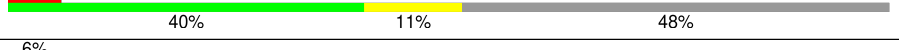


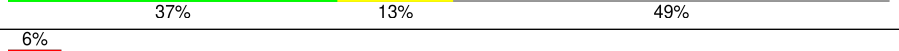
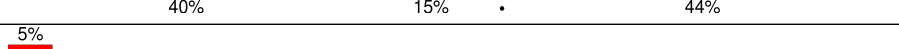
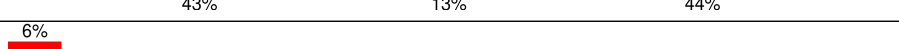
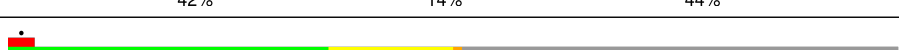


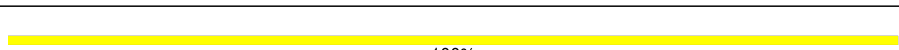
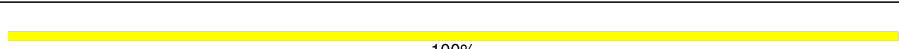
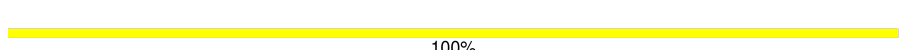




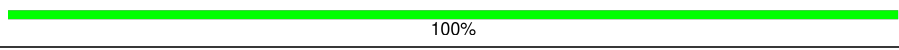


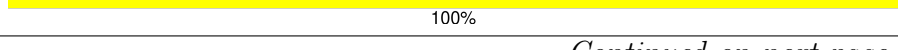

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 ( 2.51 - 3.51 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	B	153	
1	C	153	
1	J	153	
2	A	481	


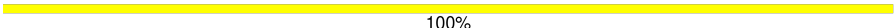

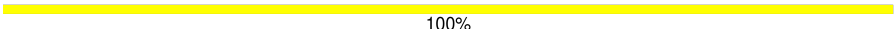
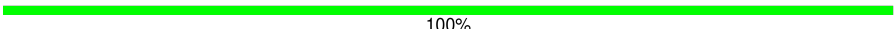
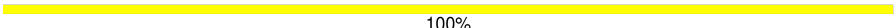
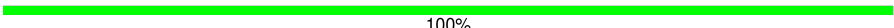


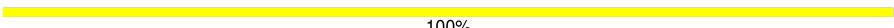

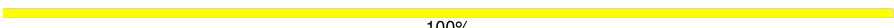

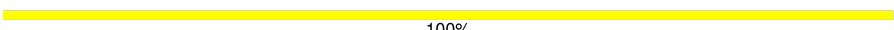
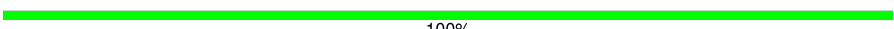

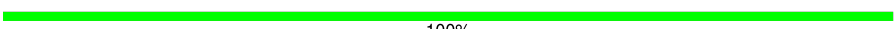


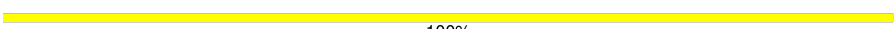

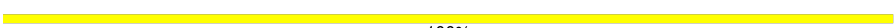



*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	481	
2	I	481	
3	D	229	
3	H	229	
3	K	229	
4	E	215	
4	L	215	
4	M	215	
5	d	235	
5	h	235	
5	k	235	
6	e	213	
6	l	213	
6	m	213	
7	N	4	
7	b	4	
7	v	4	
8	O	3	
8	c	3	
8	w	3	
9	1	2	
9	2	2	
9	3	2	
9	4	2	
9	5	2	

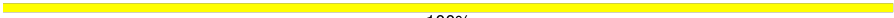
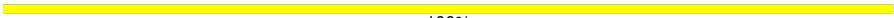

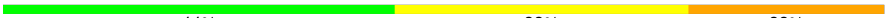


Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	7	2	 50% 50%
9	8	2	 100%
9	P	2	 50% 50%
9	Q	2	 100%
9	R	2	 100%
9	T	2	 100%
9	U	2	 100%
9	V	2	 50% 50%
9	W	2	 50% 50%
9	X	2	 100%
9	Z	2	 50% 50%
9	a	2	 100%
9	f	2	 50% 50%
9	g	2	 100%
9	i	2	 100%
9	n	2	 50% 50%
9	o	2	 100%
9	p	2	 50% 50%
9	q	2	 50% 50%
9	r	2	 100%
9	t	2	 50% 50%
9	u	2	 100%
9	x	2	 50% 50%
9	y	2	 50% 50%
9	z	2	 100%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
10	0	6	 100%
10	S	6	 100%
10	j	6	 100%
11	6	9	 44%33%22%
11	Y	9	 56%22%22%
11	s	9	 56%22%22%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26619 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 BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	128	Total	C	N	O	S	3	0
			1040	657	179	198	6		
1	C	128	Total	C	N	O	S	3	0
			1040	657	179	198	6		
1	J	128	Total	C	N	O	S	3	0
			1040	657	179	198	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5
C	559	PRO	ILE	engineered mutation	UNP Q2N0S5
C	605	CYS	THR	engineered mutation	UNP Q2N0S5
J	559	PRO	ILE	engineered mutation	UNP Q2N0S5
J	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	452	Total	C	N	O	S	5	0
			3605	2260	642	675	28		
2	A	452	Total	C	N	O	S	5	0
			3605	2260	642	675	28		
2	I	452	Total	C	N	O	S	5	0
			3605	2260	642	675	28		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5
G	509	ARG	GLU	engineered mutation	UNP Q2N0S5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	510	ARG	LYS	engineered mutation	UNP Q2N0S5
G	512	ARG	-	insertion	UNP Q2N0S5
G	513	ARG	-	insertion	UNP Q2N0S5
A	332	ASN	THR	engineered mutation	UNP Q2N0S5
A	501	CYS	ALA	engineered mutation	UNP Q2N0S5
A	509	ARG	GLU	engineered mutation	UNP Q2N0S5
A	510	ARG	LYS	engineered mutation	UNP Q2N0S5
A	512	ARG	-	insertion	UNP Q2N0S5
A	513	ARG	-	insertion	UNP Q2N0S5
I	332	ASN	THR	engineered mutation	UNP Q2N0S5
I	501	CYS	ALA	engineered mutation	UNP Q2N0S5
I	509	ARG	GLU	engineered mutation	UNP Q2N0S5
I	510	ARG	LYS	engineered mutation	UNP Q2N0S5
I	512	ARG	-	insertion	UNP Q2N0S5
I	513	ARG	-	insertion	UNP Q2N0S5

- Molecule 3 is a protein called Ab 4 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	118	Total	C	N	O	S	0	0
			919	586	153	177	3		
3	D	118	Total	C	N	O	S	0	0
			919	586	153	177	3		
3	K	118	Total	C	N	O	S	0	0
			919	586	153	177	3		

- Molecule 4 is a protein called Ab 4 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	1	0
			806	510	137	156	3		
4	E	109	Total	C	N	O	S	1	0
			806	510	137	156	3		
4	M	109	Total	C	N	O	S	1	0
			806	510	137	156	3		

- Molecule 5 is a protein called PGT121 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	131	Total	C	N	O	S	1	0
			1026	650	175	197	4		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	131	Total	C	N	O	S	1	0
			1026	650	175	197	4		
5	k	131	Total	C	N	O	S	1	0
			1026	650	175	197	4		

- Molecule 6 is a protein called PGT121 Fab light chain.

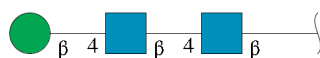
Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	108	Total	C	N	O	S	1	0
			833	522	145	164	2		
6	e	108	Total	C	N	O	S	1	0
			833	522	145	164	2		
6	m	108	Total	C	N	O	S	1	0
			833	522	145	164	2		

- Molecule 7 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
7	N	4	Total	C	N	O	0	0
			50	28	2	20		
7	b	4	Total	C	N	O	0	0
			50	28	2	20		
7	v	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 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
8	O	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
8	c	3	Total	C	N	O	0	0
			39	22	2	15		
8	w	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



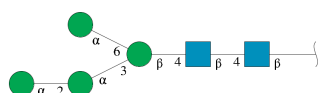
Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	2	Total	C	N	O	0	0
			28	16	2	10		
9	Q	2	Total	C	N	O	0	0
			28	16	2	10		
9	R	2	Total	C	N	O	0	0
			28	16	2	10		
9	T	2	Total	C	N	O	0	0
			28	16	2	10		
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	W	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	f	2	Total	C	N	O	0	0
			28	16	2	10		
9	g	2	Total	C	N	O	0	0
			28	16	2	10		
9	i	2	Total	C	N	O	0	0
			28	16	2	10		
9	n	2	Total	C	N	O	0	0
			28	16	2	10		
9	o	2	Total	C	N	O	0	0
			28	16	2	10		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
9	p	2	Total	C	N	O	0	0
			28	16	2	10		
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	r	2	Total	C	N	O	0	0
			28	16	2	10		
9	t	2	Total	C	N	O	0	0
			28	16	2	10		
9	u	2	Total	C	N	O	0	0
			28	16	2	10		
9	x	2	Total	C	N	O	0	0
			28	16	2	10		
9	y	2	Total	C	N	O	0	0
			28	16	2	10		
9	z	2	Total	C	N	O	0	0
			28	16	2	10		
9	1	2	Total	C	N	O	0	0
			28	16	2	10		
9	2	2	Total	C	N	O	0	0
			28	16	2	10		
9	3	2	Total	C	N	O	0	0
			28	16	2	10		
9	4	2	Total	C	N	O	0	0
			28	16	2	10		
9	5	2	Total	C	N	O	0	0
			28	16	2	10		
9	7	2	Total	C	N	O	0	0
			28	16	2	10		
9	8	2	Total	C	N	O	0	0
			28	16	2	10		

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



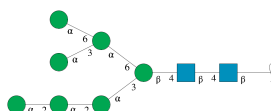
Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	6	Total	C	N	O	0	0
			72	40	2	30		

*Continued on next page...*

Continued from previous page...

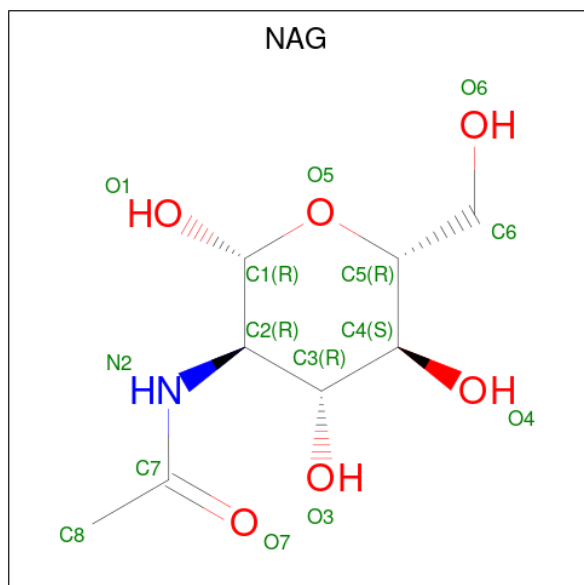
Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	6	Total	C	N	O	0	0
			72	40	2	30		
10	0	6	Total	C	N	O	0	0
			72	40	2	30		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	9	Total	C	N	O	0	0
			105	58	2	45		
11	s	9	Total	C	N	O	0	0
			105	58	2	45		
11	6	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

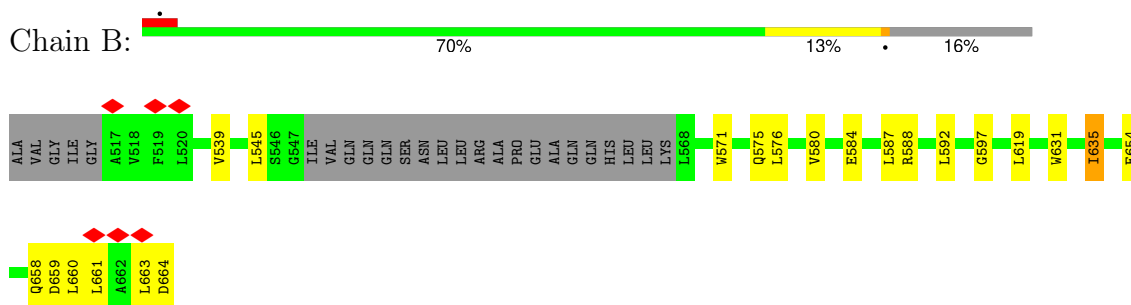


Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total 14	C 8	N 1	O 5	0
12	B	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	C	1	Total 14	C 8	N 1	O 5	0
12	C	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	J	1	Total 14	C 8	N 1	O 5	0
12	J	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0

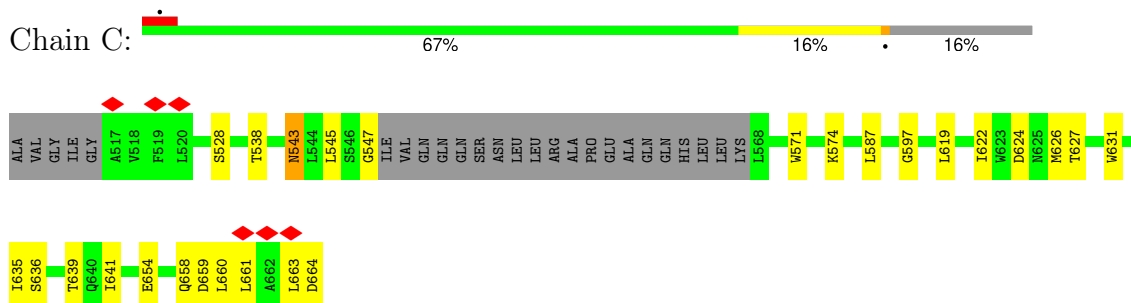
### 3 Residue-property plots [i](#)

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

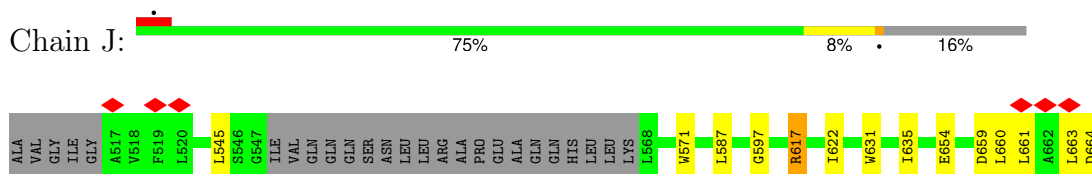
- Molecule 1: BG505 SOSIP.664 gp41



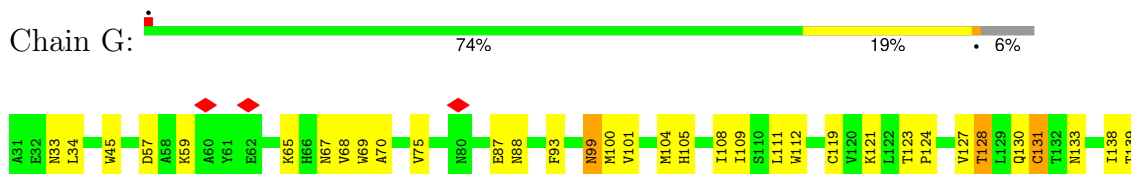
- Molecule 1: BG505 SOSIP.664 gp41

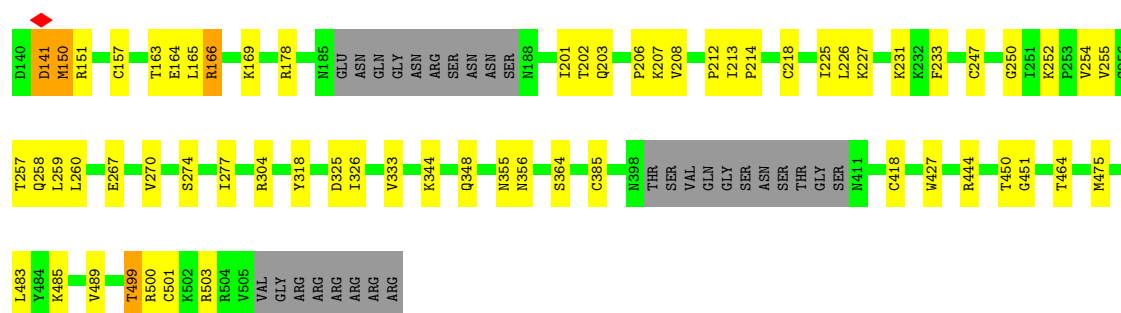


- Molecule 1: BG505 SOSIP.664 gp41

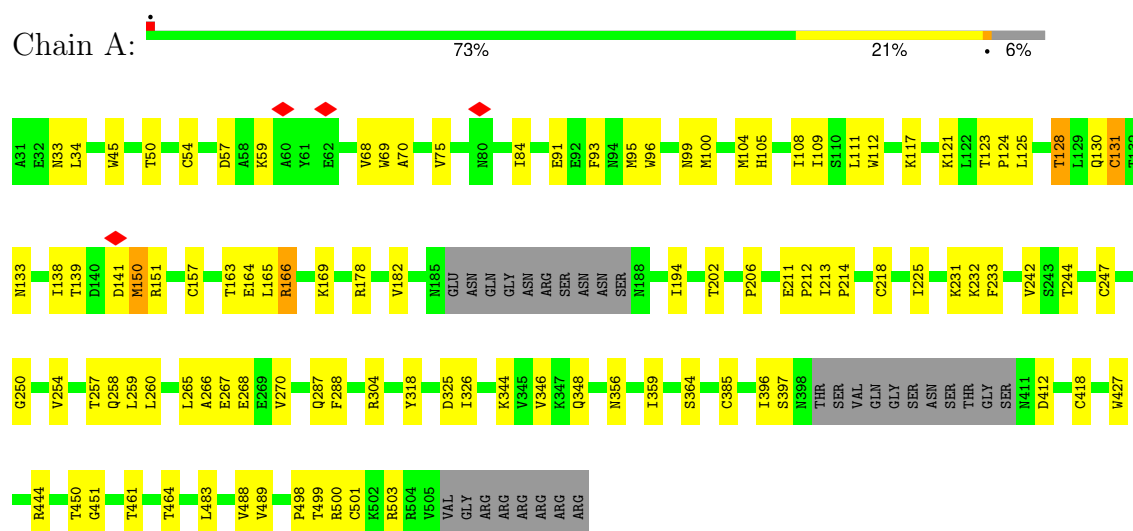


- Molecule 2: BG505 SOSIP.664 gp120

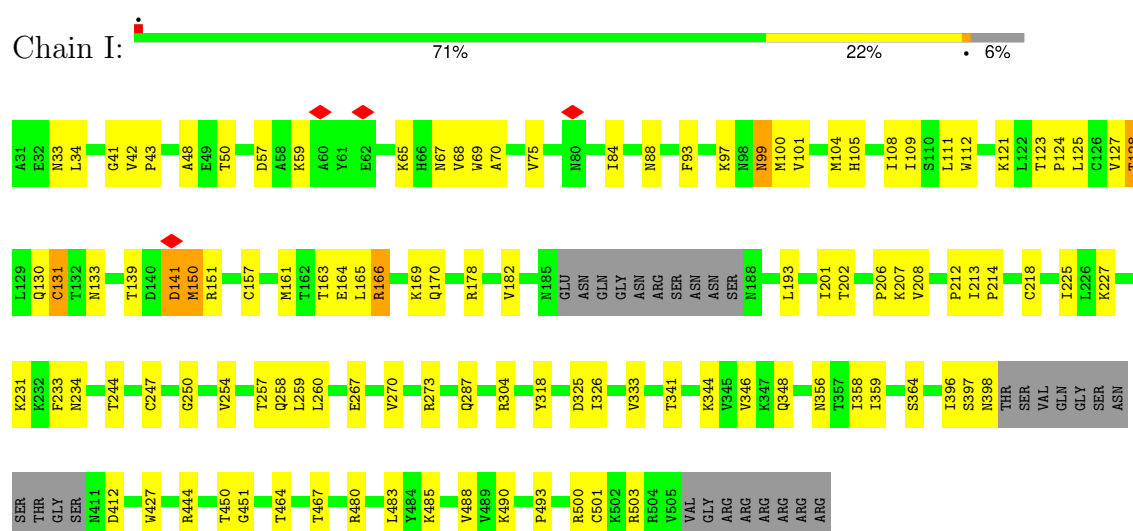




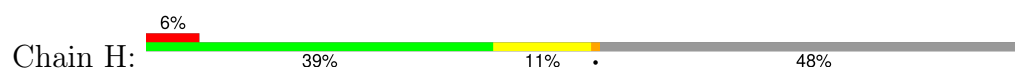
• Molecule 2: BG505 SOSIP.664 gp120

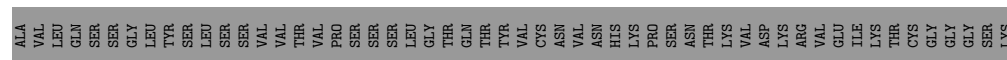
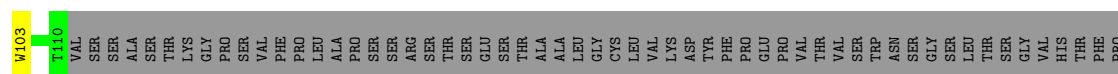
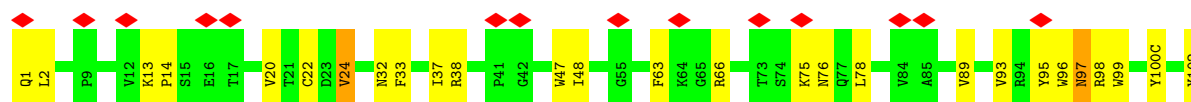


• Molecule 2: BG505 SOSIP.664 gp120

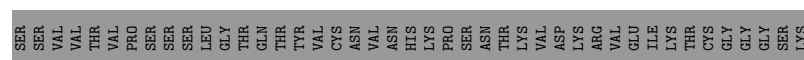
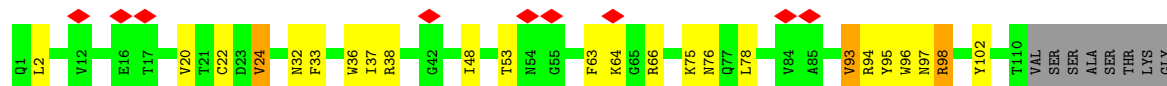


• Molecule 3: Ab 4 Fab heavy chain

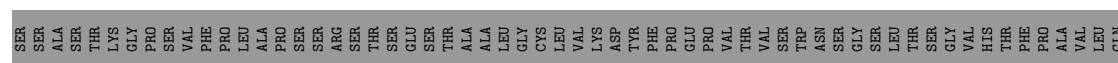
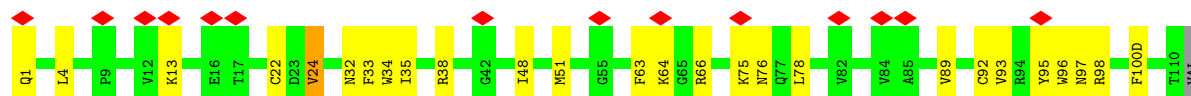
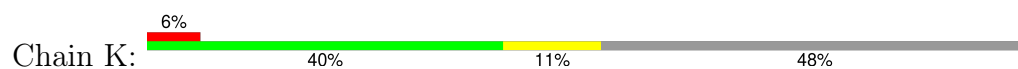




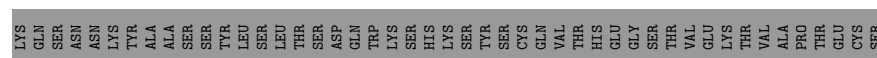
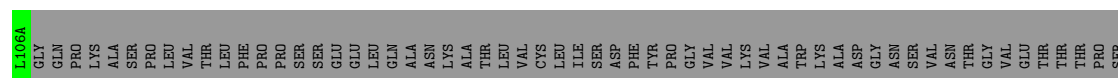
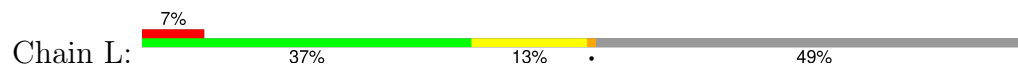
• Molecule 3: Ab 4 Fab heavy chain



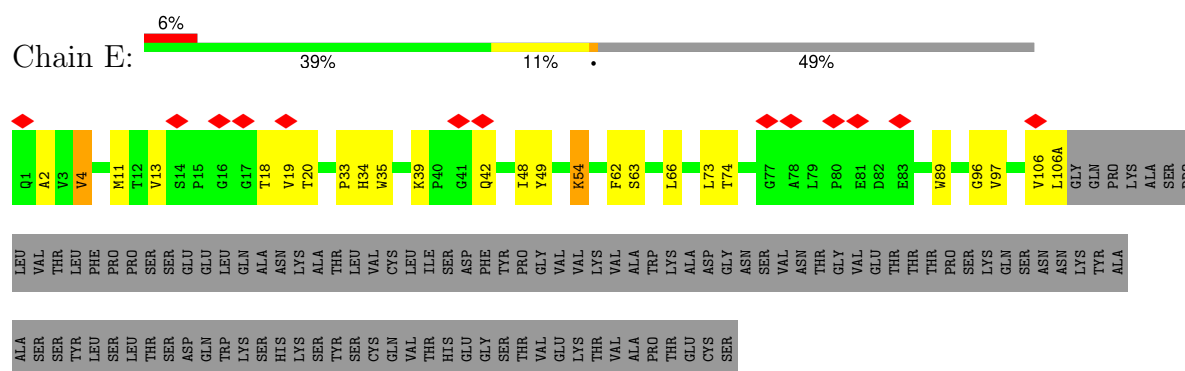
• Molecule 3: Ab 4 Fab heavy chain



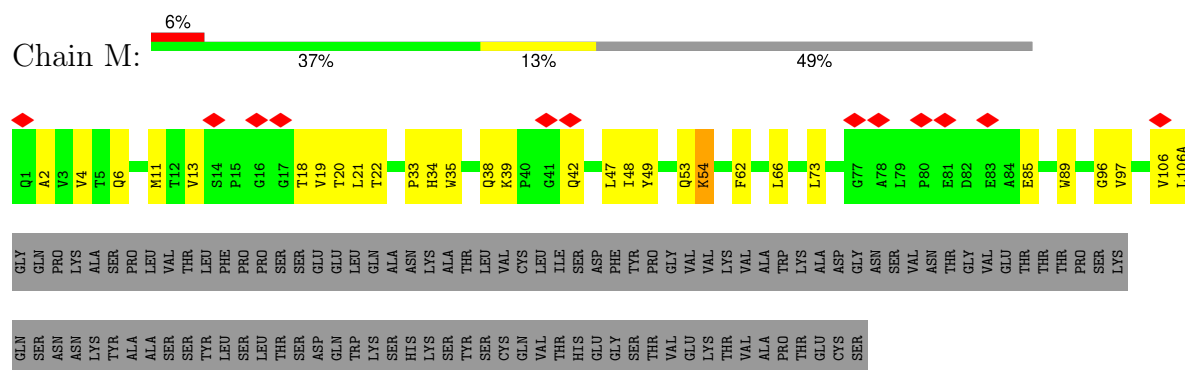
• Molecule 4: Ab 4 Fab light chain



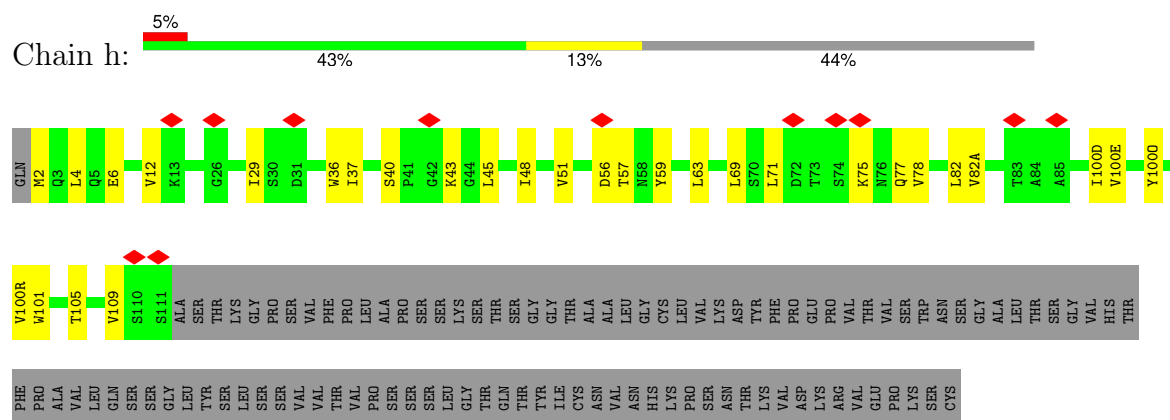
• Molecule 4: Ab 4 Fab light chain



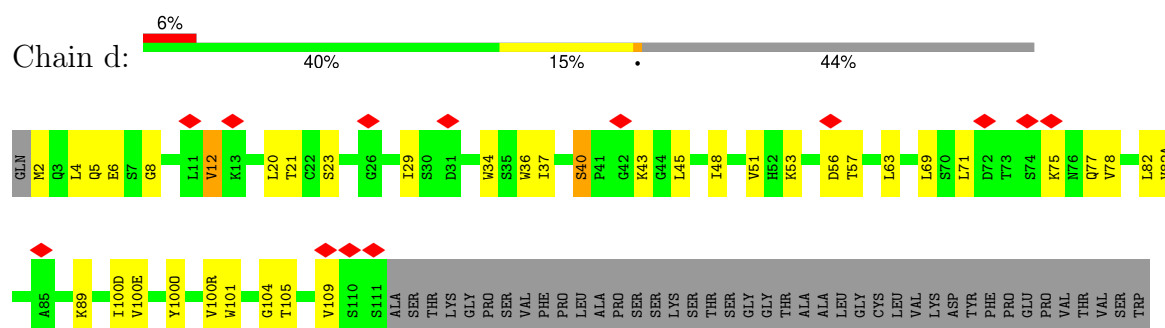
- Molecule 4: Ab 4 Fab light chain



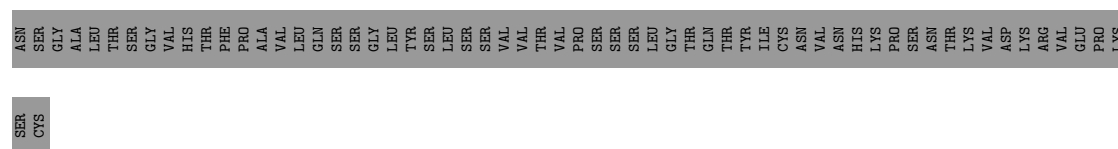
- Molecule 5: PGT121 Fab heavy chain



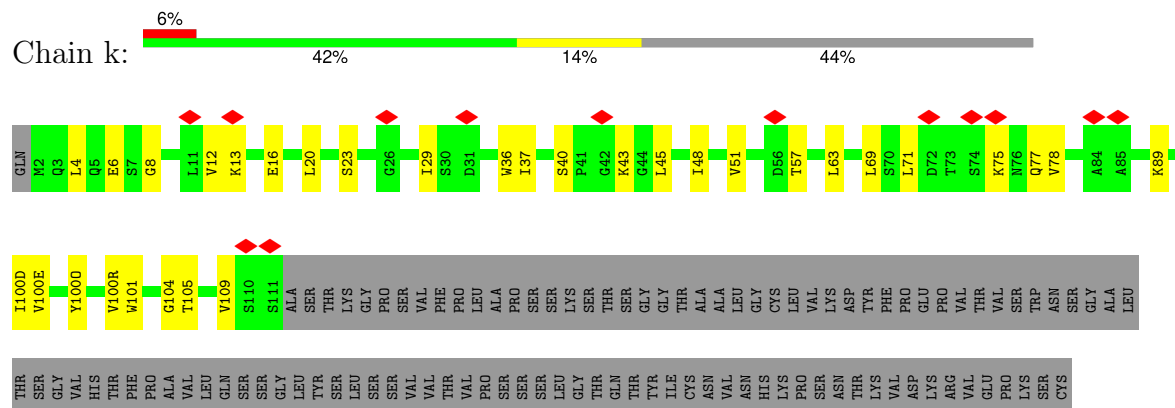
- Molecule 5: PGT121 Fab heavy chain



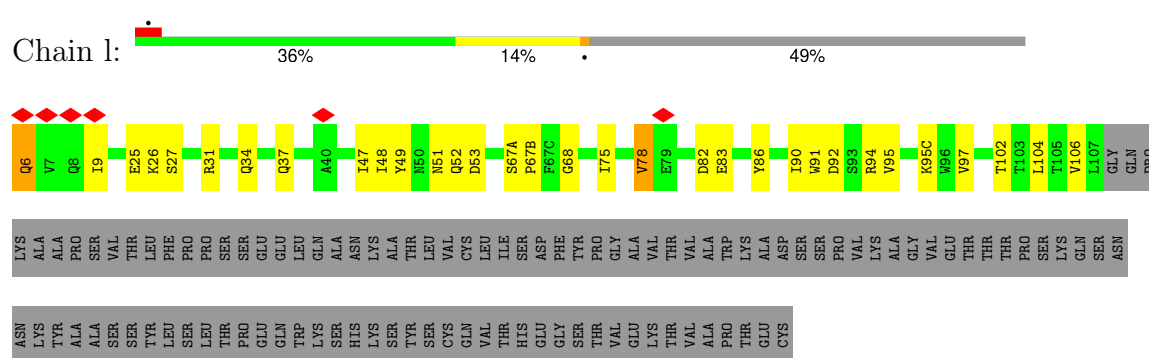




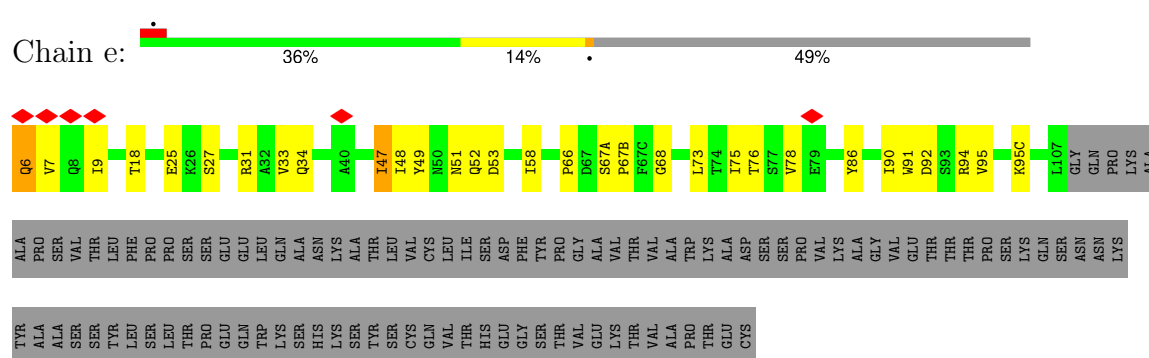
### • Molecule 5: PGT121 Fab heavy chain



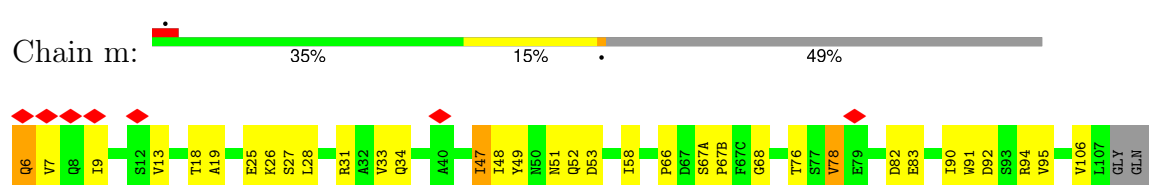
### • Molecule 6: PGT121 Fab light chain



### • Molecule 6: PGT121 Fab light chain



### • Molecule 6: PGT121 Fab light chain



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

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

- Molecule 7: 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 N:  100%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain b:  100%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain v:  100%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain O:  67%  33%

MAG1  
MAG2  
BMA3

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

Chain c:  33%  67%

MAG1  
MAG2  
BMA3

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

Chain w:  33%  67%

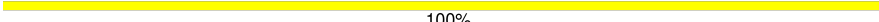
MAG1  
MAG2  
BMA3

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

Chain P:  50% 50%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  100%

MAG1  
MAG2

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

Chain T:  100%

MAG1  
MAG2

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

Chain U:  100%

MAG1  
MAG2

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

Chain V:  50% 50%

MAG1  
MAG2

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

Chain W:  50% 50%



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

Chain X:  100%



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

Chain Z:  50% 50%



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

Chain a:  100%



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

Chain f:  50% 50%



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

Chain g:  100%



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

Chain i:  100%



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

Chain n:  50% 50%

MAG1  
MAG2

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

Chain o:  100%

MAG1  
MAG2

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

Chain p:  50% 50%

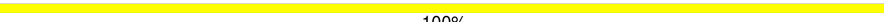
MAG1  
MAG2

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

Chain q:  50% 50%

MAG1  
MAG2

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

Chain r:  100%

MAG1  
MAG2

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

Chain t:  50% 50%

MAG1  
MAG2

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

Chain u:  100%

NAG1  
NAG2

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

Chain x:  50% 50%

NAG1  
NAG2

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

Chain y:  50% 50%

NAG1  
NAG2

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

Chain z:  100%

NAG1  
NAG2

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

Chain 1:  100%

NAG1  
NAG2

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

Chain 2:  100%

NAG1  
NAG2

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

Chain 3:  50% 50%

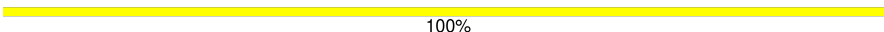
NAG1  
NAG2

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

Chain 4:  50% 50%

MAG1  
MAG2

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

Chain 5:  100%

MAG1  
MAG2

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

Chain 7:  50% 50%

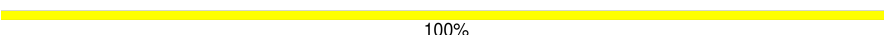
MAG1  
MAG2

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

Chain 8:  100%

MAG1  
MAG2

- Molecule 10: 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 S:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 10: 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 j:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 10: 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

mido-2-deoxy-beta-D-glucopyranose

Chain 0:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain Y:  56% 22% 22%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

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

Chain s:  56% 22% 22%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

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

Chain 6:  44% 33% 22%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	436694, 436694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.692	Depositor
Minimum map value	-1.949	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.155	Depositor
Map size (Å)	368.52, 368.52, 368.52	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9213, 0.9213, 0.9213	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.17	0/1058	0.39	0/1434
1	C	0.15	0/1058	0.37	0/1434
1	J	0.15	0/1058	0.39	0/1434
2	A	0.21	0/3679	0.41	0/4991
2	G	0.20	0/3679	0.41	0/4991
2	I	0.20	0/3679	0.42	0/4991
3	D	0.11	0/944	0.33	0/1289
3	H	0.12	0/944	0.33	0/1289
3	K	0.11	0/944	0.32	0/1289
4	E	0.10	0/827	0.31	0/1127
4	L	0.11	0/827	0.31	0/1127
4	M	0.10	0/827	0.31	0/1127
5	d	0.13	0/1052	0.36	0/1428
5	h	0.14	0/1052	0.35	0/1428
5	k	0.13	0/1052	0.34	0/1428
6	e	0.12	0/854	0.33	0/1165
6	l	0.13	0/854	0.36	0/1165
6	m	0.12	0/854	0.36	0/1165
All	All	0.17	0/25242	0.38	0/34302

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1040	0	1014	14	0
1	C	1040	0	1014	16	0
1	J	1040	0	1014	11	0
2	A	3605	0	3541	59	0
2	G	3605	0	3541	58	0
2	I	3605	0	3541	63	0
3	D	919	0	876	19	0
3	H	919	0	876	19	0
3	K	919	0	876	18	0
4	E	806	0	788	11	0
4	L	806	0	788	16	0
4	M	806	0	788	14	0
5	d	1026	0	995	27	0
5	h	1026	0	995	23	0
5	k	1026	0	995	24	0
6	e	833	0	797	21	0
6	l	833	0	797	20	0
6	m	833	0	797	22	0
7	N	50	0	43	1	0
7	b	50	0	43	1	0
7	v	50	0	43	1	0
8	O	39	0	34	0	0
8	c	39	0	34	0	0
8	w	39	0	34	0	0
9	1	28	0	25	0	0
9	2	28	0	25	0	0
9	3	28	0	25	2	0
9	4	28	0	25	1	0
9	5	28	0	25	0	0
9	7	28	0	25	0	0
9	8	28	0	25	0	0
9	P	28	0	25	0	0
9	Q	28	0	25	1	0
9	R	28	0	25	0	0
9	T	28	0	25	0	0
9	U	28	0	25	0	0
9	V	28	0	25	2	0
9	W	28	0	25	1	0
9	X	28	0	25	0	0
9	Z	28	0	25	0	0
9	a	28	0	25	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	i	28	0	25	0	0
9	n	28	0	25	0	0
9	o	28	0	25	0	0
9	p	28	0	25	2	0
9	q	28	0	25	1	0
9	r	28	0	25	0	0
9	t	28	0	25	0	0
9	u	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
9	z	28	0	25	0	0
10	0	72	0	61	0	0
10	S	72	0	61	0	0
10	j	72	0	61	0	0
11	6	105	0	88	3	0
11	Y	105	0	88	4	0
11	s	105	0	88	3	0
12	A	70	0	65	0	0
12	B	28	0	26	0	0
12	C	28	0	26	0	0
12	G	70	0	65	2	0
12	I	70	0	65	1	0
12	J	28	0	26	0	0
All	All	26619	0	25734	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 422 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:33:PHE:HB2	3:D:95:TYR:HB3	1.42	1.01
2:I:218:CYS:HA	2:I:247:CYS:HB3	1.57	0.86
3:K:33:PHE:HB2	3:K:95:TYR:HB3	1.57	0.85
2:G:218:CYS:HA	2:G:247:CYS:HB3	1.58	0.85
2:A:218:CYS:HA	2:A:247:CYS:HB3	1.58	0.85

There are no symmetry-related clashes.

## 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	B	127/153 (83%)	120 (94%)	7 (6%)	0	100	100
1	C	127/153 (83%)	122 (96%)	5 (4%)	0	100	100
1	J	127/153 (83%)	121 (95%)	6 (5%)	0	100	100
2	A	451/481 (94%)	424 (94%)	27 (6%)	0	100	100
2	G	451/481 (94%)	426 (94%)	25 (6%)	0	100	100
2	I	451/481 (94%)	423 (94%)	28 (6%)	0	100	100
3	D	116/229 (51%)	107 (92%)	8 (7%)	1 (1%)	14	46
3	H	116/229 (51%)	107 (92%)	8 (7%)	1 (1%)	14	46
3	K	116/229 (51%)	108 (93%)	7 (6%)	1 (1%)	14	46
4	E	108/215 (50%)	102 (94%)	5 (5%)	1 (1%)	14	46
4	L	108/215 (50%)	102 (94%)	5 (5%)	1 (1%)	14	46
4	M	108/215 (50%)	100 (93%)	7 (6%)	1 (1%)	14	46
5	d	130/235 (55%)	114 (88%)	16 (12%)	0	100	100
5	h	130/235 (55%)	116 (89%)	14 (11%)	0	100	100
5	k	130/235 (55%)	117 (90%)	13 (10%)	0	100	100
6	e	107/213 (50%)	100 (94%)	6 (6%)	1 (1%)	14	46
6	l	107/213 (50%)	100 (94%)	6 (6%)	1 (1%)	14	46
6	m	107/213 (50%)	101 (94%)	5 (5%)	1 (1%)	14	46
All	All	3117/4578 (68%)	2910 (93%)	198 (6%)	9 (0%)	37	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	98	ARG
3	K	98	ARG
4	L	4	VAL
4	E	4	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	e	25	GLU

### 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	B	112/129 (87%)	107 (96%)	5 (4%)	24	57
1	C	112/129 (87%)	106 (95%)	6 (5%)	20	52
1	J	112/129 (87%)	110 (98%)	2 (2%)	51	76
2	A	408/428 (95%)	381 (93%)	27 (7%)	15	44
2	G	408/428 (95%)	383 (94%)	25 (6%)	17	47
2	I	408/428 (95%)	380 (93%)	28 (7%)	14	43
3	D	99/196 (50%)	95 (96%)	4 (4%)	28	60
3	H	99/196 (50%)	91 (92%)	8 (8%)	11	36
3	K	99/196 (50%)	94 (95%)	5 (5%)	21	54
4	E	86/178 (48%)	80 (93%)	6 (7%)	14	42
4	L	86/178 (48%)	81 (94%)	5 (6%)	18	49
4	M	86/178 (48%)	80 (93%)	6 (7%)	14	42
5	d	113/202 (56%)	106 (94%)	7 (6%)	16	47
5	h	113/202 (56%)	109 (96%)	4 (4%)	32	64
5	k	113/202 (56%)	112 (99%)	1 (1%)	70	84
6	e	90/179 (50%)	86 (96%)	4 (4%)	25	58
6	l	90/179 (50%)	86 (96%)	4 (4%)	25	58
6	m	90/179 (50%)	85 (94%)	5 (6%)	19	51
All	All	2724/3936 (69%)	2572 (94%)	152 (6%)	23	51

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	133	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	M	54[B]	LYS
2	I	166[B]	ARG
2	I	412	ASP
6	m	83	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	432	GLN
3	K	39	GLN
6	m	37	GLN
2	A	302	ASN
2	A	287	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

126 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	$\# Z  > 2$
10	NAG	0	1	2,10	14,14,15	0.67	0	17,19,21	2.02	2 (11%)
10	NAG	0	2	10	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
10	BMA	0	3	10	11,11,12	0.83	0	15,15,17	2.36	5 (33%)
10	MAN	0	4	10	11,11,12	0.63	0	15,15,17	1.44	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	0	5	10	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
10	MAN	0	6	10	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
9	NAG	1	1	2,9	14,14,15	0.78	0	17,19,21	1.01	1 (5%)
9	NAG	1	2	9	14,14,15	0.71	0	17,19,21	1.20	1 (5%)
9	NAG	2	1	2,9	14,14,15	0.76	0	17,19,21	0.89	0
9	NAG	2	2	9	14,14,15	0.72	0	17,19,21	0.85	0
9	NAG	3	1	2,9	14,14,15	0.73	0	17,19,21	0.98	1 (5%)
9	NAG	3	2	9	14,14,15	0.73	0	17,19,21	0.90	0
9	NAG	4	1	2,9	14,14,15	0.72	0	17,19,21	1.26	2 (11%)
9	NAG	4	2	9	14,14,15	0.86	0	17,19,21	1.25	2 (11%)
9	NAG	5	1	2,9	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
9	NAG	5	2	9	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
11	NAG	6	1	2,11	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
11	NAG	6	2	11	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
11	BMA	6	3	11	11,11,12	0.52	0	15,15,17	1.41	1 (6%)
11	MAN	6	4	11	11,11,12	0.49	0	15,15,17	0.59	0
11	MAN	6	5	11	11,11,12	0.54	0	15,15,17	1.21	1 (6%)
11	MAN	6	6	11	11,11,12	0.36	0	15,15,17	0.59	0
11	MAN	6	7	11	11,11,12	0.33	0	15,15,17	0.55	0
11	MAN	6	8	11	11,11,12	0.34	0	15,15,17	0.52	0
11	MAN	6	9	11	11,11,12	0.26	0	15,15,17	0.55	0
9	NAG	7	1	2,9	14,14,15	0.71	0	17,19,21	1.31	2 (11%)
9	NAG	7	2	9	14,14,15	0.73	0	17,19,21	0.85	0
9	NAG	8	1	2,9	14,14,15	0.81	0	17,19,21	1.26	2 (11%)
9	NAG	8	2	9	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
7	NAG	N	1	2,7	14,14,15	0.75	0	17,19,21	0.97	0
7	NAG	N	2	7	14,14,15	0.73	0	17,19,21	0.88	1 (5%)
7	BMA	N	3	7	11,11,12	0.81	0	15,15,17	2.70	5 (33%)
7	MAN	N	4	7	11,11,12	0.71	0	15,15,17	1.12	1 (6%)
8	NAG	O	1	2,8	14,14,15	0.75	0	17,19,21	0.99	0
8	NAG	O	2	8	14,14,15	0.72	0	17,19,21	0.89	0
8	BMA	O	3	8	11,11,12	0.84	0	15,15,17	2.11	3 (20%)
9	NAG	P	1	2,9	14,14,15	0.77	0	17,19,21	1.19	2 (11%)
9	NAG	P	2	9	14,14,15	0.73	0	17,19,21	0.83	0
9	NAG	Q	1	2,9	14,14,15	0.75	0	17,19,21	0.92	0
9	NAG	Q	2	9	14,14,15	0.77	0	17,19,21	1.12	2 (11%)
9	NAG	R	1	2,9	14,14,15	0.76	0	17,19,21	0.92	0
9	NAG	R	2	9	14,14,15	0.70	0	17,19,21	0.84	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	S	1	2,10	14,14,15	0.67	0	17,19,21	1.98	2 (11%)
10	NAG	S	2	10	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
10	BMA	S	3	10	11,11,12	0.83	0	15,15,17	2.36	5 (33%)
10	MAN	S	4	10	11,11,12	0.62	0	15,15,17	1.45	1 (6%)
10	MAN	S	5	10	11,11,12	0.72	0	15,15,17	1.10	1 (6%)
10	MAN	S	6	10	11,11,12	0.69	0	15,15,17	1.12	1 (6%)
9	NAG	T	1	2,9	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
9	NAG	T	2	9	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
9	NAG	U	1	2,9	14,14,15	0.74	0	17,19,21	0.88	0
9	NAG	U	2	9	14,14,15	0.72	0	17,19,21	0.84	0
9	NAG	V	1	2,9	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
9	NAG	V	2	9	14,14,15	0.73	0	17,19,21	0.90	0
9	NAG	W	1	2,9	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
9	NAG	W	2	9	14,14,15	0.86	1 (7%)	17,19,21	1.26	2 (11%)
9	NAG	X	1	2,9	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
9	NAG	X	2	9	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
11	NAG	Y	1	2,11	14,14,15	0.41	0	17,19,21	0.75	0
11	NAG	Y	2	11	14,14,15	0.47	0	17,19,21	1.21	1 (5%)
11	BMA	Y	3	11	11,11,12	0.52	0	15,15,17	1.41	1 (6%)
11	MAN	Y	4	11	11,11,12	0.48	0	15,15,17	0.57	0
11	MAN	Y	5	11	11,11,12	0.55	0	15,15,17	1.19	1 (6%)
11	MAN	Y	6	11	11,11,12	0.38	0	15,15,17	0.57	0
11	MAN	Y	7	11	11,11,12	0.34	0	15,15,17	0.55	0
11	MAN	Y	8	11	11,11,12	0.36	0	15,15,17	0.51	0
11	MAN	Y	9	11	11,11,12	0.28	0	15,15,17	0.54	0
9	NAG	Z	1	2,9	14,14,15	0.71	0	17,19,21	1.32	2 (11%)
9	NAG	Z	2	9	14,14,15	0.72	0	17,19,21	0.84	0
9	NAG	a	1	2,9	14,14,15	0.83	0	17,19,21	1.20	1 (5%)
9	NAG	a	2	9	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
7	NAG	b	1	2,7	14,14,15	0.76	0	17,19,21	0.99	0
7	NAG	b	2	7	14,14,15	0.74	0	17,19,21	0.90	1 (5%)
7	BMA	b	3	7	11,11,12	0.81	0	15,15,17	2.71	5 (33%)
7	MAN	b	4	7	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
8	NAG	c	1	2,8	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
8	NAG	c	2	8	14,14,15	0.74	0	17,19,21	0.89	0
8	BMA	c	3	8	11,11,12	0.85	0	15,15,17	2.13	3 (20%)
9	NAG	f	1	2,9	14,14,15	0.78	0	17,19,21	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	f	2	9	14,14,15	0.73	0	17,19,21	0.85	0
9	NAG	g	1	2,9	14,14,15	0.74	0	17,19,21	0.97	1 (5%)
9	NAG	g	2	9	14,14,15	0.77	0	17,19,21	1.15	2 (11%)
9	NAG	i	1	2,9	14,14,15	0.73	0	17,19,21	0.94	0
9	NAG	i	2	9	14,14,15	0.70	0	17,19,21	0.85	0
10	NAG	j	1	2,10	14,14,15	0.68	0	17,19,21	1.99	2 (11%)
10	NAG	j	2	10	14,14,15	0.71	0	17,19,21	1.06	2 (11%)
10	BMA	j	3	10	11,11,12	0.83	0	15,15,17	2.34	5 (33%)
10	MAN	j	4	10	11,11,12	0.63	0	15,15,17	1.43	1 (6%)
10	MAN	j	5	10	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
10	MAN	j	6	10	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
9	NAG	n	1	2,9	14,14,15	0.78	0	17,19,21	0.98	0
9	NAG	n	2	9	14,14,15	0.72	0	17,19,21	1.20	1 (5%)
9	NAG	o	1	2,9	14,14,15	0.76	0	17,19,21	0.87	0
9	NAG	o	2	9	14,14,15	0.71	0	17,19,21	0.85	0
9	NAG	p	1	2,9	14,14,15	0.75	0	17,19,21	0.97	1 (5%)
9	NAG	p	2	9	14,14,15	0.74	0	17,19,21	0.91	0
9	NAG	q	1	2,9	14,14,15	0.72	0	17,19,21	1.24	2 (11%)
9	NAG	q	2	9	14,14,15	0.88	1 (7%)	17,19,21	1.37	3 (17%)
9	NAG	r	1	2,9	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
9	NAG	r	2	9	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
11	NAG	s	1	2,11	14,14,15	0.41	0	17,19,21	0.78	0
11	NAG	s	2	11	14,14,15	0.47	0	17,19,21	1.23	2 (11%)
11	BMA	s	3	11	11,11,12	0.52	0	15,15,17	1.43	1 (6%)
11	MAN	s	4	11	11,11,12	0.48	0	15,15,17	0.59	0
11	MAN	s	5	11	11,11,12	0.56	0	15,15,17	1.19	1 (6%)
11	MAN	s	6	11	11,11,12	0.36	0	15,15,17	0.57	0
11	MAN	s	7	11	11,11,12	0.33	0	15,15,17	0.56	0
11	MAN	s	8	11	11,11,12	0.35	0	15,15,17	0.52	0
11	MAN	s	9	11	11,11,12	0.27	0	15,15,17	0.55	0
9	NAG	t	1	2,9	14,14,15	0.70	0	17,19,21	1.32	2 (11%)
9	NAG	t	2	9	14,14,15	0.73	0	17,19,21	0.85	0
9	NAG	u	1	2,9	14,14,15	0.81	0	17,19,21	1.26	2 (11%)
9	NAG	u	2	9	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
7	NAG	v	1	2,7	14,14,15	0.76	0	17,19,21	0.97	0
7	NAG	v	2	7	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
7	BMA	v	3	7	11,11,12	0.82	0	15,15,17	2.68	5 (33%)
7	MAN	v	4	7	11,11,12	0.71	0	15,15,17	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	w	1	2,8	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
8	NAG	w	2	8	14,14,15	0.72	0	17,19,21	0.89	0
8	BMA	w	3	8	11,11,12	0.84	0	15,15,17	2.11	3 (20%)
9	NAG	x	1	2,9	14,14,15	0.78	0	17,19,21	1.19	2 (11%)
9	NAG	x	2	9	14,14,15	0.73	0	17,19,21	0.83	0
9	NAG	y	1	2,9	14,14,15	0.75	0	17,19,21	0.91	0
9	NAG	y	2	9	14,14,15	0.77	0	17,19,21	1.09	1 (5%)
9	NAG	z	1	2,9	14,14,15	0.75	0	17,19,21	0.96	0
9	NAG	z	2	9	14,14,15	0.70	0	17,19,21	0.85	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
10	NAG	0	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	0	2	10	-	1/6/23/26	0/1/1/1
10	BMA	0	3	10	-	0/2/19/22	0/1/1/1
10	MAN	0	4	10	-	0/2/19/22	0/1/1/1
10	MAN	0	5	10	-	2/2/19/22	0/1/1/1
10	MAN	0	6	10	-	2/2/19/22	0/1/1/1
9	NAG	1	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	1	2	9	-	4/6/23/26	0/1/1/1
9	NAG	2	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	2	2	9	-	0/6/23/26	0/1/1/1
9	NAG	3	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	3	2	9	-	0/6/23/26	0/1/1/1
9	NAG	4	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	4	2	9	-	1/6/23/26	0/1/1/1
9	NAG	5	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	5	2	9	-	2/6/23/26	0/1/1/1
11	NAG	6	1	2,11	-	3/6/23/26	0/1/1/1
11	NAG	6	2	11	-	4/6/23/26	0/1/1/1
11	BMA	6	3	11	-	2/2/19/22	1/1/1/1
11	MAN	6	4	11	-	2/2/19/22	0/1/1/1
11	MAN	6	5	11	-	1/2/19/22	0/1/1/1
11	MAN	6	6	11	-	1/2/19/22	1/1/1/1
11	MAN	6	7	11	-	2/2/19/22	1/1/1/1

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	Y	5	11	-	1/2/19/22	0/1/1/1
11	MAN	Y	6	11	-	1/2/19/22	1/1/1/1
11	MAN	Y	7	11	-	2/2/19/22	1/1/1/1
11	MAN	Y	8	11	-	2/2/19/22	0/1/1/1
11	MAN	Y	9	11	-	1/2/19/22	1/1/1/1
9	NAG	Z	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	1/6/23/26	0/1/1/1
9	NAG	a	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	1/6/23/26	0/1/1/1
7	NAG	b	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	MAN	b	4	7	-	1/2/19/22	1/1/1/1
8	NAG	c	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
9	NAG	f	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
9	NAG	g	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
9	NAG	i	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	-	0/6/23/26	0/1/1/1
10	NAG	j	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	j	2	10	-	1/6/23/26	0/1/1/1
10	BMA	j	3	10	-	0/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
10	MAN	j	5	10	-	2/2/19/22	0/1/1/1
10	MAN	j	6	10	-	2/2/19/22	0/1/1/1
9	NAG	n	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	4/6/23/26	0/1/1/1
9	NAG	o	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	o	2	9	-	0/6/23/26	0/1/1/1
9	NAG	p	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	p	2	9	-	0/6/23/26	0/1/1/1
9	NAG	q	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	q	2	9	-	1/6/23/26	0/1/1/1
9	NAG	r	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	r	2	9	-	2/6/23/26	0/1/1/1
11	NAG	s	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	s	2	11	-	3/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	s	3	11	-	2/2/19/22	1/1/1/1
11	MAN	s	4	11	-	2/2/19/22	0/1/1/1
11	MAN	s	5	11	-	1/2/19/22	0/1/1/1
11	MAN	s	6	11	-	1/2/19/22	1/1/1/1
11	MAN	s	7	11	-	1/2/19/22	1/1/1/1
11	MAN	s	8	11	-	2/2/19/22	0/1/1/1
11	MAN	s	9	11	-	1/2/19/22	1/1/1/1
9	NAG	t	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	1/6/23/26	0/1/1/1
9	NAG	u	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	u	2	9	-	1/6/23/26	0/1/1/1
7	NAG	v	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
7	BMA	v	3	7	-	0/2/19/22	0/1/1/1
7	MAN	v	4	7	-	1/2/19/22	1/1/1/1
8	NAG	w	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	0/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
9	NAG	x	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	x	2	9	-	0/6/23/26	0/1/1/1
9	NAG	y	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	y	2	9	-	2/6/23/26	0/1/1/1
9	NAG	z	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	2	NAG	C1-C2	2.07	1.55	1.52
9	W	2	NAG	C1-C2	2.02	1.55	1.52

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	3	BMA	C1-O5-C5	8.45	123.52	112.19
7	N	3	BMA	C1-O5-C5	8.44	123.50	112.19
7	v	3	BMA	C1-O5-C5	8.41	123.45	112.19
10	0	1	NAG	C1-O5-C5	7.30	121.97	112.19
10	j	1	NAG	C1-O5-C5	7.17	121.79	112.19

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	T	2	NAG	C1-C2-N2-C7
9	n	2	NAG	C1-C2-N2-C7
9	1	2	NAG	C1-C2-N2-C7
11	Y	2	NAG	C8-C7-N2-C2
11	Y	2	NAG	O7-C7-N2-C2

5 of 15 ring outliers are listed below:

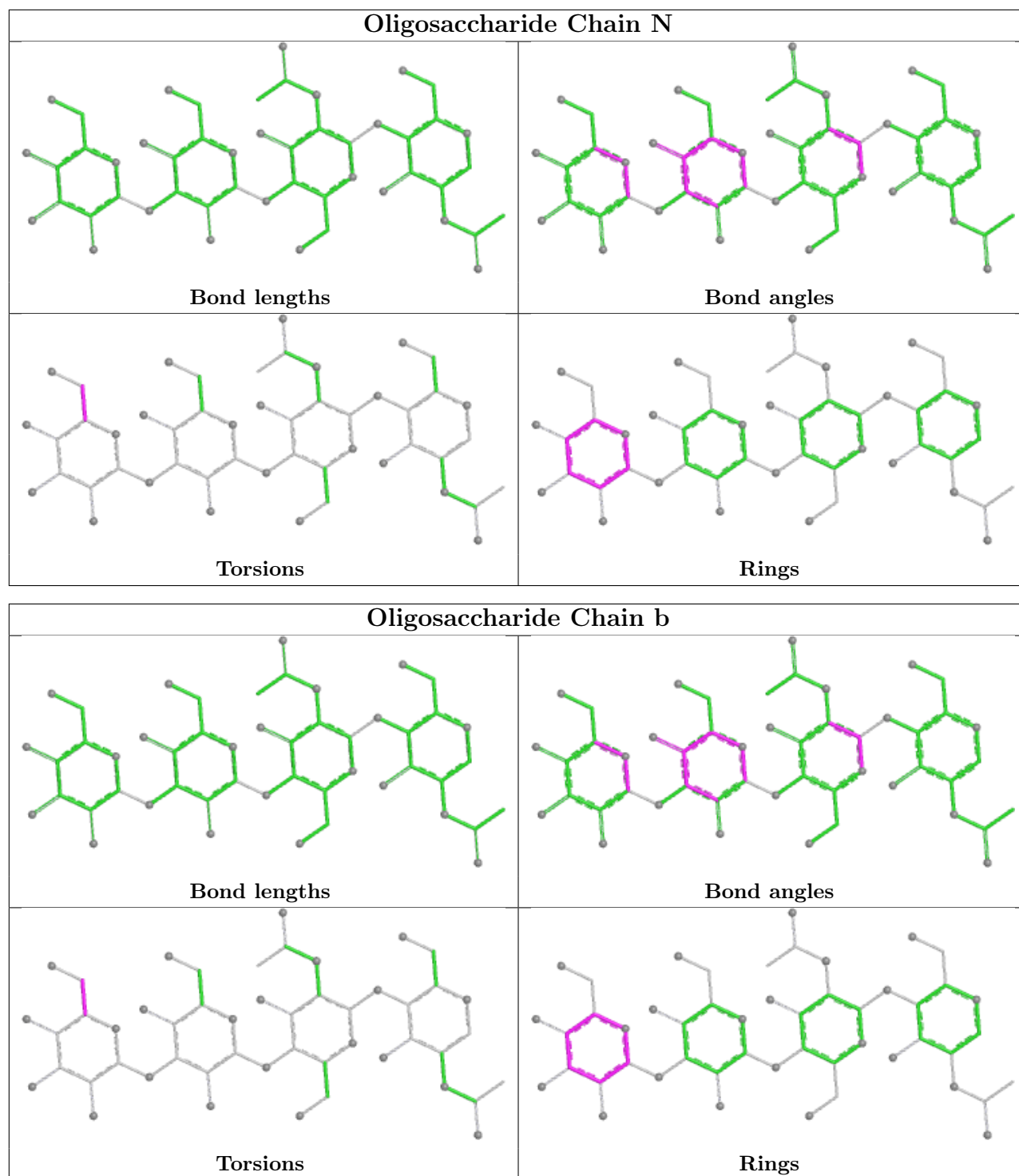
Mol	Chain	Res	Type	Atoms
11	s	7	MAN	C1-C2-C3-C4-C5-O5
11	6	7	MAN	C1-C2-C3-C4-C5-O5
11	Y	7	MAN	C1-C2-C3-C4-C5-O5
11	s	3	BMA	C1-C2-C3-C4-C5-O5
11	Y	3	BMA	C1-C2-C3-C4-C5-O5

22 monomers are involved in 20 short contacts:

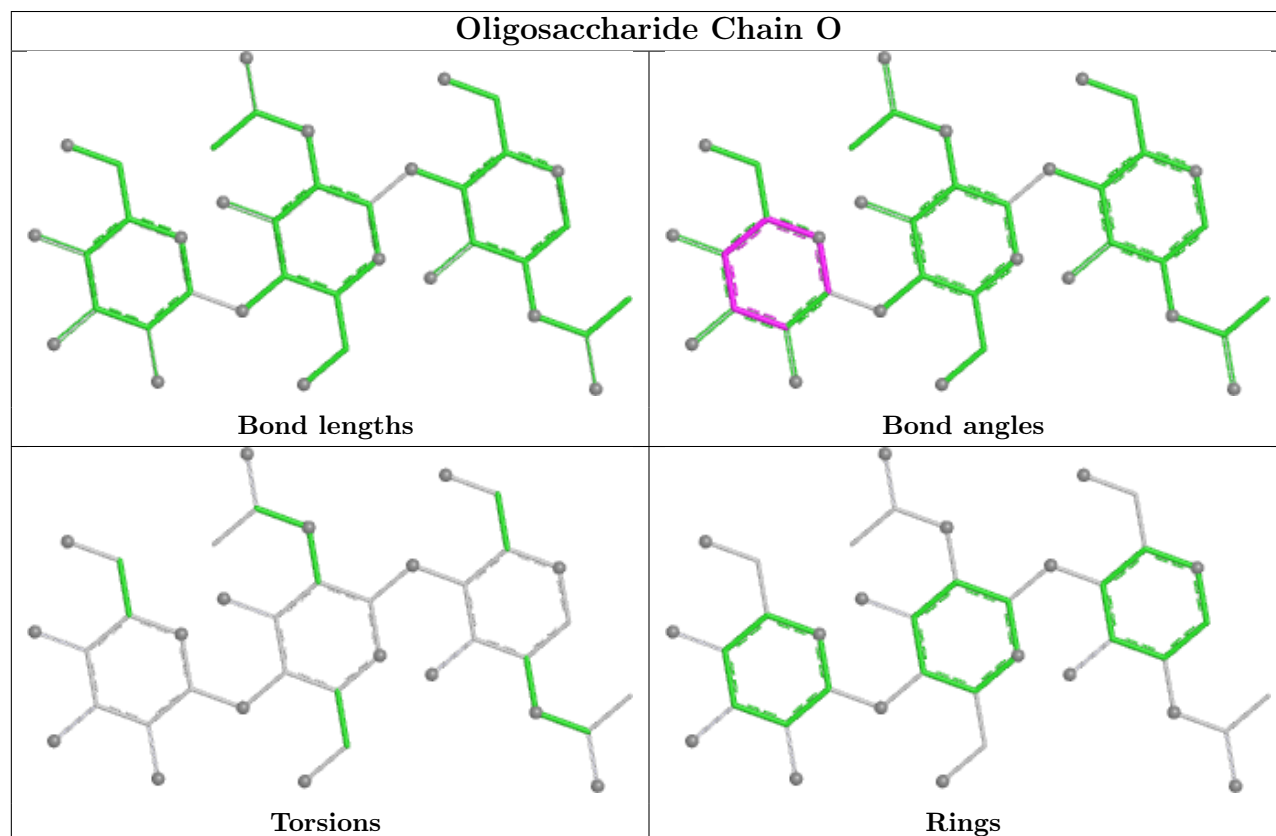
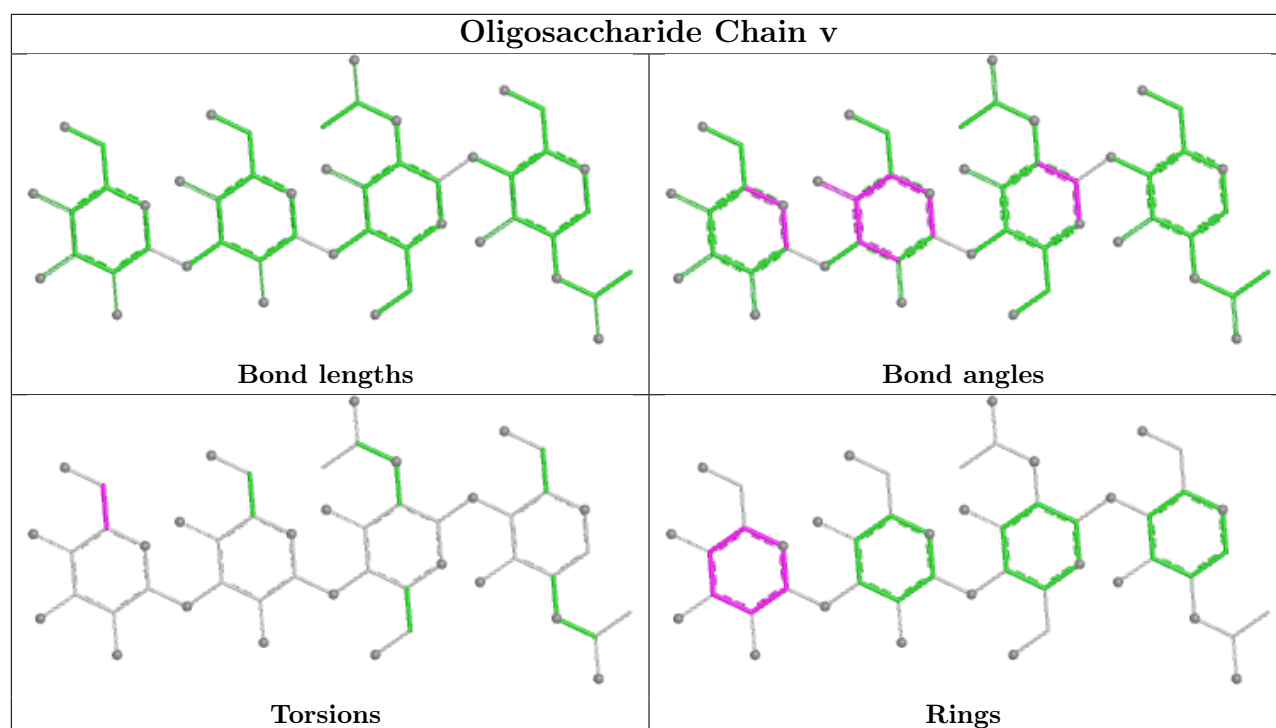
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	6	7	MAN	1	0
7	N	1	NAG	1	0
11	s	3	BMA	1	0
9	3	2	NAG	1	0
9	4	2	NAG	1	0
11	6	2	NAG	2	0
9	p	1	NAG	1	0
9	p	2	NAG	1	0
7	b	1	NAG	1	0
7	v	1	NAG	1	0
11	s	2	NAG	2	0
11	Y	7	MAN	1	0
11	Y	3	BMA	1	0
9	3	1	NAG	1	0
9	Q	1	NAG	1	0
9	V	1	NAG	1	0
11	s	7	MAN	1	0
9	W	2	NAG	1	0
9	q	2	NAG	1	0
11	6	3	BMA	1	0
11	Y	2	NAG	3	0
9	V	2	NAG	1	0

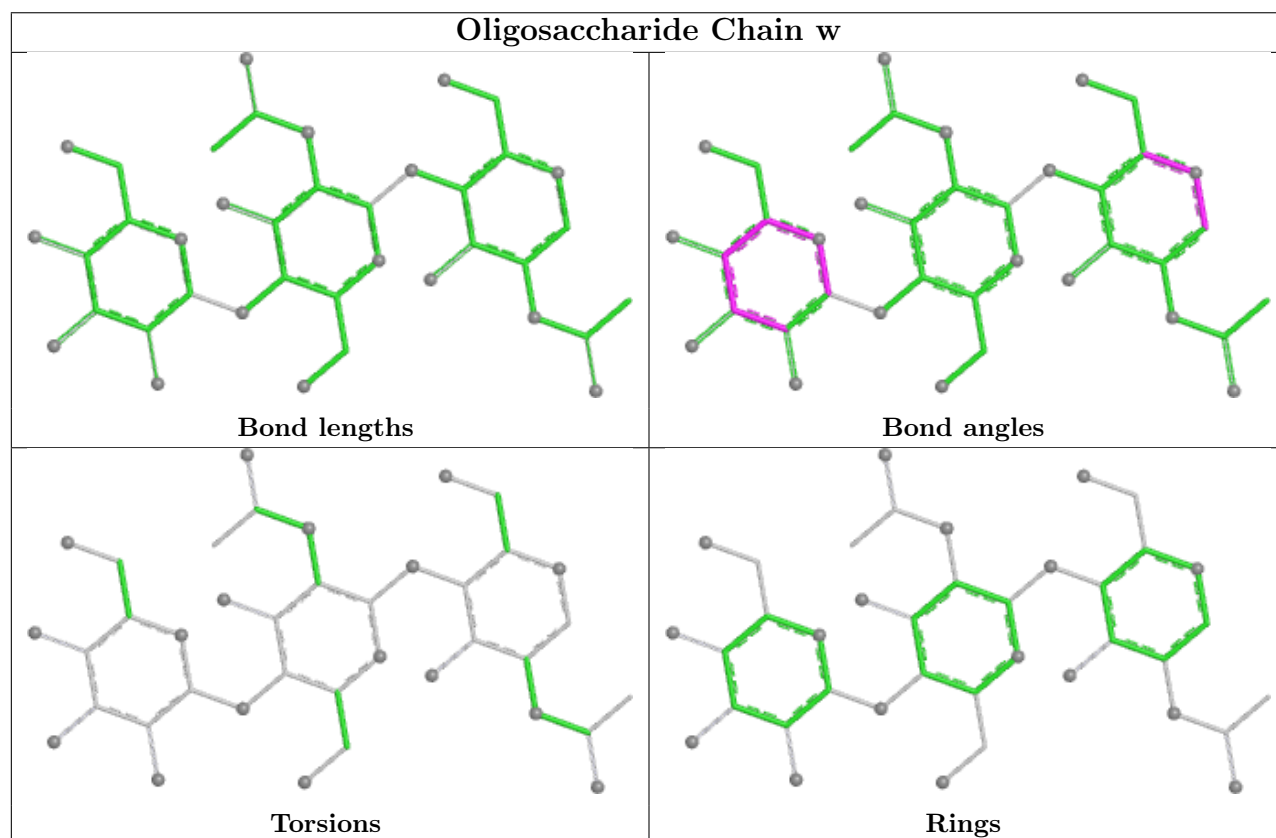
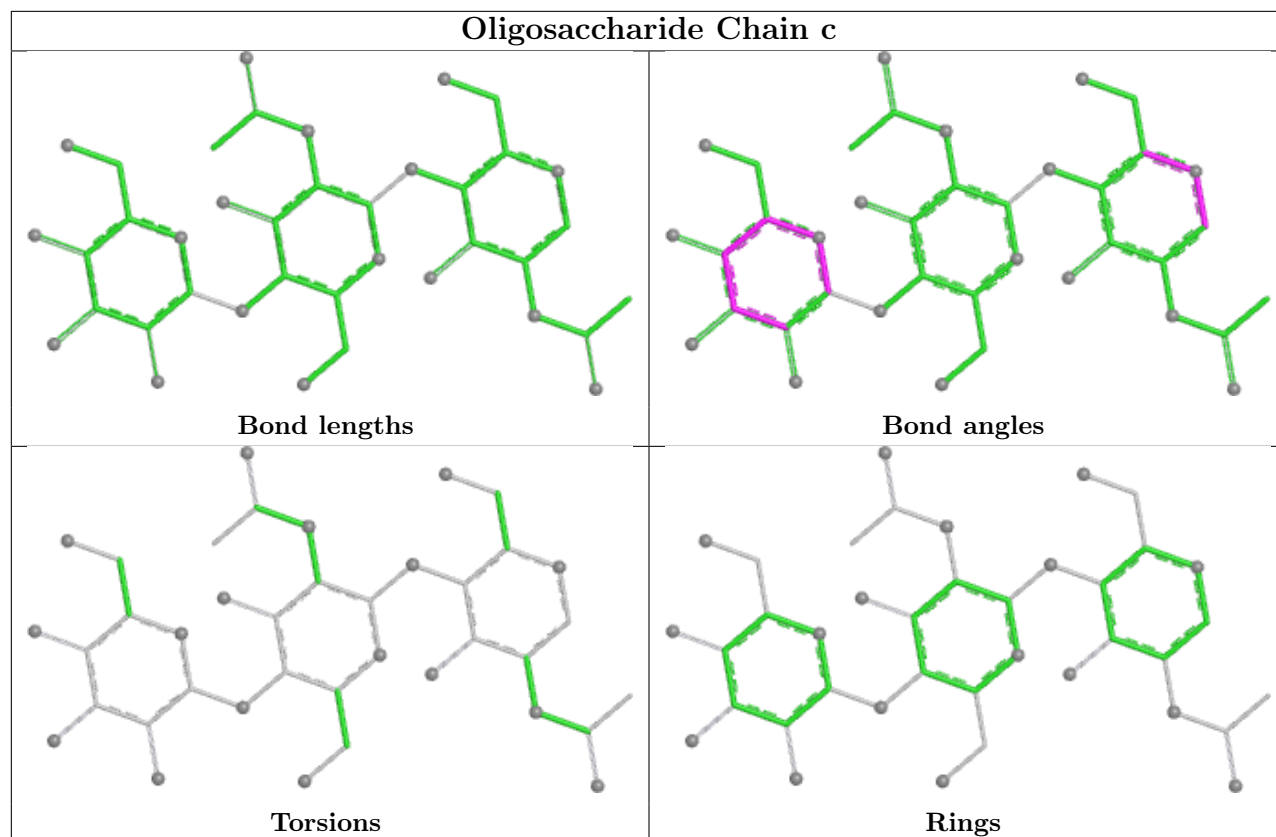
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

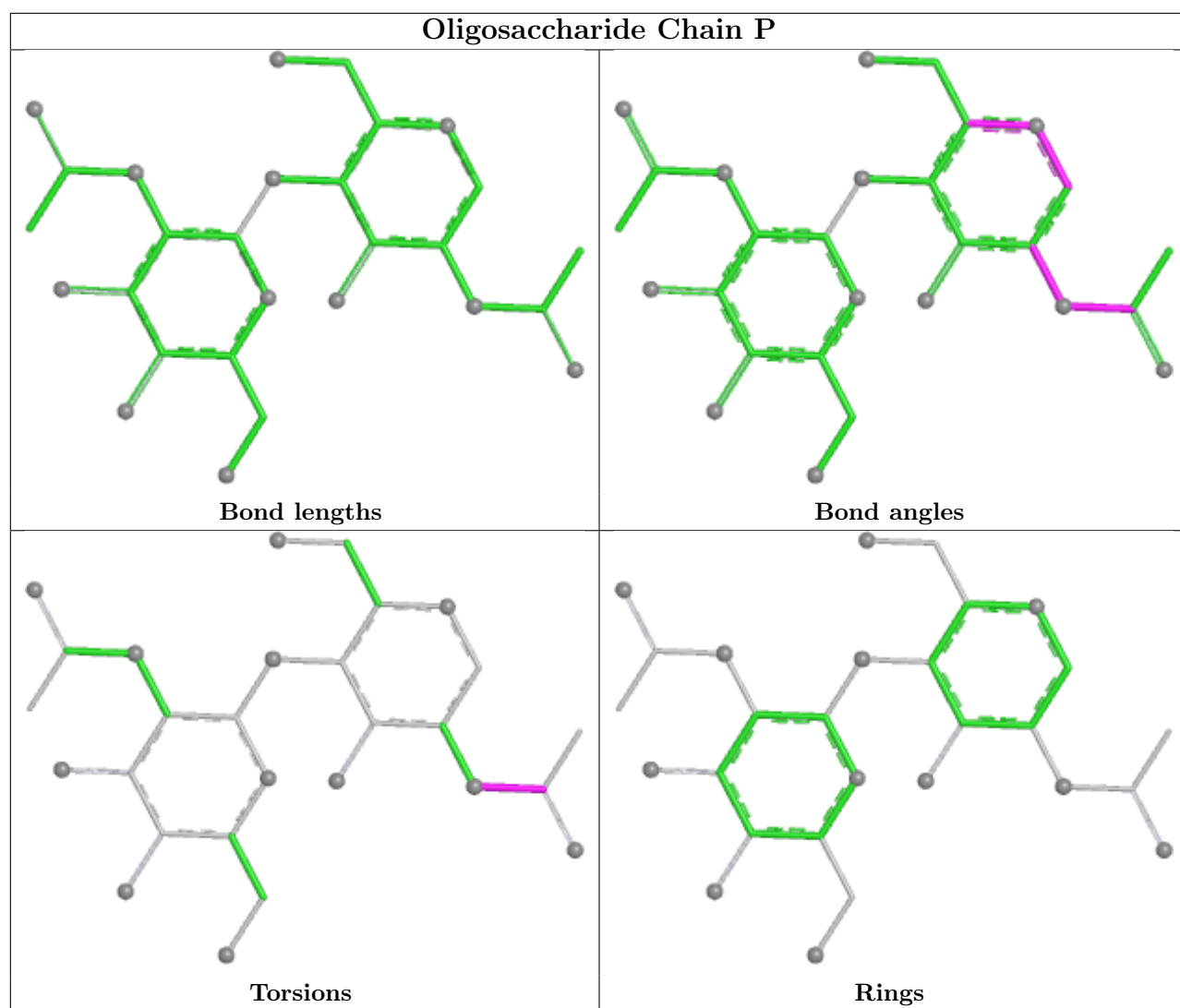
bond angles, torsion angles, and ring geometry for oligosaccharide.

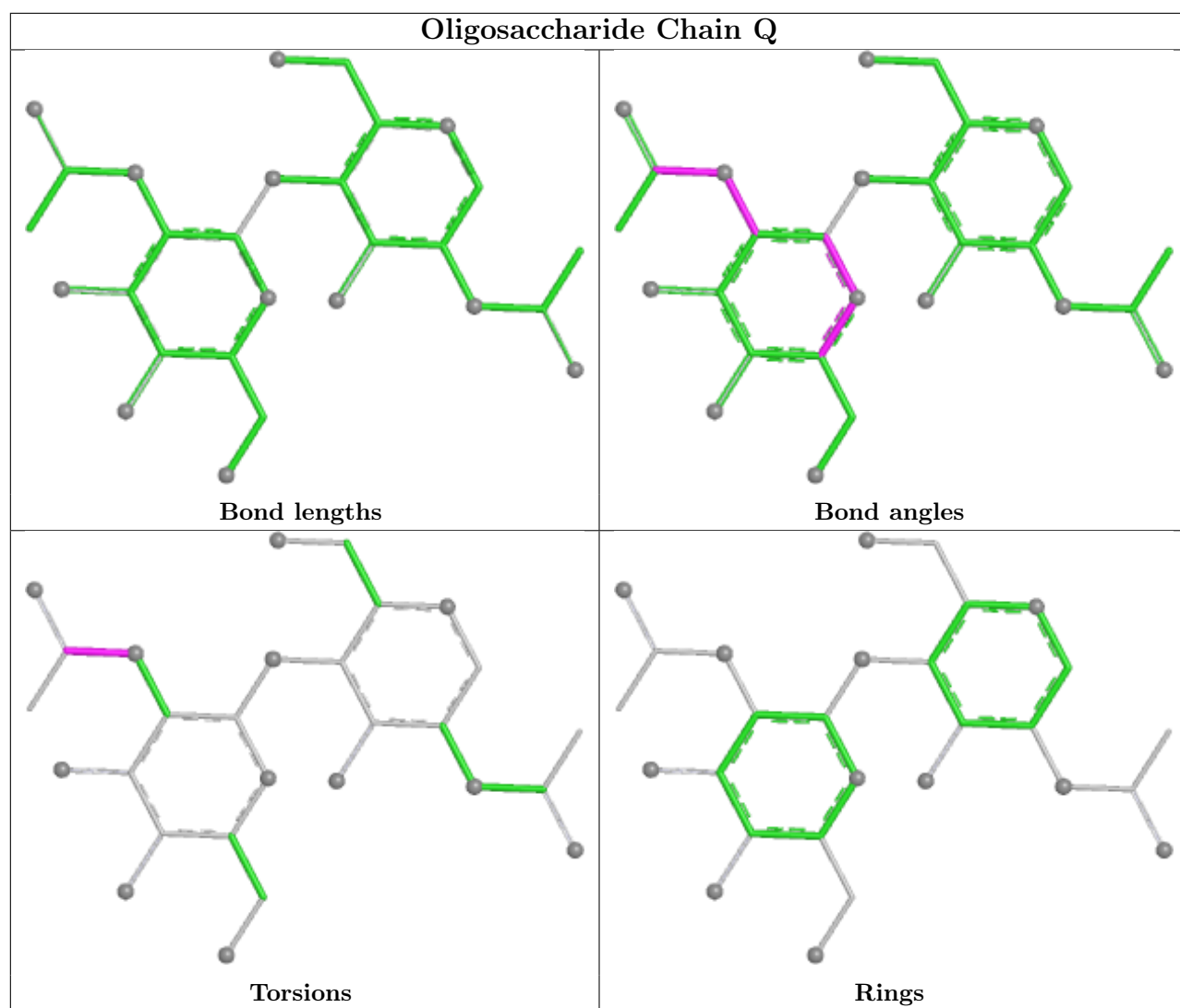


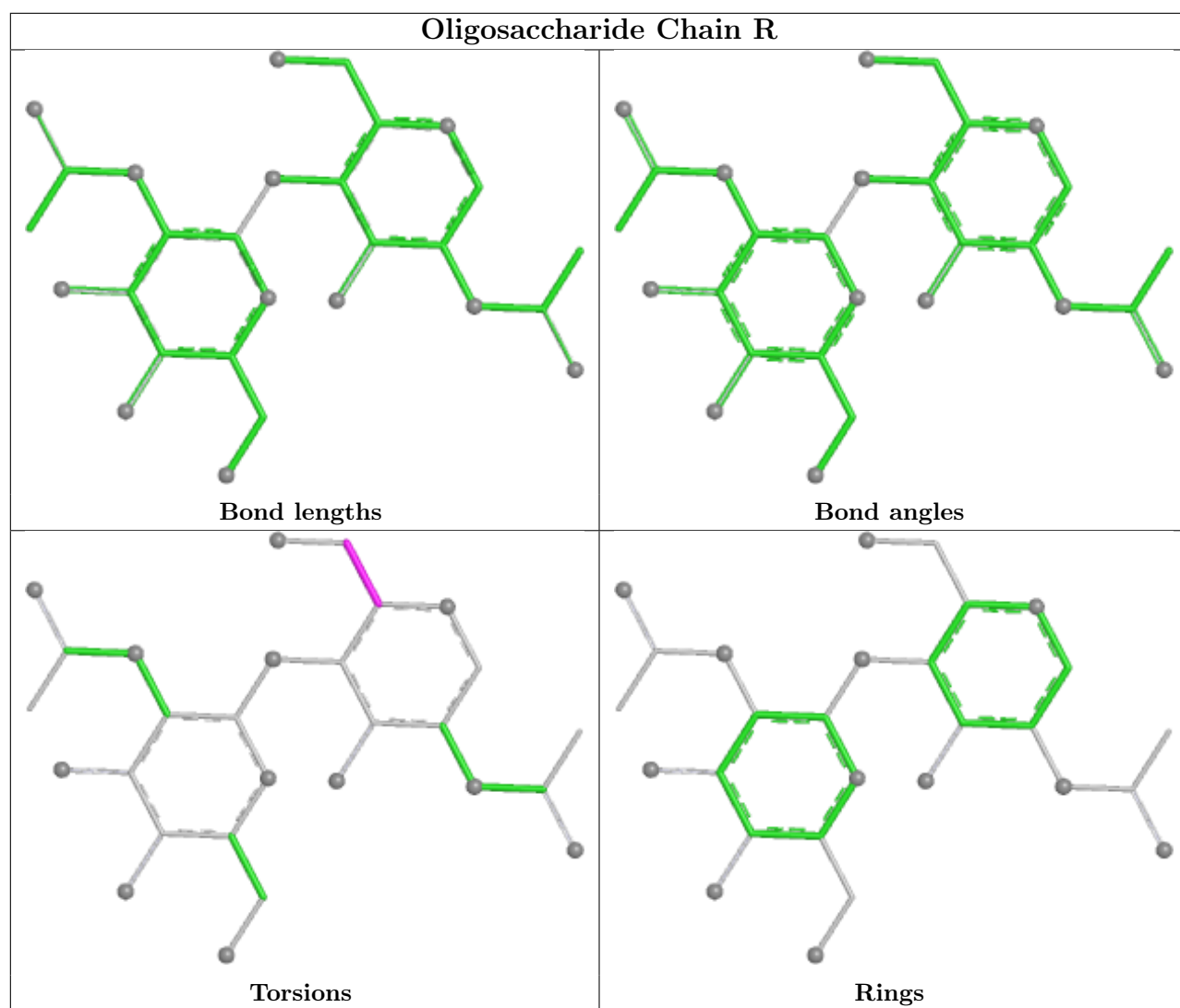


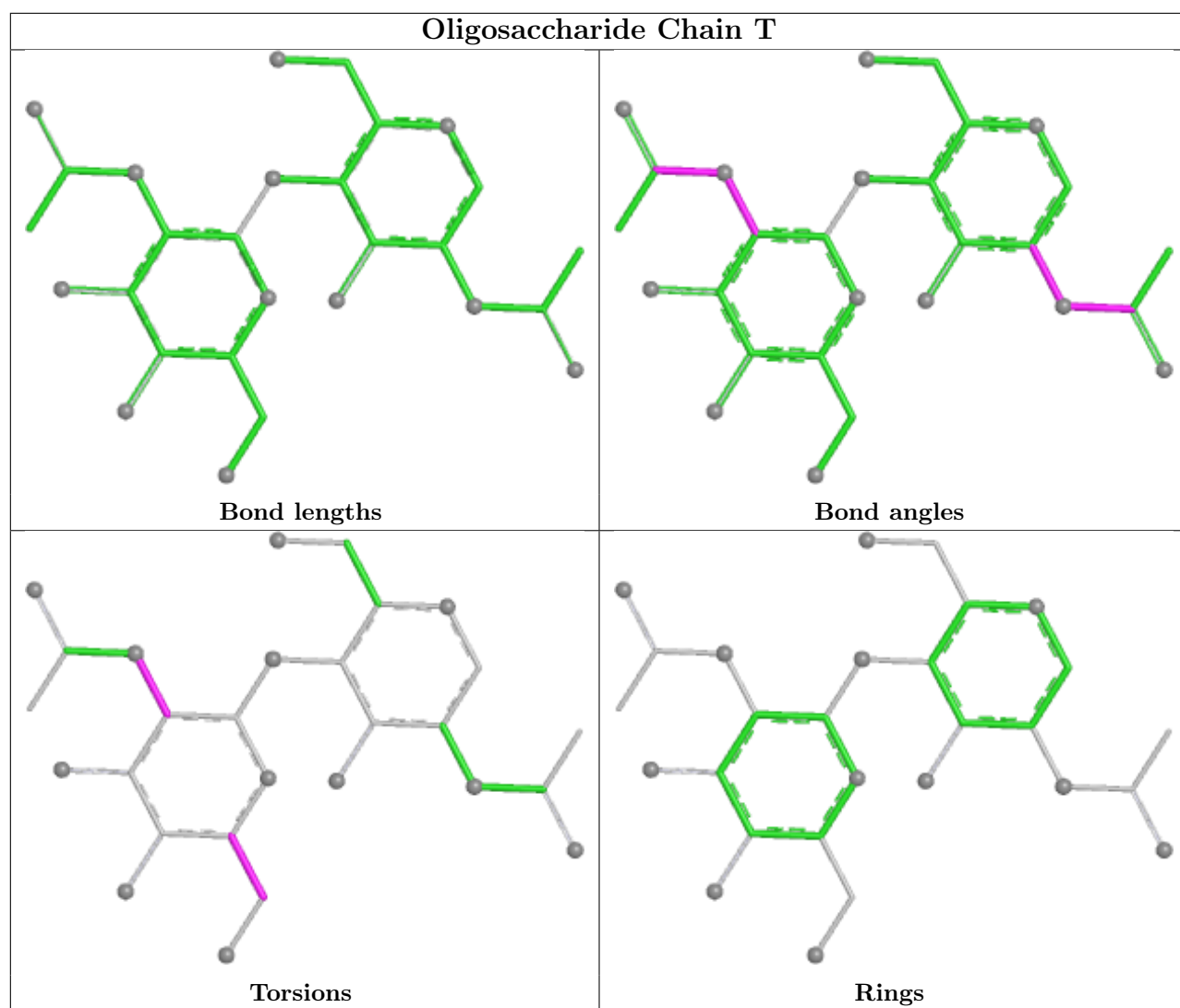


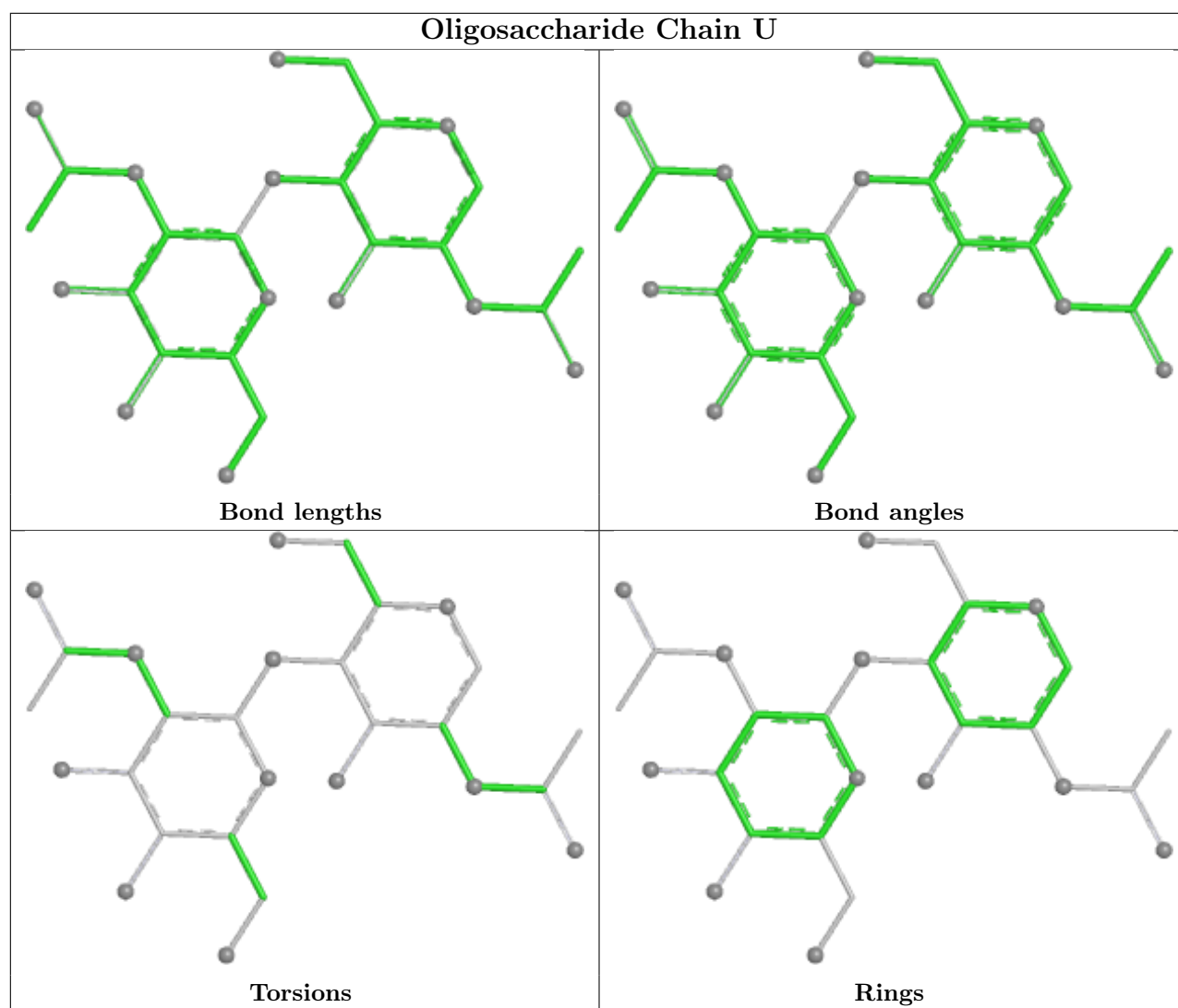


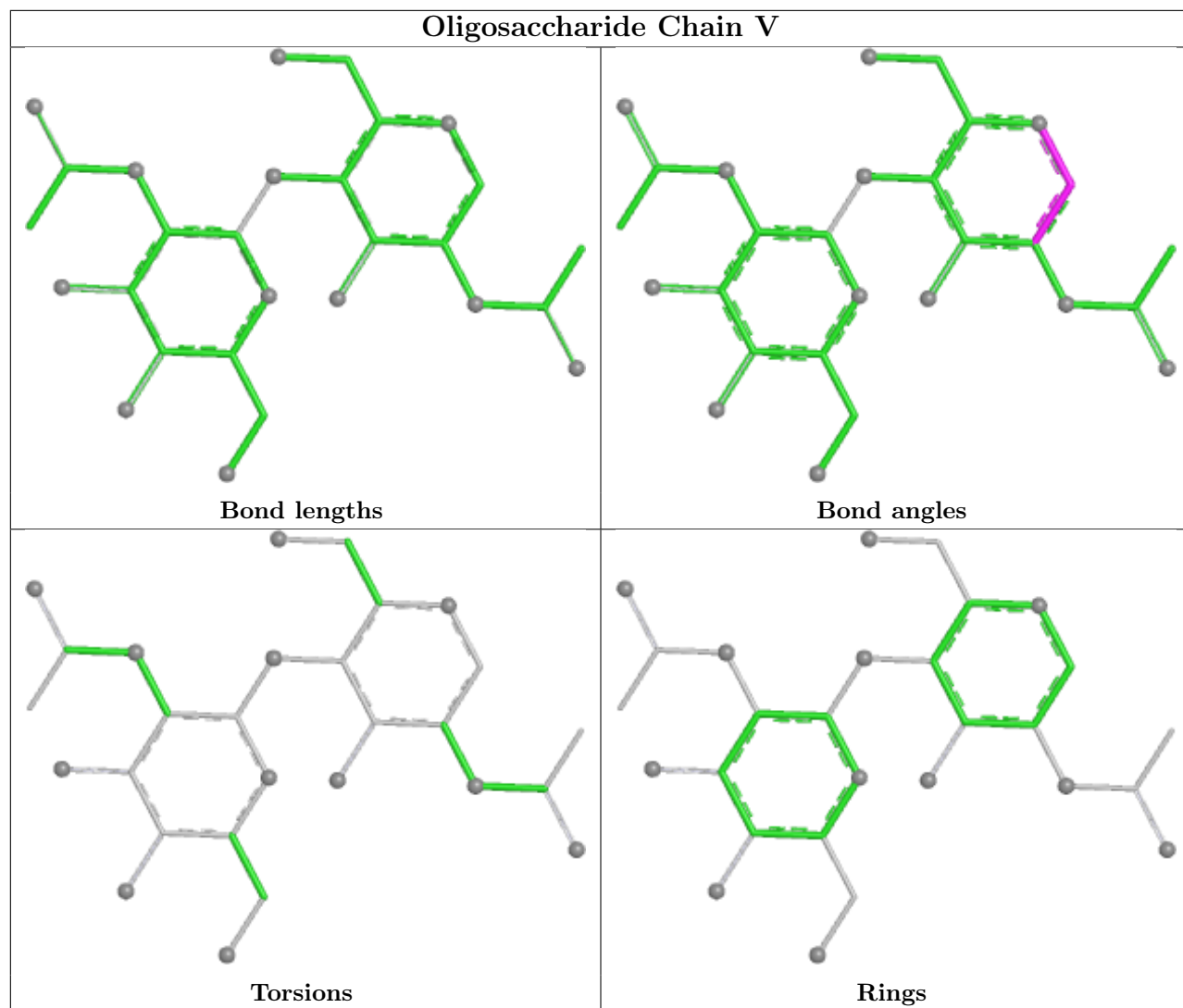




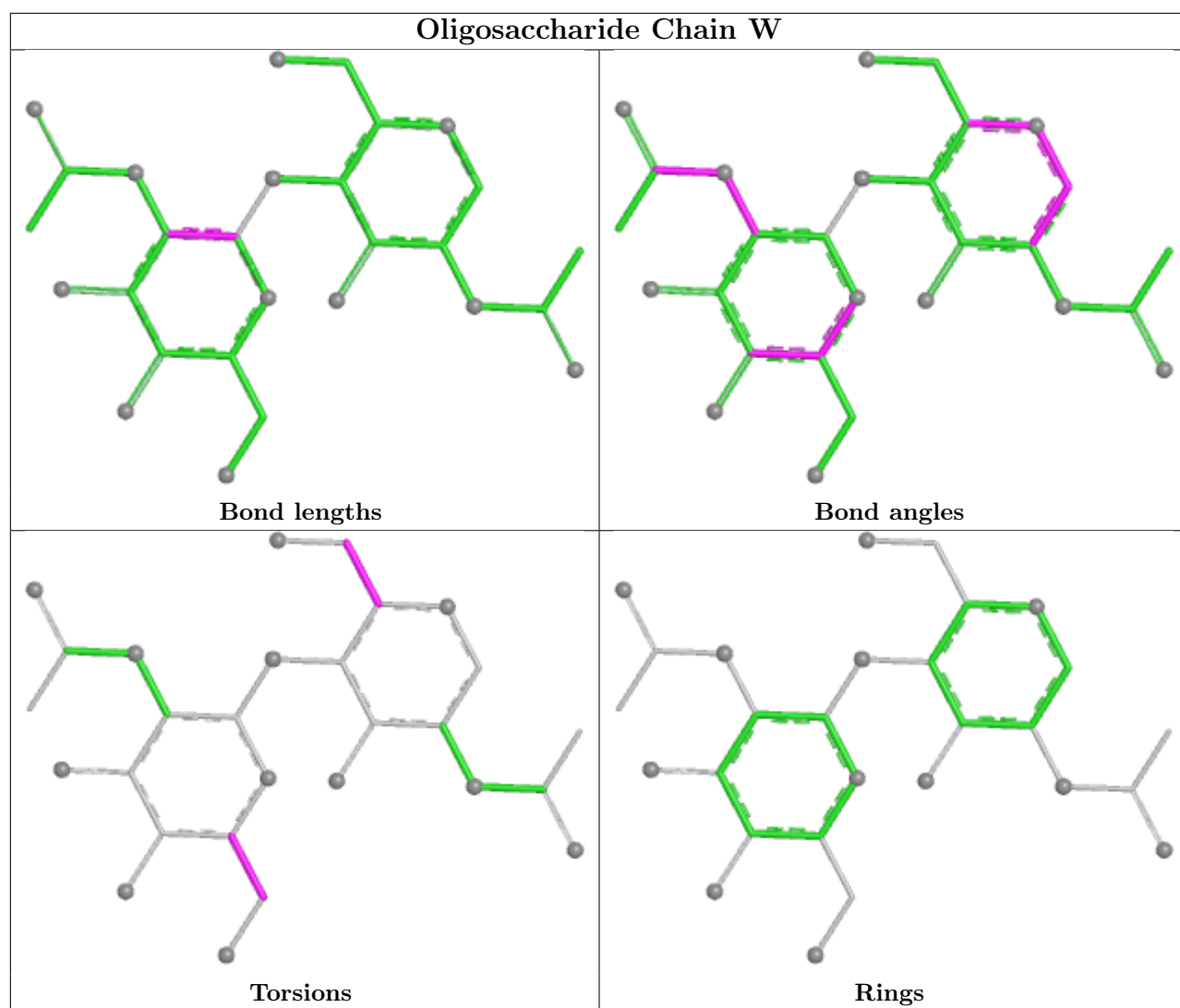


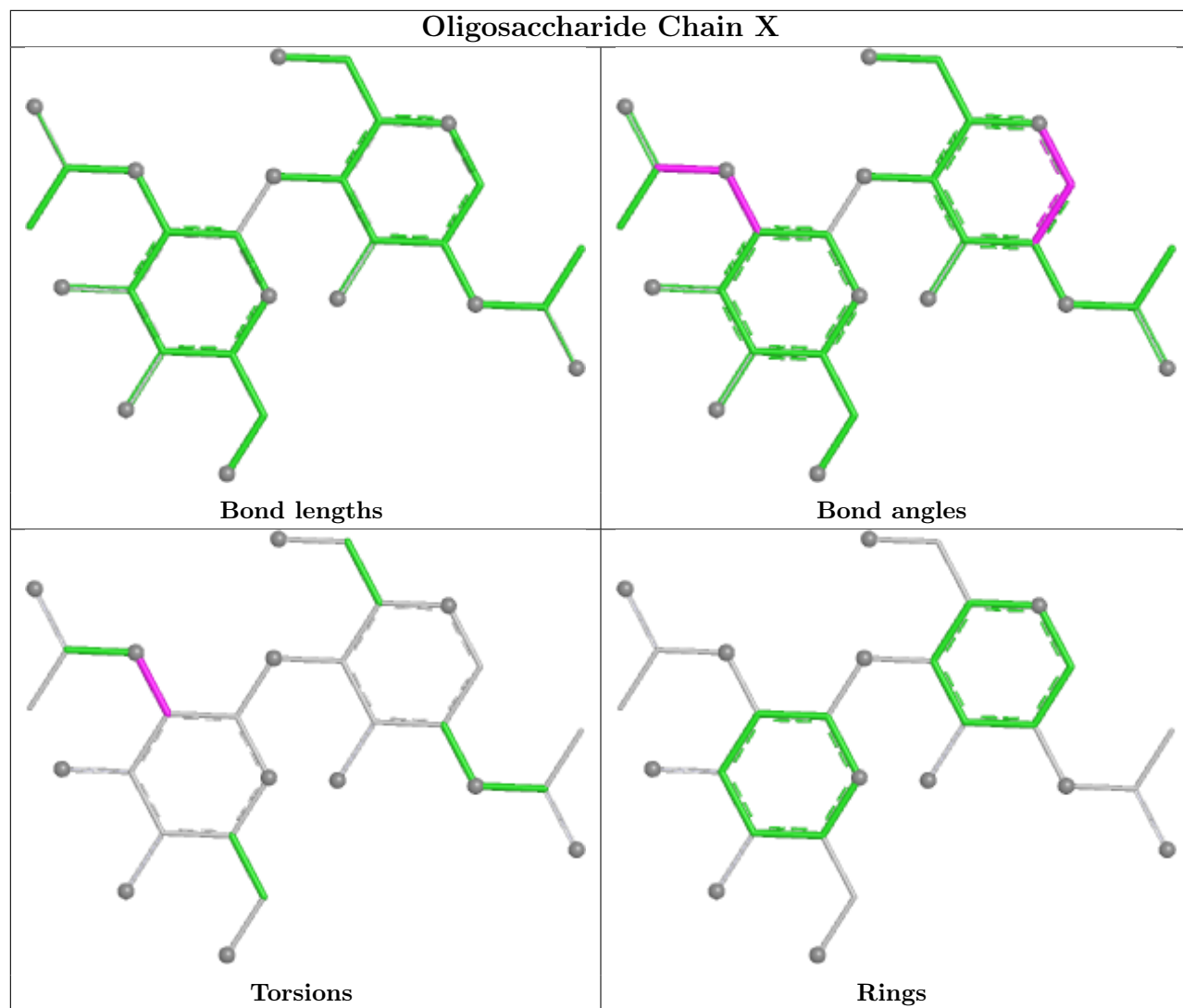


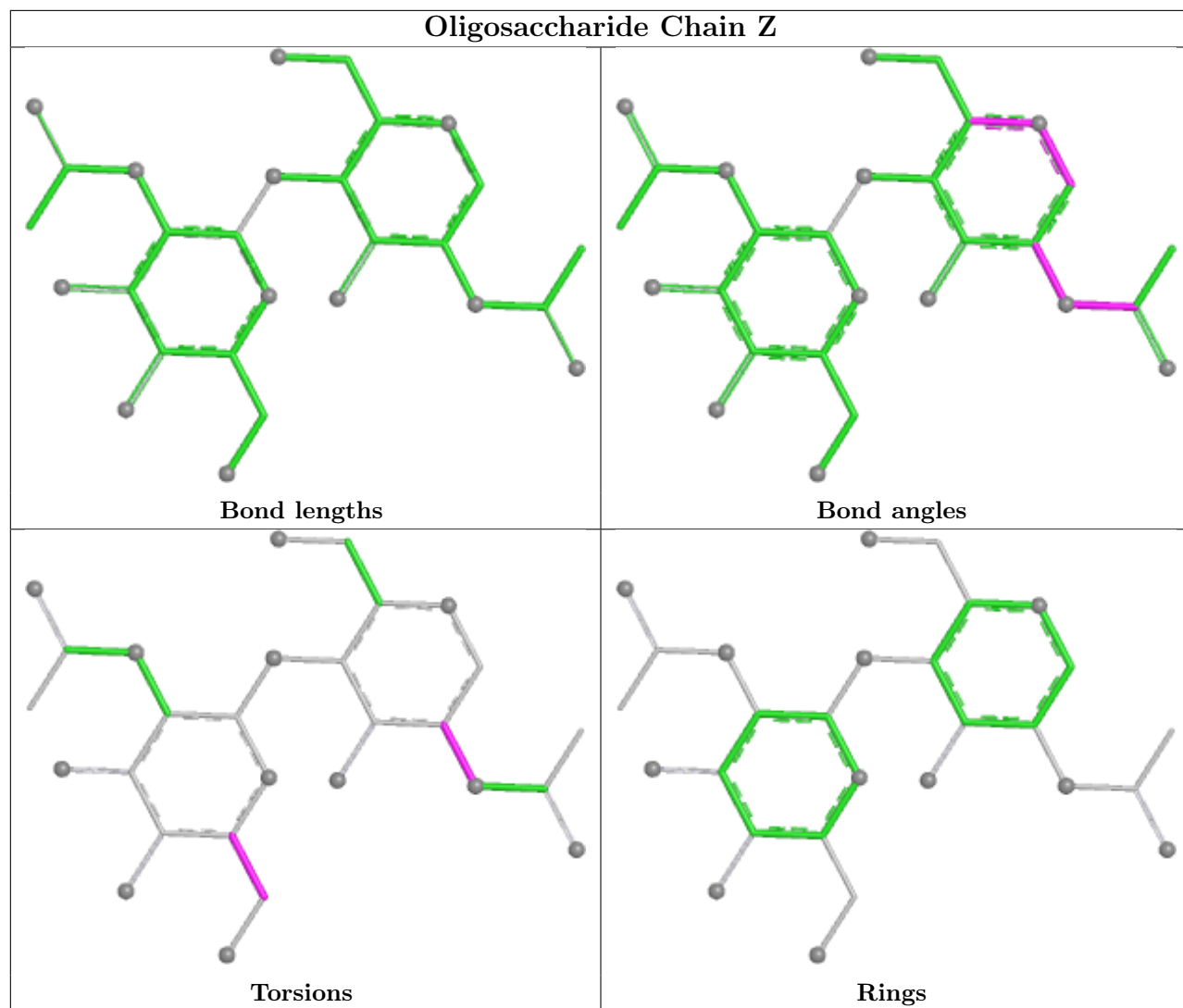


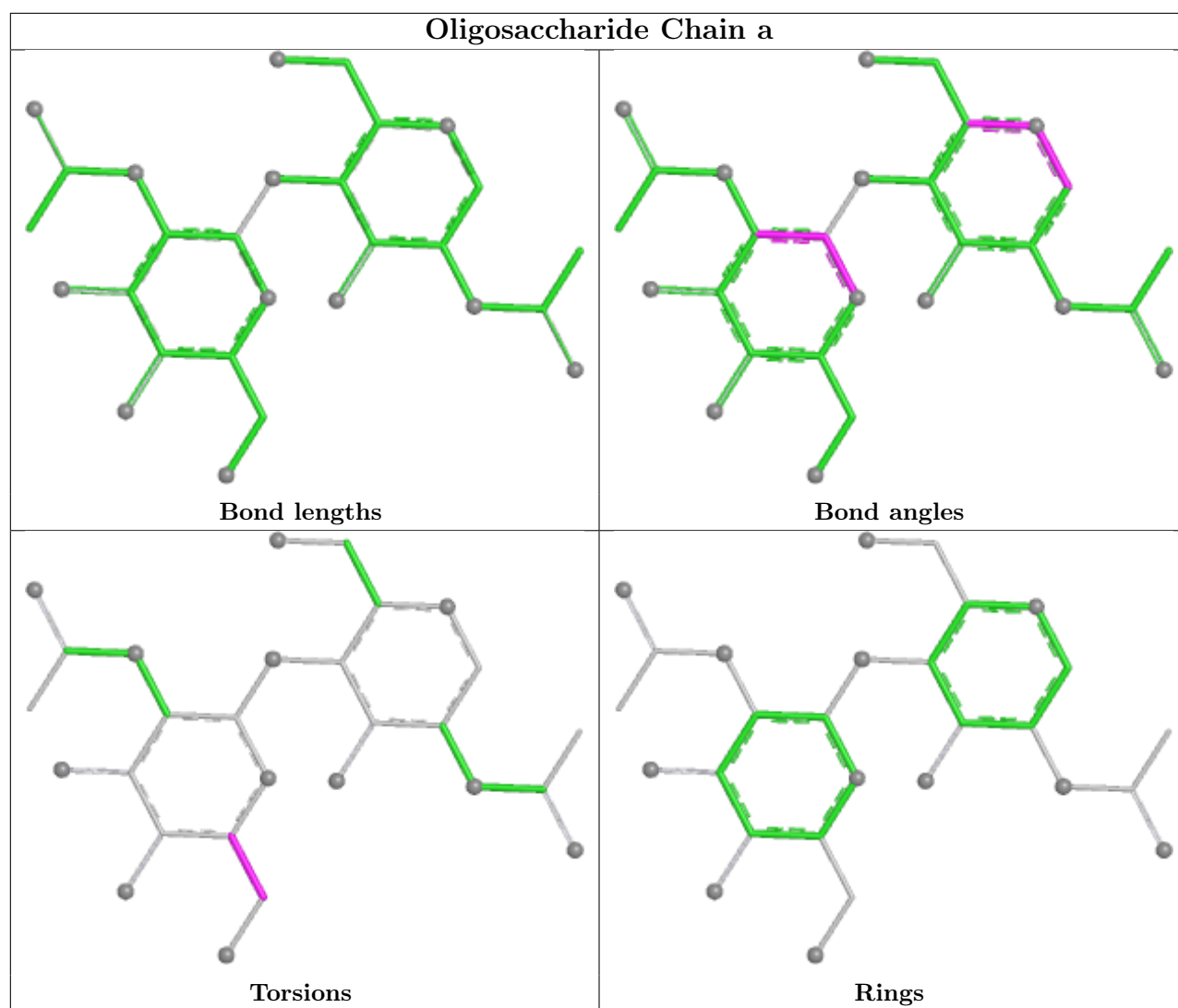


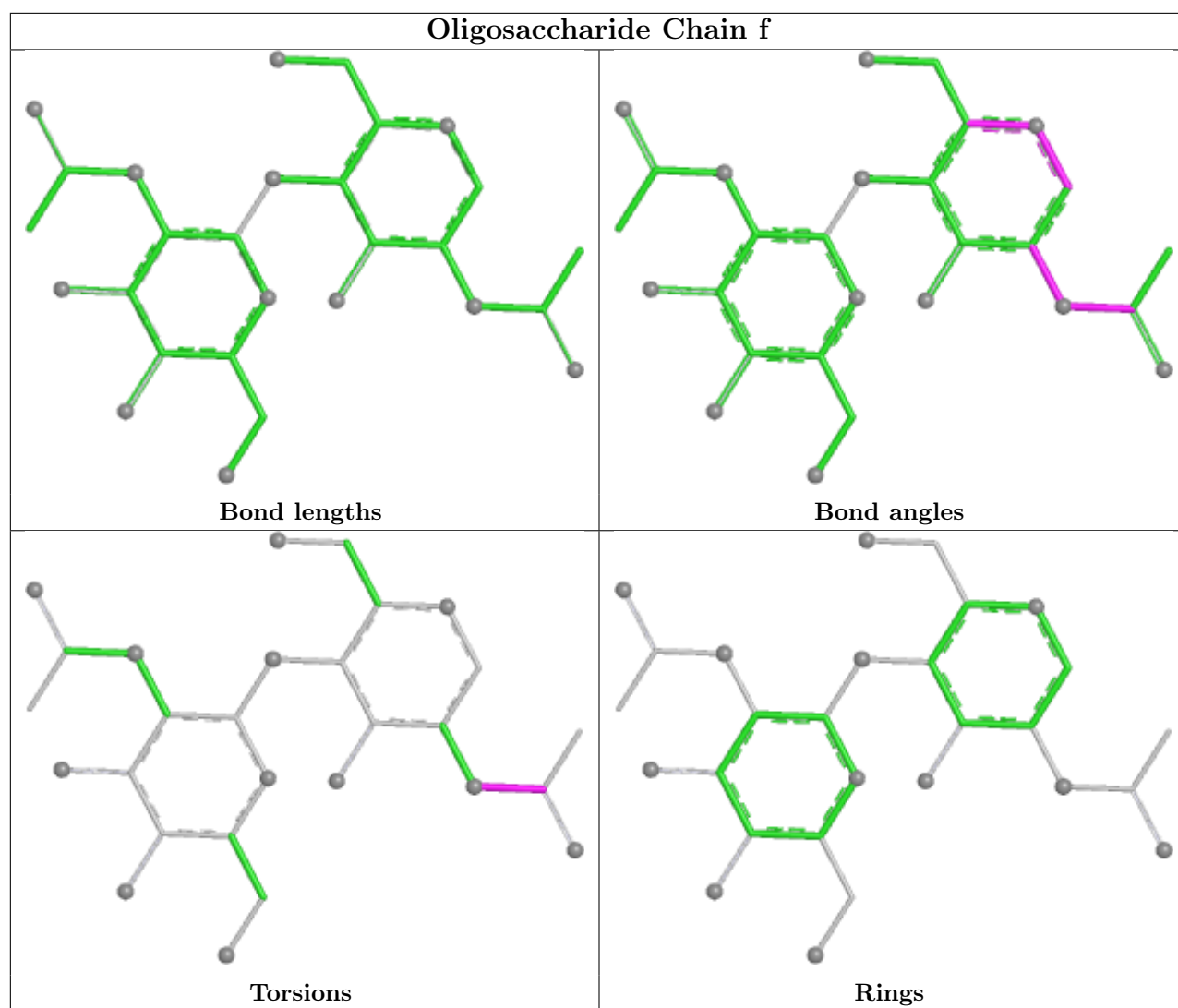


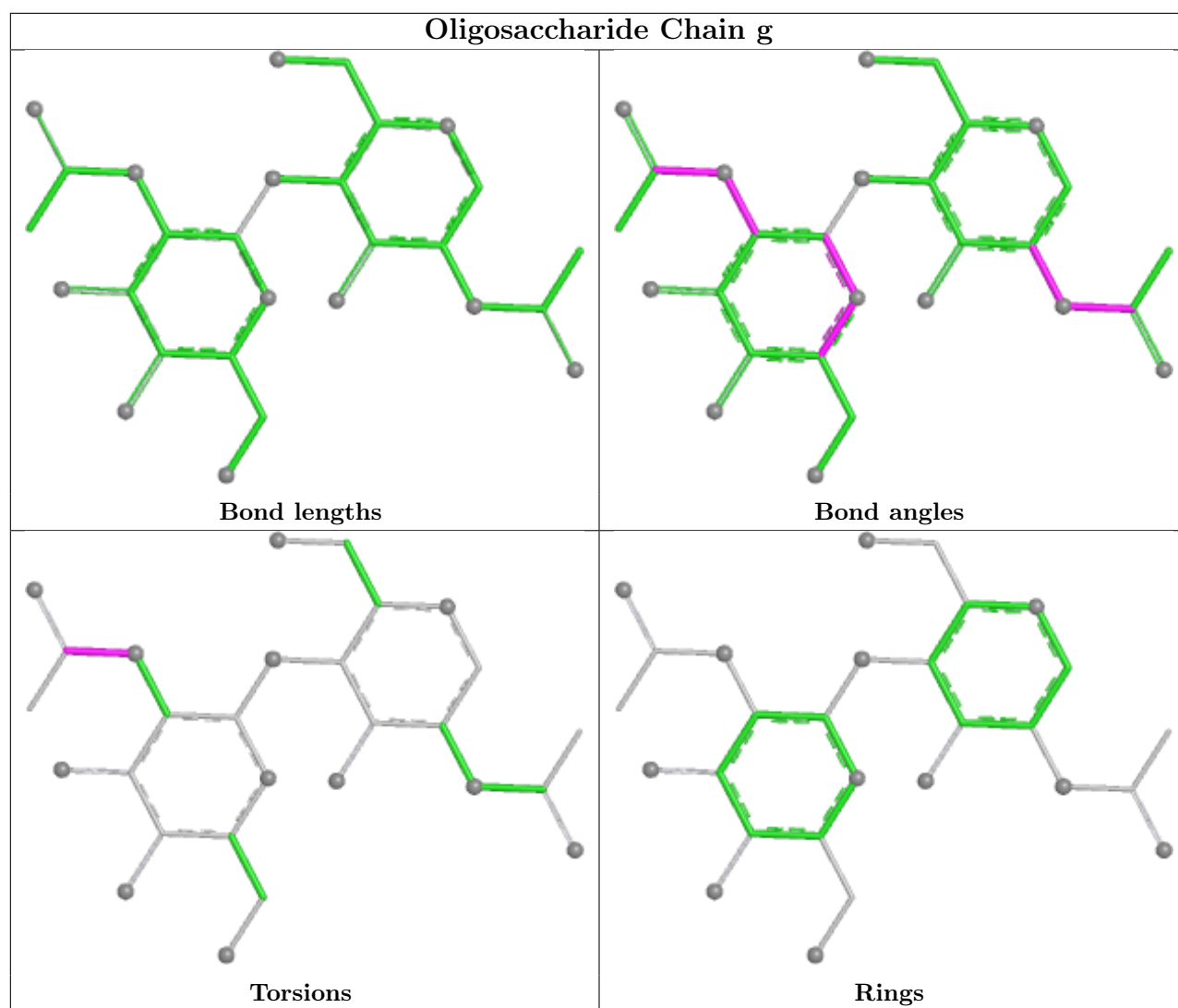


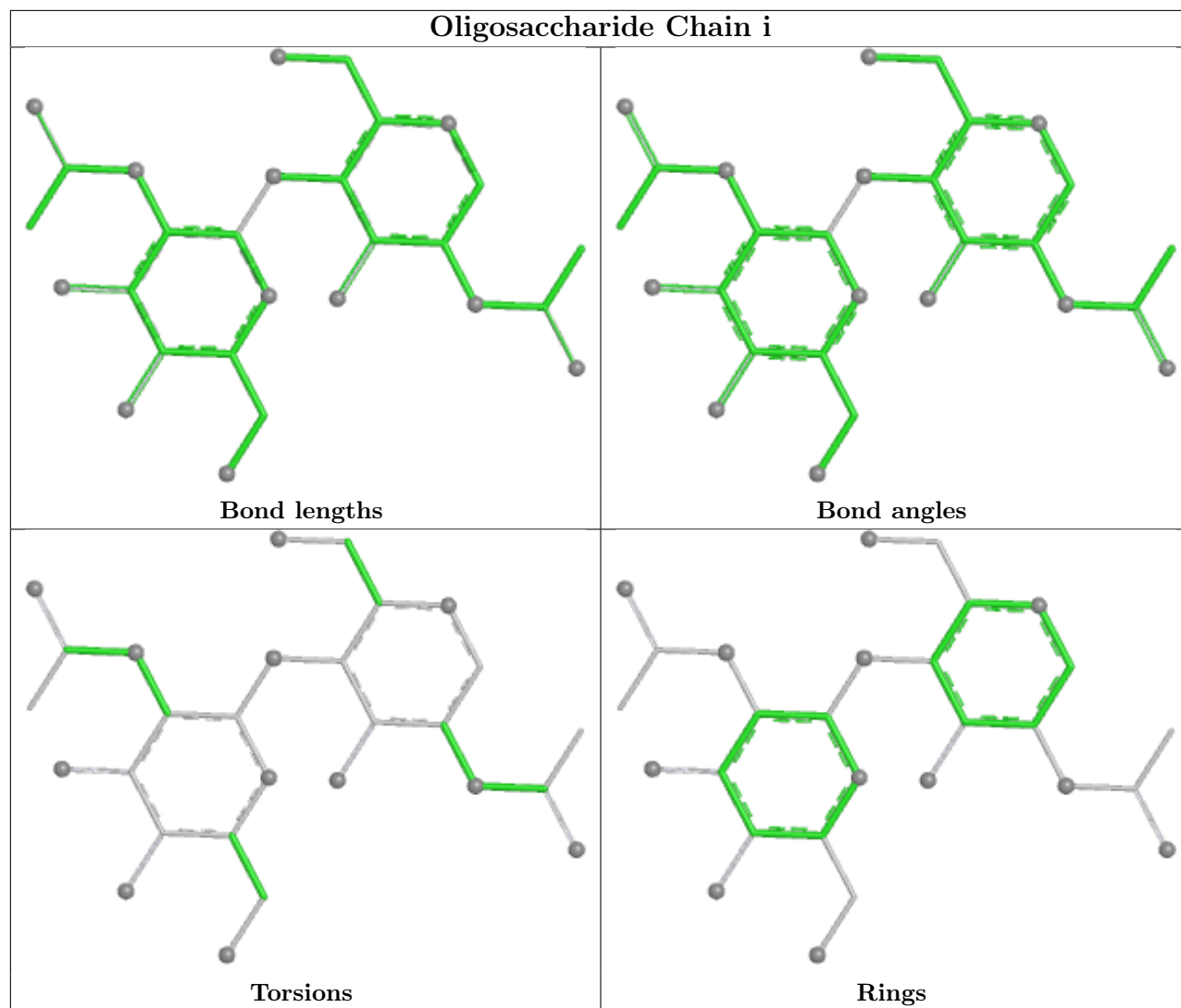


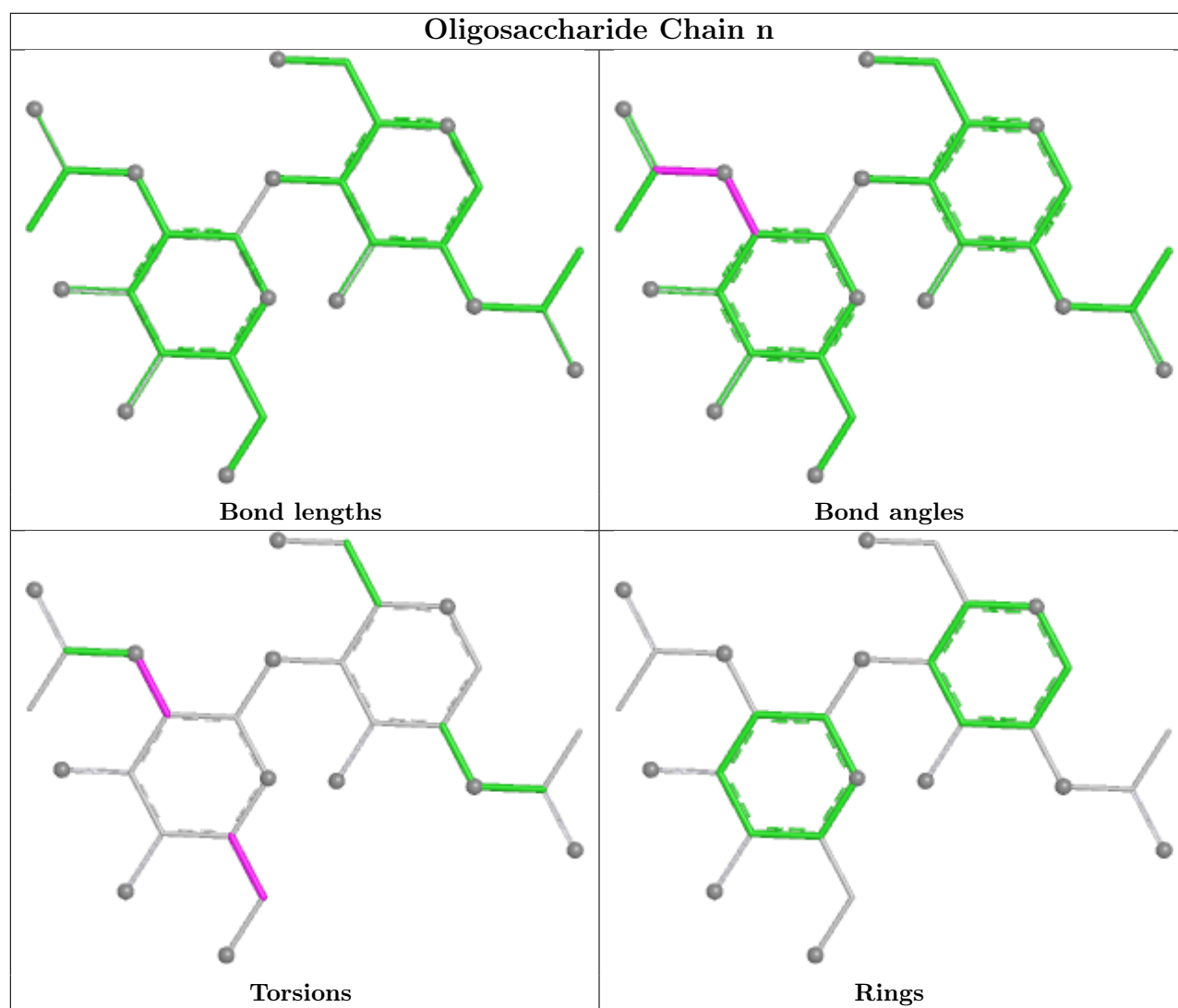




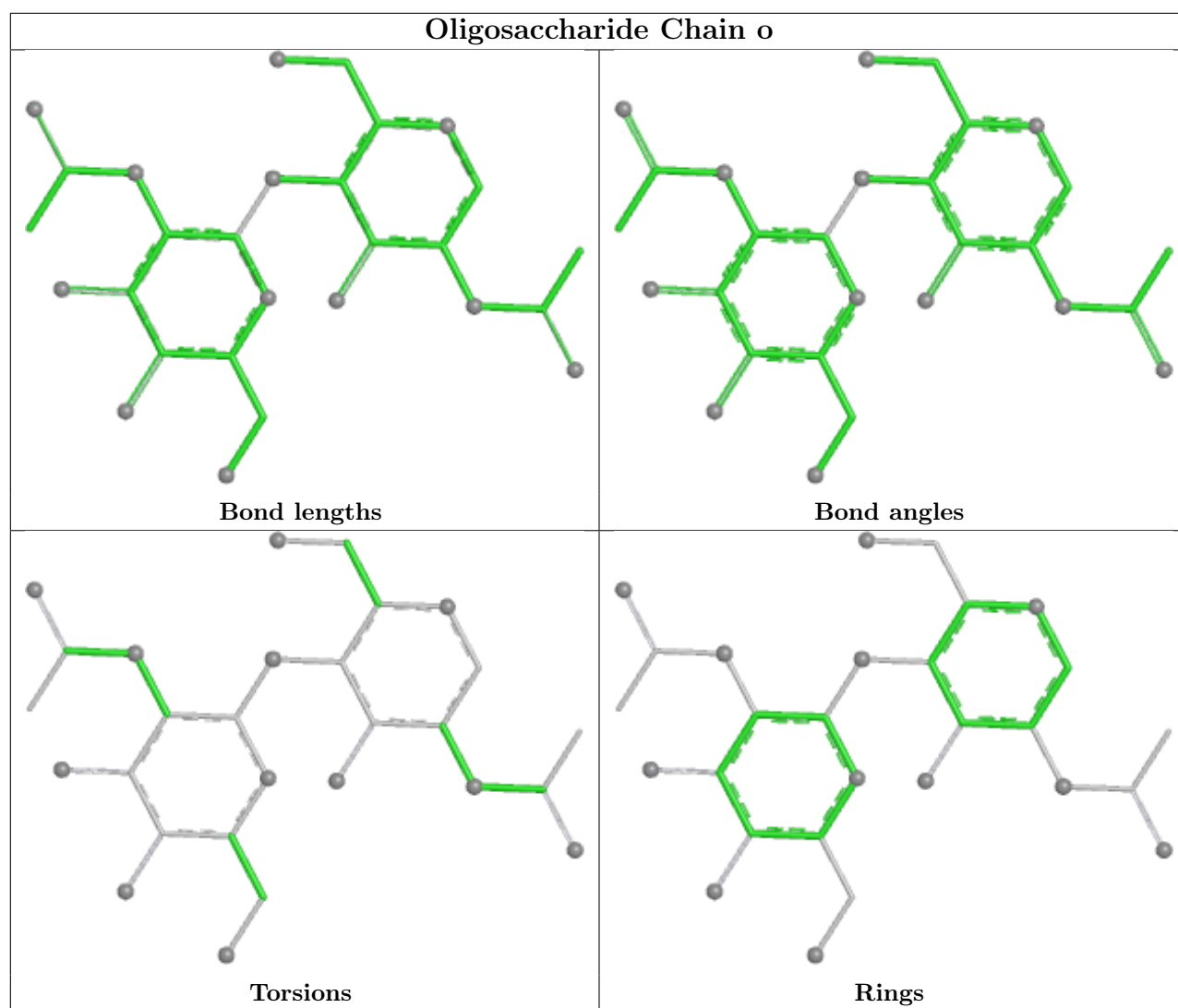


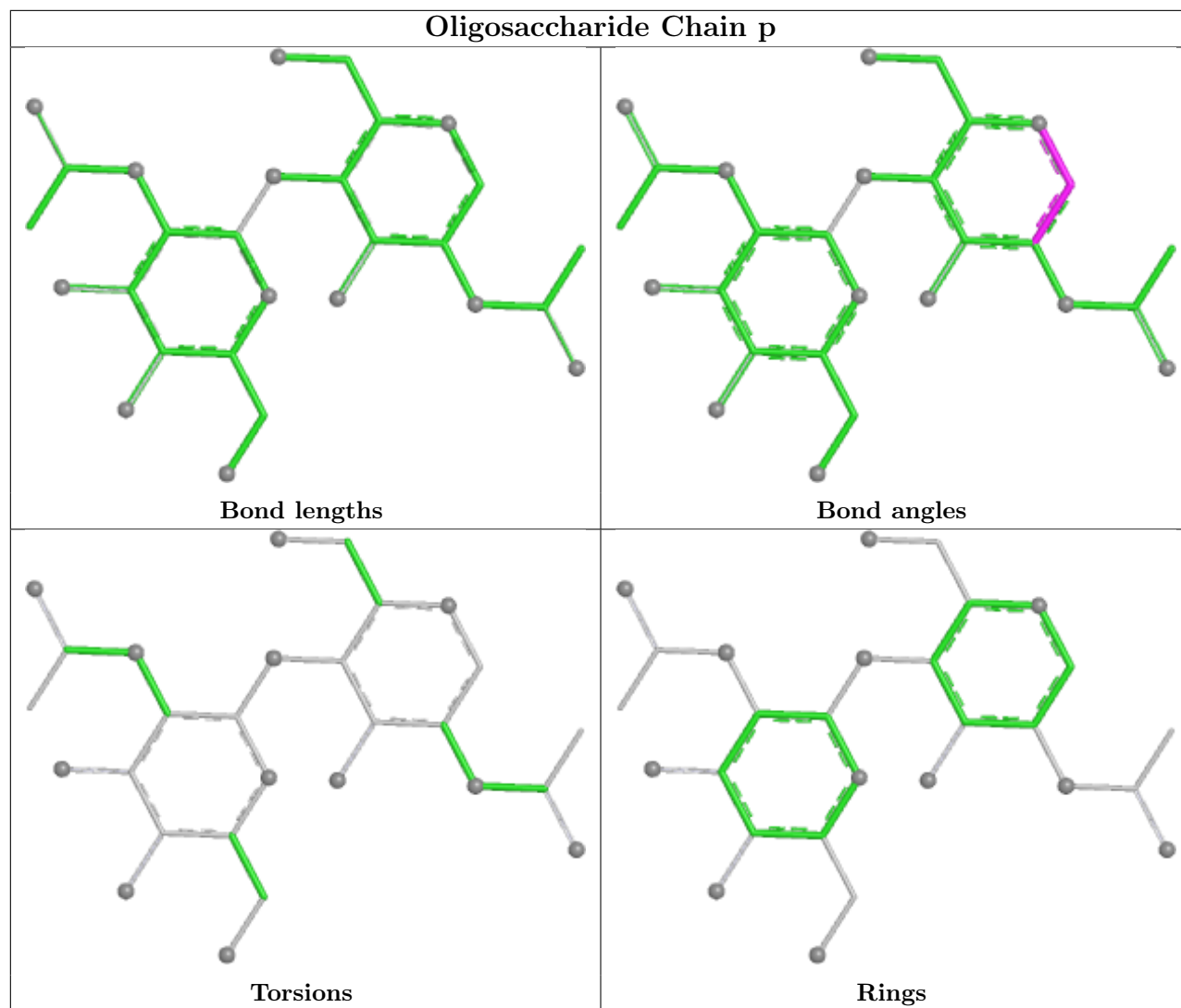


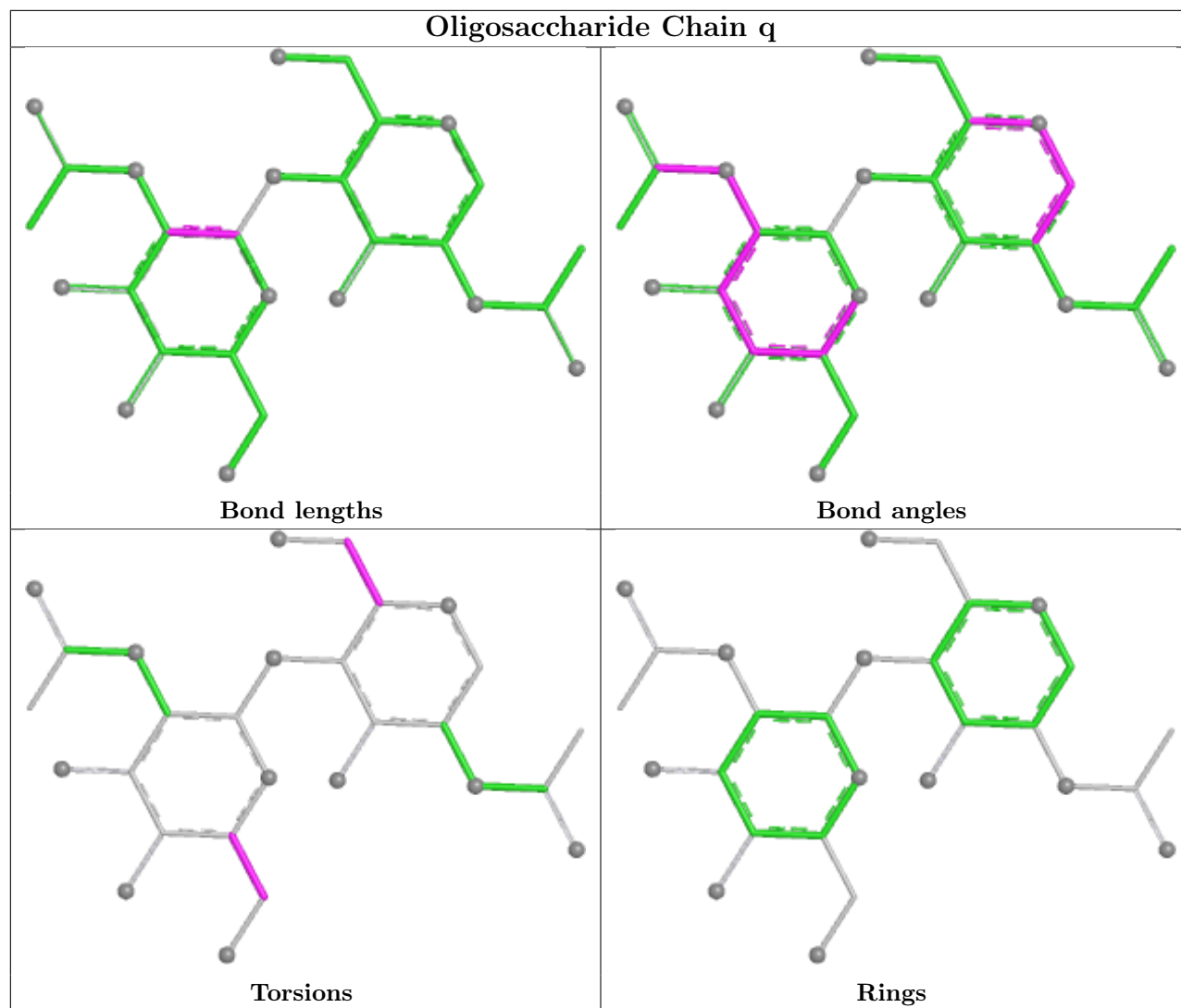


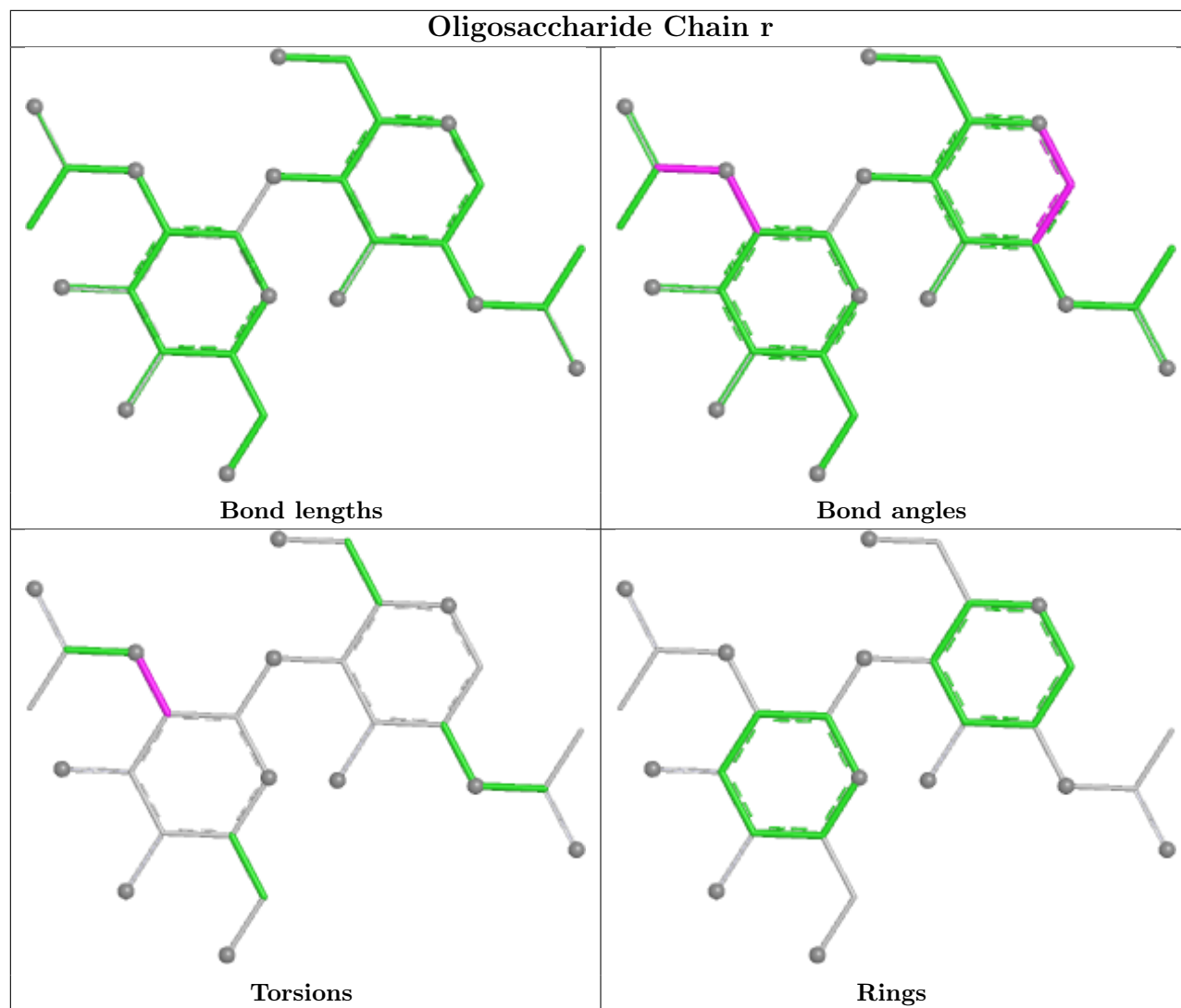


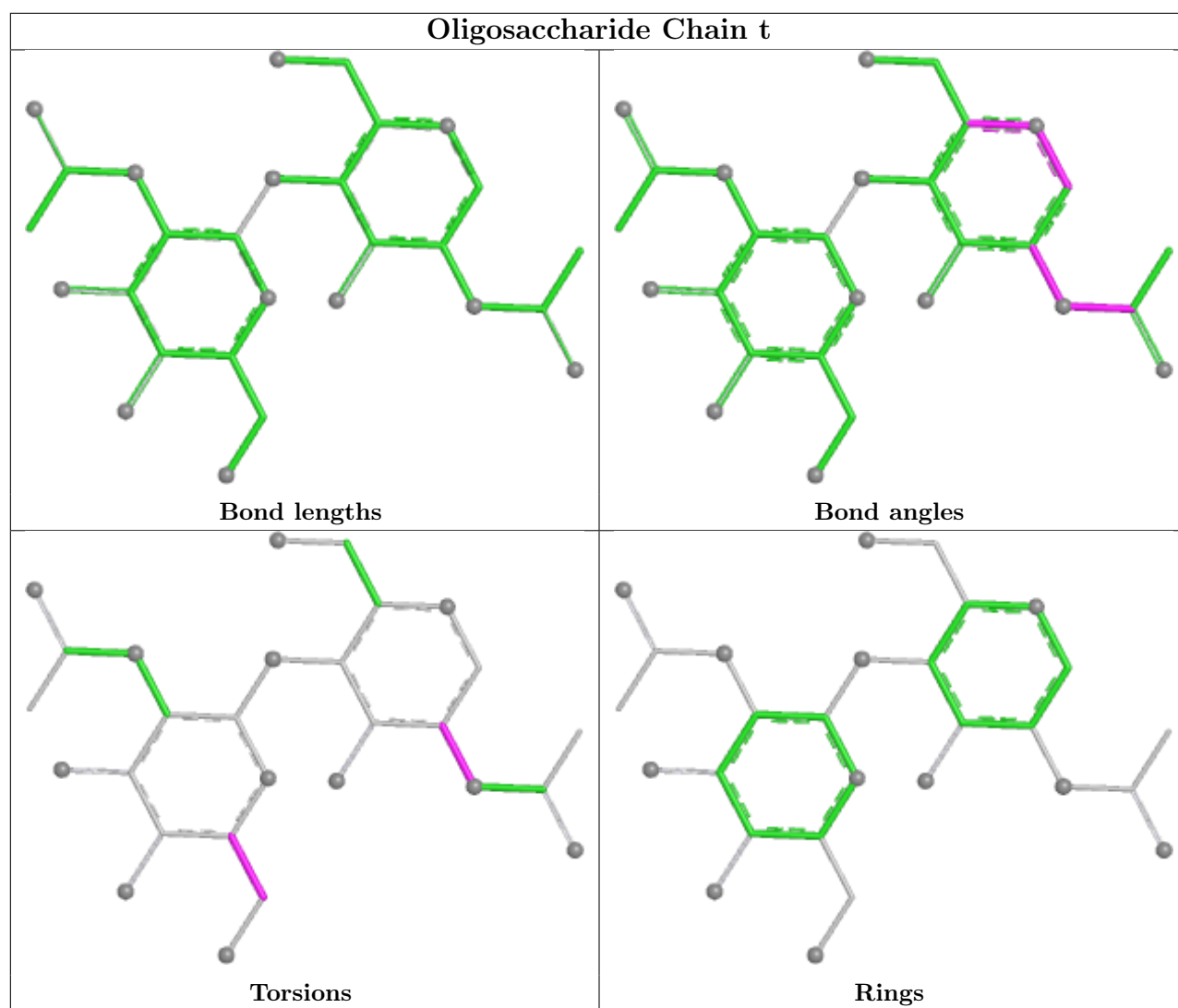


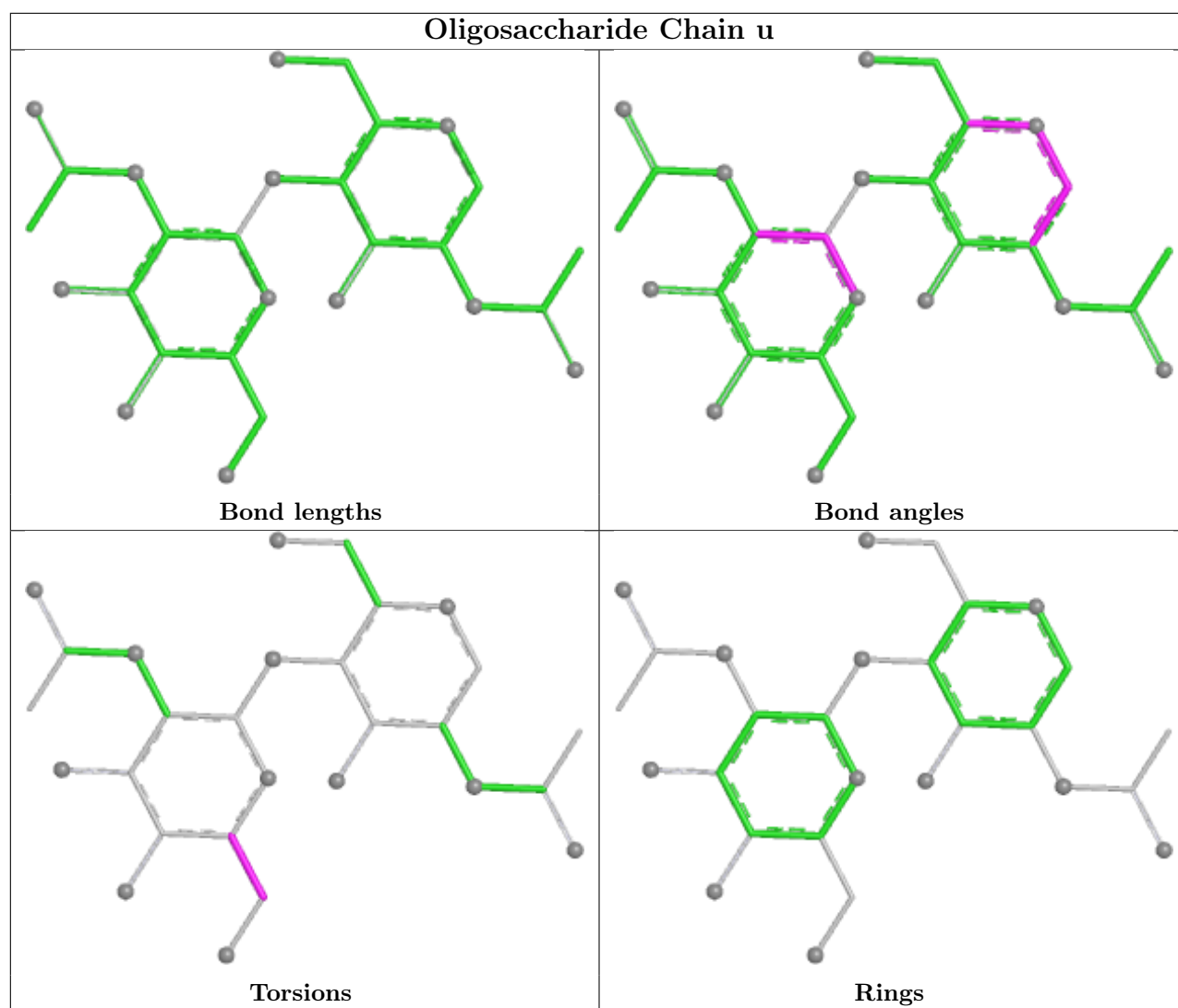


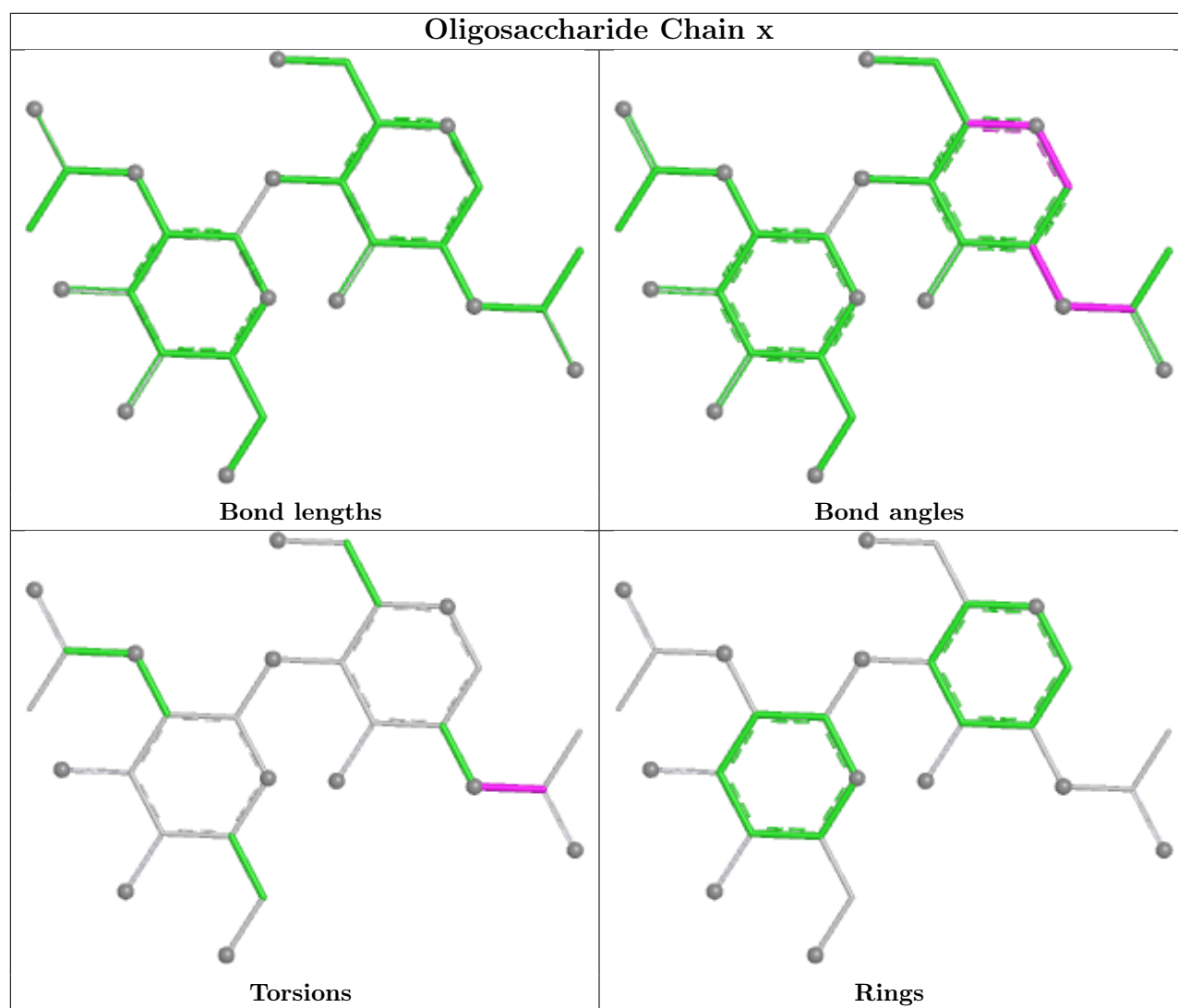


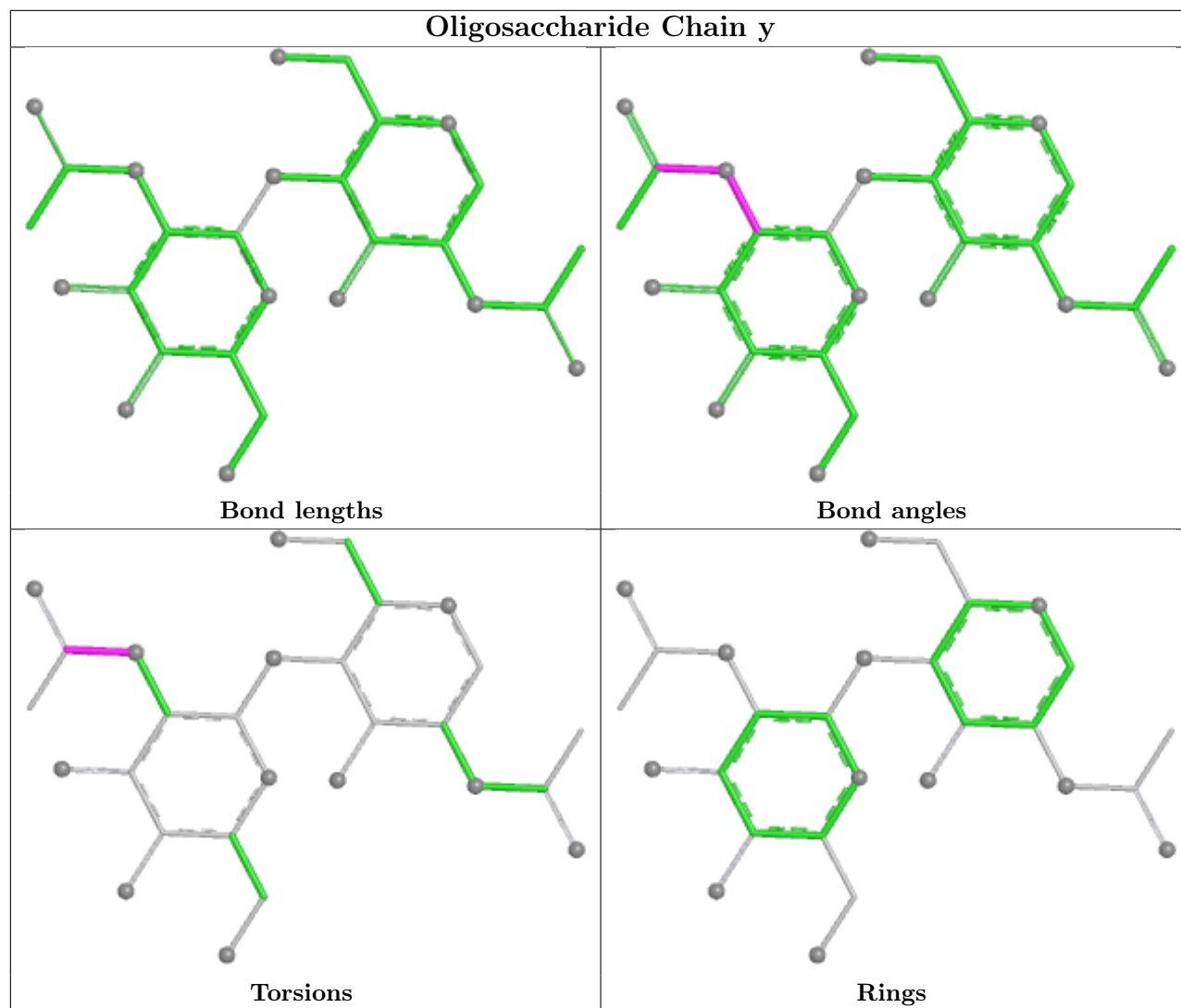




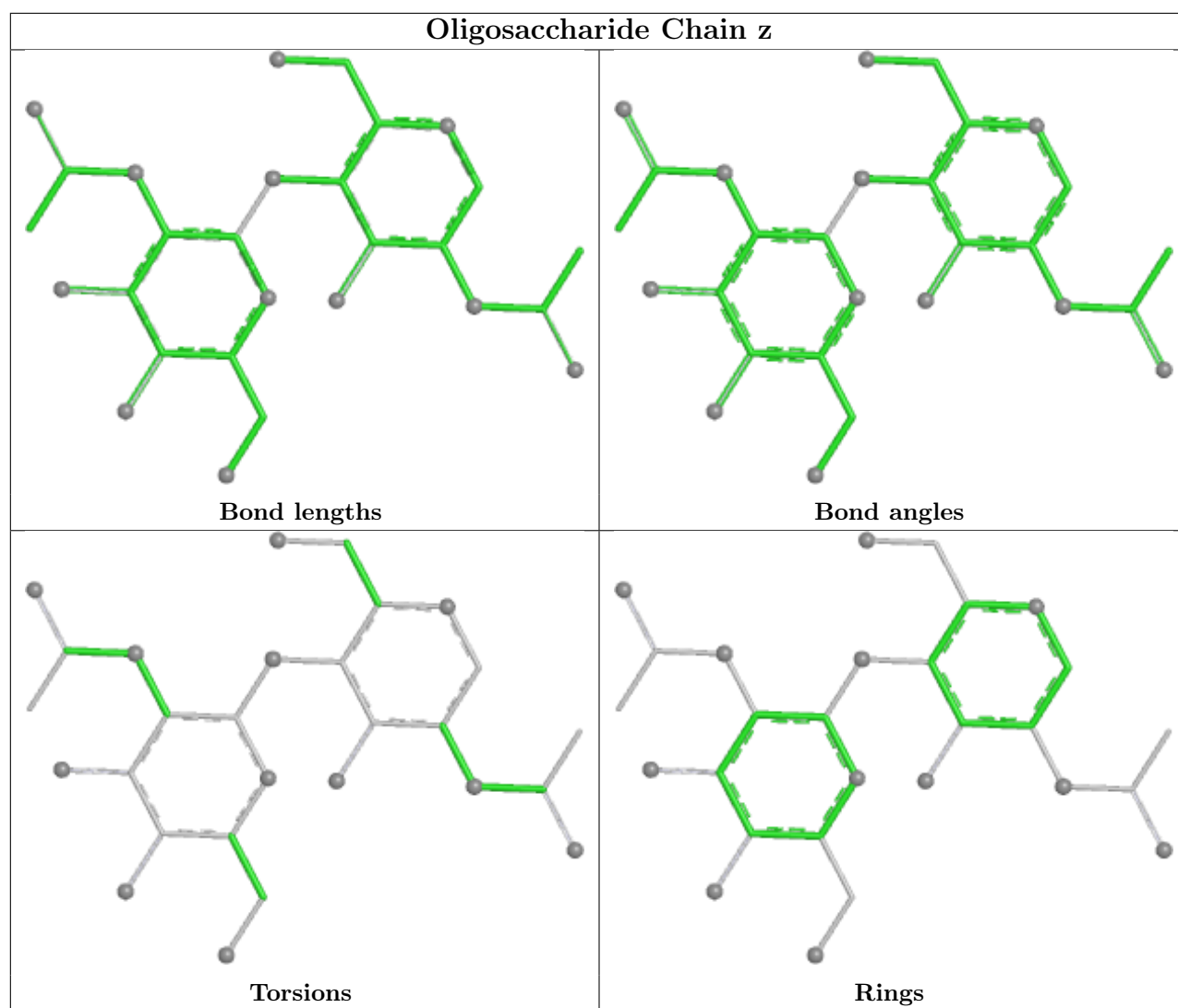


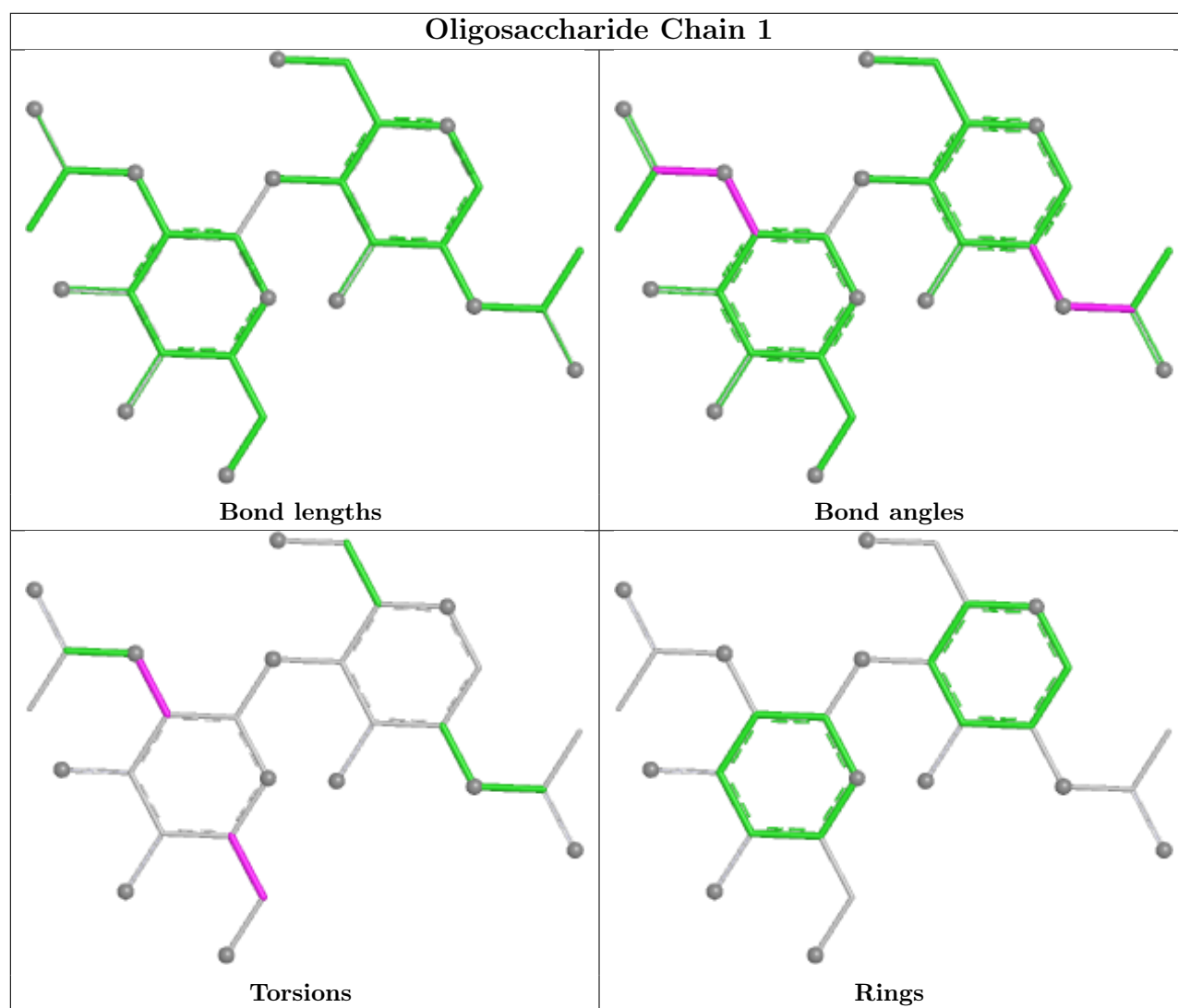


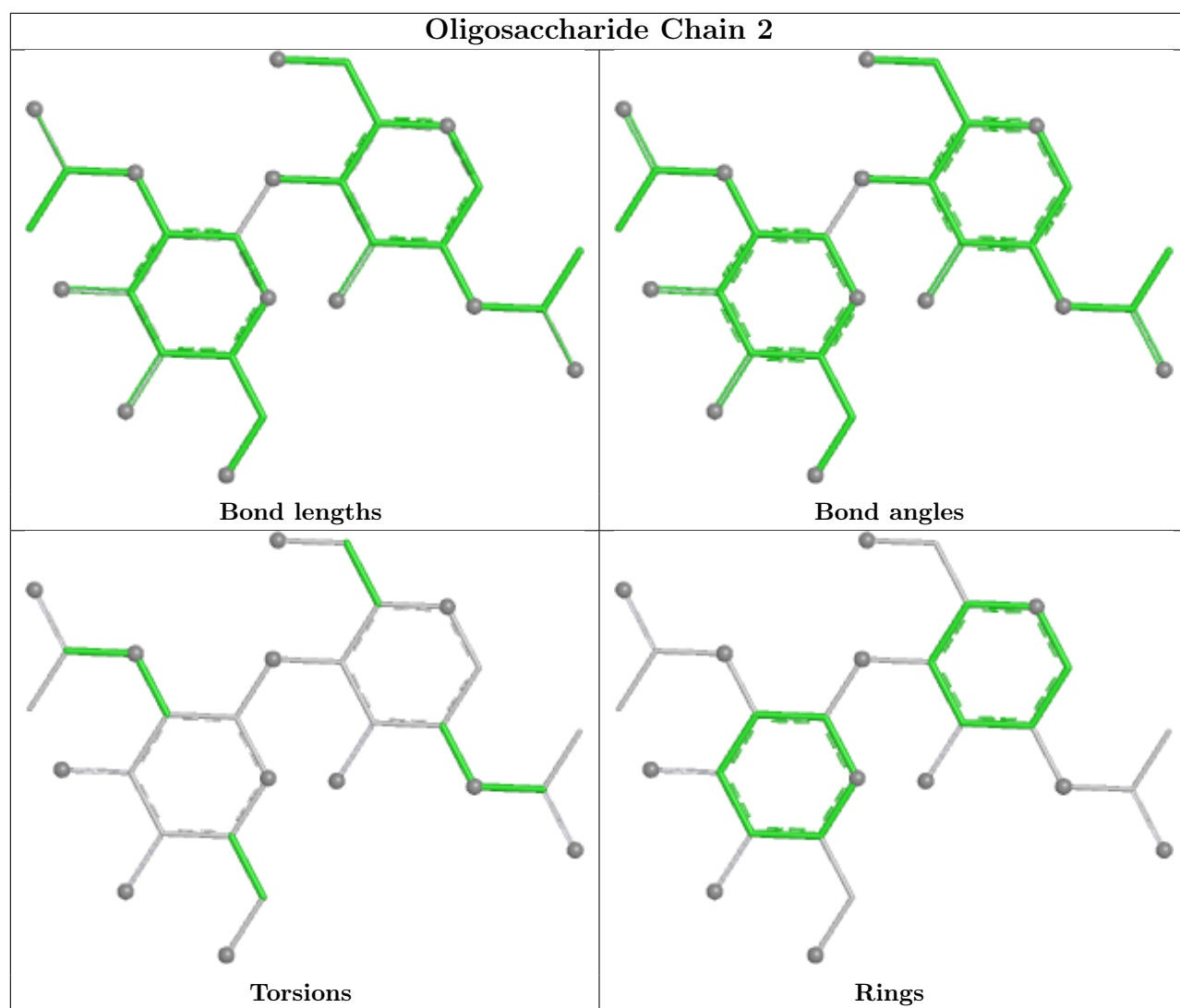


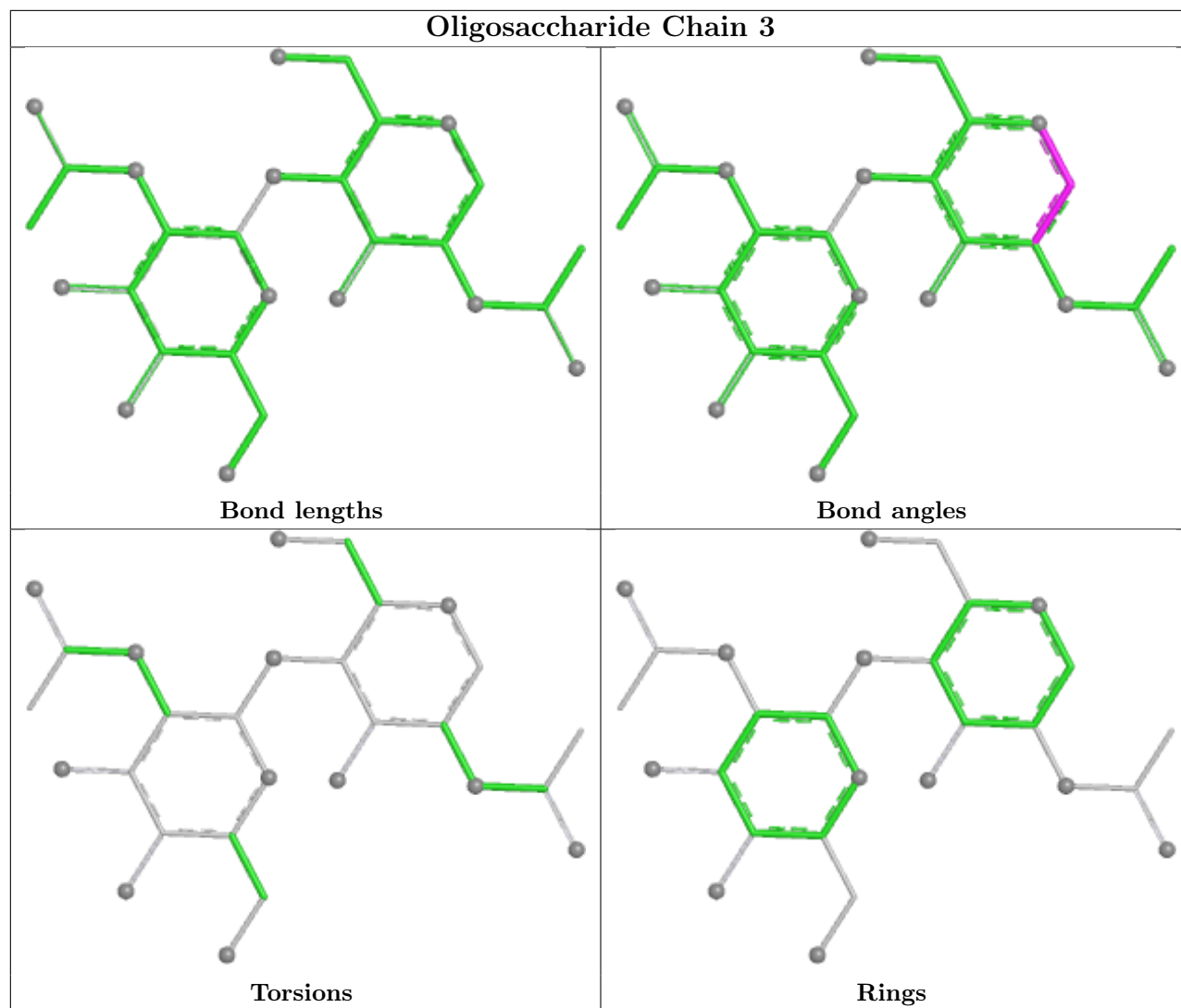


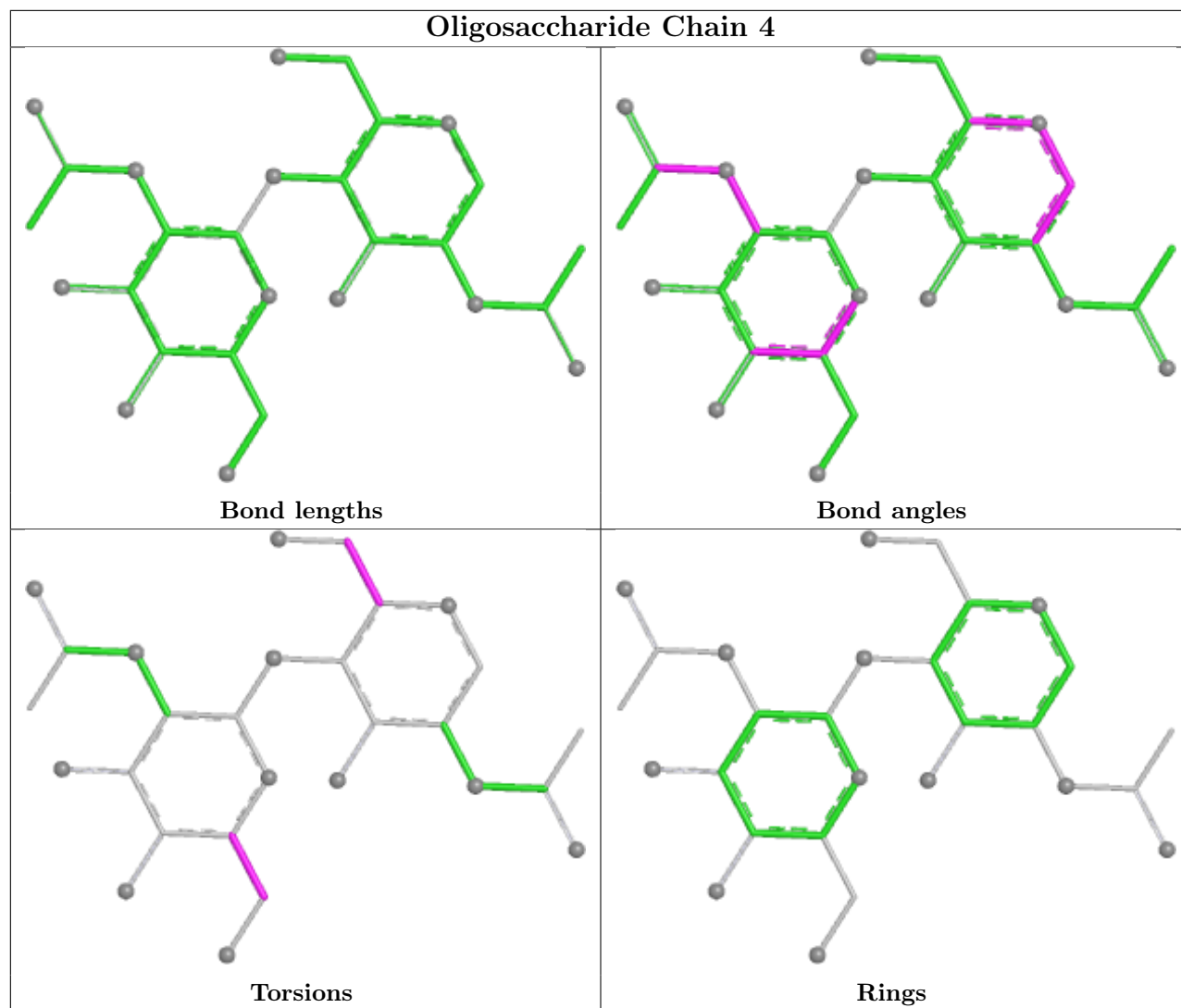


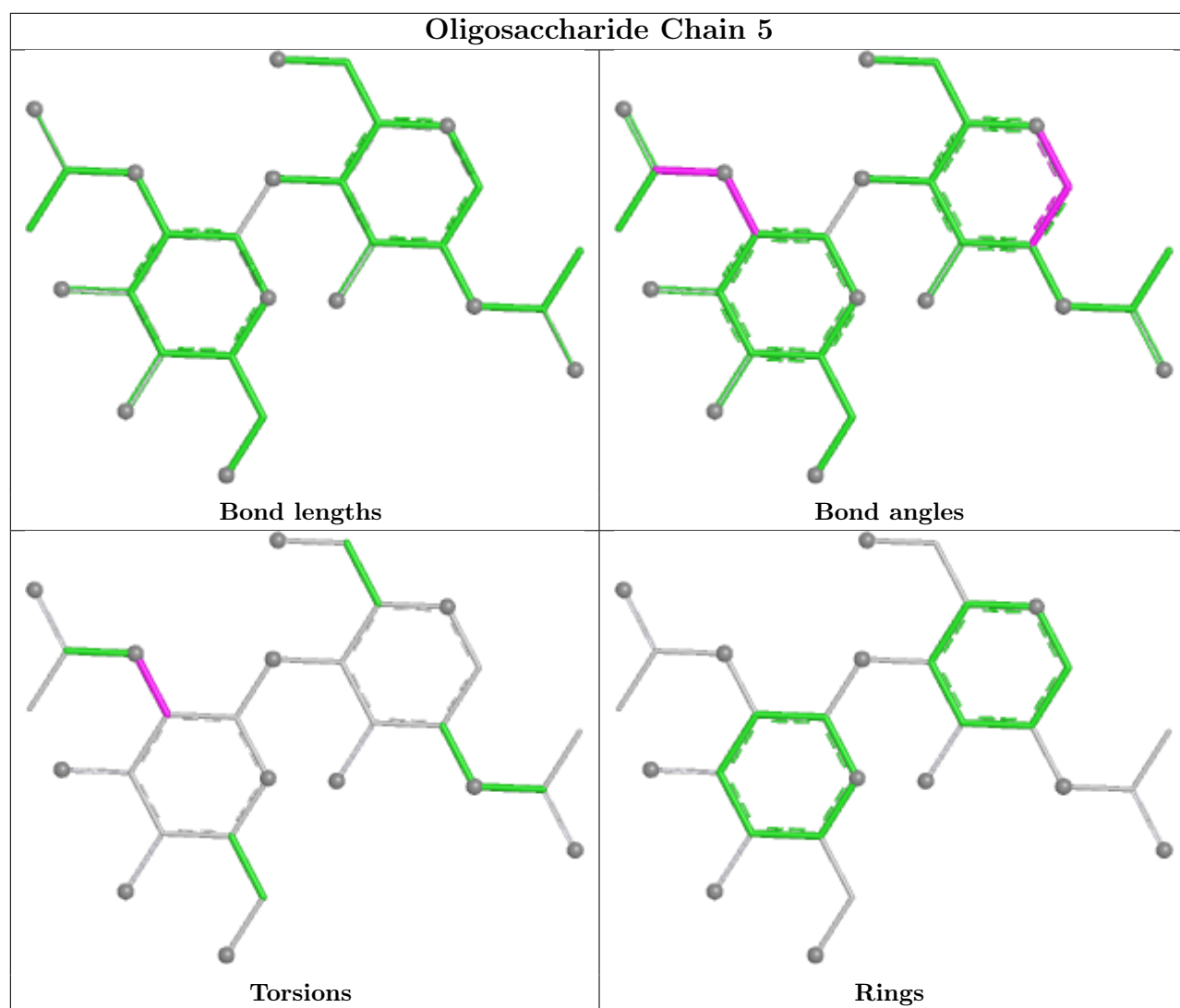


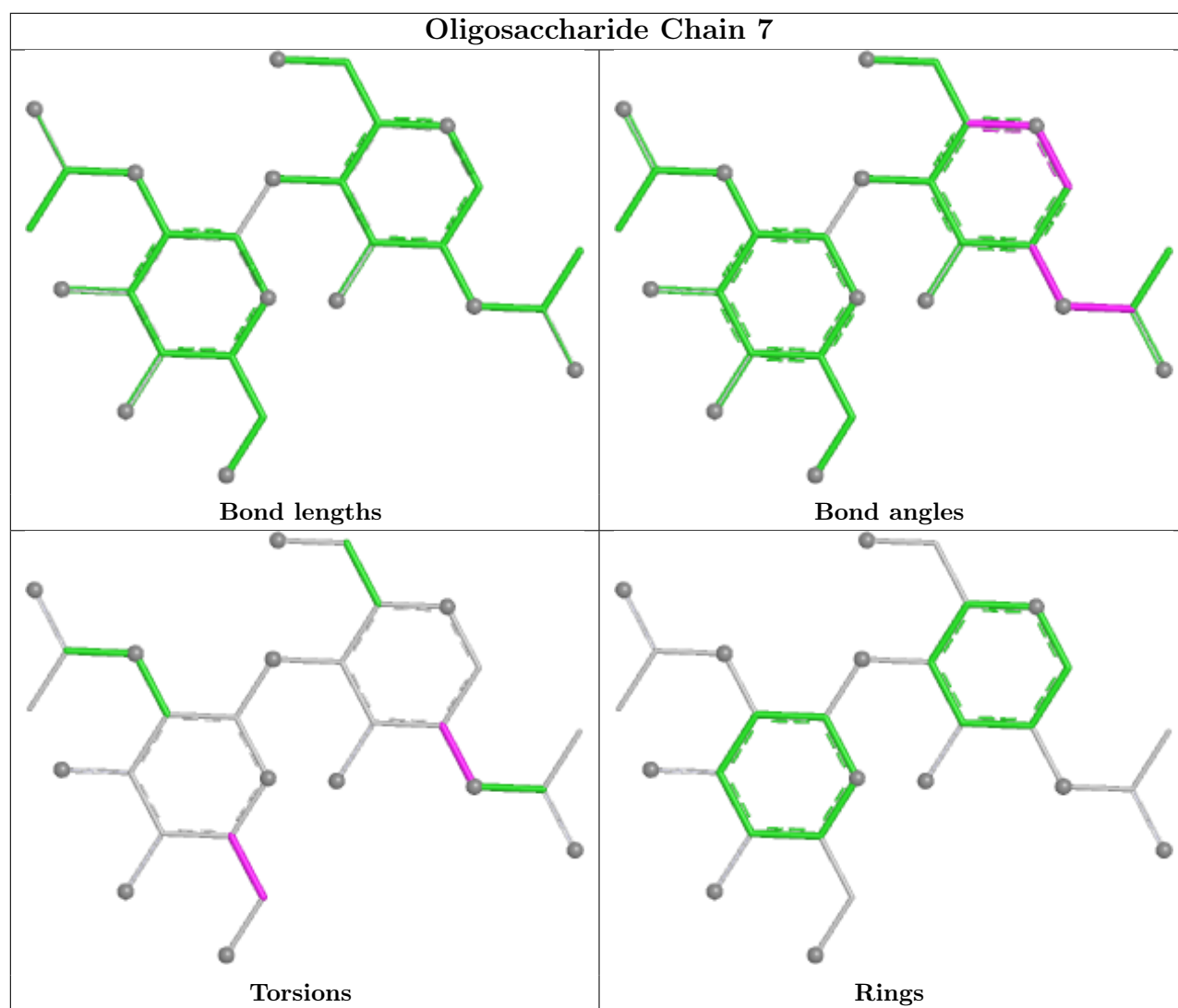


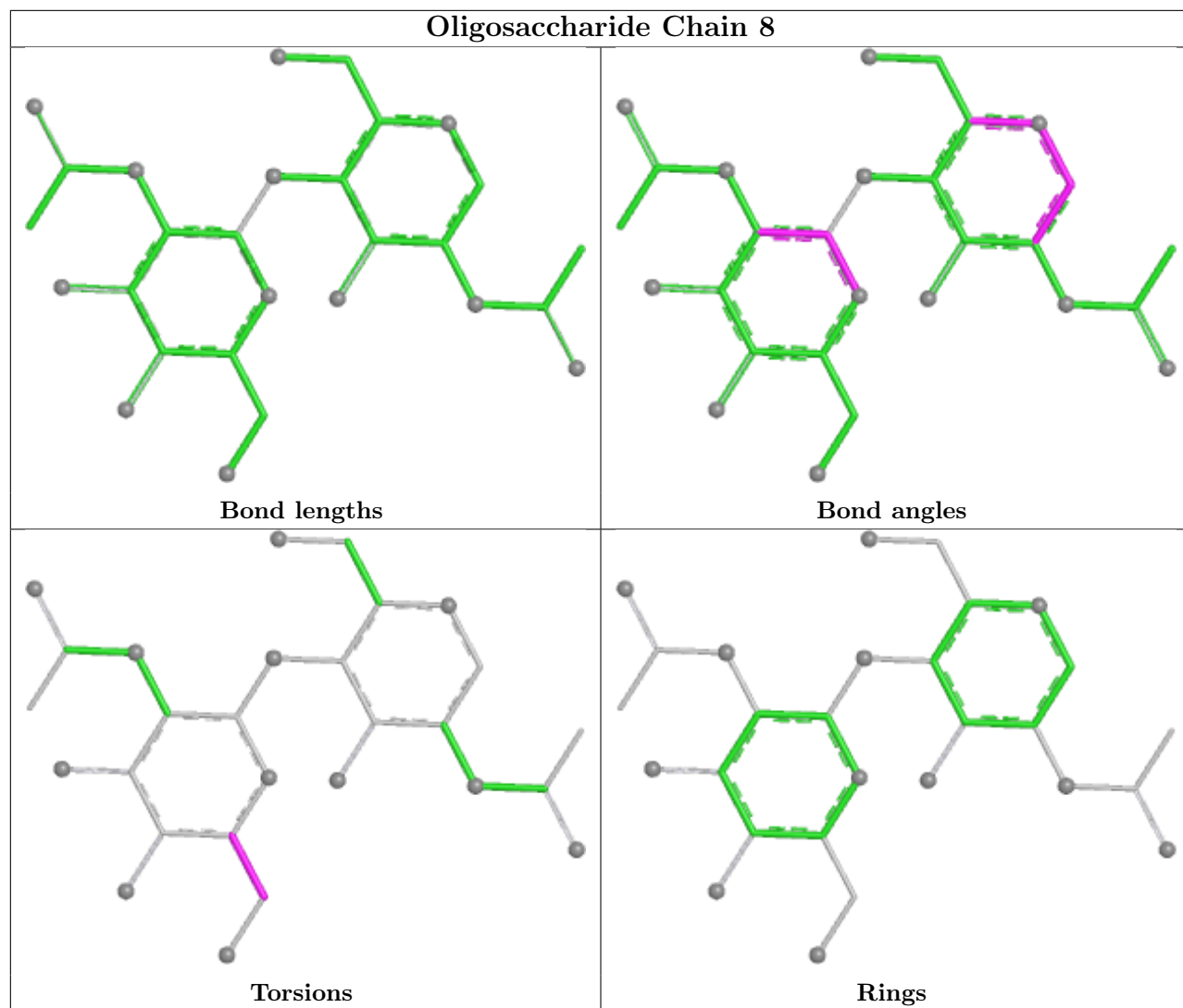




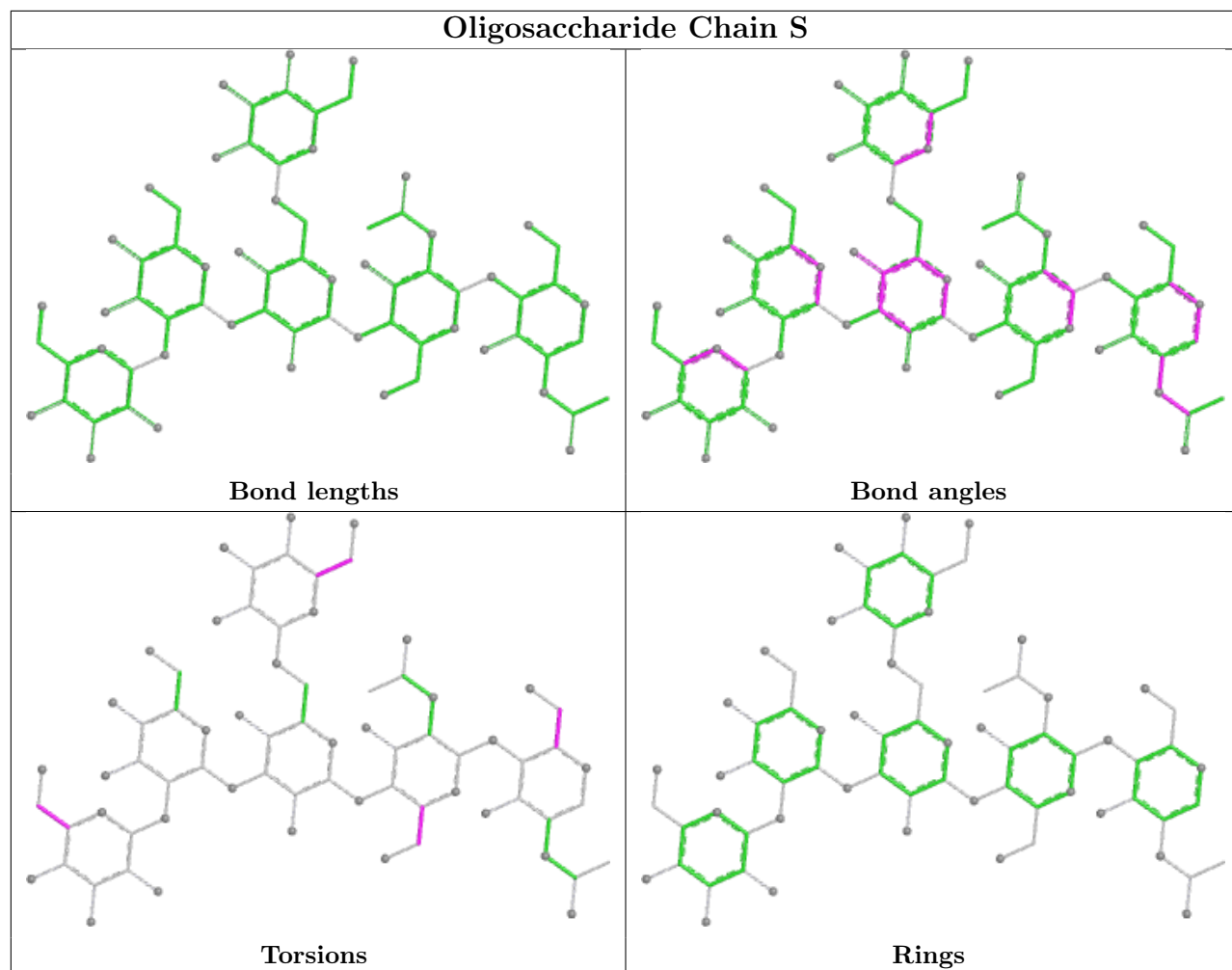


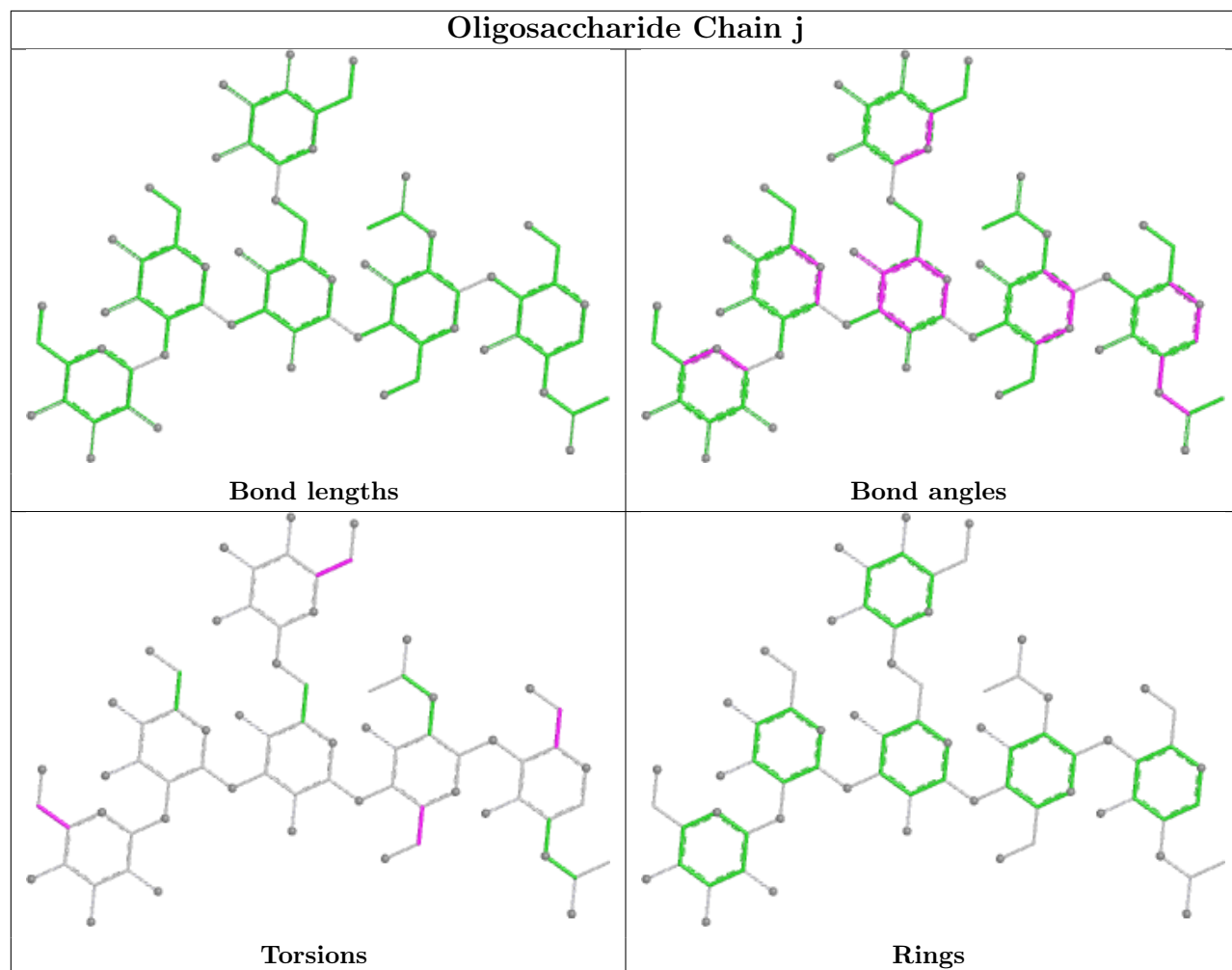


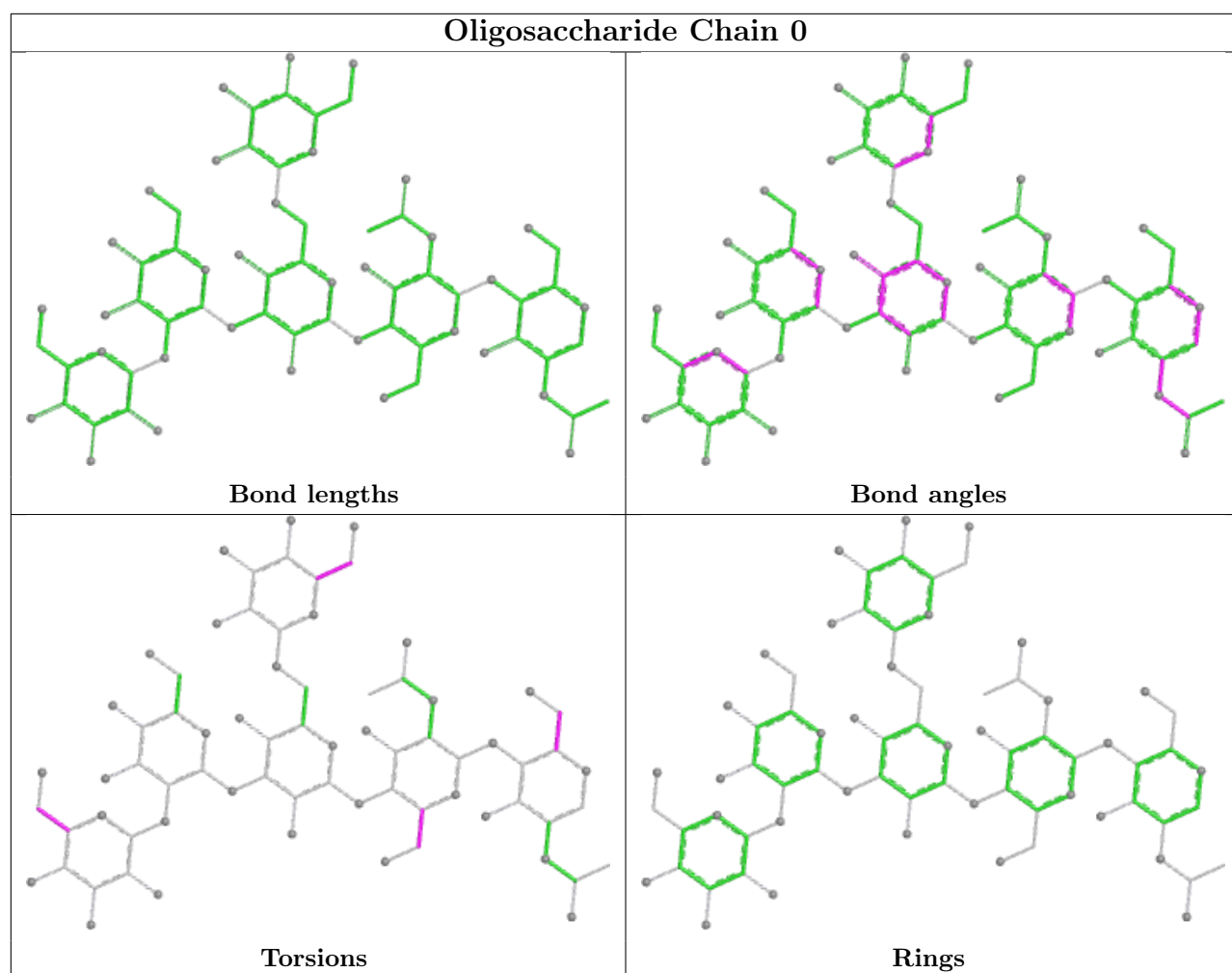


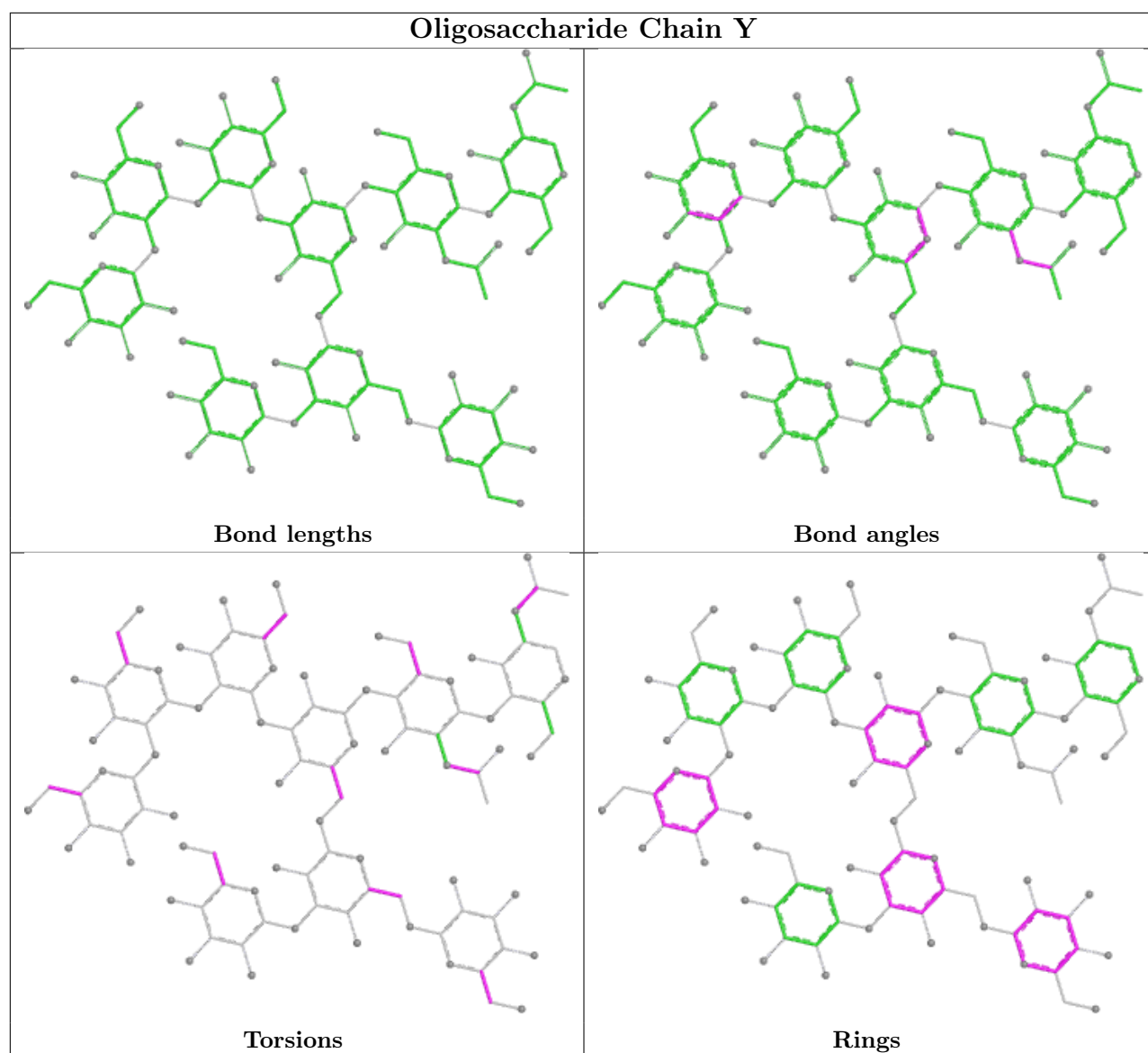


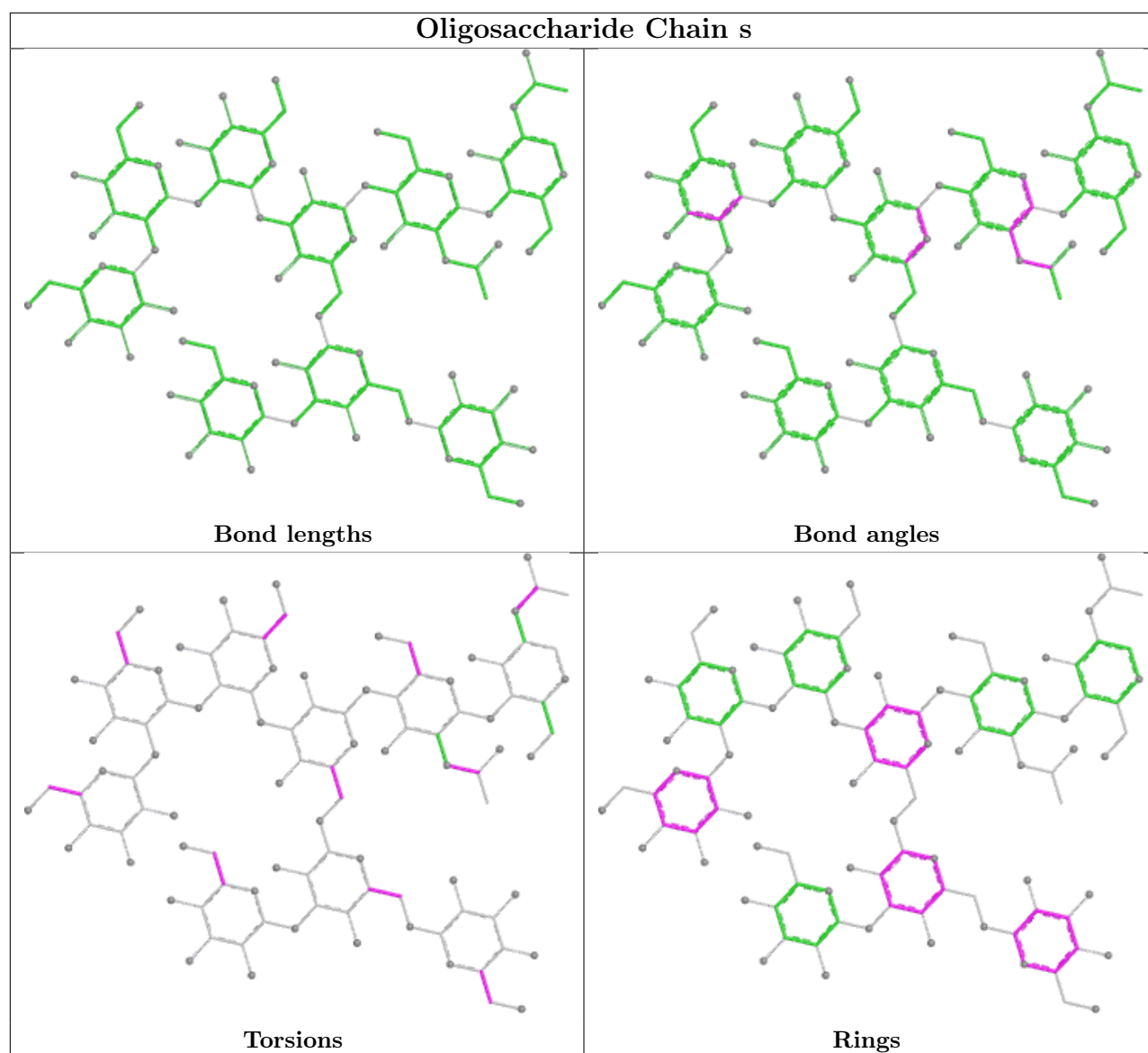


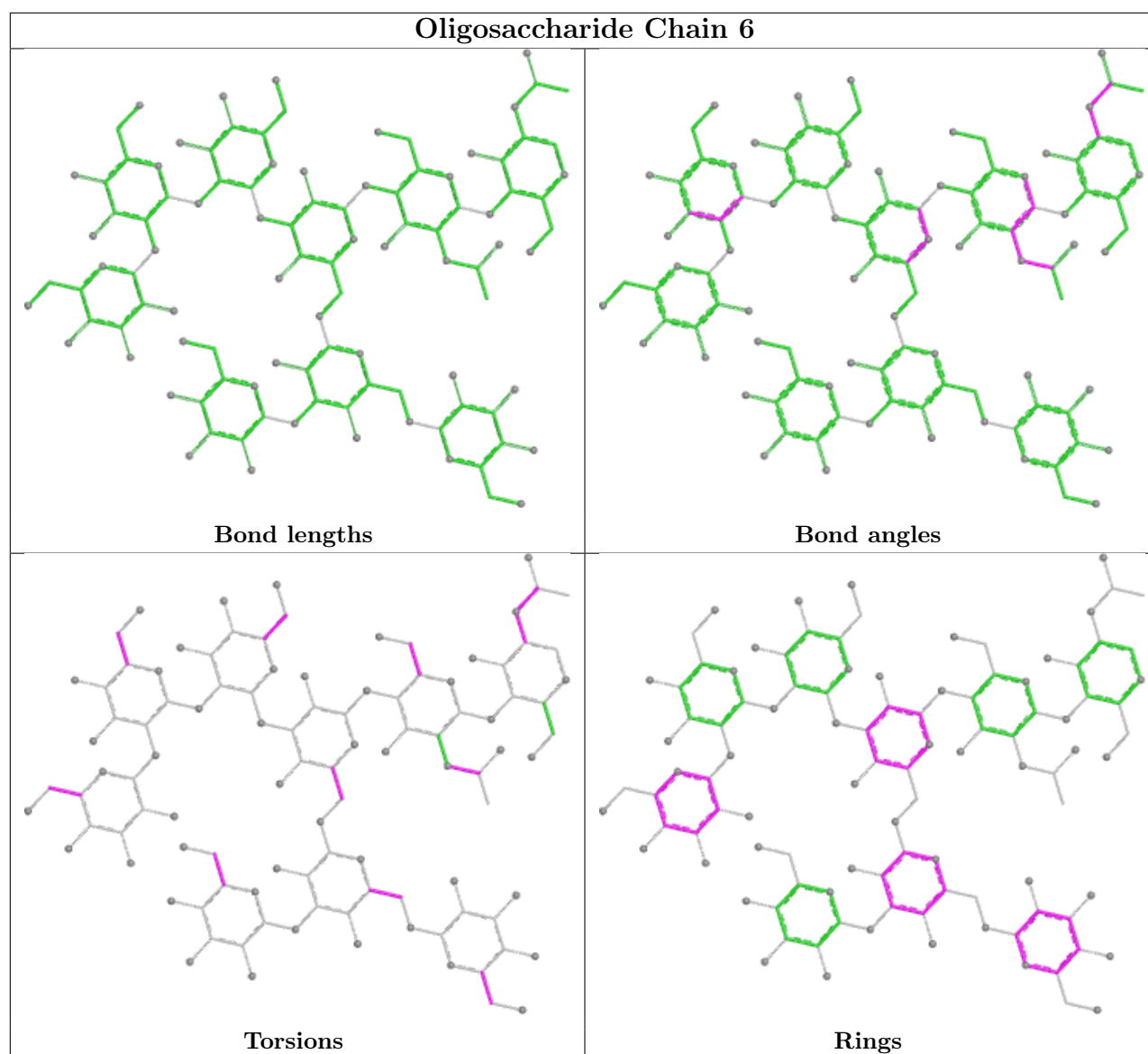












## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	NAG	I	601	2	14,14,15	0.73	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	C	702	1	14,14,15	0.69	0	17,19,21	0.87	0
12	NAG	I	602	2	14,14,15	0.69	0	17,19,21	1.98	2 (11%)
12	NAG	J	702	1	14,14,15	0.70	0	17,19,21	0.86	0
12	NAG	I	605	2	14,14,15	0.77	0	17,19,21	0.85	0
12	NAG	G	602	2	14,14,15	0.70	0	17,19,21	2.00	2 (11%)
12	NAG	G	603	2	14,14,15	0.72	0	17,19,21	0.90	0
12	NAG	G	604	2	14,14,15	0.72	0	17,19,21	0.89	0
12	NAG	J	701	1	14,14,15	0.86	1 (7%)	17,19,21	1.42	3 (17%)
12	NAG	A	603	2	14,14,15	0.74	0	17,19,21	0.90	1 (5%)
12	NAG	C	701	1	14,14,15	0.86	1 (7%)	17,19,21	1.42	3 (17%)
12	NAG	I	603	2	14,14,15	0.73	0	17,19,21	0.90	0
12	NAG	A	602	2	14,14,15	0.70	0	17,19,21	2.04	2 (11%)
12	NAG	G	605	2	14,14,15	0.77	0	17,19,21	0.84	0
12	NAG	A	605	2	14,14,15	0.77	0	17,19,21	0.86	0
12	NAG	G	601	2	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
12	NAG	B	702	1	14,14,15	0.69	0	17,19,21	0.87	0
12	NAG	I	604	2	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
12	NAG	B	701	1	14,14,15	0.87	1 (7%)	17,19,21	1.43	3 (17%)
12	NAG	A	604	2	14,14,15	0.77	0	17,19,21	1.93	3 (17%)
12	NAG	A	601	2	14,14,15	0.73	0	17,19,21	0.93	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
12	NAG	I	601	2	-	2/6/23/26	0/1/1/1
12	NAG	C	702	1	-	3/6/23/26	0/1/1/1
12	NAG	I	602	2	-	1/6/23/26	0/1/1/1
12	NAG	J	702	1	-	3/6/23/26	0/1/1/1
12	NAG	I	605	2	-	0/6/23/26	0/1/1/1
12	NAG	G	602	2	-	1/6/23/26	0/1/1/1
12	NAG	G	603	2	-	0/6/23/26	0/1/1/1
12	NAG	G	604	2	-	2/6/23/26	0/1/1/1
12	NAG	J	701	1	-	2/6/23/26	0/1/1/1
12	NAG	A	603	2	-	0/6/23/26	0/1/1/1
12	NAG	C	701	1	-	2/6/23/26	0/1/1/1
12	NAG	I	603	2	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	602	2	-	1/6/23/26	0/1/1/1
12	NAG	G	605	2	-	0/6/23/26	0/1/1/1
12	NAG	A	605	2	-	0/6/23/26	0/1/1/1
12	NAG	G	601	2	-	1/6/23/26	0/1/1/1
12	NAG	B	702	1	-	3/6/23/26	0/1/1/1
12	NAG	I	604	2	-	2/6/23/26	0/1/1/1
12	NAG	B	701	1	-	2/6/23/26	0/1/1/1
12	NAG	A	604	2	-	2/6/23/26	0/1/1/1
12	NAG	A	601	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	701	NAG	C1-C2	2.20	1.55	1.52
12	C	701	NAG	C1-C2	2.14	1.55	1.52
12	J	701	NAG	C1-C2	2.14	1.55	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	602	NAG	C1-O5-C5	6.87	121.39	112.19
12	G	602	NAG	C1-O5-C5	6.73	121.21	112.19
12	I	602	NAG	C1-O5-C5	6.64	121.08	112.19
12	A	604	NAG	C1-O5-C5	6.60	121.03	112.19
12	B	701	NAG	C2-N2-C7	3.43	127.50	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	701	NAG	C8-C7-N2-C2
12	B	701	NAG	O7-C7-N2-C2
12	G	604	NAG	C8-C7-N2-C2
12	G	604	NAG	O7-C7-N2-C2
12	C	701	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	601	NAG	1	0
12	G	601	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

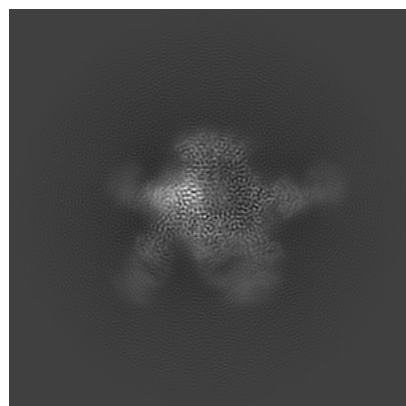
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72206. These allow visual inspection of the internal detail of the map and identification of artifacts.

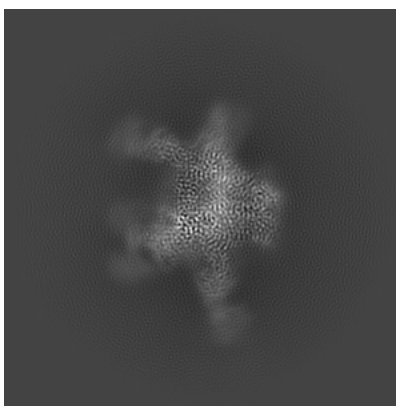
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

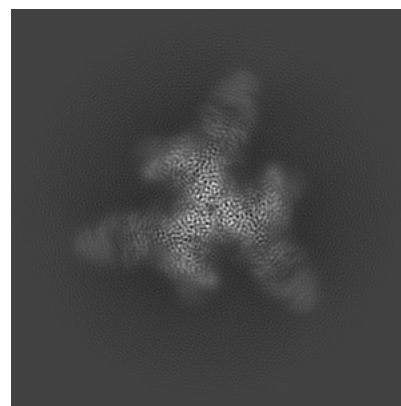
#### 6.1.1 Primary map



X

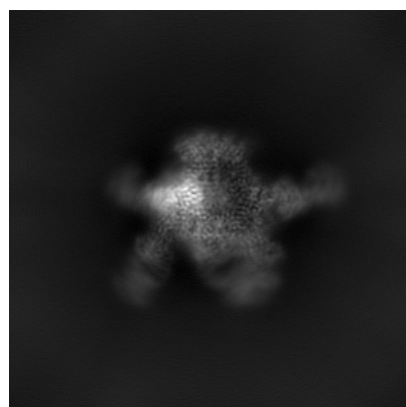


Y

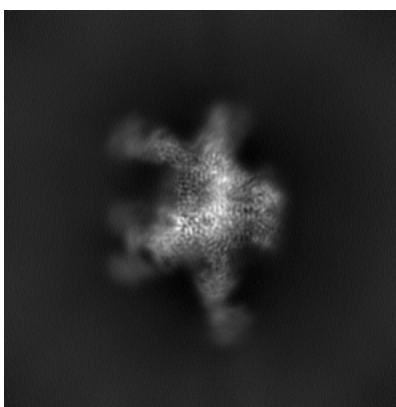


Z

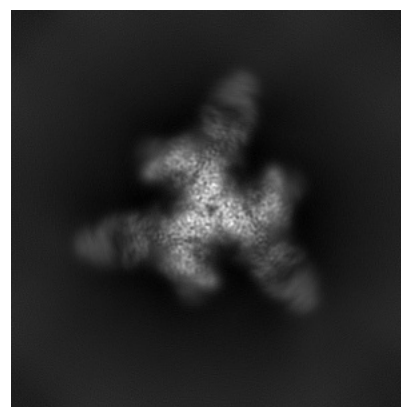
#### 6.1.2 Raw map



X



Y

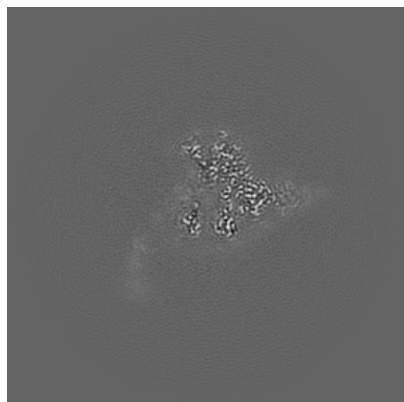


Z

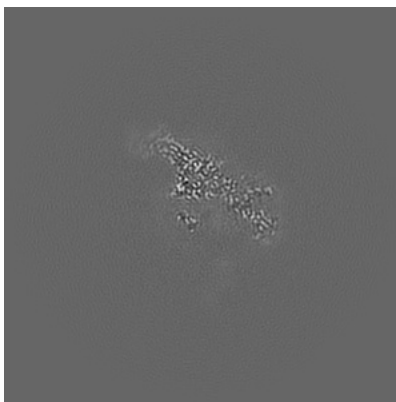
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

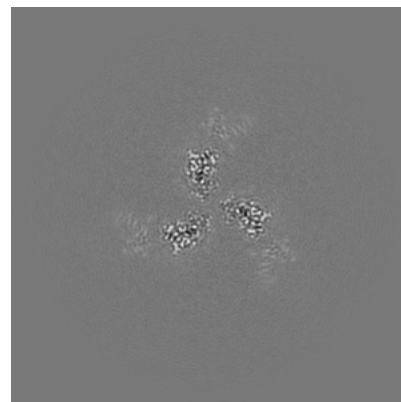
### 6.2.1 Primary map



X Index: 200

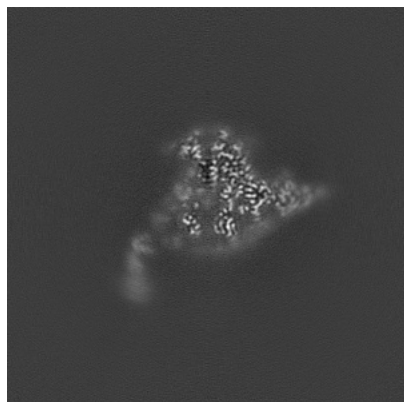


Y Index: 200

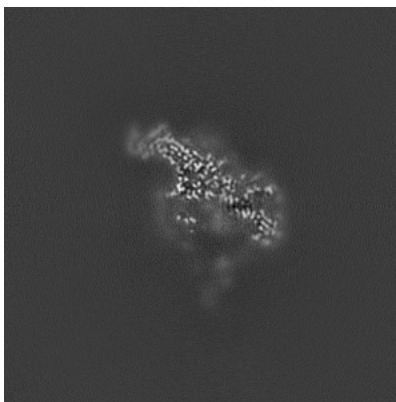


Z Index: 200

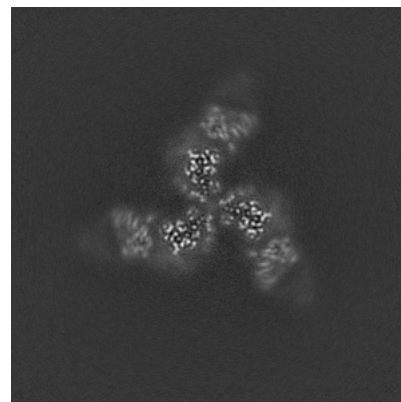
### 6.2.2 Raw map



X Index: 200



Y Index: 200

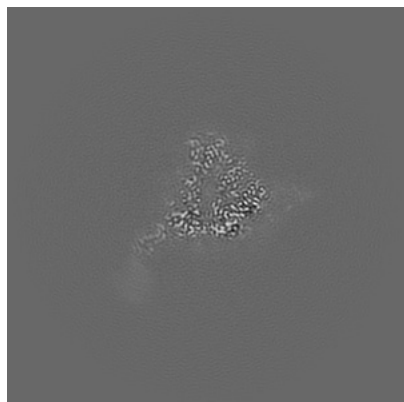


Z Index: 200

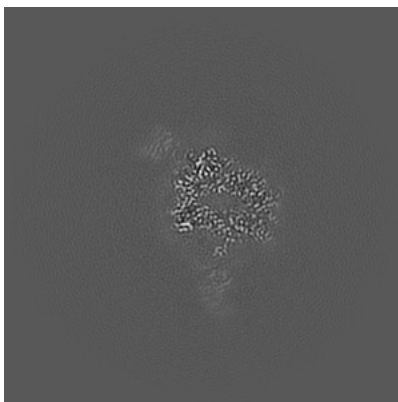
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

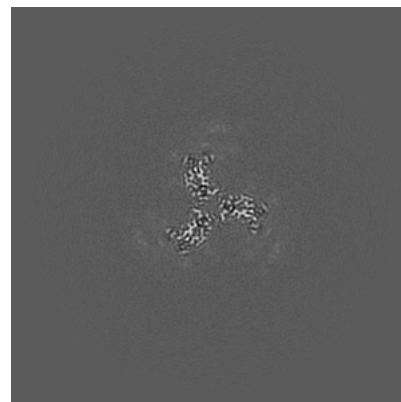
### 6.3.1 Primary map



X Index: 191

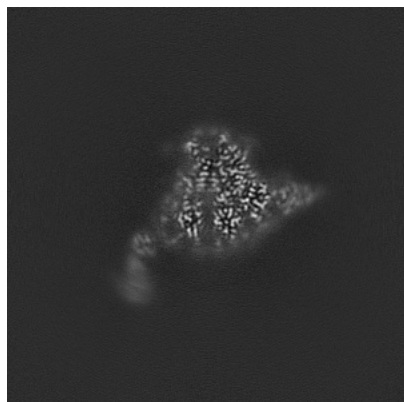


Y Index: 189

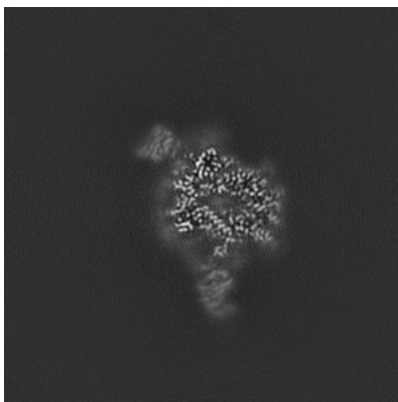


Z Index: 192

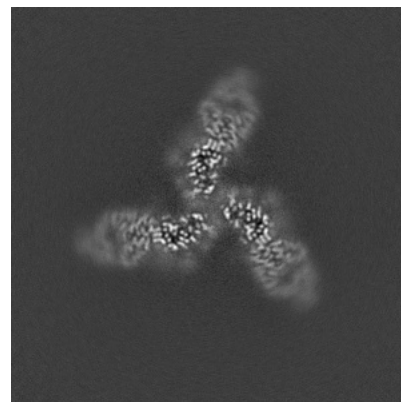
### 6.3.2 Raw map



X Index: 196



Y Index: 189

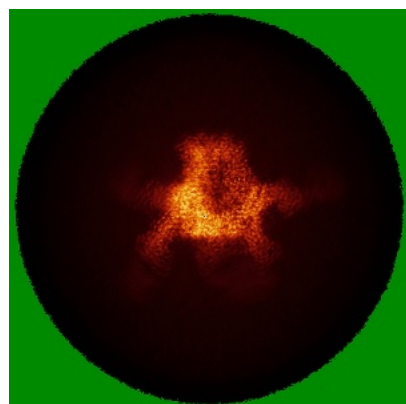


Z Index: 210

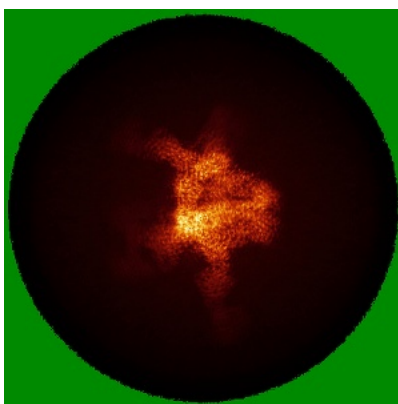
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

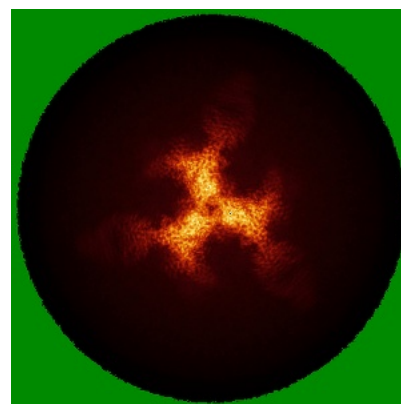
### 6.4.1 Primary map



X

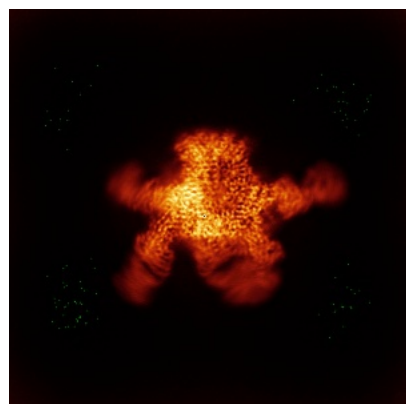


Y

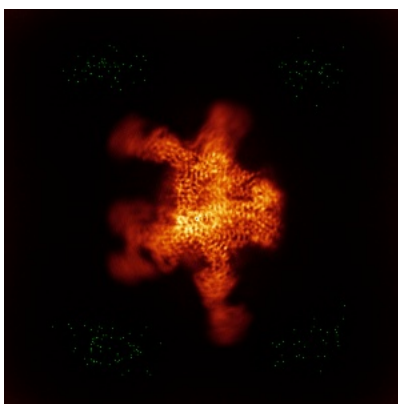


Z

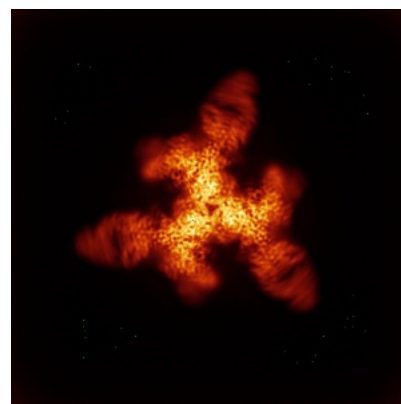
### 6.4.2 Raw map



X



Y

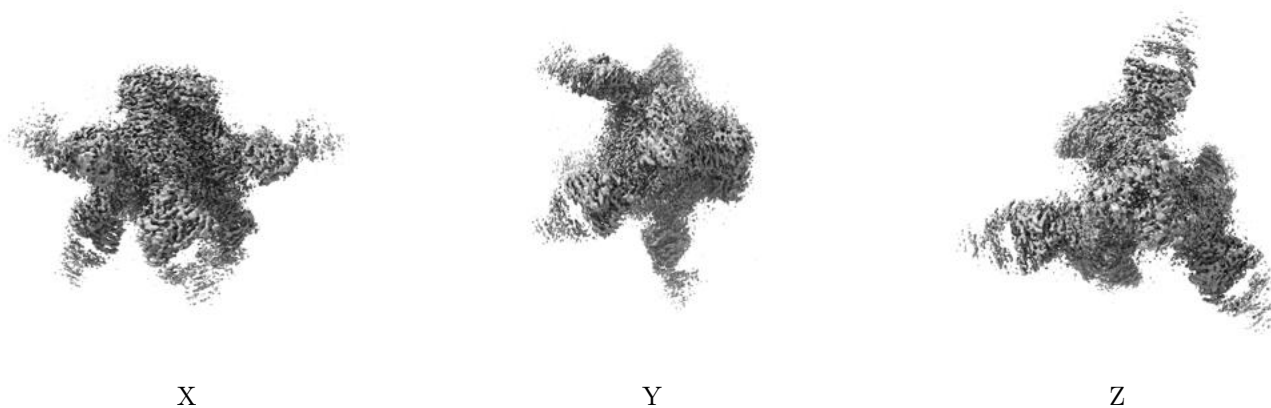


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.155. 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



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

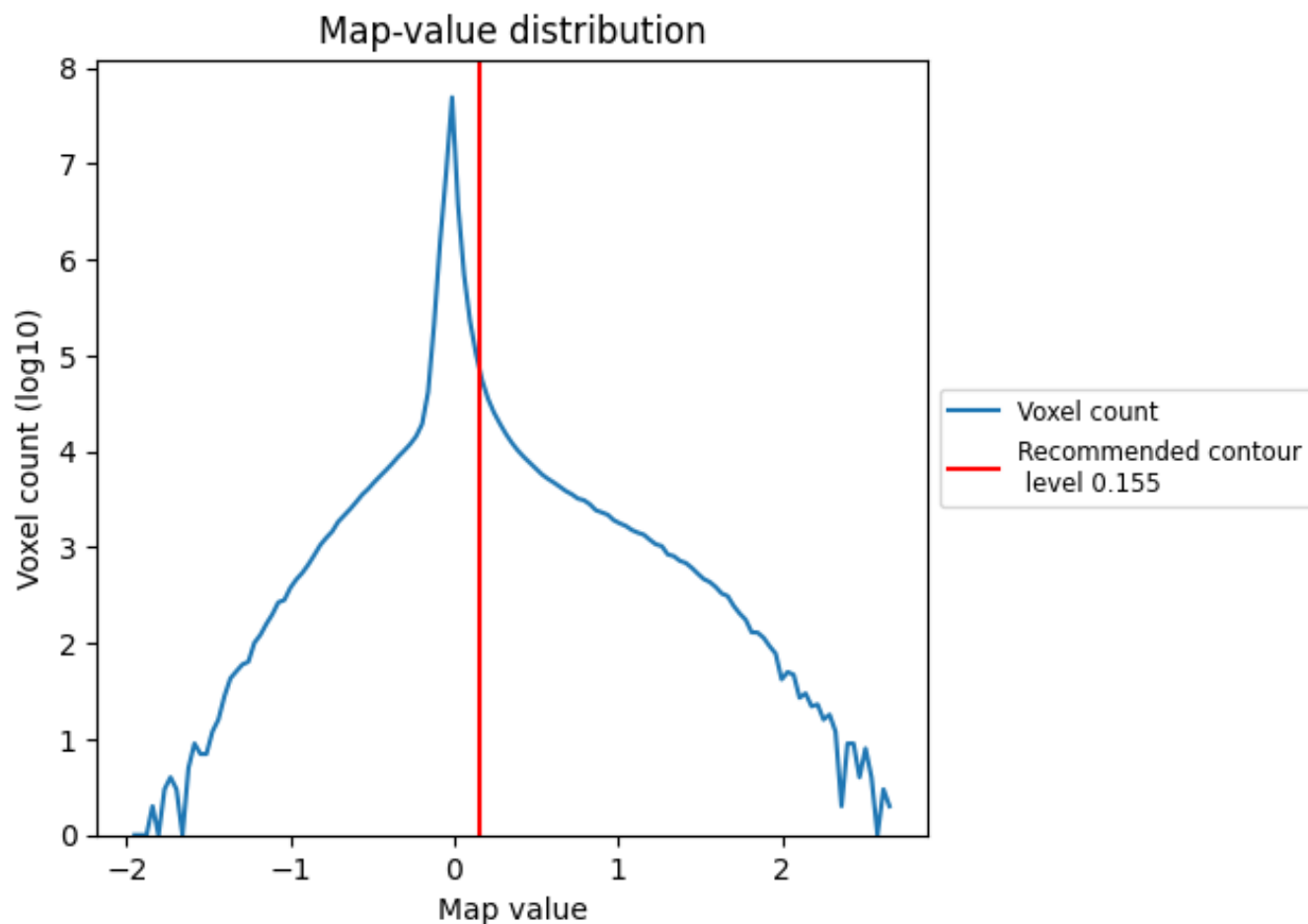
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

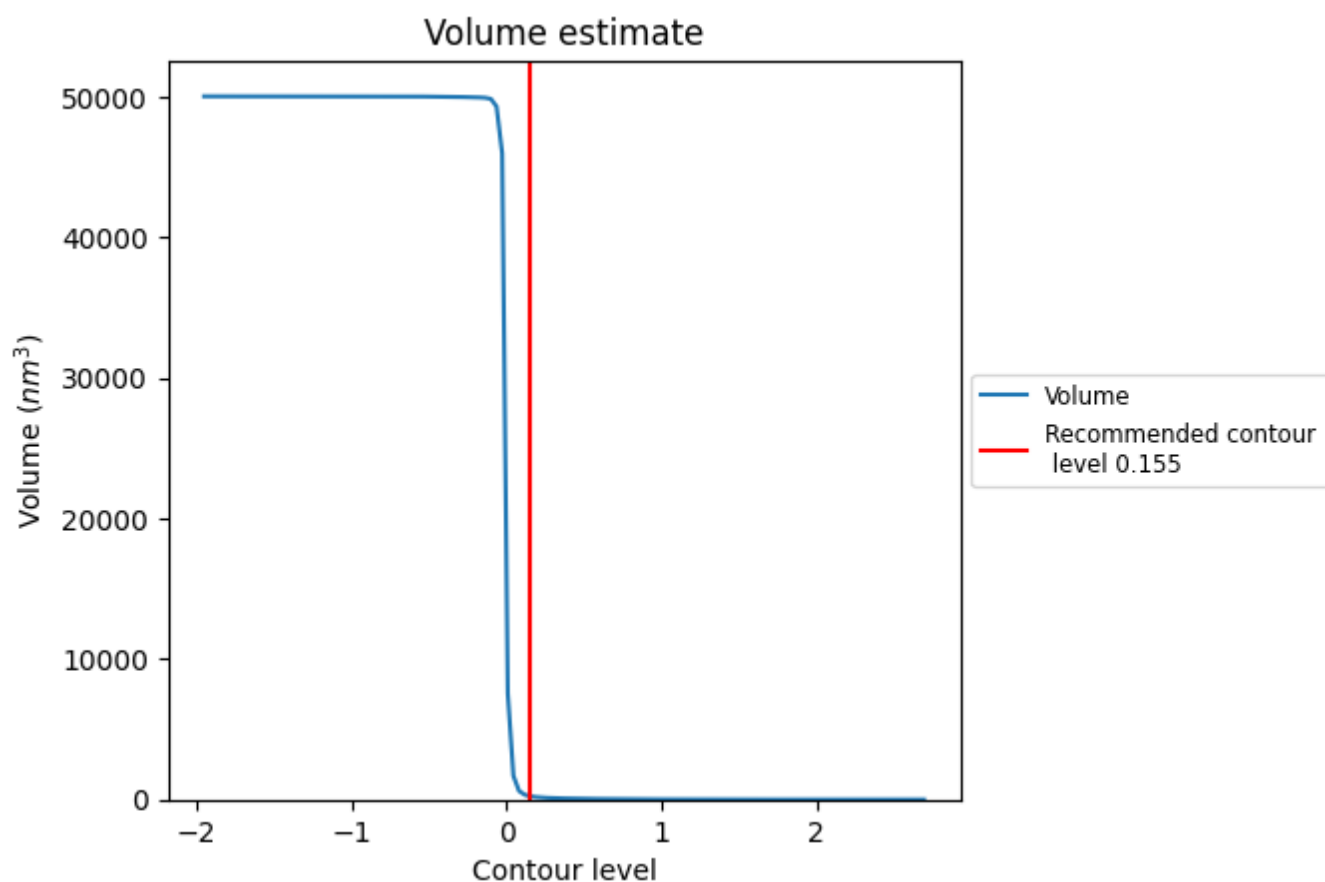
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

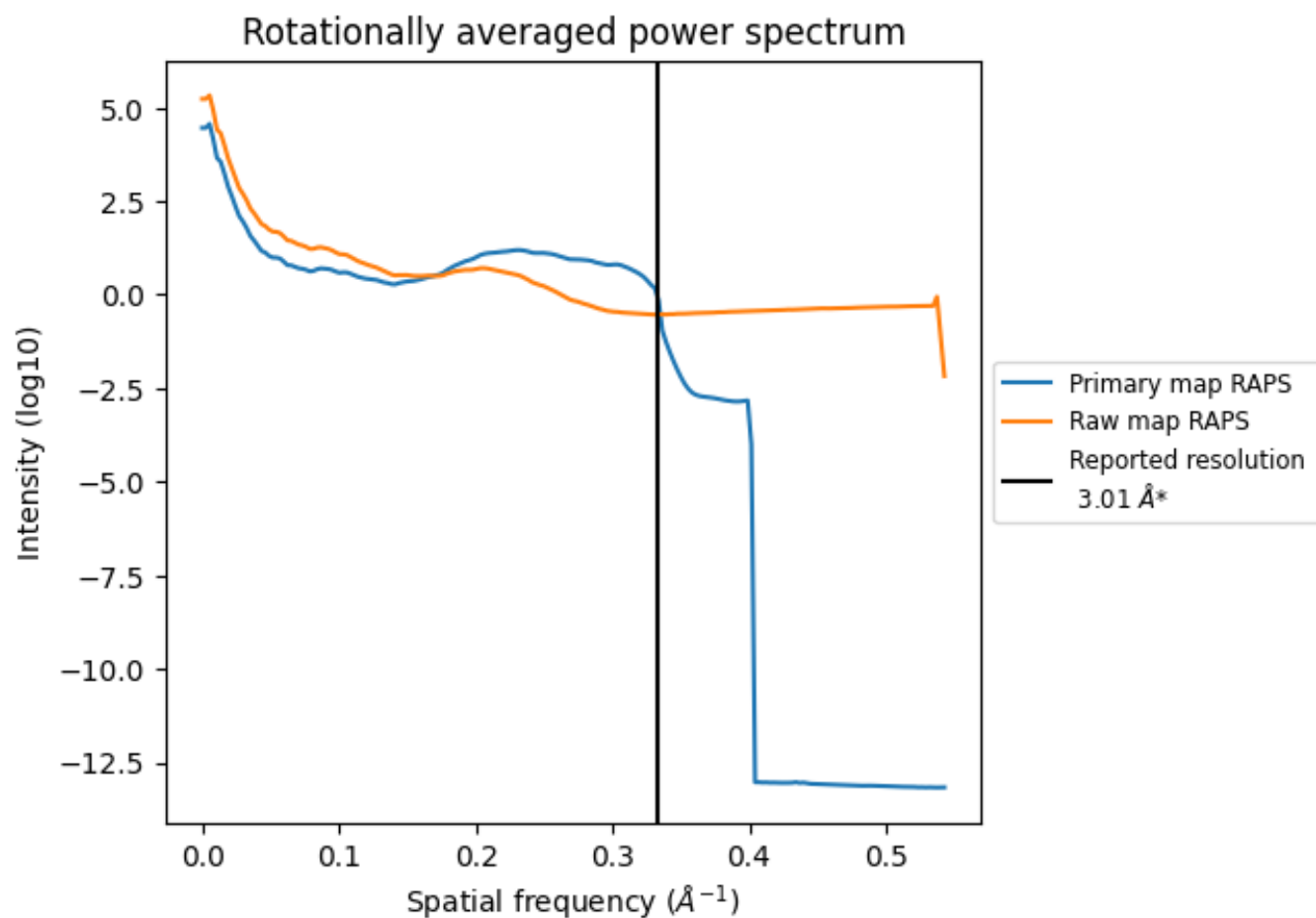


The volume at the recommended contour level is 231 nm<sup>3</sup>; this corresponds to an approximate mass of 209 kDa.

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 ⓘ

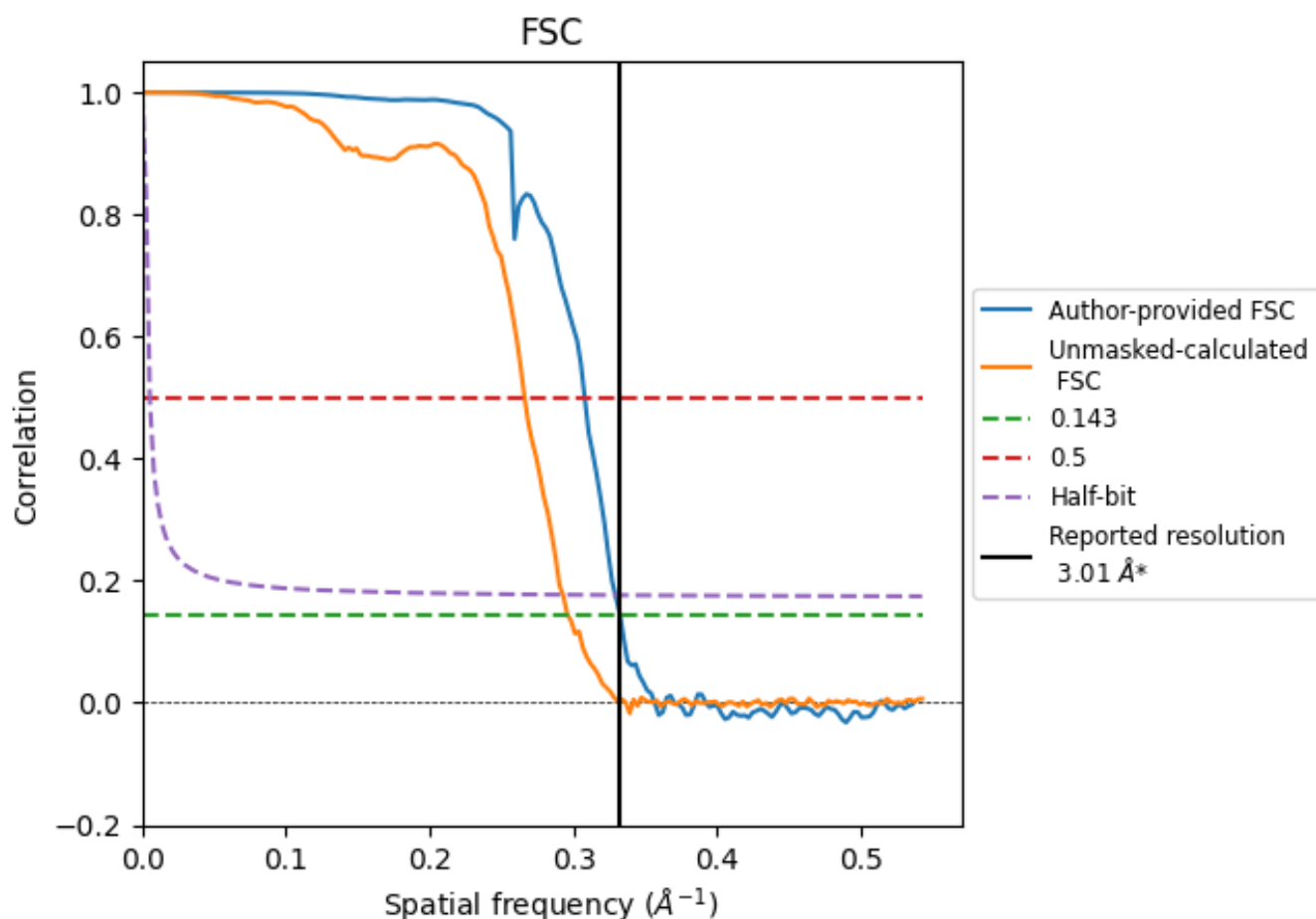


\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

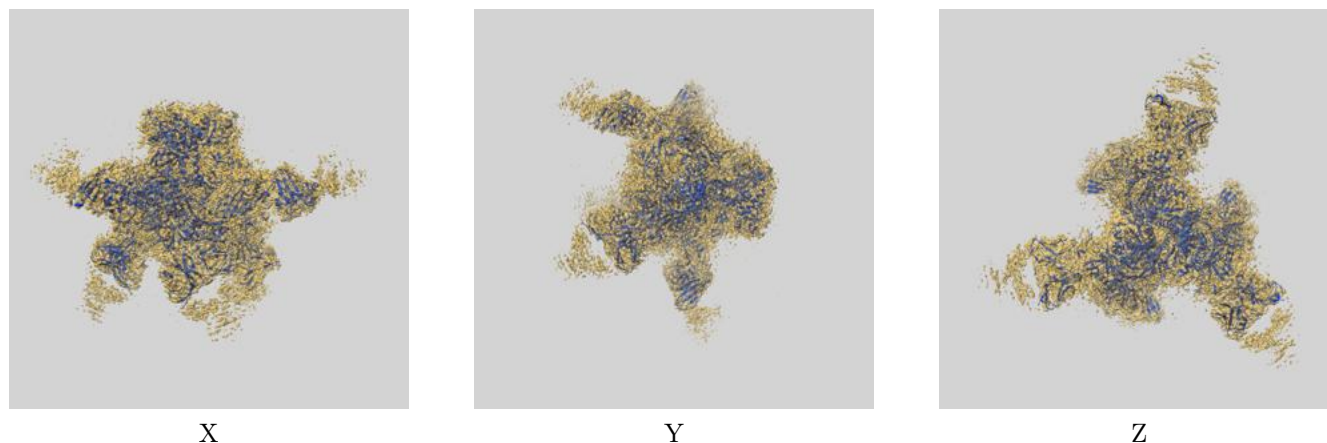
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.01	3.25	3.04
Unmasked-calculated*	3.38	3.76	3.42

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

## 9 Map-model fit [i](#)

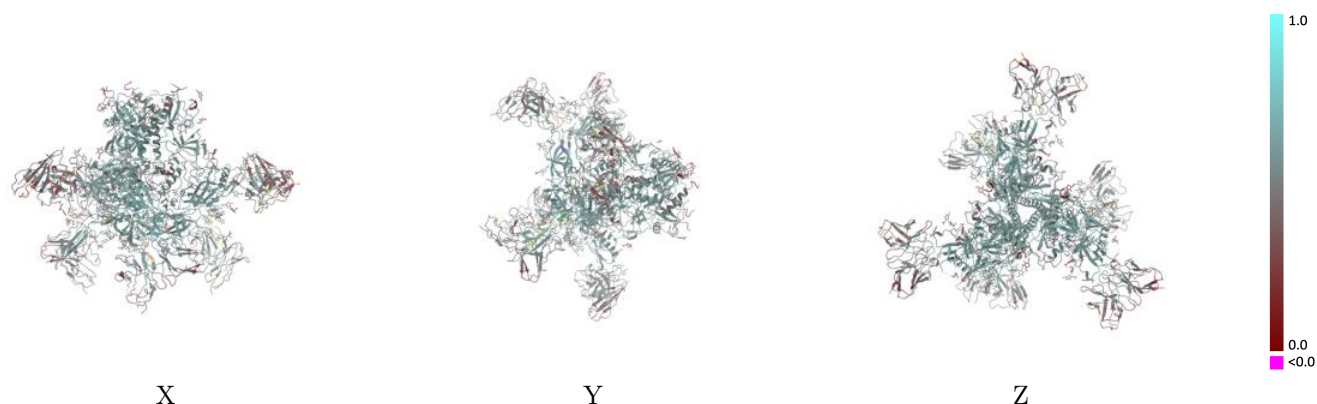
This section contains information regarding the fit between EMDB map EMD-72206 and PDB model 9Q3S. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



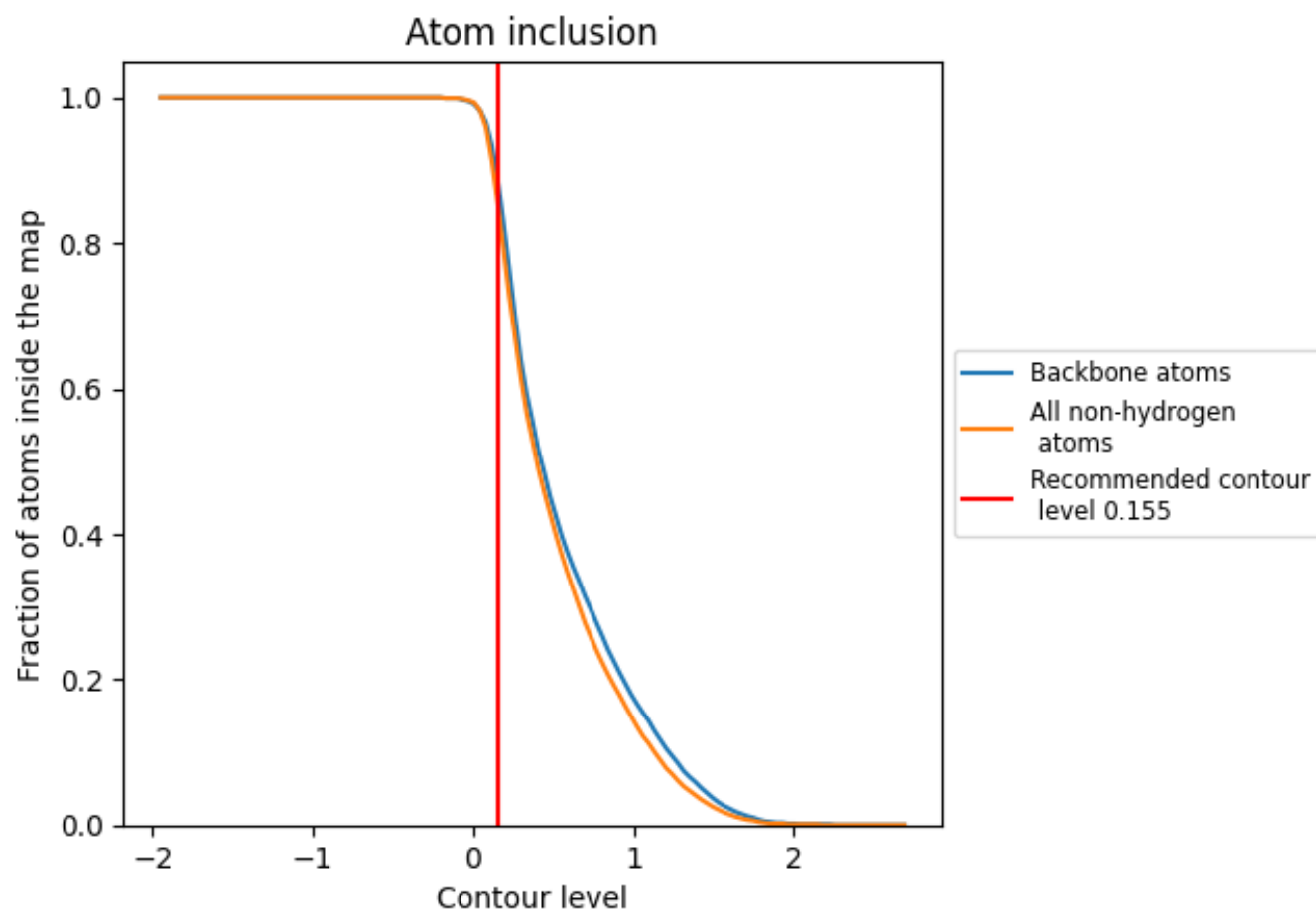
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.155).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.5270
0	 0.8190	 0.5020
1	 0.7860	 0.4640
2	 0.8210	 0.5200
3	 0.8570	 0.4870
4	 0.8930	 0.4990
5	 0.7140	 0.4710
6	 0.9140	 0.5420
7	 0.8570	 0.4730
8	 0.7860	 0.4540
A	 0.9430	 0.5820
B	 0.8810	 0.5340
C	 0.8820	 0.5320
D	 0.7340	 0.4420
E	 0.7150	 0.4430
G	 0.9430	 0.5820
H	 0.7310	 0.4410
I	 0.9450	 0.5820
J	 0.8800	 0.5320
K	 0.7160	 0.4420
L	 0.7260	 0.4470
M	 0.7250	 0.4430
N	 0.8000	 0.5110
O	 0.8970	 0.5850
P	 0.7860	 0.5480
Q	 0.7500	 0.4720
R	 0.8210	 0.5360
S	 0.8060	 0.5060
T	 0.7860	 0.4720
U	 0.8210	 0.5190
V	 0.8210	 0.4820
W	 0.9290	 0.5050
X	 0.7500	 0.4700
Y	 0.9140	 0.5410
Z	 0.8930	 0.4770



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
a	 0.7860	 0.4370
b	 0.7600	 0.5220
c	 0.8720	 0.5810
d	 0.7830	 0.4960
e	 0.8000	 0.5030
f	 0.8210	 0.5400
g	 0.8210	 0.4760
h	 0.7770	 0.4930
i	 0.8210	 0.5180
j	 0.8190	 0.4920
k	 0.7840	 0.4960
l	 0.8050	 0.5040
m	 0.7990	 0.5050
n	 0.7860	 0.4550
o	 0.8210	 0.5150
p	 0.8210	 0.4880
q	 0.9290	 0.4970
r	 0.7500	 0.4760
s	 0.9050	 0.5480
t	 0.8570	 0.4710
u	 0.7860	 0.4340
v	 0.7800	 0.5190
w	 0.8970	 0.5720
x	 0.8210	 0.5450
y	 0.7500	 0.4700
z	 0.8210	 0.5360