



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 06:31 AM EDT

PDB ID : 8G4M
EMDB ID : EMD-29725
Title : Vaccine-elicited human antibody 2C06 in complex with HIV-1 envelope trimer BG505 DS-SOSIP
Authors : Wang, S.; Morano, N.C.; Shapiro, L.; Kwong, P.D.
Deposited on : 2023-02-10
Resolution : 2.95 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

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:

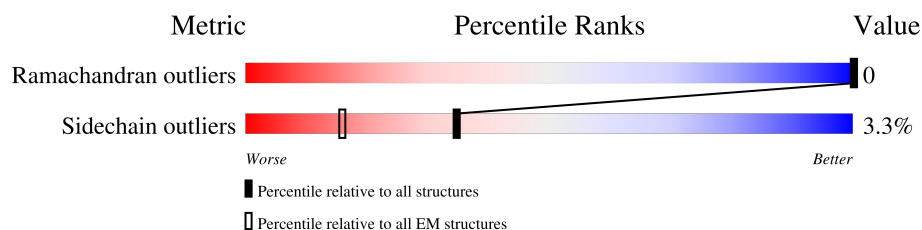
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 2.95 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.










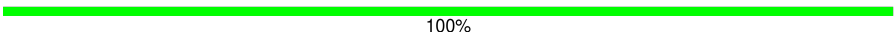
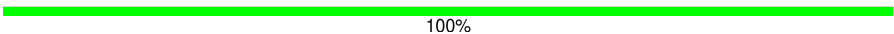
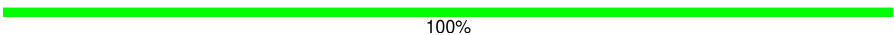



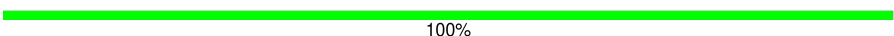

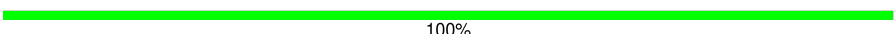

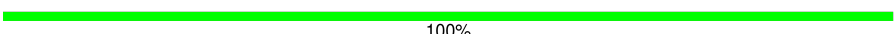
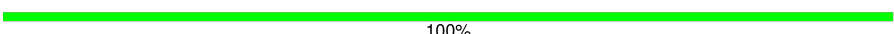
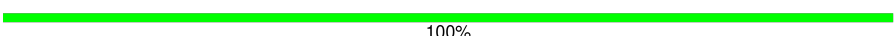

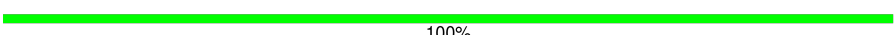
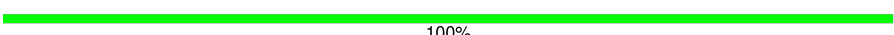
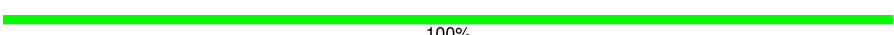
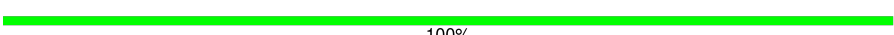
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	C	473	93% 5%
1	G	473	93% 5%
1	I	473	92% 5%
2	A	153	86% 13%
2	B	153	81% 5% 14%
2	F	153	84% 14%
3	D	236	50% 47%
3	H	236	50% 47%
3	J	236	49% 47%


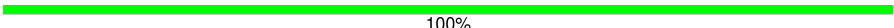
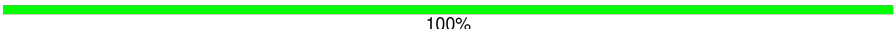
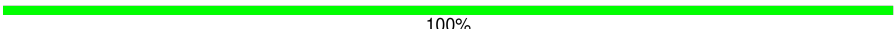
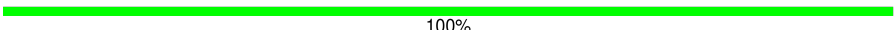
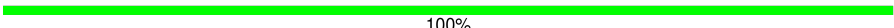

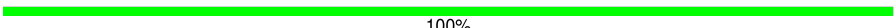

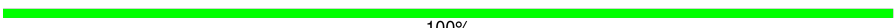
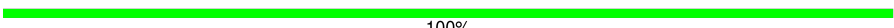
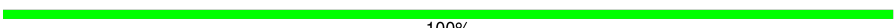
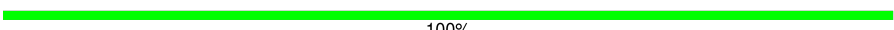
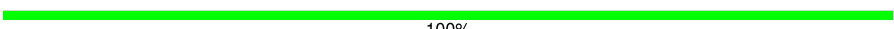
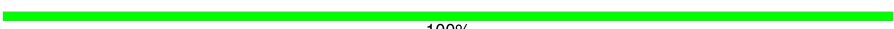
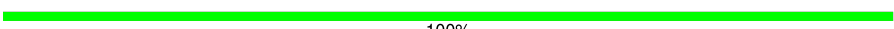

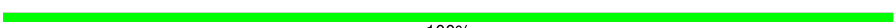



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Mol	Chain	Length	Quality of chain
4	E	214	
4	K	214	
4	L	214	
5	M	5	
5	a	5	
5	o	5	
6	0	2	
6	1	2	
6	2	2	
6	N	2	
6	P	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	b	2	
6	c	2	
6	d	2	
6	f	2	
6	g	2	

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Mol	Chain	Length	Quality of chain
6	h	2	 50%50%
6	i	2	 100%
6	j	2	 100%
6	k	2	 100%
6	l	2	 100%
6	m	2	 100%
6	n	2	 50%50%
6	p	2	 100%
6	q	2	 50%50%
6	r	2	 100%
6	s	2	 100%
6	u	2	 100%
6	v	2	 100%
6	w	2	 100%
6	x	2	 100%
6	y	2	 100%
6	z	2	 50%50%
7	O	3	 100%
8	Q	6	 50%50%
8	t	6	 50%50%
9	e	5	 60%40%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20584 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
1	C	448	Total	C	N	O	S	0	0
			3521	2207	625	659	30		
1	G	448	Total	C	N	O	S	0	0
			3521	2207	625	659	30		
1	I	448	Total	C	N	O	S	0	0
			3521	2207	625	659	30		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	CYS	ILE	engineered mutation	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	433	CYS	ALA	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	201	CYS	ILE	engineered mutation	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	433	CYS	ALA	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	133	Total	C	N	O	S	0	0
			1042	660	179	197	6		
2	B	131	Total	C	N	O	S	0	0
			1030	652	177	195	6		
2	F	131	Total	C	N	O	S	0	0
			1030	652	177	195	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	CYS	THR	engineered mutation	UNP Q2N0S7
B	605	CYS	THR	engineered mutation	UNP Q2N0S7
F	605	CYS	THR	engineered mutation	UNP Q2N0S7

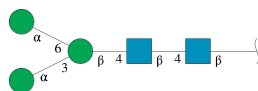
- Molecule 3 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	124	Total	C	N	O	S	0	0
			952	596	161	189	6		
3	H	124	Total	C	N	O	S	0	0
			952	596	161	189	6		
3	J	124	Total	C	N	O	S	0	0
			952	596	161	189	6		

- Molecule 4 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	107	Total	C	N	O	S	0	0
			820	518	140	159	3		
4	L	107	Total	C	N	O	S	0	0
			820	518	140	159	3		
4	K	107	Total	C	N	O	S	0	0
			820	518	140	159	3		

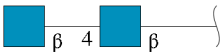
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	5	Total	C	N	O	0	0
			61	34	2	25		
5	a	5	Total	C	N	O	0	0
			61	34	2	25		
5	o	5	Total	C	N	O	0	0
			61	34	2	25		

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

cetamido-2-deoxy-beta-D-glucopyranose.



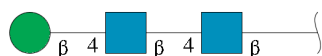
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	d	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		
6	i	2	Total	C	N	O	0	0
			28	16	2	10		
6	j	2	Total	C	N	O	0	0
			28	16	2	10		

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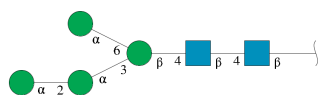
Mol	Chain	Residues	Atoms				AltConf	Trace
6	k	2	Total	C	N	O	0	0
			28	16	2	10		
6	l	2	Total	C	N	O	0	0
			28	16	2	10		
6	m	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	p	2	Total	C	N	O	0	0
			28	16	2	10		
6	q	2	Total	C	N	O	0	0
			28	16	2	10		
6	r	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	u	2	Total	C	N	O	0	0
			28	16	2	10		
6	v	2	Total	C	N	O	0	0
			28	16	2	10		
6	w	2	Total	C	N	O	0	0
			28	16	2	10		
6	x	2	Total	C	N	O	0	0
			28	16	2	10		
6	y	2	Total	C	N	O	0	0
			28	16	2	10		
6	z	2	Total	C	N	O	0	0
			28	16	2	10		
6	0	2	Total	C	N	O	0	0
			28	16	2	10		
6	1	2	Total	C	N	O	0	0
			28	16	2	10		
6	2	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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.



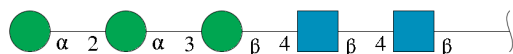
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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.



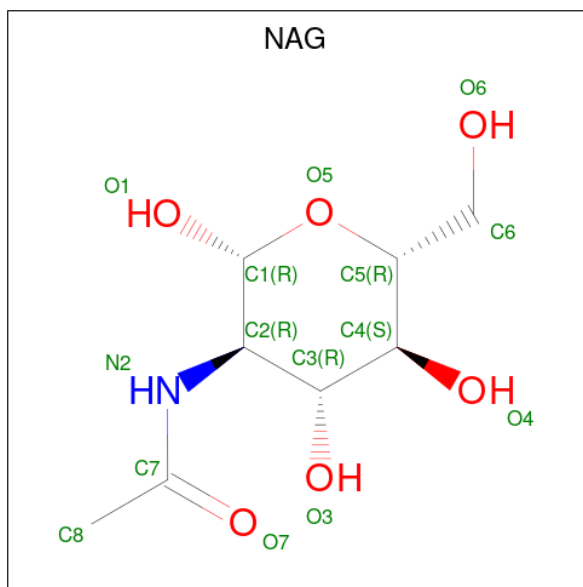
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	6	Total	C	N	O	0	0
			72	40	2	30		
8	t	6	Total	C	N	O	0	0
			72	40	2	30		

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



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



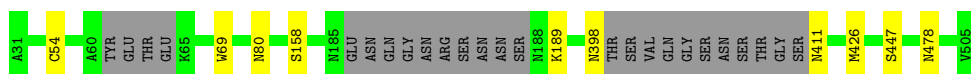
Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14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

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.

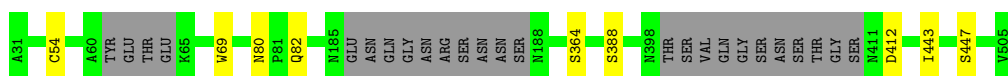
- Molecule 1: Envelope glycoprotein gp120

Chain C: 




- Molecule 1: Envelope glycoprotein gp120

Chain G: 




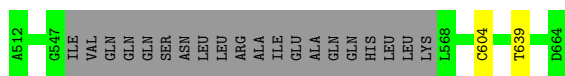
- Molecule 1: Envelope glycoprotein gp120

Chain I: 




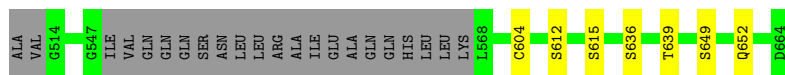
- Molecule 2: Envelope glycoprotein gp41

Chain A: 



- Molecule 2: Envelope glycoprotein gp41

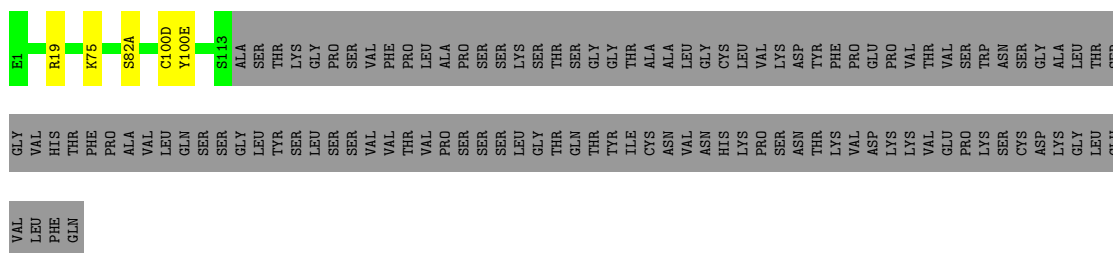
Chain B: 



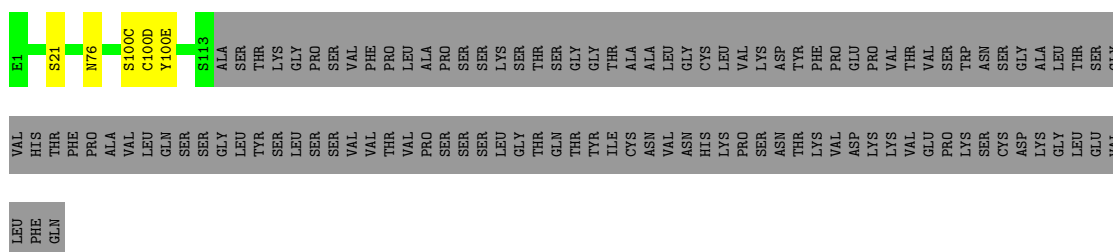
- Molecule 2: Envelope glycoprotein gp41

ALA VAL GS14 GS47 TLE VAL GLN GLN GLN SER ASN LEU LEU ARG ALA TLE GLU ALA GLN GLN HIS LEU LEU LYS L668 C604 E654 L663 D664

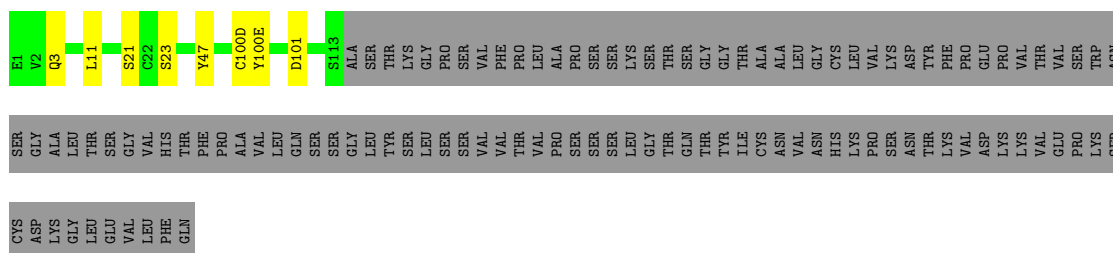
Chain D:  50% . 47%



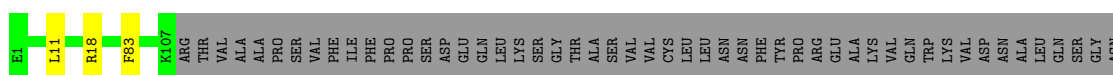
Chain H:  50% 47%



Chain J: 49% 1% 47%



Chain E: 49% 50%



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

- Molecule 4: antibody light chain

Chain L:  48% 50%

E1 E17 R18 S22 E81 D82 F83 K107 ARG THR VAL ALA PRO SER SER VAL PHE PHE ILE PHE PRO SER ASP ASP GLN LYS THR SER GLY THR ALA ALA SER VAL VAL CYS LEU ASN LEU ASN PHE THR PRO ARG GLU LYS VAL VAL GLN TRP LYS ASP ASN ALA LEU GLN

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

- Molecule 4: antibody light chain

Chain K:  49% 50%

E1 S65 F83 K107 ARG THR VAL ALA PRO SER SER VAL PHE ILE PHE PRO SER SER LEU SER PHE THR THR LEU THR LEU SER SER LYS THR ALA ASP TYR GLU LYS HIS VAL TYR VAL ALA CYS THR VAL HIS GLN GLY LEU SER SER PRO VAL THR LYS PHE SER ASN ARG GLY CYS

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

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

Chain M:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: 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 a:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain o:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain N:  100%



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

Chain P:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  50% 50%



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

Chain X:  100%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain b:  50% 50%



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

Chain c:  100%



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

Chain d:  100%



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

Chain f:  100%



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

Chain g:  100%



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

Chain h:  50% 50%



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

Chain i:  100%



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

Chain j:  100%



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

Chain k:  100%



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

Chain l:  100%

MAG1
MAG2

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

Chain m:  100%

MAG1
MAG2

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

Chain n:  50% 50%

MAG1
MAG2

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

Chain p:  100%

MAG1
MAG2

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

Chain q:  50% 50%

MAG1
MAG2

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

Chain r:  100%

MAG1
MAG2

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

Chain s:  100%

WAG1
WAG2

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

Chain u:  100%

WAG1
WAG2

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

Chain v:  100%

WAG1
WAG2

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

Chain w:  100%

WAG1
WAG2

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

Chain x:  100%

WAG1
WAG2

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

Chain y:  100%

WAG1
WAG2

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

Chain z:  50% 50%

WAG1
WAG2

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

Chain 0:  100%

MAG1
MAG2

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

Chain 1:  100%

MAG1
MAG2

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

Chain 2:  100%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2
BMA3

- Molecule 8: 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 Q:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 8: 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 t:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: alpha-D-mannopyranose-(1-2)-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

nose



MAG1	MAG2	MAN4	MAN5
MAG3			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	645442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.06	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.220	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	0.26	0/3593	0.49	0/4876
1	G	0.26	0/3593	0.49	0/4876
1	I	0.26	0/3593	0.49	0/4876
2	A	0.24	0/1060	0.44	0/1438
2	B	0.25	0/1048	0.45	0/1421
2	F	0.24	0/1048	0.45	0/1421
3	D	0.29	0/973	0.53	0/1318
3	H	0.28	0/973	0.52	0/1318
3	J	0.29	0/973	0.52	0/1318
4	E	0.27	0/840	0.50	0/1140
4	K	0.27	0/840	0.51	0/1140
4	L	0.28	0/840	0.53	0/1140
All	All	0.26	0/19374	0.49	0/26282

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](#)

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	C	440/473 (93%)	430 (98%)	10 (2%)	0	100	100
1	G	440/473 (93%)	429 (98%)	11 (2%)	0	100	100
1	I	440/473 (93%)	429 (98%)	11 (2%)	0	100	100
2	A	129/153 (84%)	128 (99%)	1 (1%)	0	100	100
2	B	127/153 (83%)	126 (99%)	1 (1%)	0	100	100
2	F	127/153 (83%)	126 (99%)	1 (1%)	0	100	100
3	D	122/236 (52%)	117 (96%)	5 (4%)	0	100	100
3	H	122/236 (52%)	119 (98%)	3 (2%)	0	100	100
3	J	122/236 (52%)	119 (98%)	3 (2%)	0	100	100
4	E	105/214 (49%)	103 (98%)	2 (2%)	0	100	100
4	K	105/214 (49%)	102 (97%)	3 (3%)	0	100	100
4	L	105/214 (49%)	103 (98%)	2 (2%)	0	100	100
All	All	2384/3228 (74%)	2331 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	400/422 (95%)	390 (98%)	10 (2%)	42	66
1	G	400/422 (95%)	391 (98%)	9 (2%)	45	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	400/422 (95%)	388 (97%)	12 (3%)	36	60
2	A	111/129 (86%)	109 (98%)	2 (2%)	54	75
2	B	110/129 (85%)	103 (94%)	7 (6%)	14	34
2	F	110/129 (85%)	108 (98%)	2 (2%)	54	75
3	D	102/199 (51%)	97 (95%)	5 (5%)	21	45
3	H	102/199 (51%)	97 (95%)	5 (5%)	21	45
3	J	102/199 (51%)	94 (92%)	8 (8%)	10	26
4	E	88/184 (48%)	85 (97%)	3 (3%)	32	57
4	K	88/184 (48%)	86 (98%)	2 (2%)	45	69
4	L	88/184 (48%)	83 (94%)	5 (6%)	17	39
All	All	2101/2802 (75%)	2031 (97%)	70 (3%)	35	58

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	22	SER
4	L	83	PHE
3	J	100(D)	CYS
2	B	636	SER
2	B	615	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	658	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 ⓘ

107 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	$\# Z > 2$
6	NAG	0	1	6,1	14,14,15	0.19	0	17,19,21	0.51	0
6	NAG	0	2	6	14,14,15	0.23	0	17,19,21	0.50	0
6	NAG	1	1	6,1	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	1	2	6	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	2	1	6,1	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	2	2	6	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	M	1	5,1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.50	0
5	BMA	M	3	5	11,11,12	0.44	0	15,15,17	0.71	0
5	MAN	M	4	5	11,11,12	0.55	0	15,15,17	0.95	2 (13%)
5	MAN	M	5	5	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.43	0	17,19,21	0.49	0
6	NAG	N	2	6	14,14,15	0.34	0	17,19,21	0.50	0
7	NAG	O	1	7,1	14,14,15	0.27	0	17,19,21	0.42	0
7	NAG	O	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	BMA	O	3	7	11,11,12	0.51	0	15,15,17	0.68	0
6	NAG	P	1	6,1	14,14,15	0.27	0	17,19,21	0.51	0
6	NAG	P	2	6	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	Q	1	8,1	14,14,15	0.24	0	17,19,21	0.49	0
8	NAG	Q	2	8	14,14,15	0.18	0	17,19,21	0.41	0
8	BMA	Q	3	8	11,11,12	0.54	0	15,15,17	0.77	0
8	MAN	Q	4	8	11,11,12	0.56	0	15,15,17	0.96	2 (13%)
8	MAN	Q	5	8	11,11,12	0.61	0	15,15,17	0.89	2 (13%)
8	MAN	Q	6	8	11,11,12	0.66	0	15,15,17	0.85	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	R	2	6	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	S	1	6,1	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	S	2	6	14,14,15	0.19	0	17,19,21	0.44	0
6	NAG	T	1	6,1	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	T	2	6	14,14,15	0.23	0	17,19,21	0.52	0
6	NAG	U	1	6,1	14,14,15	0.22	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	U	2	6	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	V	1	6,1	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	V	2	6	14,14,15	0.18	0	17,19,21	0.44	0
6	NAG	W	1	6,1	14,14,15	0.20	0	17,19,21	0.49	0
6	NAG	W	2	6	14,14,15	0.27	0	17,19,21	0.91	1 (5%)
6	NAG	X	1	6,1	14,14,15	0.24	0	17,19,21	0.53	0
6	NAG	X	2	6	14,14,15	0.20	0	17,19,21	0.51	0
6	NAG	Y	1	6,1	14,14,15	0.20	0	17,19,21	0.52	0
6	NAG	Y	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	Z	1	6,1	14,14,15	0.23	0	17,19,21	0.61	0
6	NAG	Z	2	6	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	a	1	5,1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	a	2	5	14,14,15	0.25	0	17,19,21	0.53	0
5	BMA	a	3	5	11,11,12	0.50	0	15,15,17	0.69	0
5	MAN	a	4	5	11,11,12	0.53	0	15,15,17	1.01	2 (13%)
5	MAN	a	5	5	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
6	NAG	b	1	6,1	14,14,15	0.49	0	17,19,21	0.39	0
6	NAG	b	2	6	14,14,15	0.65	1 (7%)	17,19,21	2.40	1 (5%)
6	NAG	c	1	6,1	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	c	2	6	14,14,15	0.18	0	17,19,21	0.45	0
6	NAG	d	1	6,1	14,14,15	0.25	0	17,19,21	0.51	0
6	NAG	d	2	6	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	e	1	9,1	14,14,15	0.22	0	17,19,21	0.48	0
9	NAG	e	2	9	14,14,15	0.20	0	17,19,21	0.41	0
9	BMA	e	3	9	11,11,12	0.49	0	15,15,17	0.70	0
9	MAN	e	4	9	11,11,12	0.55	0	15,15,17	0.94	2 (13%)
9	MAN	e	5	9	11,11,12	0.58	0	15,15,17	0.95	2 (13%)
6	NAG	f	1	6,1	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	f	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	g	1	6,1	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	g	2	6	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	h	1	6,1	14,14,15	0.19	0	17,19,21	0.51	0
6	NAG	h	2	6	14,14,15	0.25	0	17,19,21	0.94	1 (5%)
6	NAG	i	1	6,1	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	i	2	6	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	j	1	6,1	14,14,15	0.31	0	17,19,21	0.62	0
6	NAG	j	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	k	1	6,1	14,14,15	0.22	0	17,19,21	0.63	0
6	NAG	k	2	6	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	l	1	6,1	14,14,15	0.22	0	17,19,21	0.52	0
6	NAG	l	2	6	14,14,15	0.25	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	m	1	6,1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	m	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	n	1	6,1	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
6	NAG	n	2	6	14,14,15	0.24	0	17,19,21	0.50	0
5	NAG	o	1	5,1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	o	2	5	14,14,15	0.25	0	17,19,21	0.52	0
5	BMA	o	3	5	11,11,12	0.45	0	15,15,17	0.66	0
5	MAN	o	4	5	11,11,12	0.59	0	15,15,17	0.98	2 (13%)
5	MAN	o	5	5	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
6	NAG	p	1	6,1	14,14,15	0.33	0	17,19,21	0.48	0
6	NAG	p	2	6	14,14,15	0.35	0	17,19,21	0.41	0
6	NAG	q	1	6,1	14,14,15	0.25	0	17,19,21	0.40	0
6	NAG	q	2	6	14,14,15	0.23	0	17,19,21	0.94	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	r	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	s	1	6,1	14,14,15	0.28	0	17,19,21	0.42	0
6	NAG	s	2	6	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	t	1	8,1	14,14,15	0.26	0	17,19,21	0.54	0
8	NAG	t	2	8	14,14,15	0.21	0	17,19,21	0.41	0
8	BMA	t	3	8	11,11,12	0.63	0	15,15,17	0.68	0
8	MAN	t	4	8	11,11,12	0.56	0	15,15,17	0.81	1 (6%)
8	MAN	t	5	8	11,11,12	0.57	0	15,15,17	1.17	2 (13%)
8	MAN	t	6	8	11,11,12	0.66	0	15,15,17	0.89	2 (13%)
6	NAG	u	1	6,1	14,14,15	0.19	0	17,19,21	0.46	0
6	NAG	u	2	6	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	v	1	6,1	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	v	2	6	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	w	1	6,1	14,14,15	0.23	0	17,19,21	0.42	0
6	NAG	w	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	x	1	6,1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	x	2	6	14,14,15	0.18	0	17,19,21	0.50	0
6	NAG	y	1	6,1	14,14,15	0.20	0	17,19,21	0.50	0
6	NAG	y	2	6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	z	1	6,1	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	z	2	6	14,14,15	0.29	0	17,19,21	0.91	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
6	NAG	0	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	0	2	6	-	2/6/23/26	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	0/6/23/26	0/1/1/1
6	NAG	2	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	2	2	6	-	2/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	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	-	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	-	2/6/23/26	0/1/1/1
7	NAG	O	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
8	NAG	Q	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	6	8	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	4/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	4/6/23/26	0/1/1/1

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	2	NAG	O5-C1	-2.21	1.40	1.43

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	2	NAG	C2-N2-C7	9.42	135.53	122.90
8	t	5	MAN	C1-O5-C5	3.53	116.92	112.19
6	h	2	NAG	C2-N2-C7	2.91	126.80	122.90
6	q	2	NAG	C2-N2-C7	2.89	126.77	122.90
6	z	2	NAG	C2-N2-C7	2.88	126.75	122.90

There are no chirality outliers.

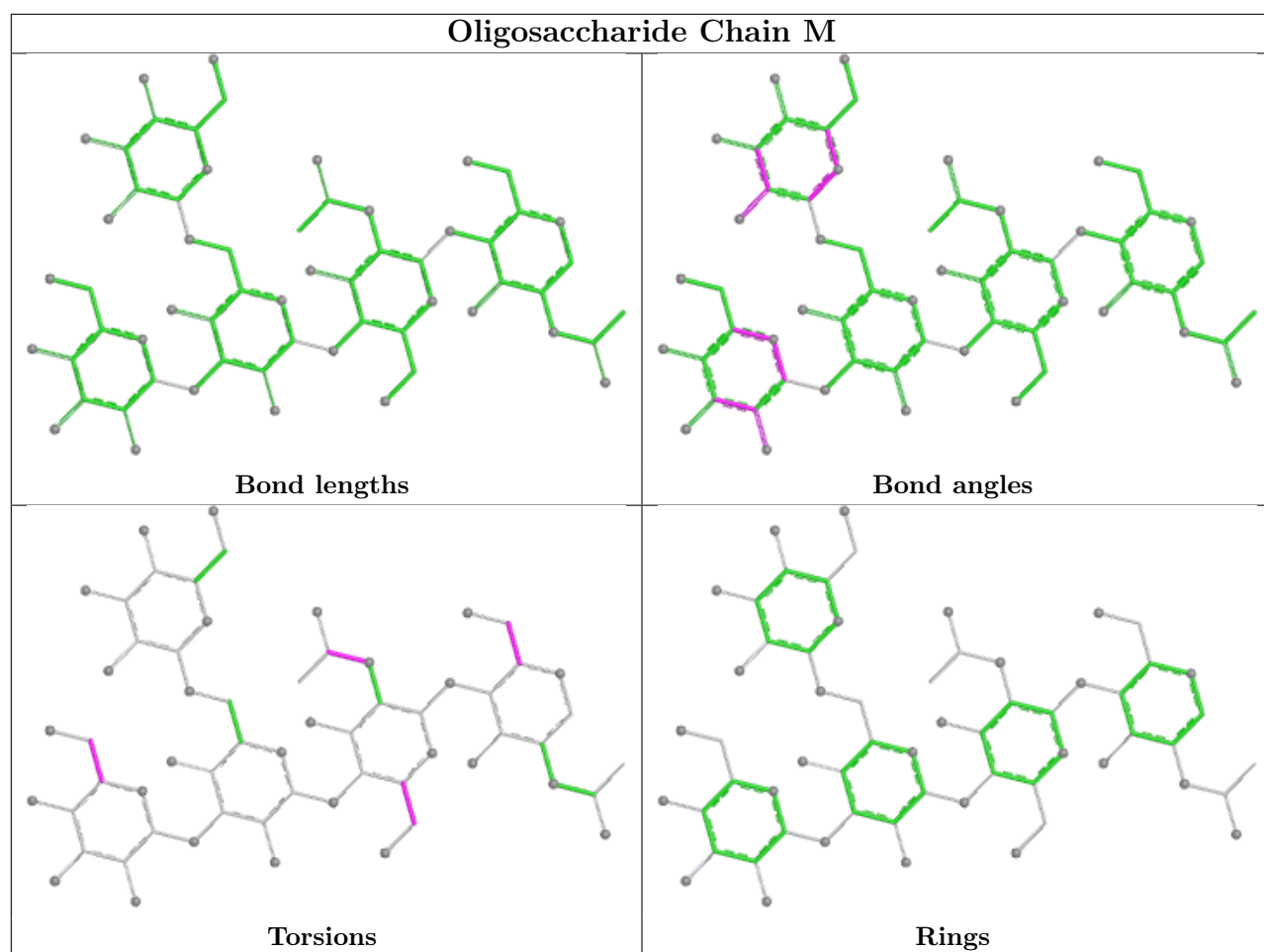
5 of 187 torsion outliers are listed below:

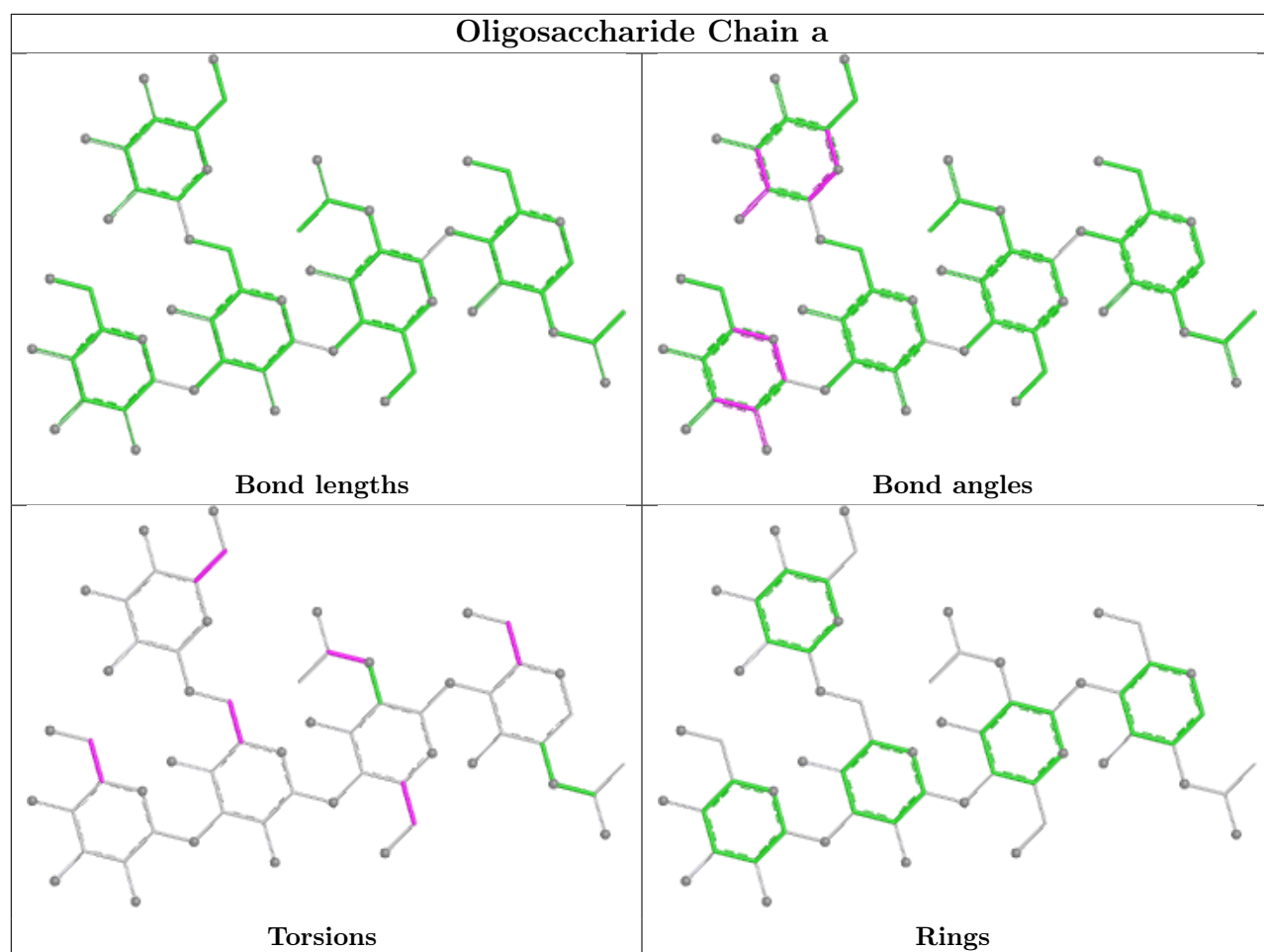
Mol	Chain	Res	Type	Atoms
6	b	2	NAG	C1-C2-N2-C7
6	j	2	NAG	C1-C2-N2-C7
6	m	1	NAG	C1-C2-N2-C7
6	n	1	NAG	C1-C2-N2-C7
6	p	2	NAG	C1-C2-N2-C7

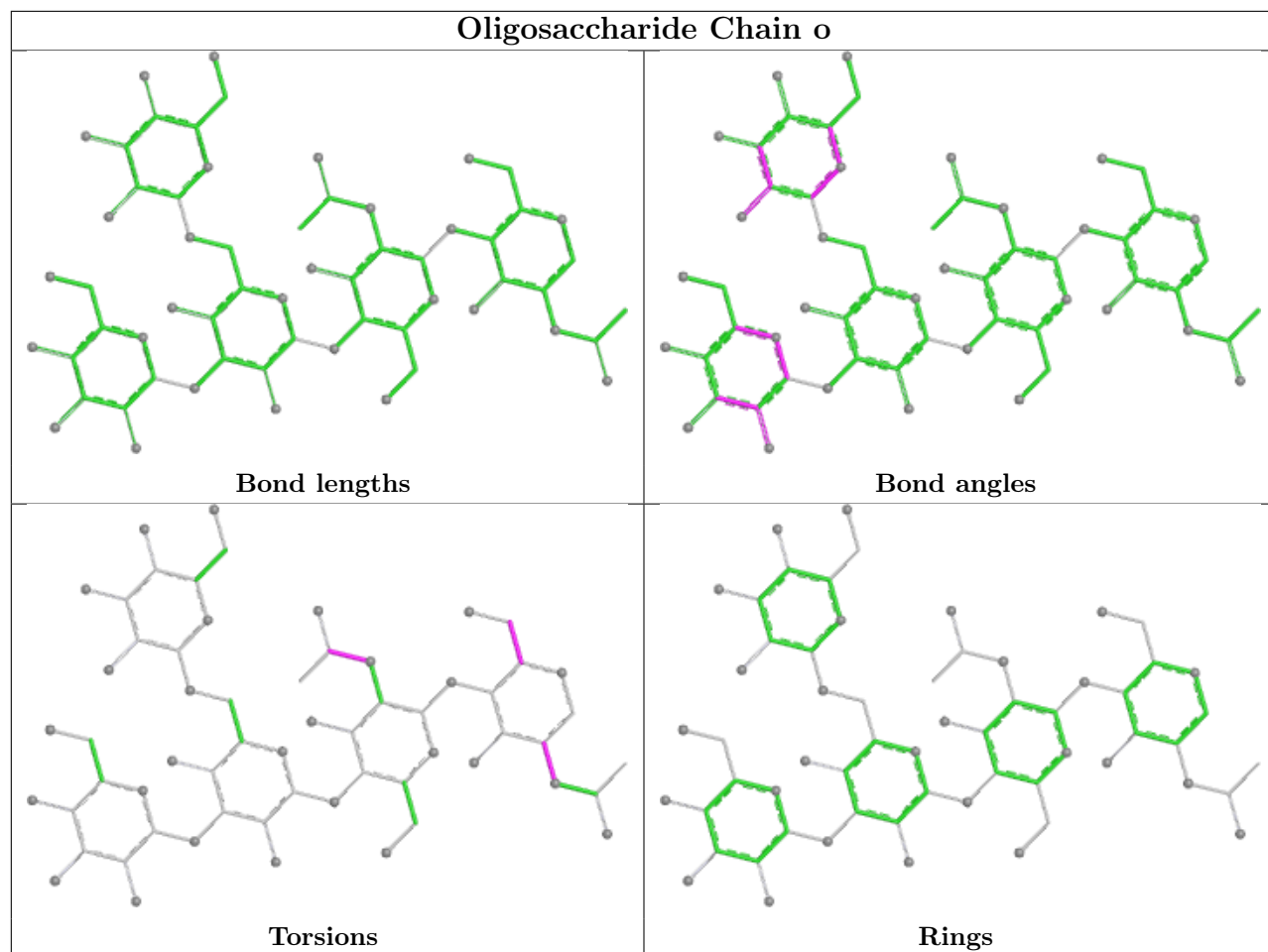
There are no ring outliers.

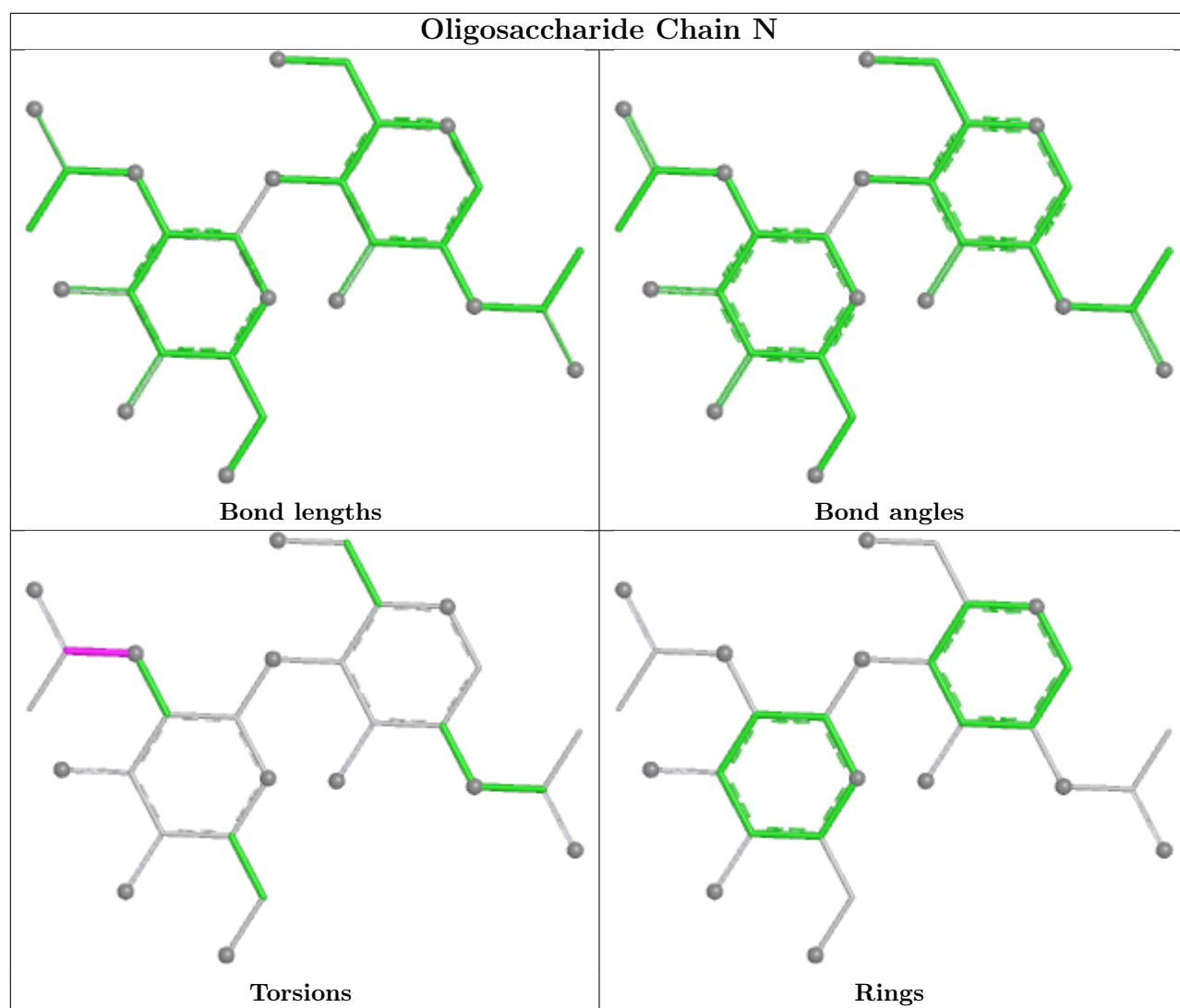
No monomer is involved in short contacts.

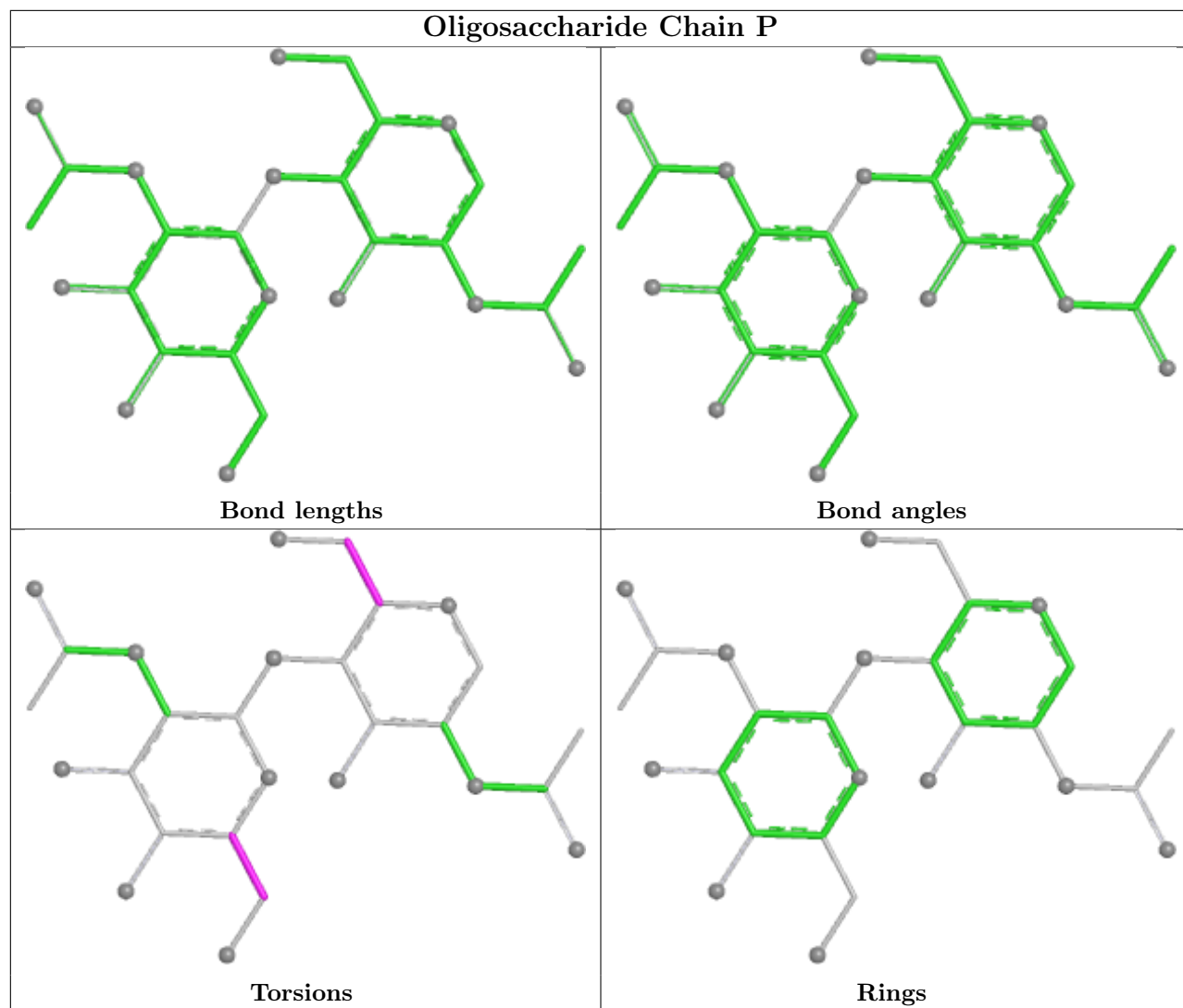
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

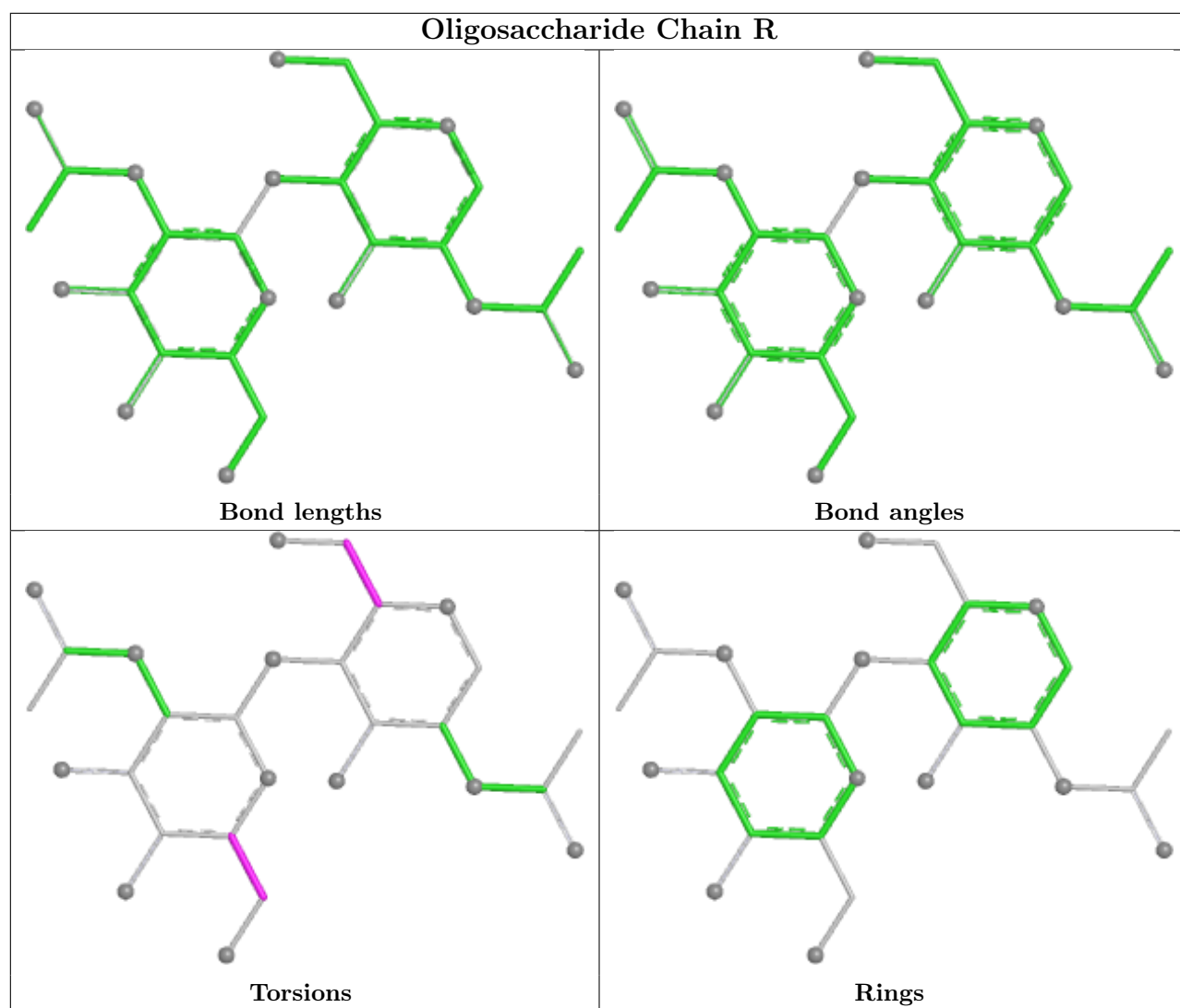


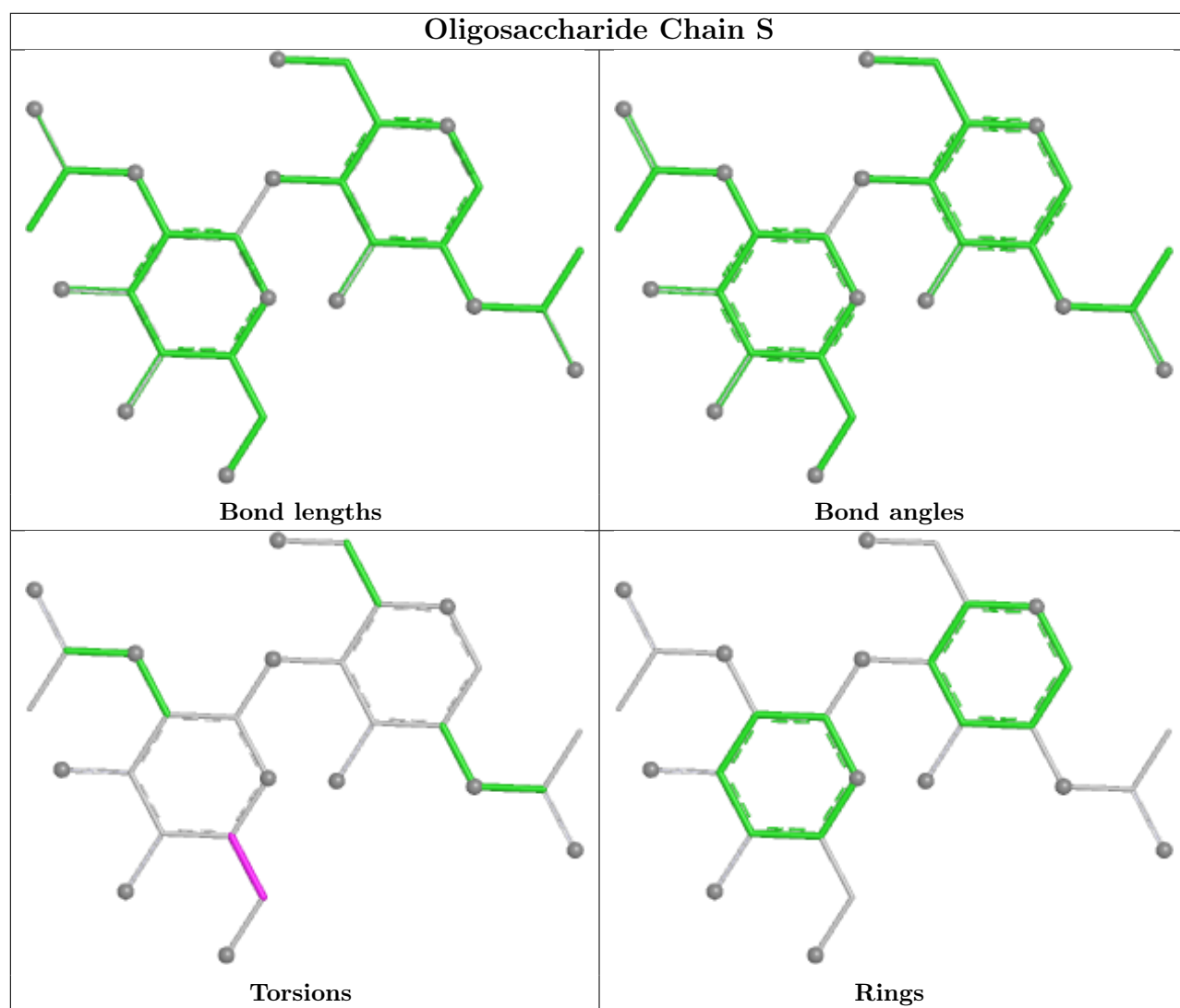


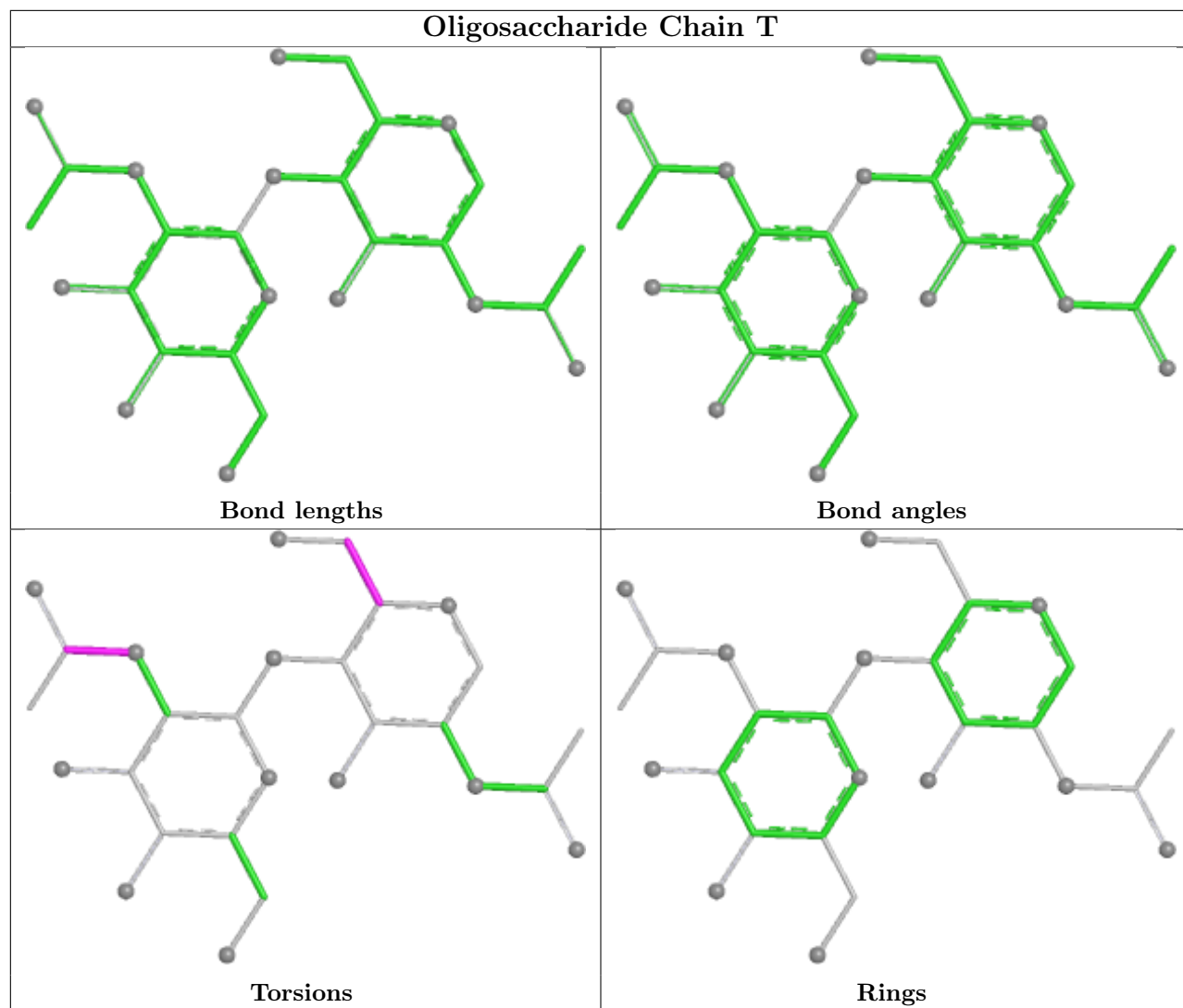


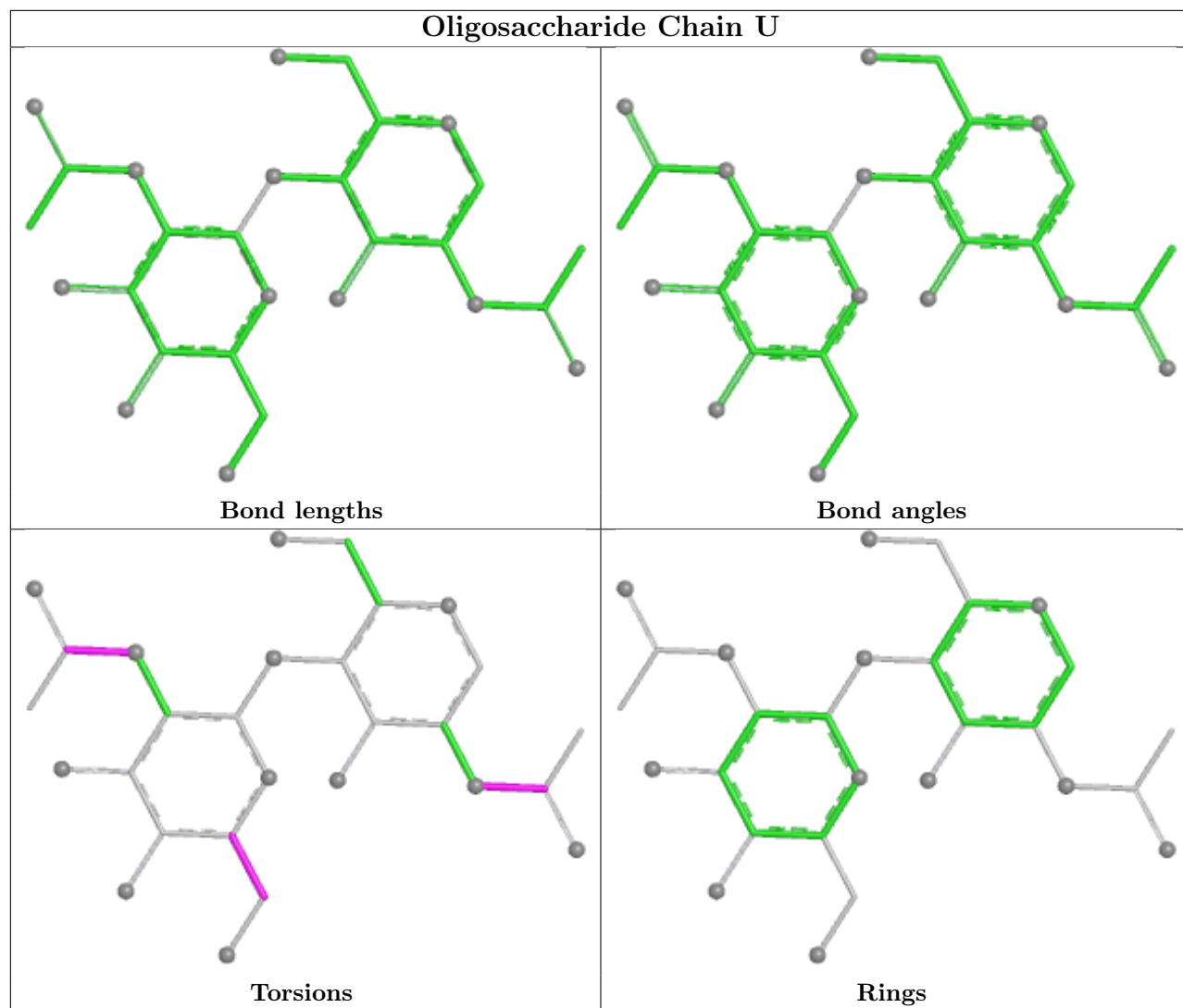


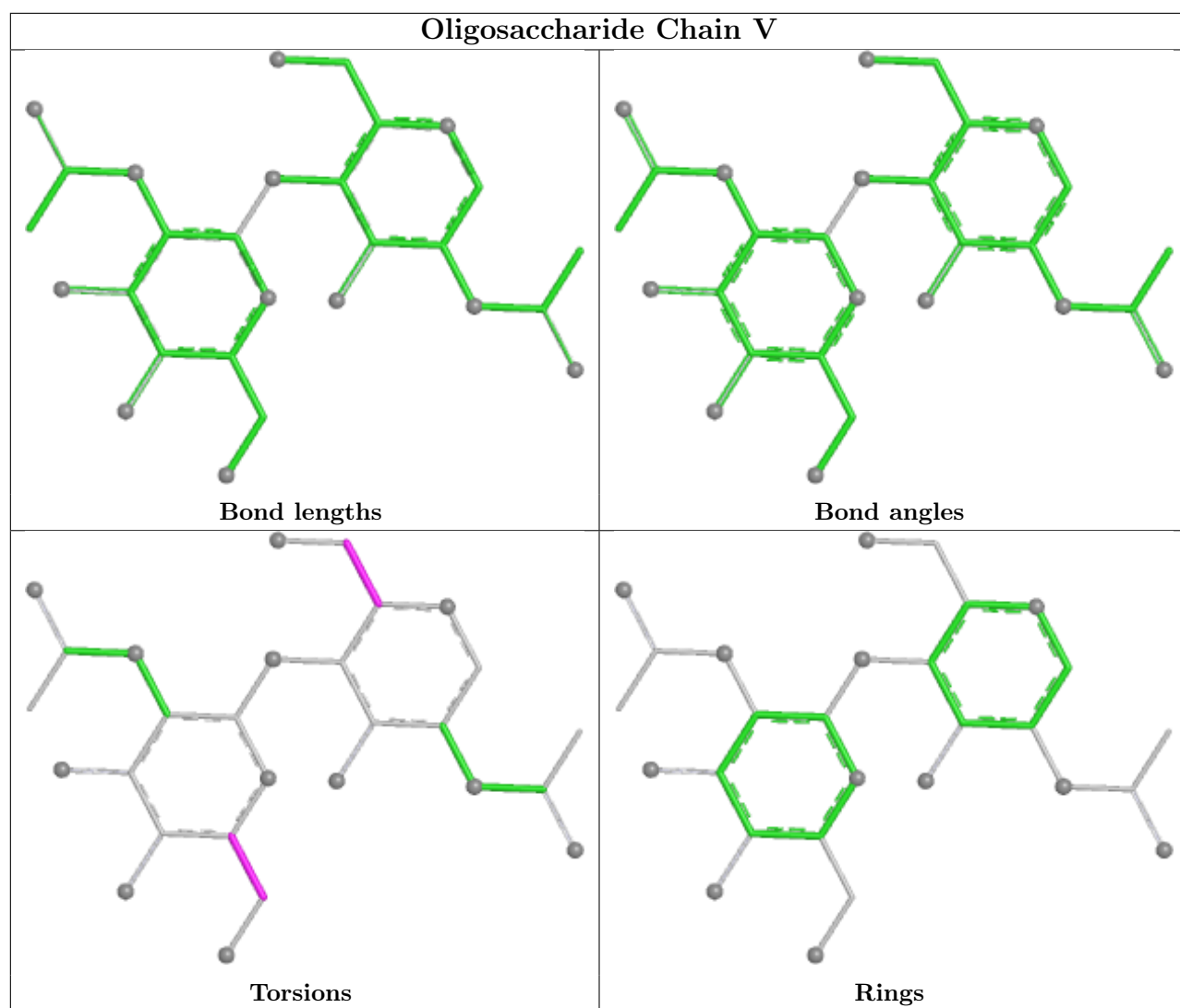


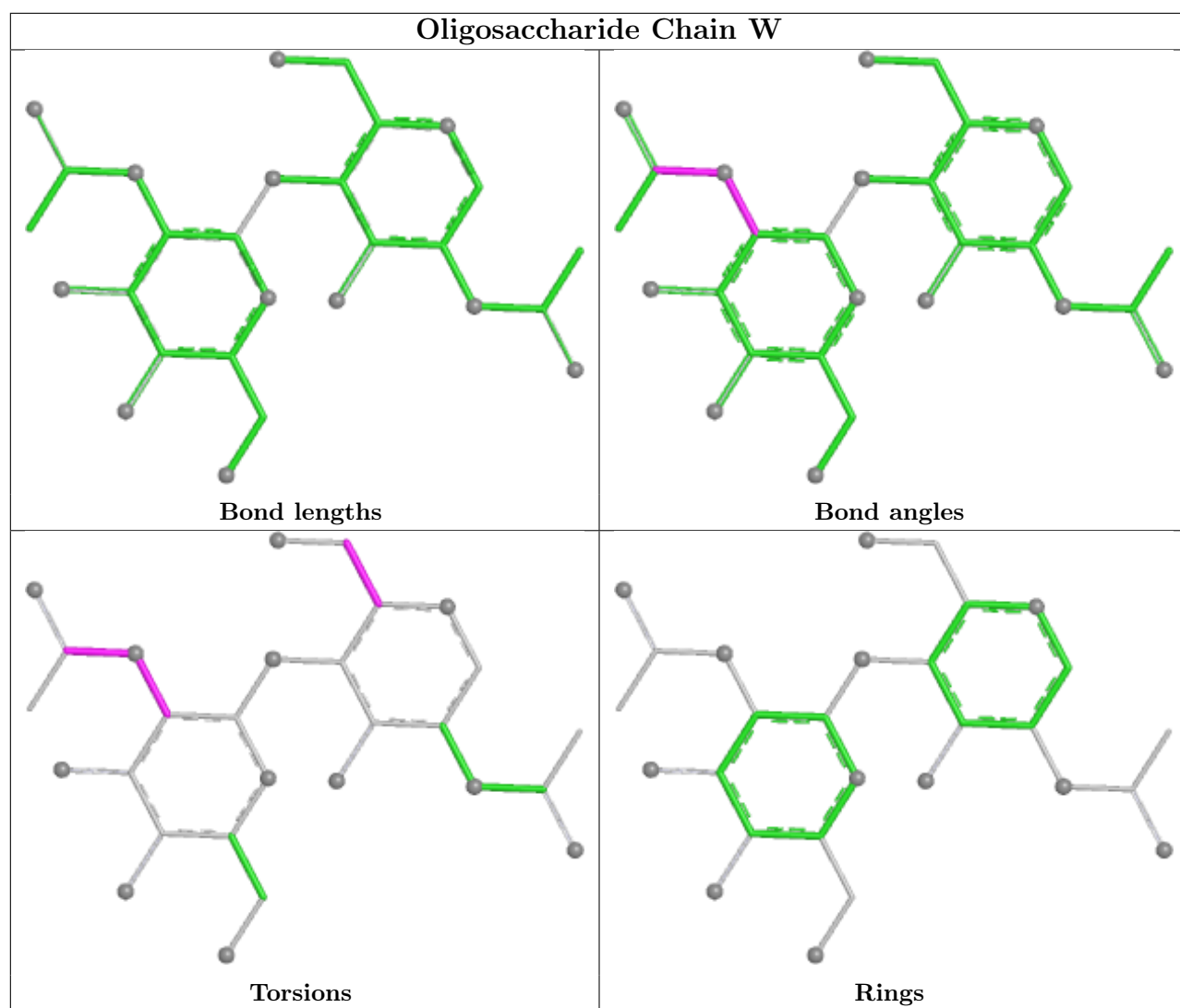


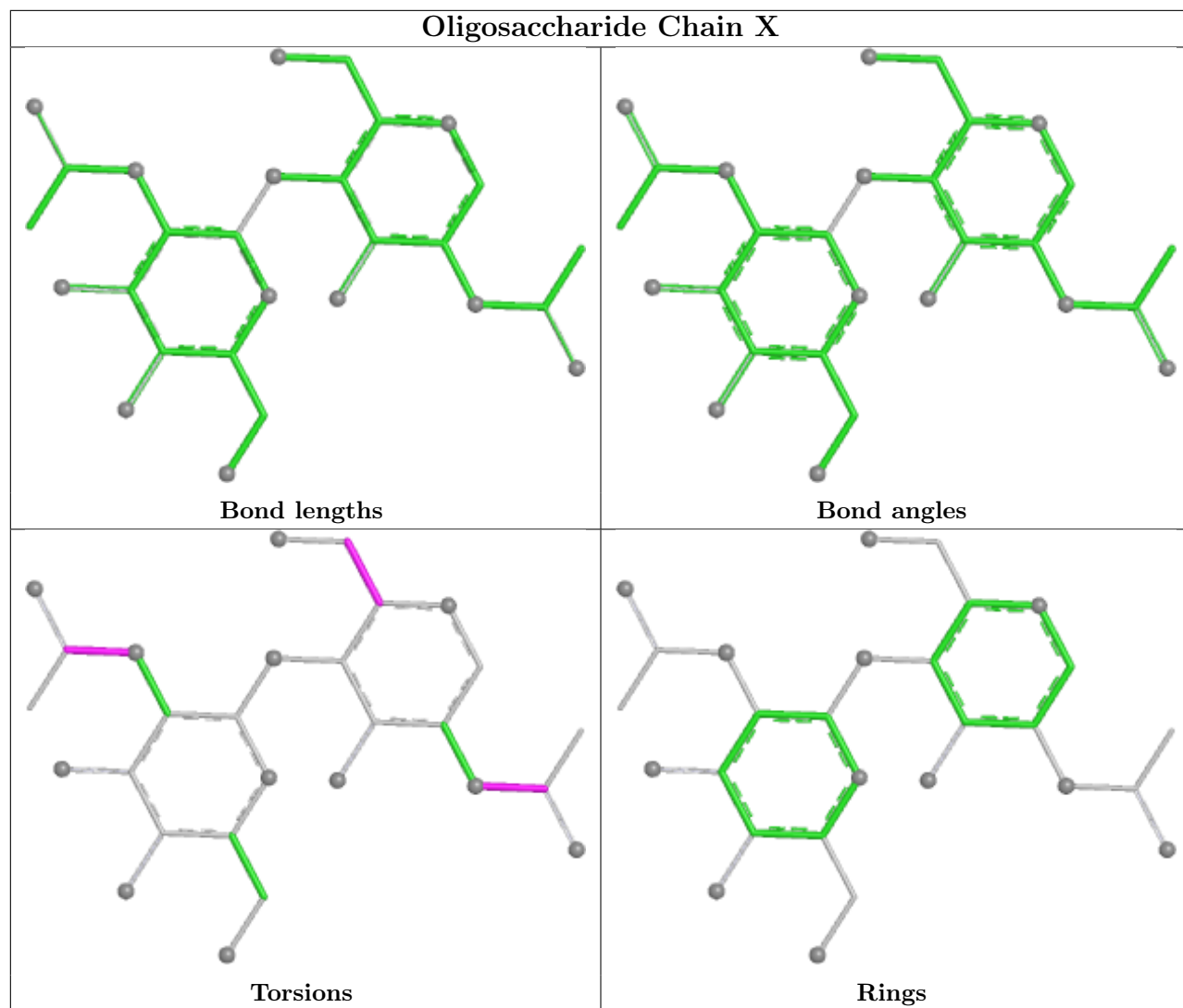


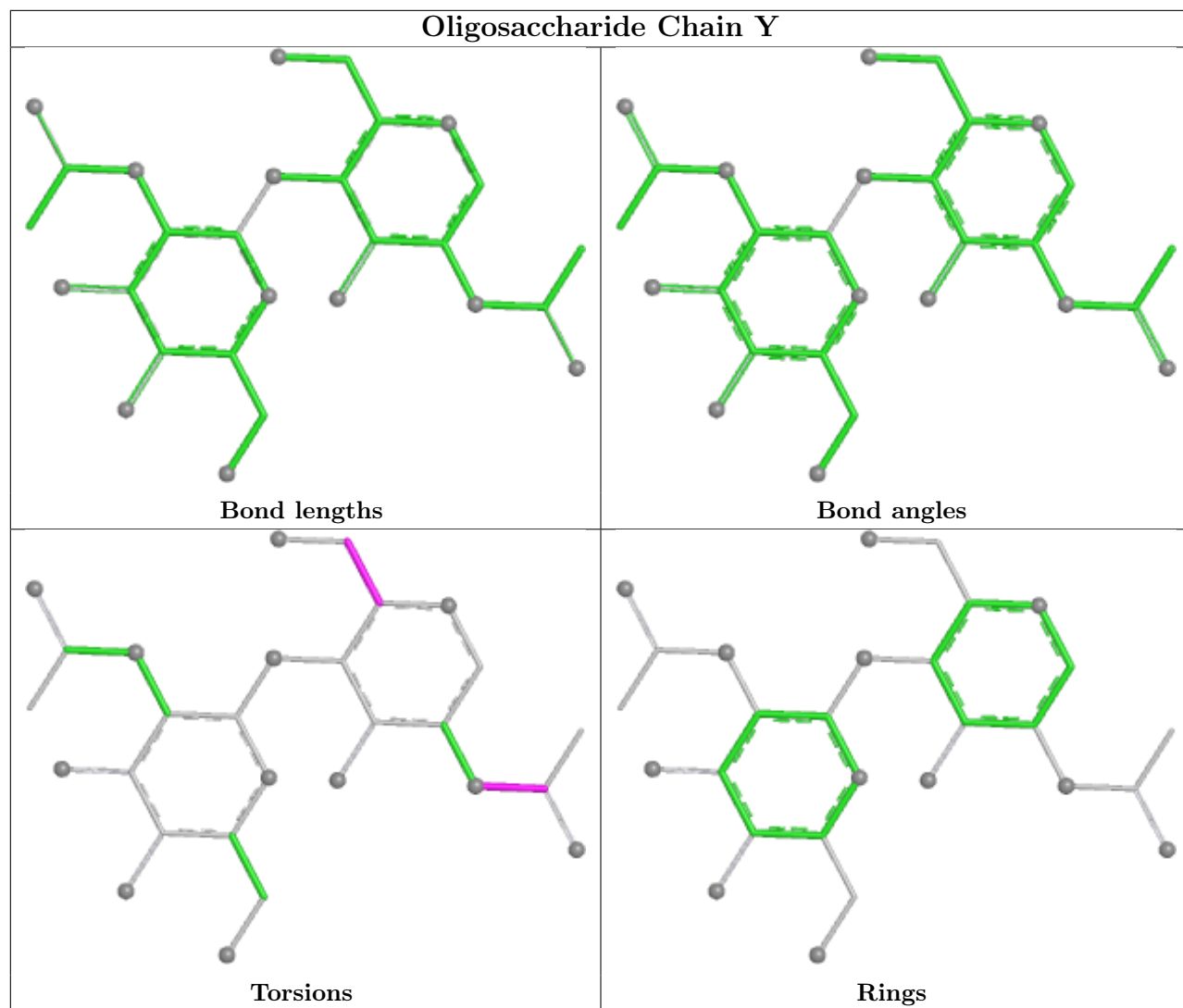


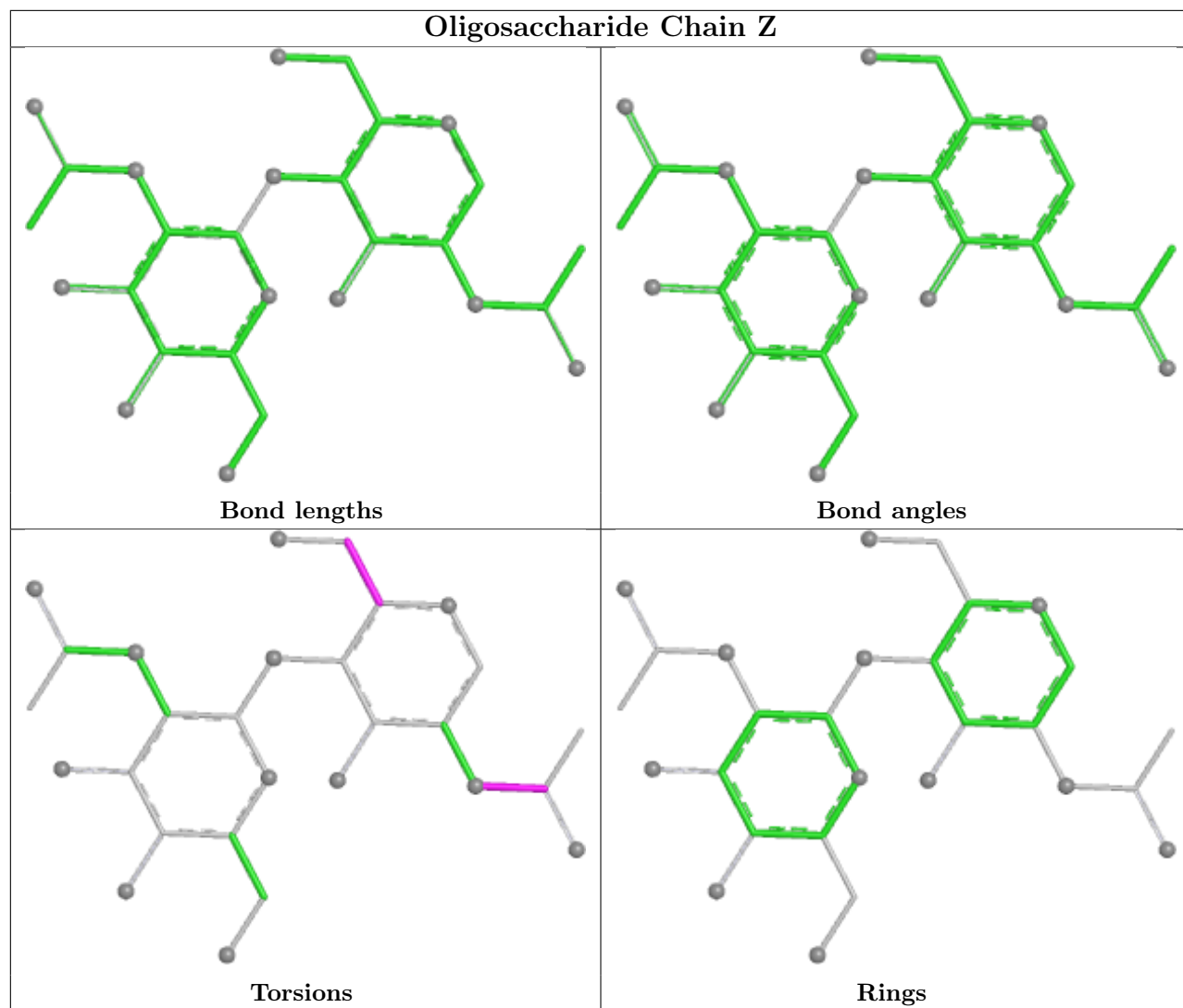


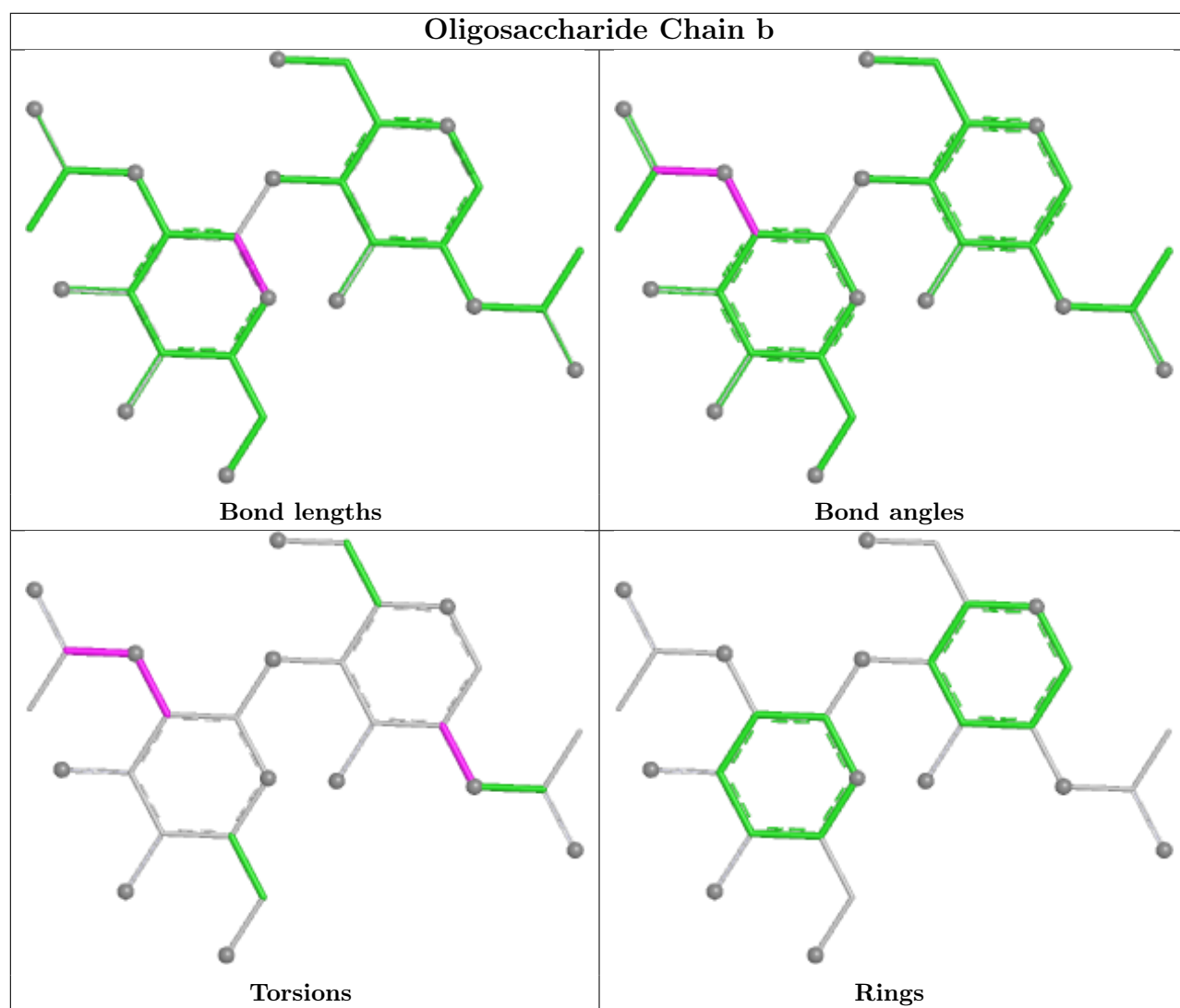


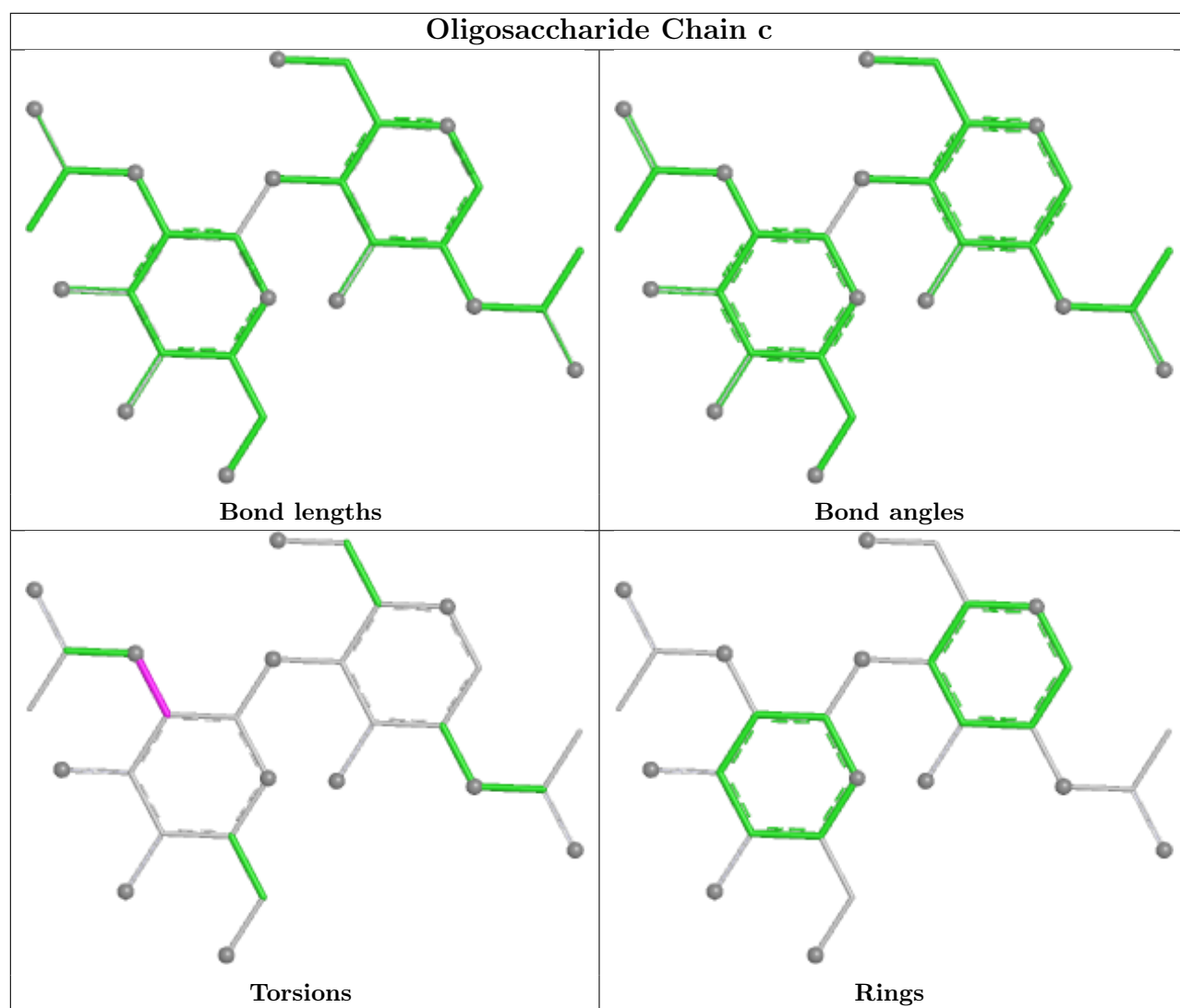


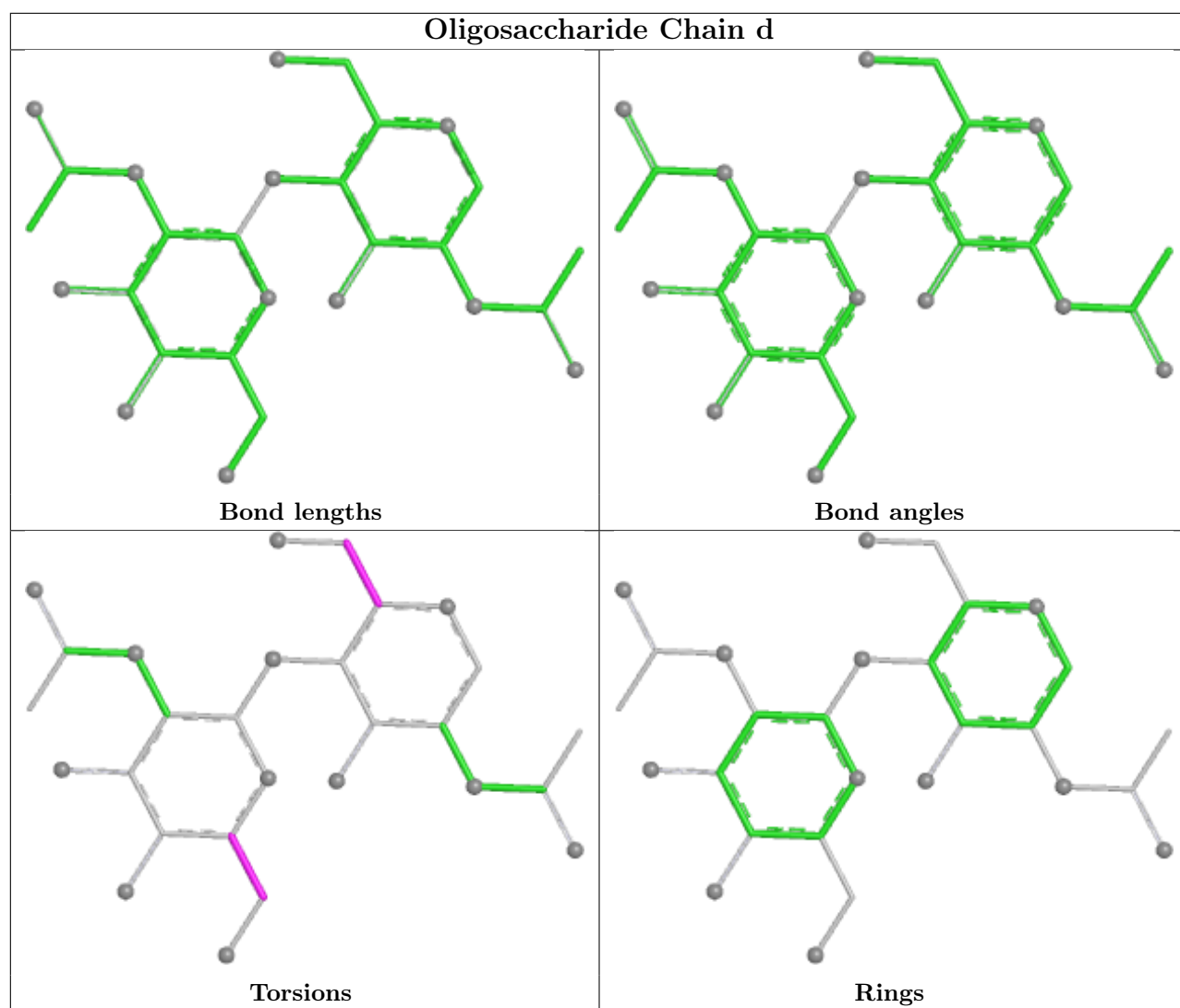


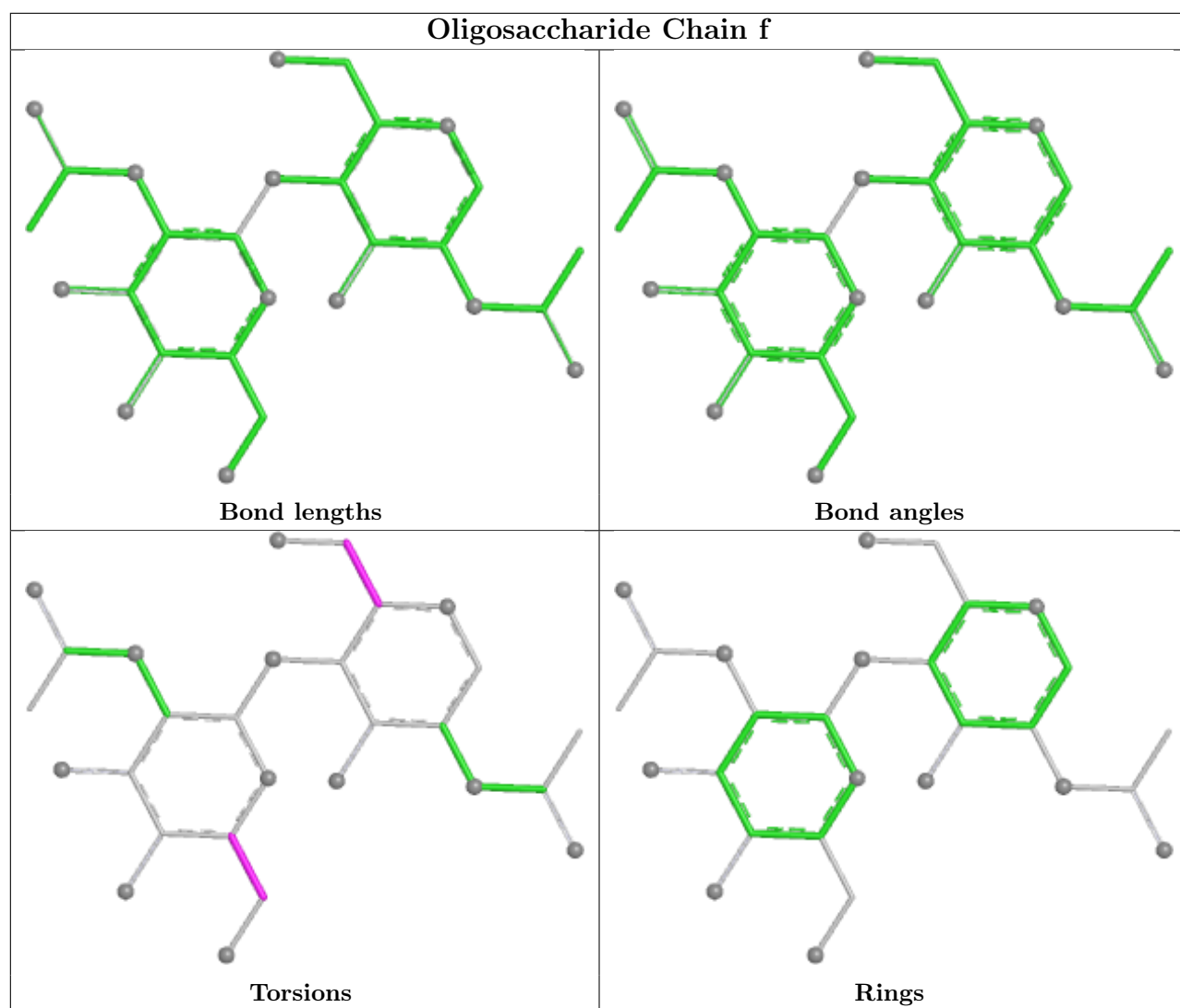


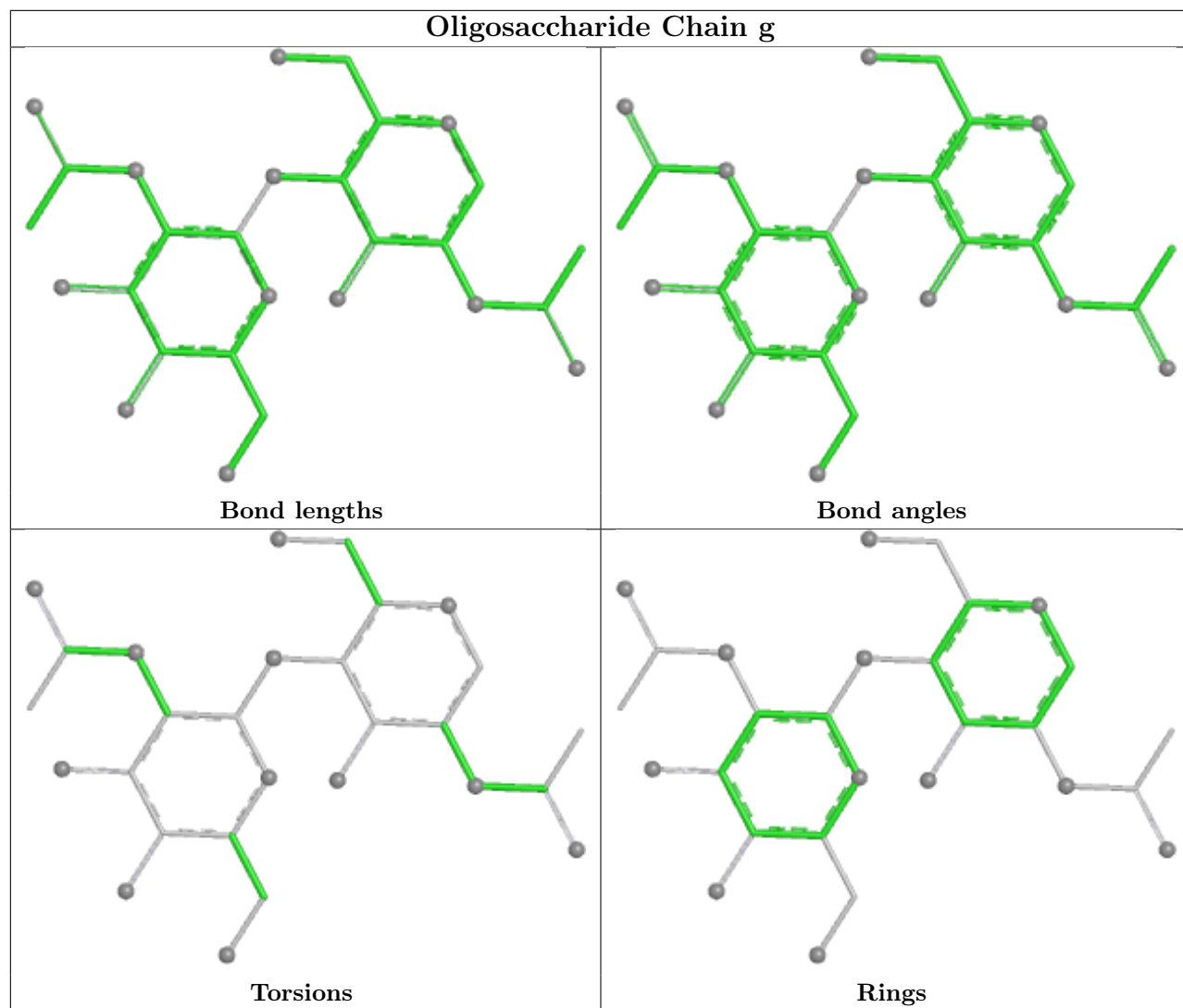


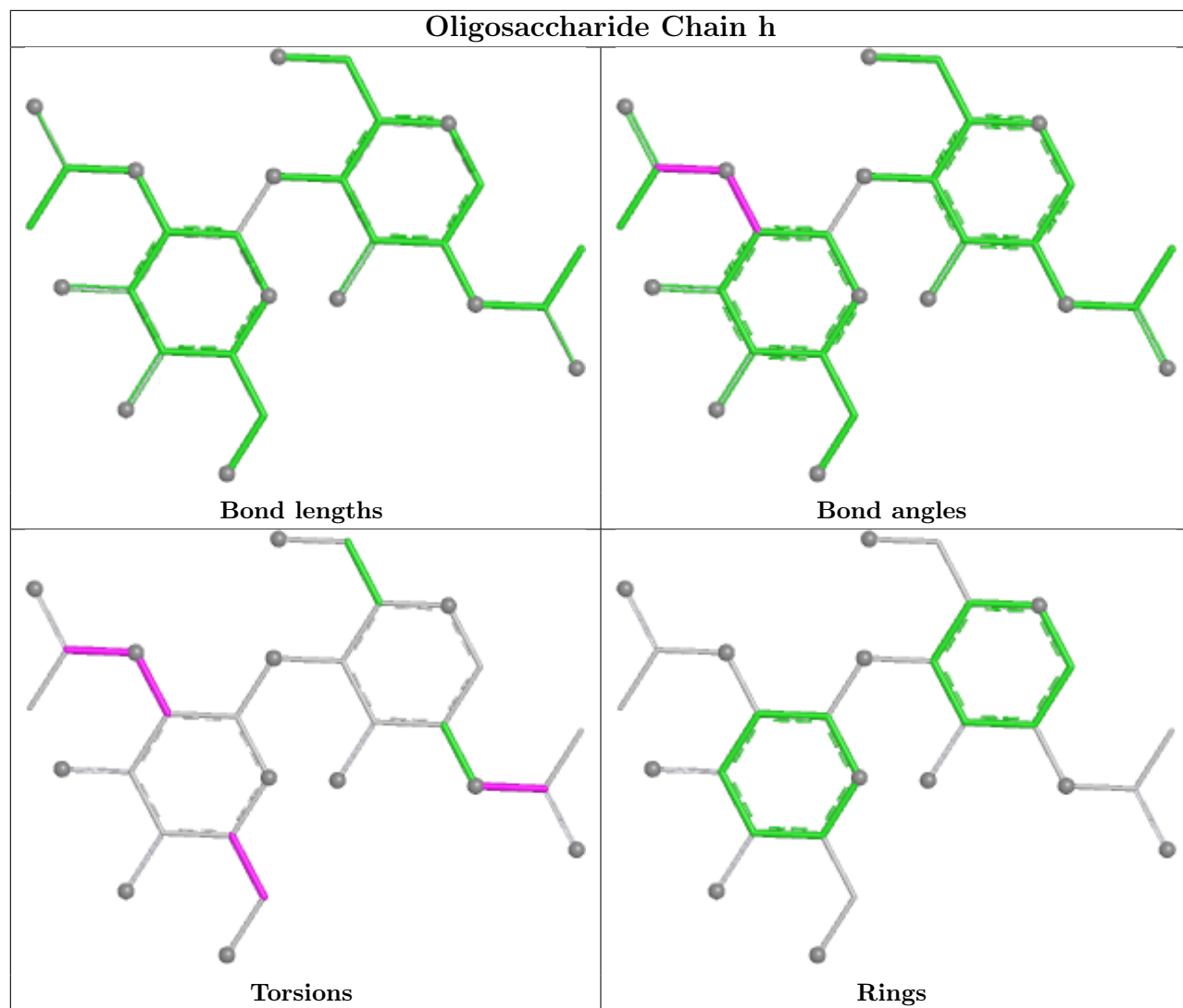


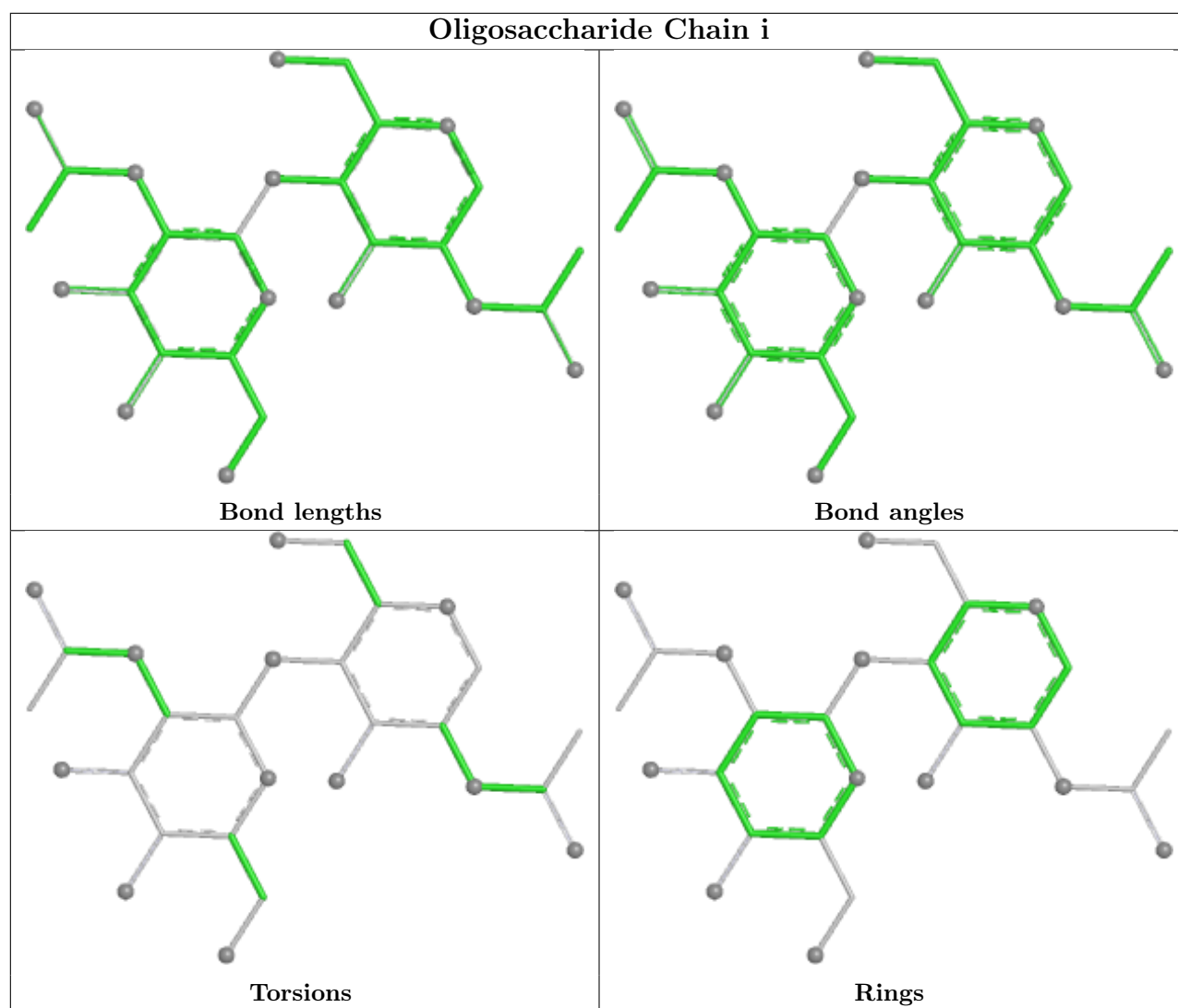


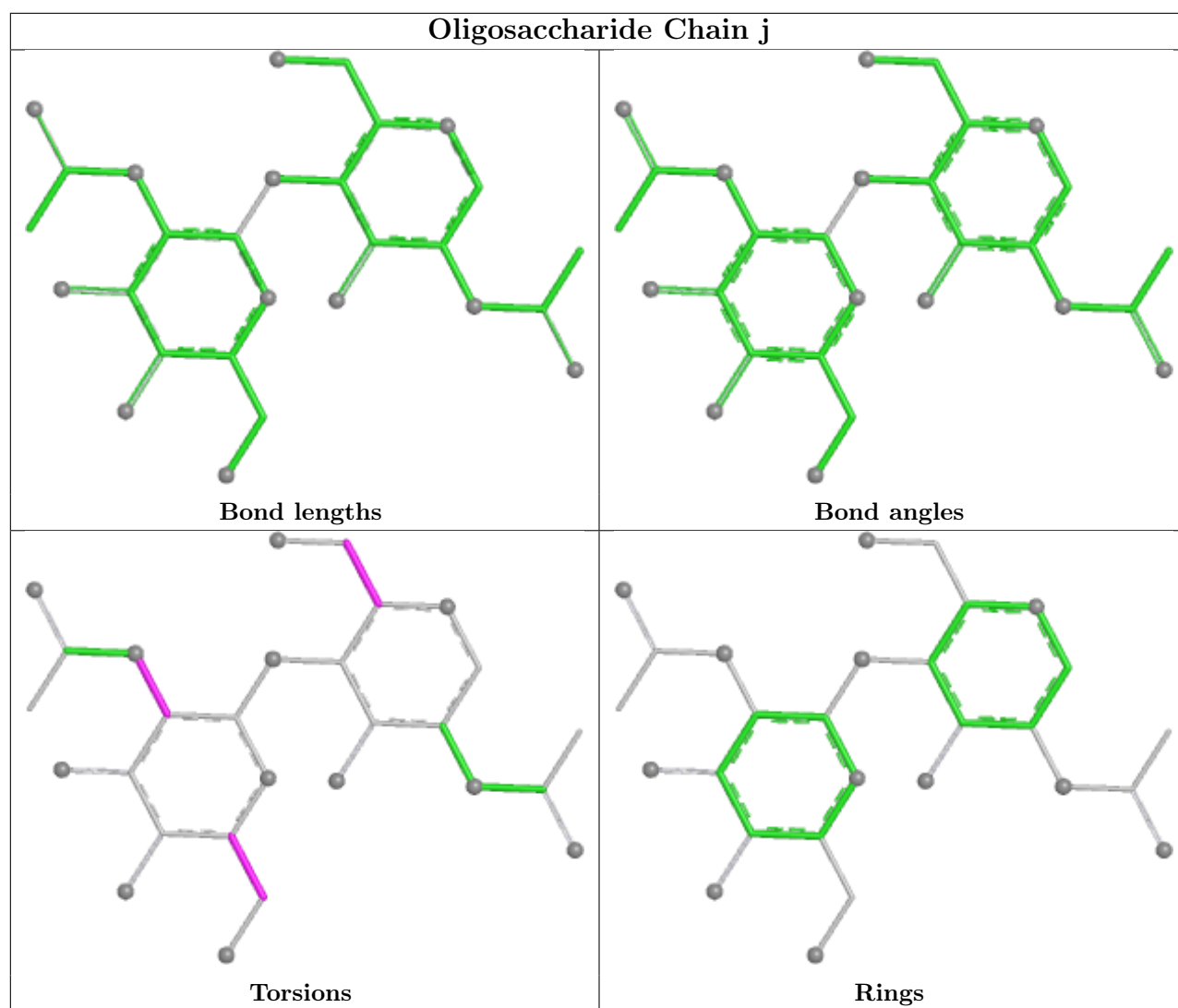


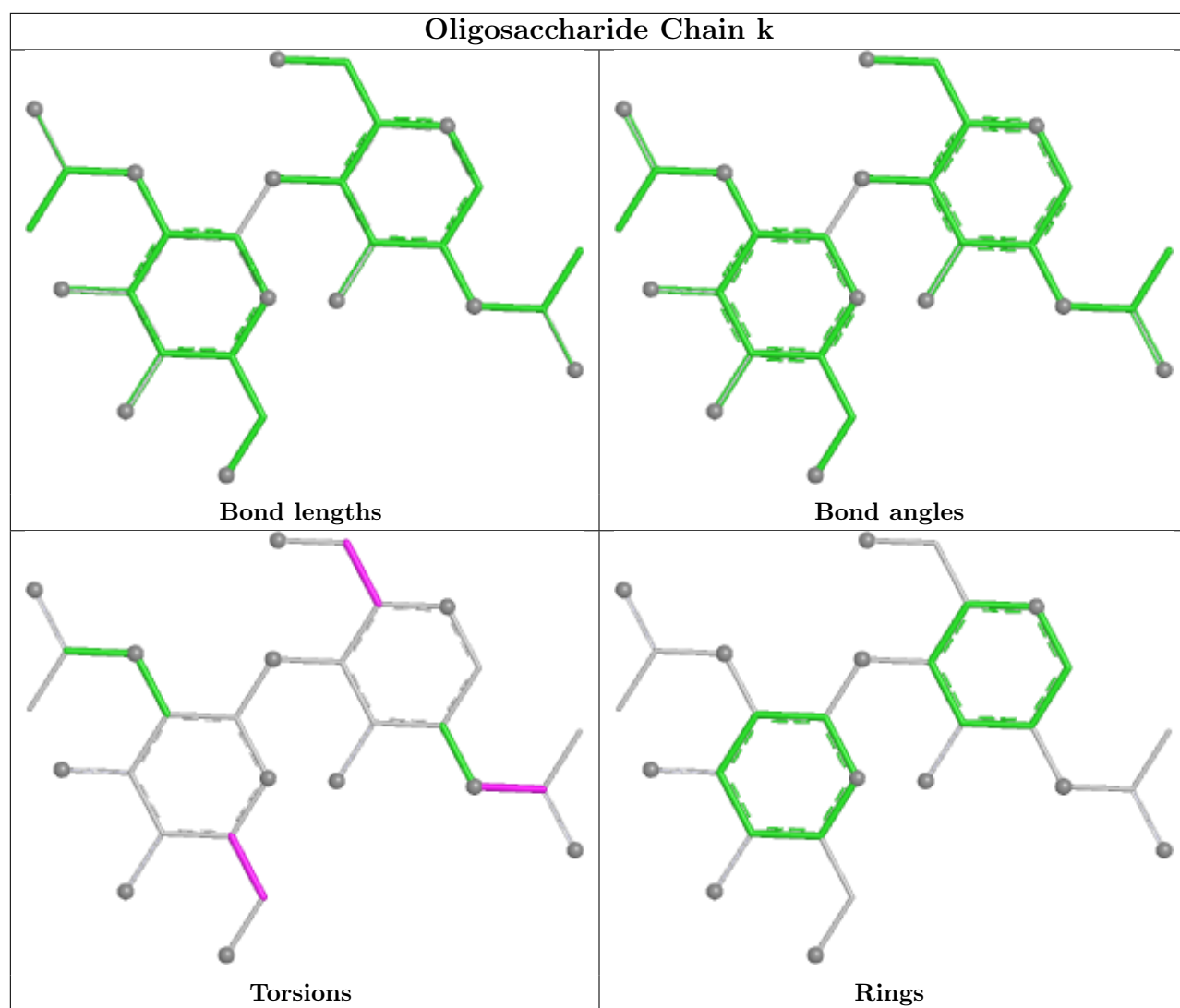


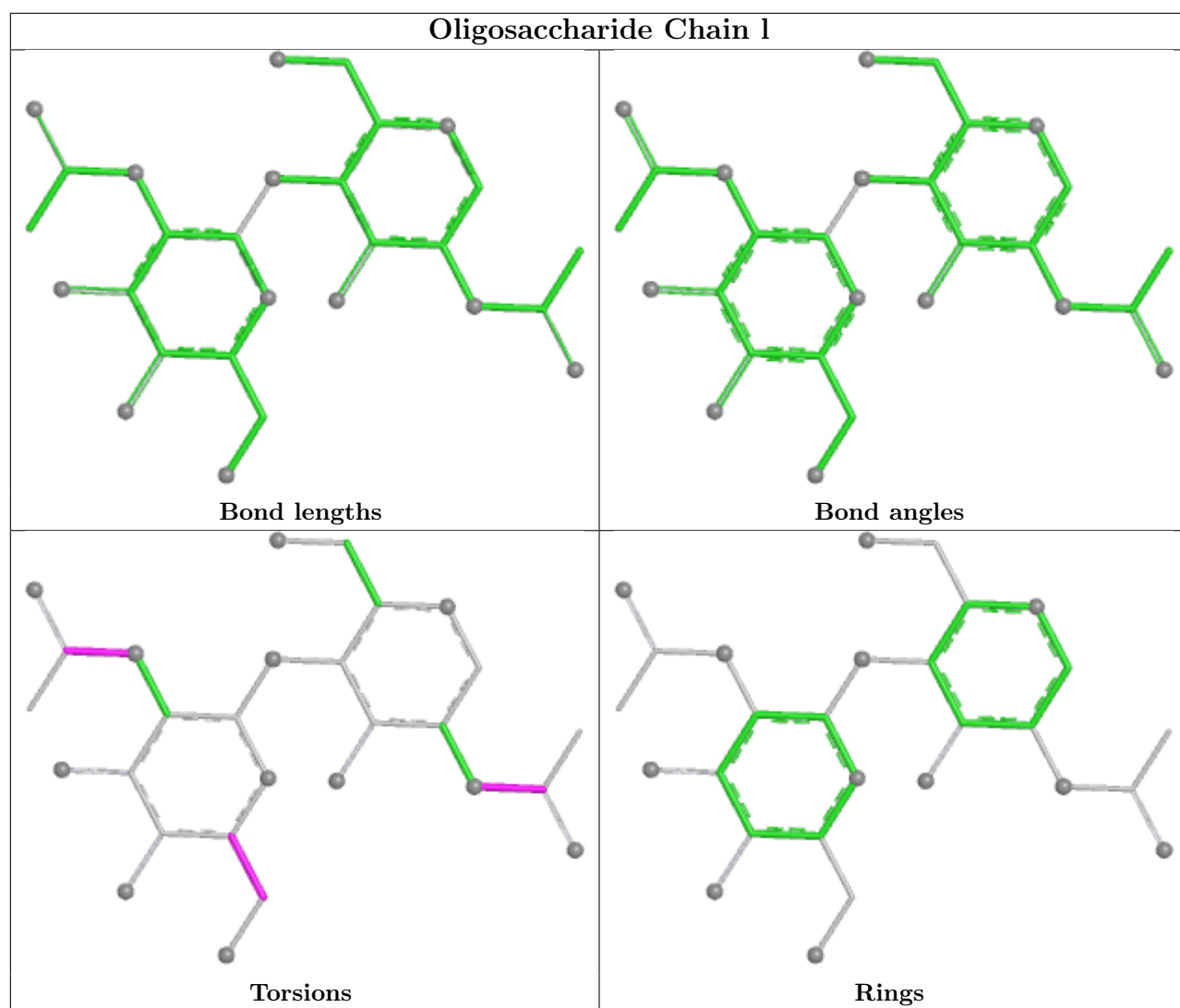


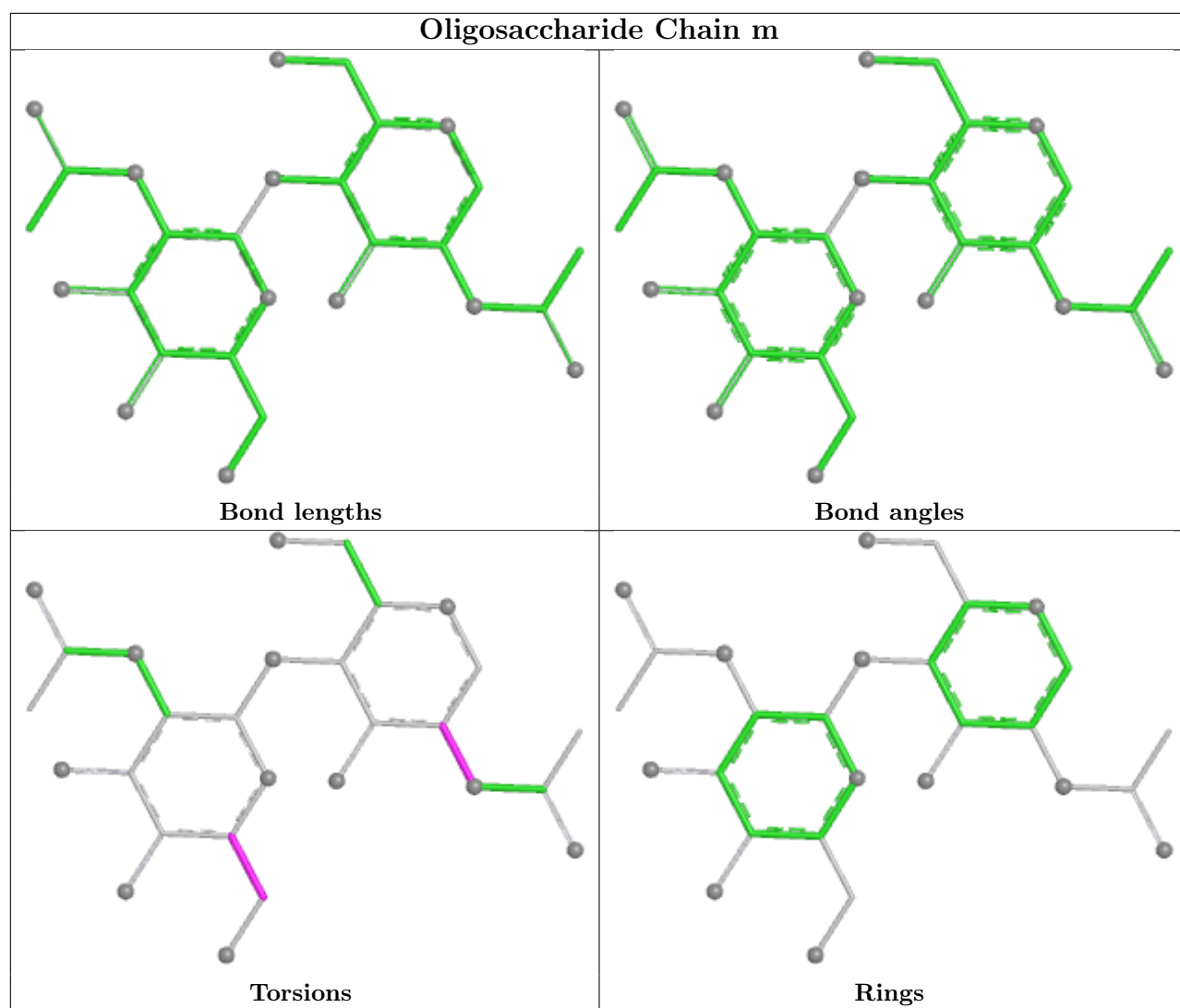


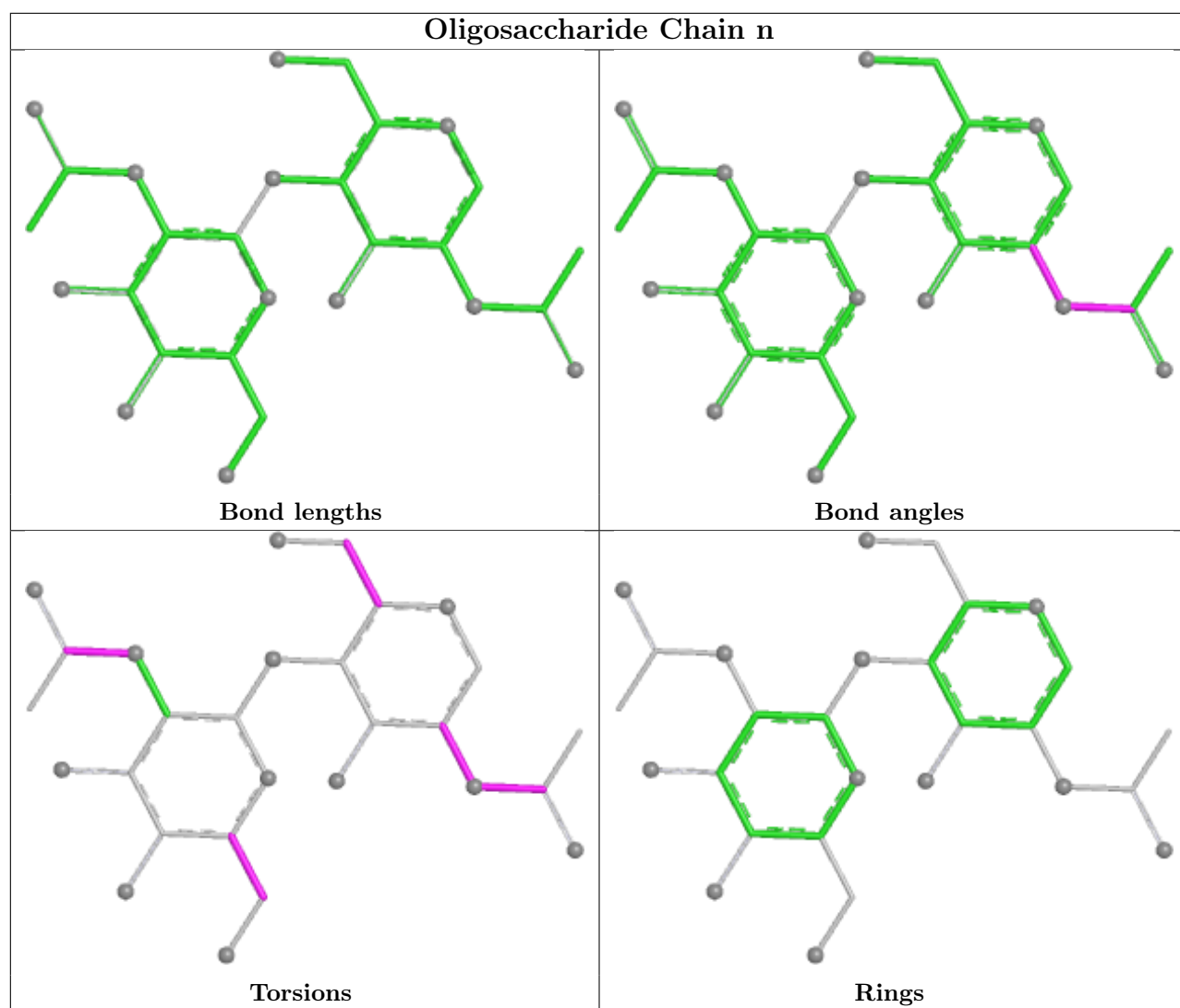


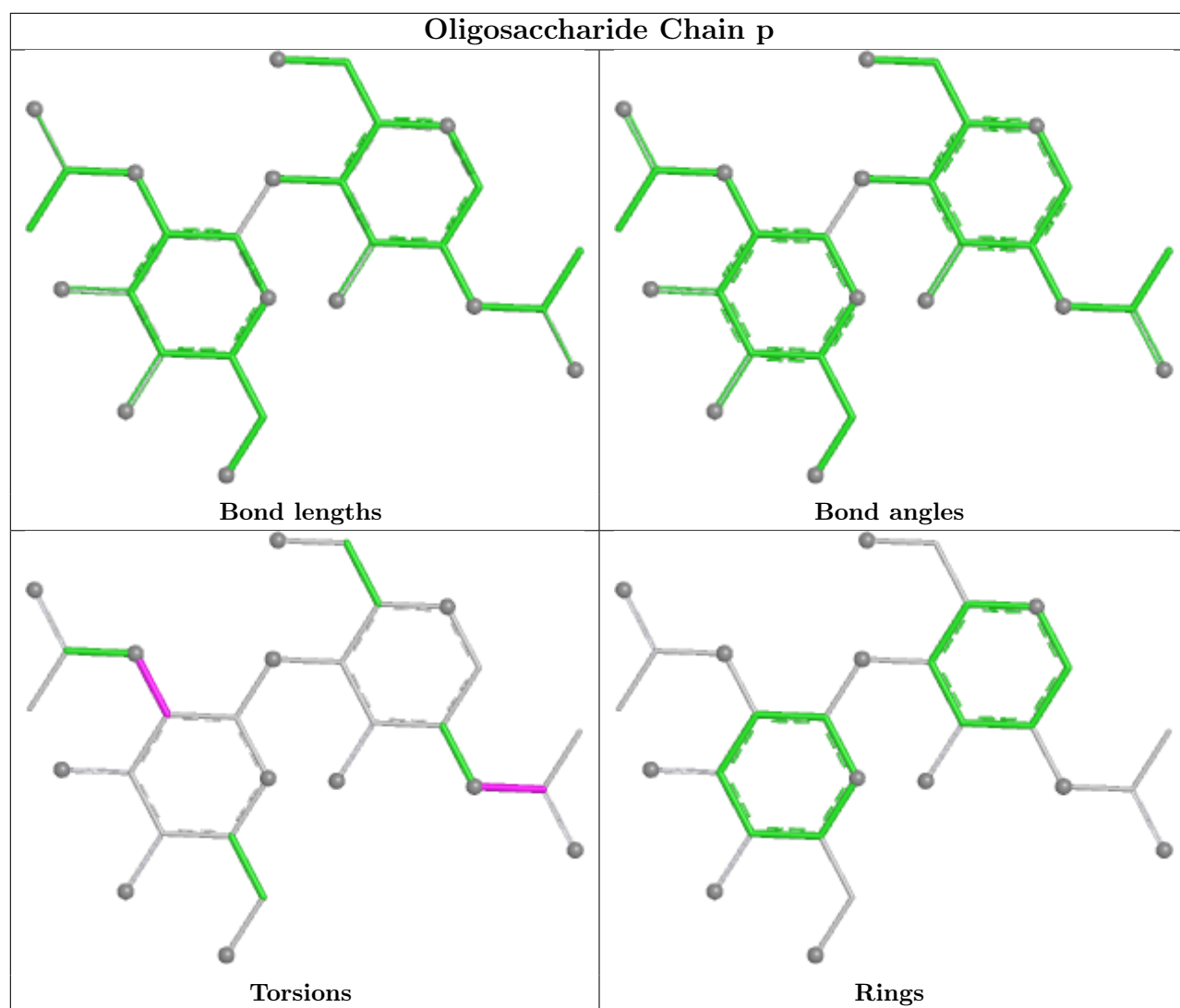


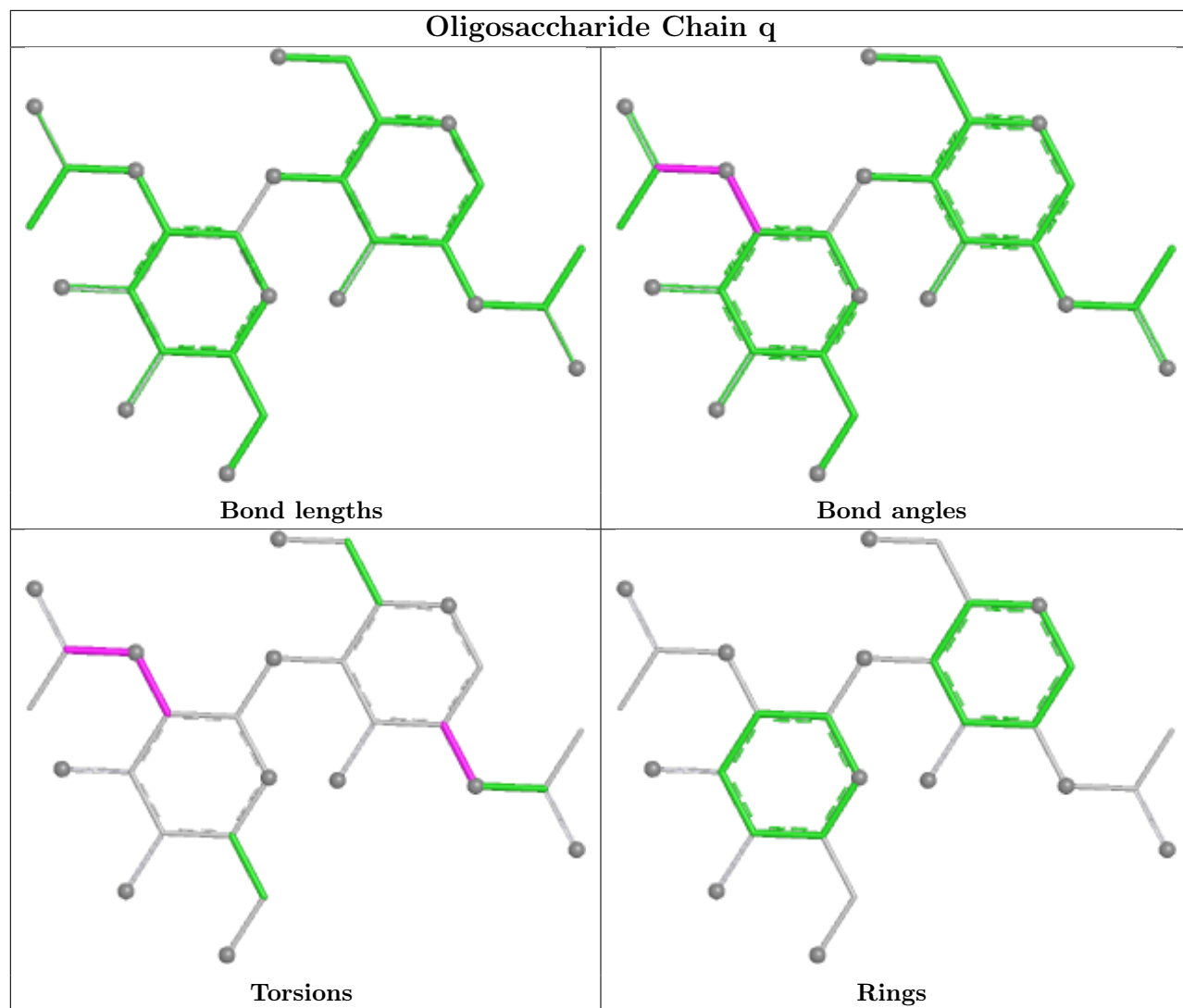


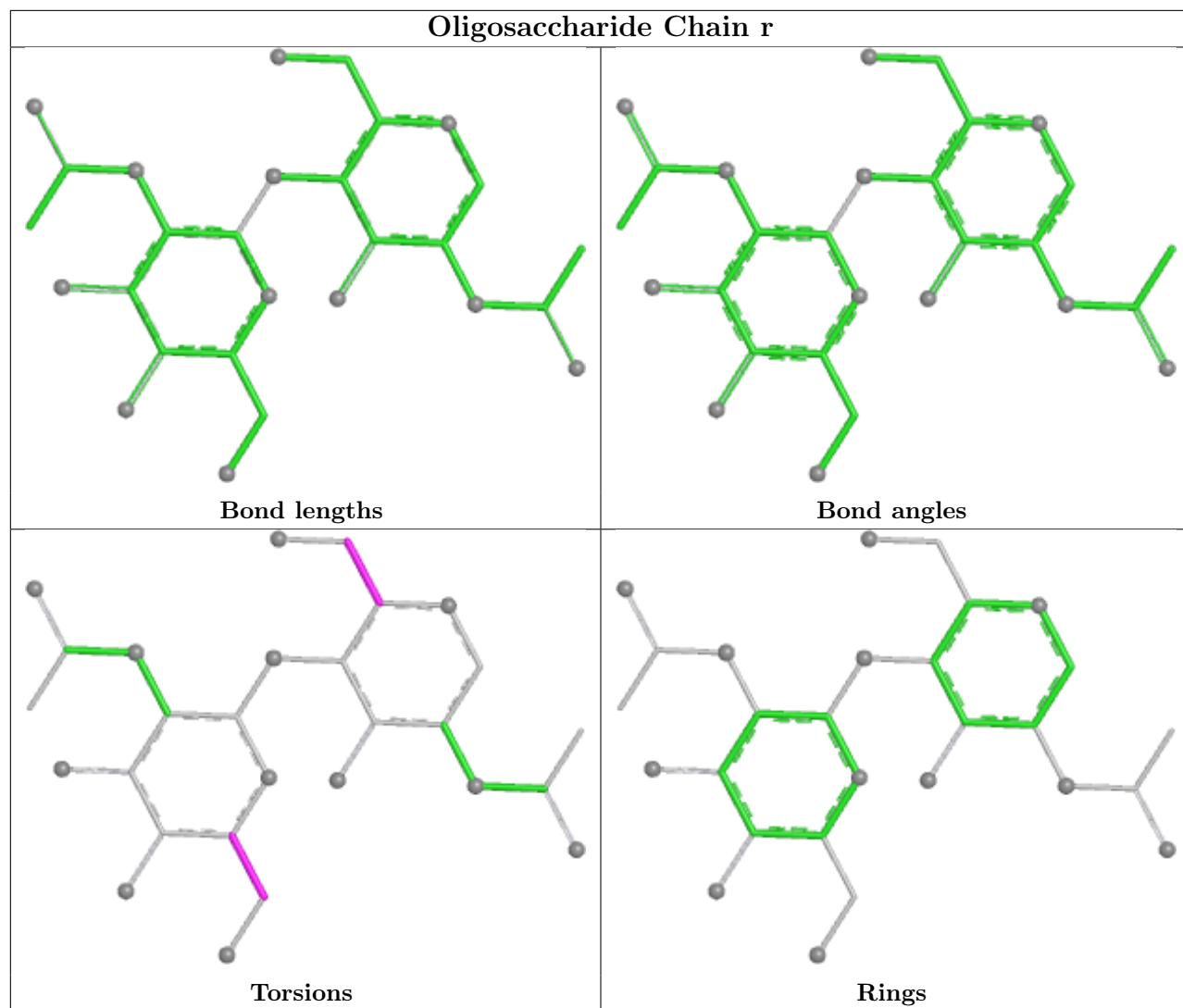


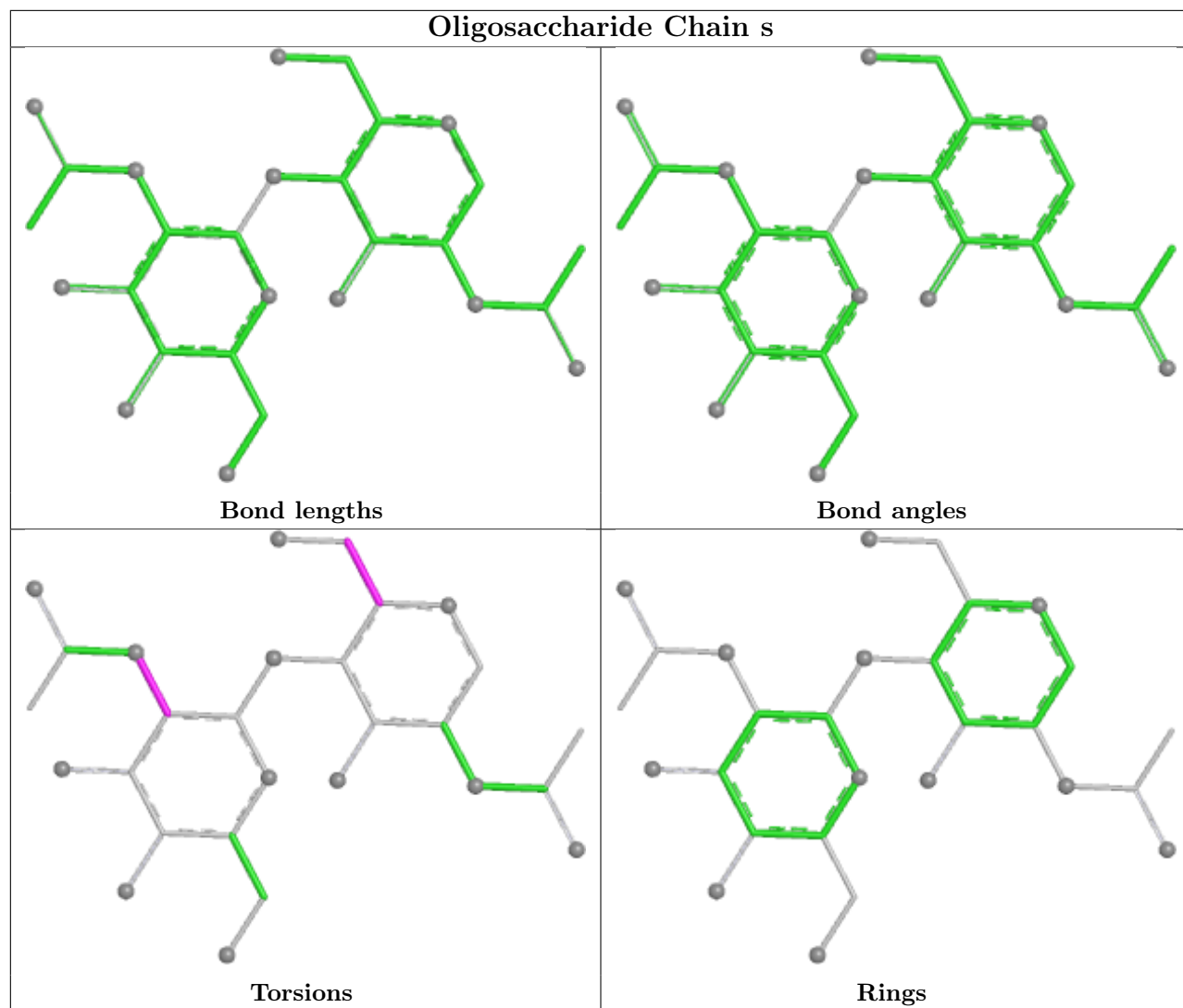


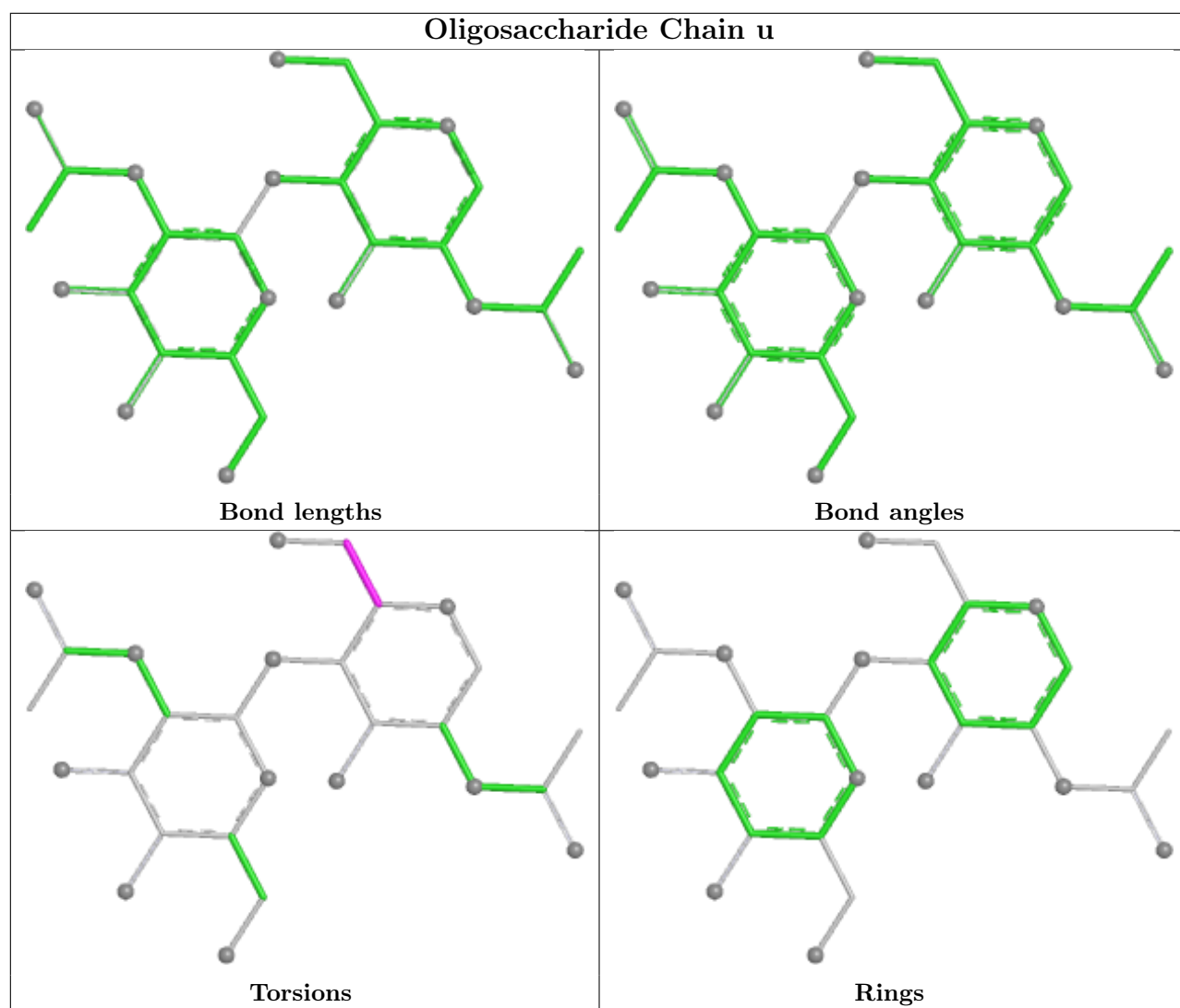


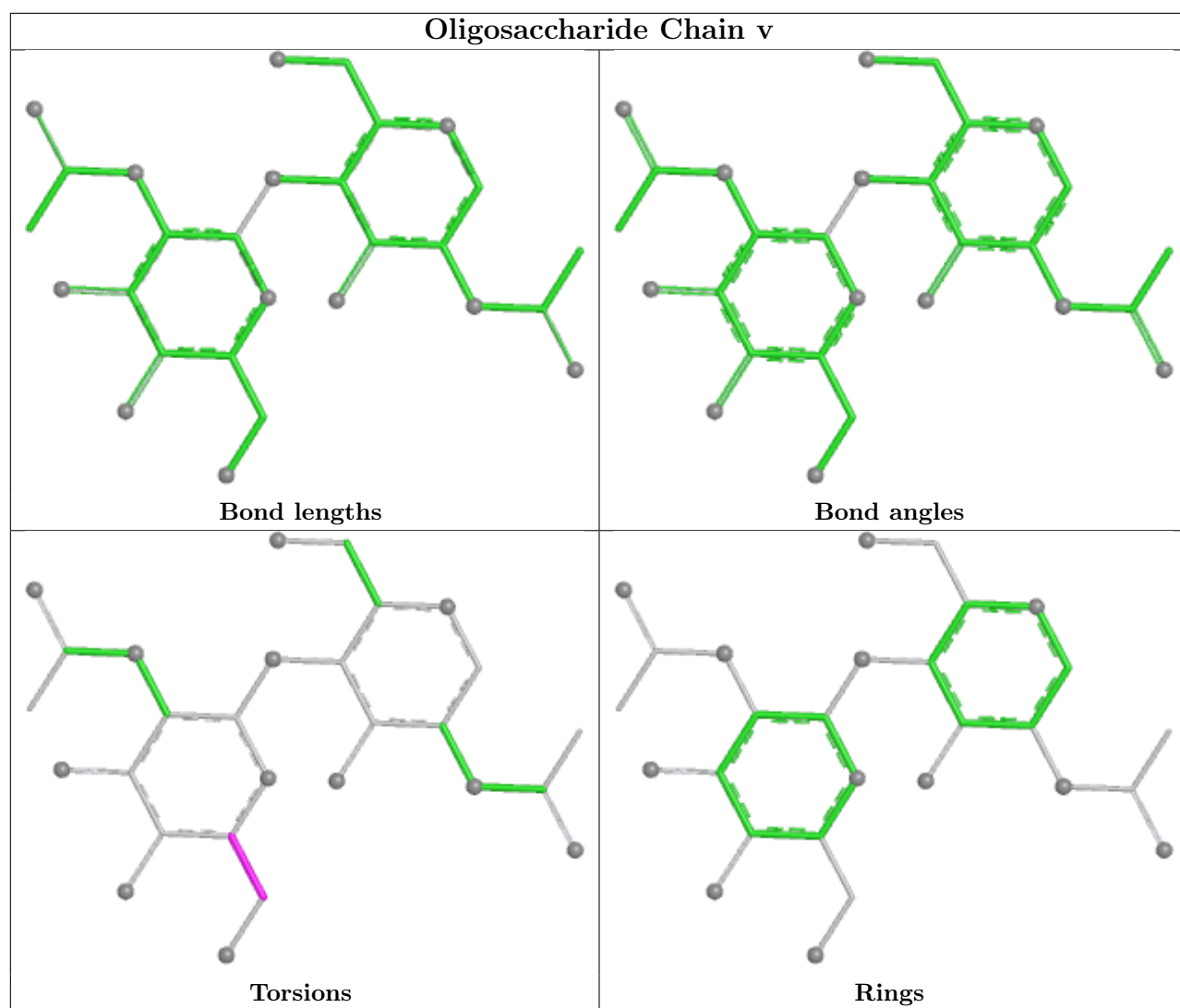


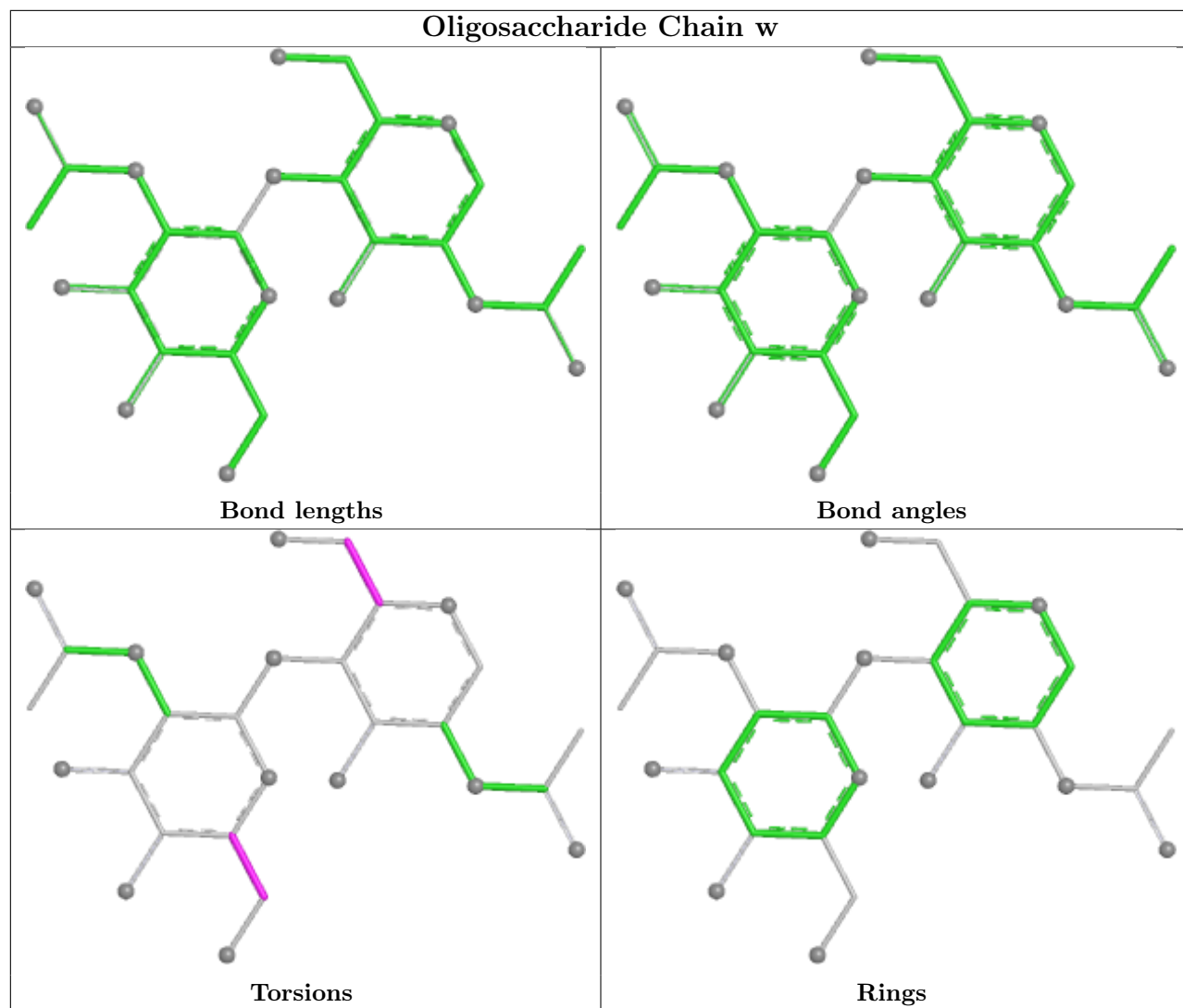


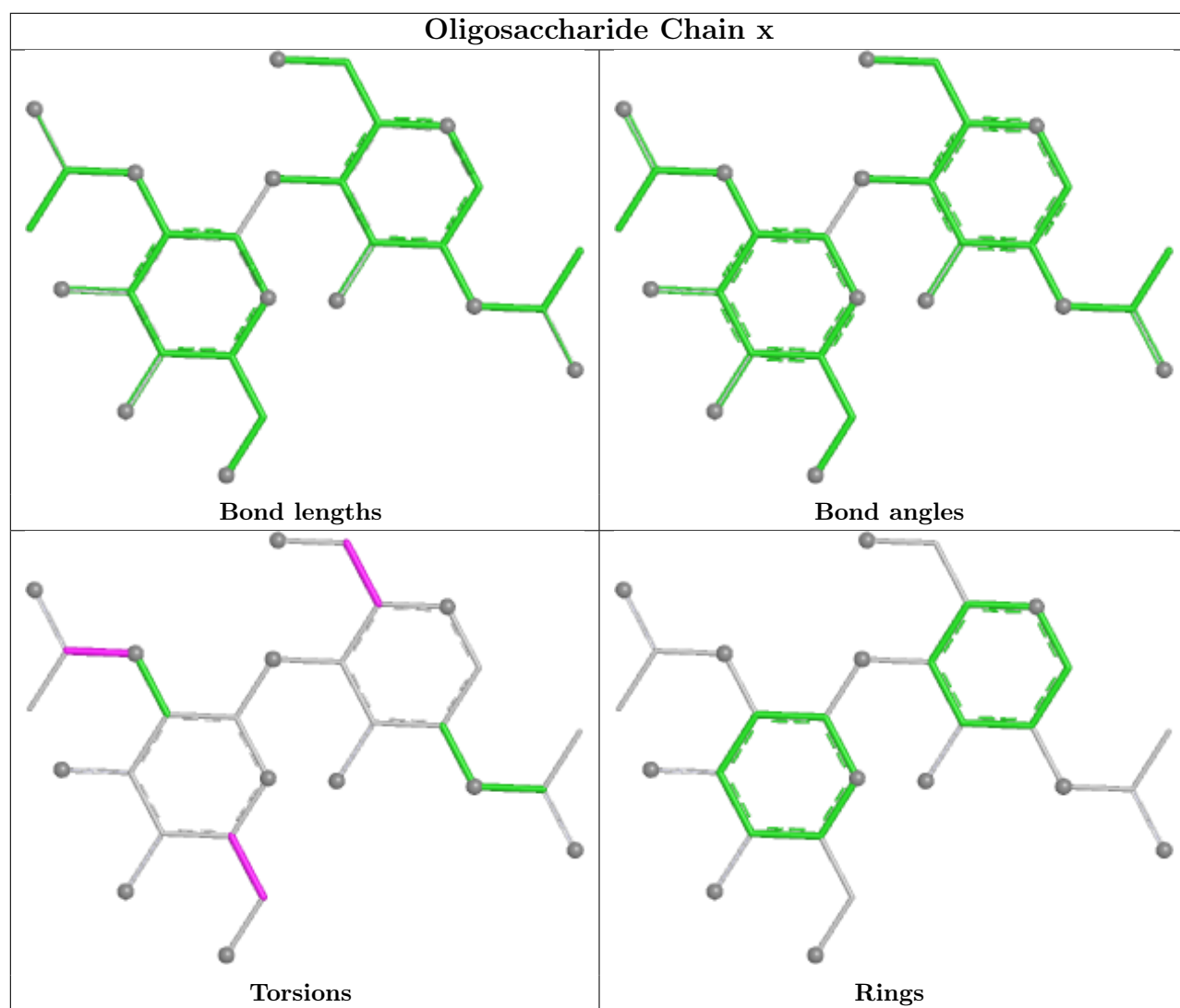


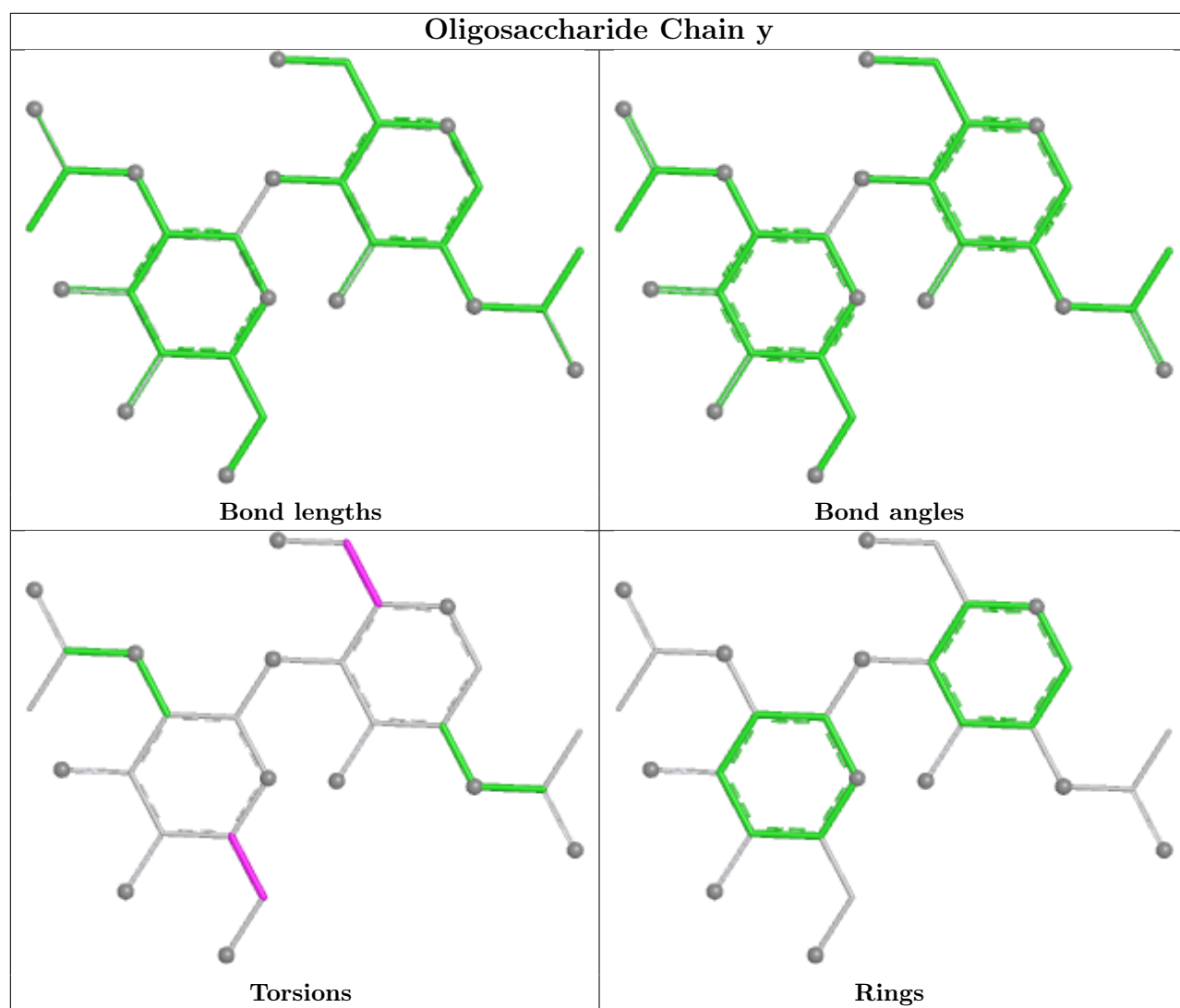


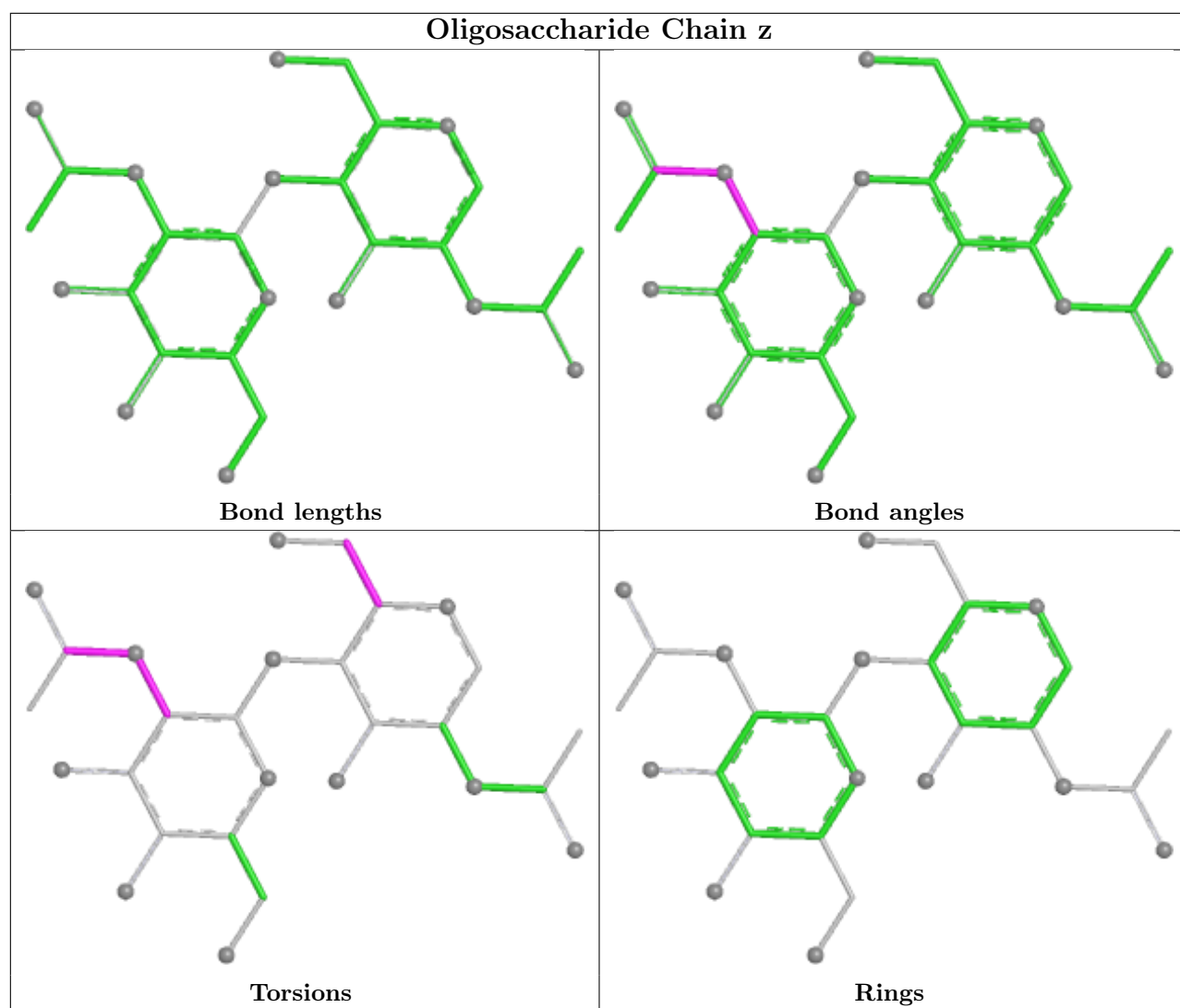


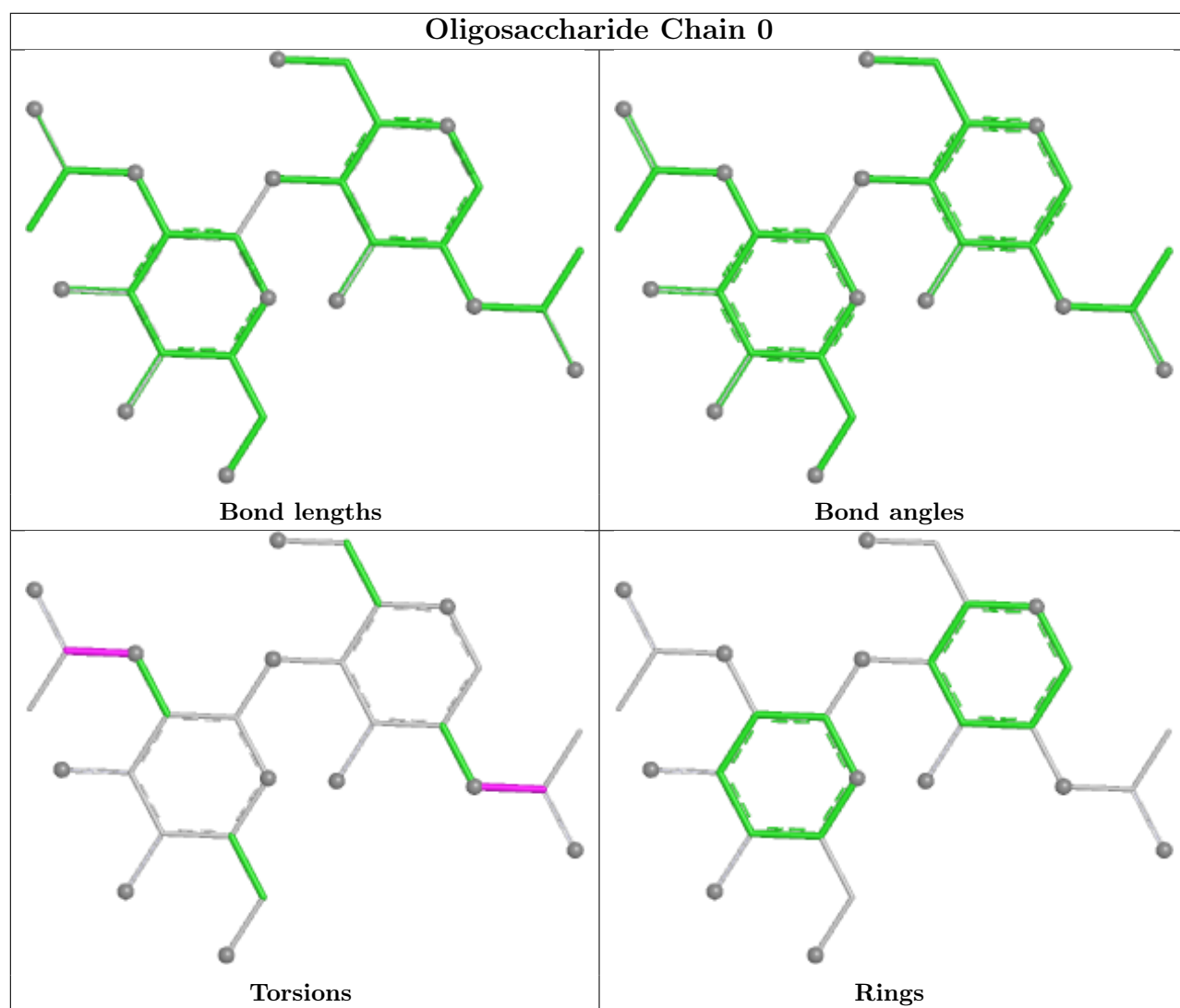


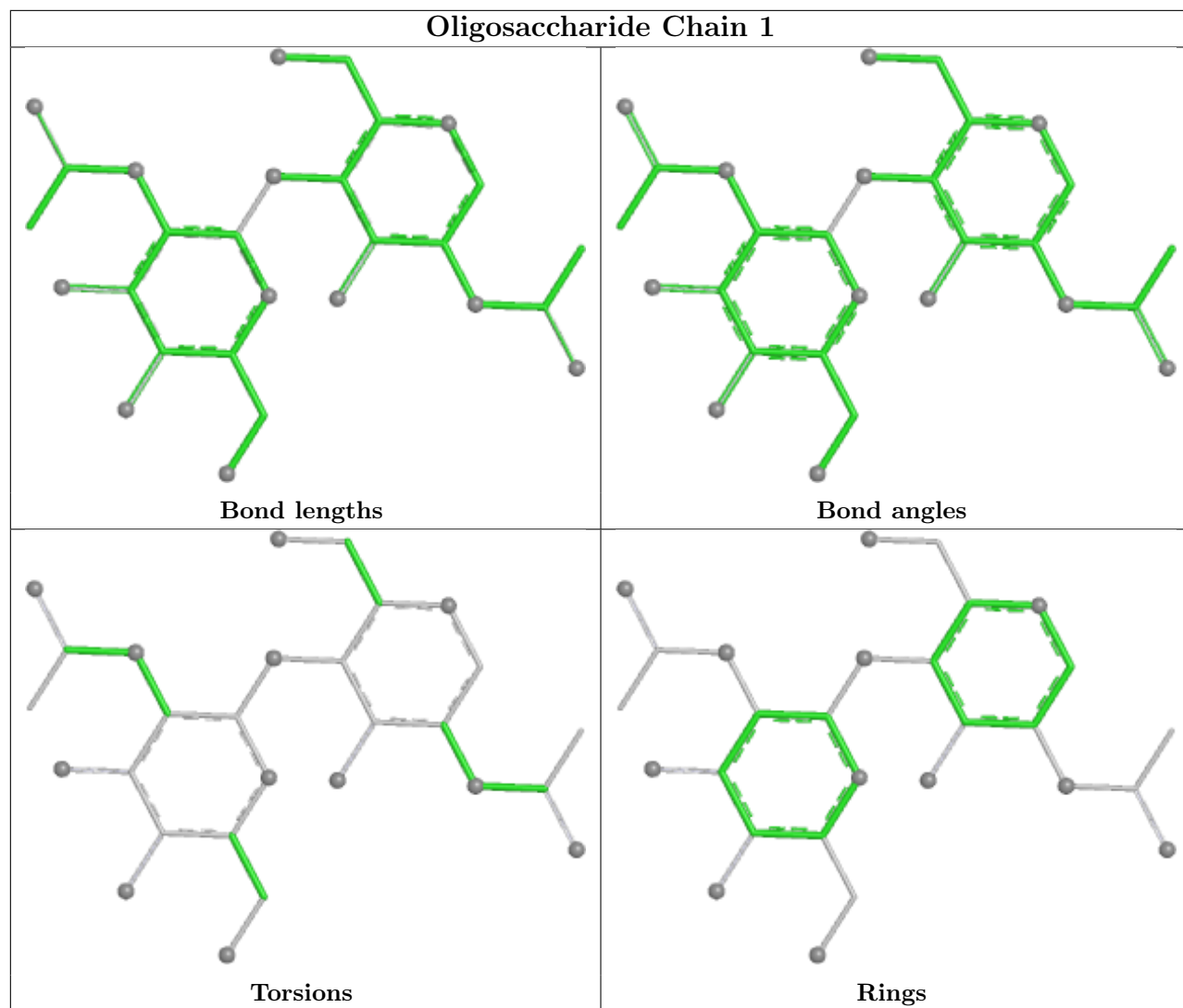


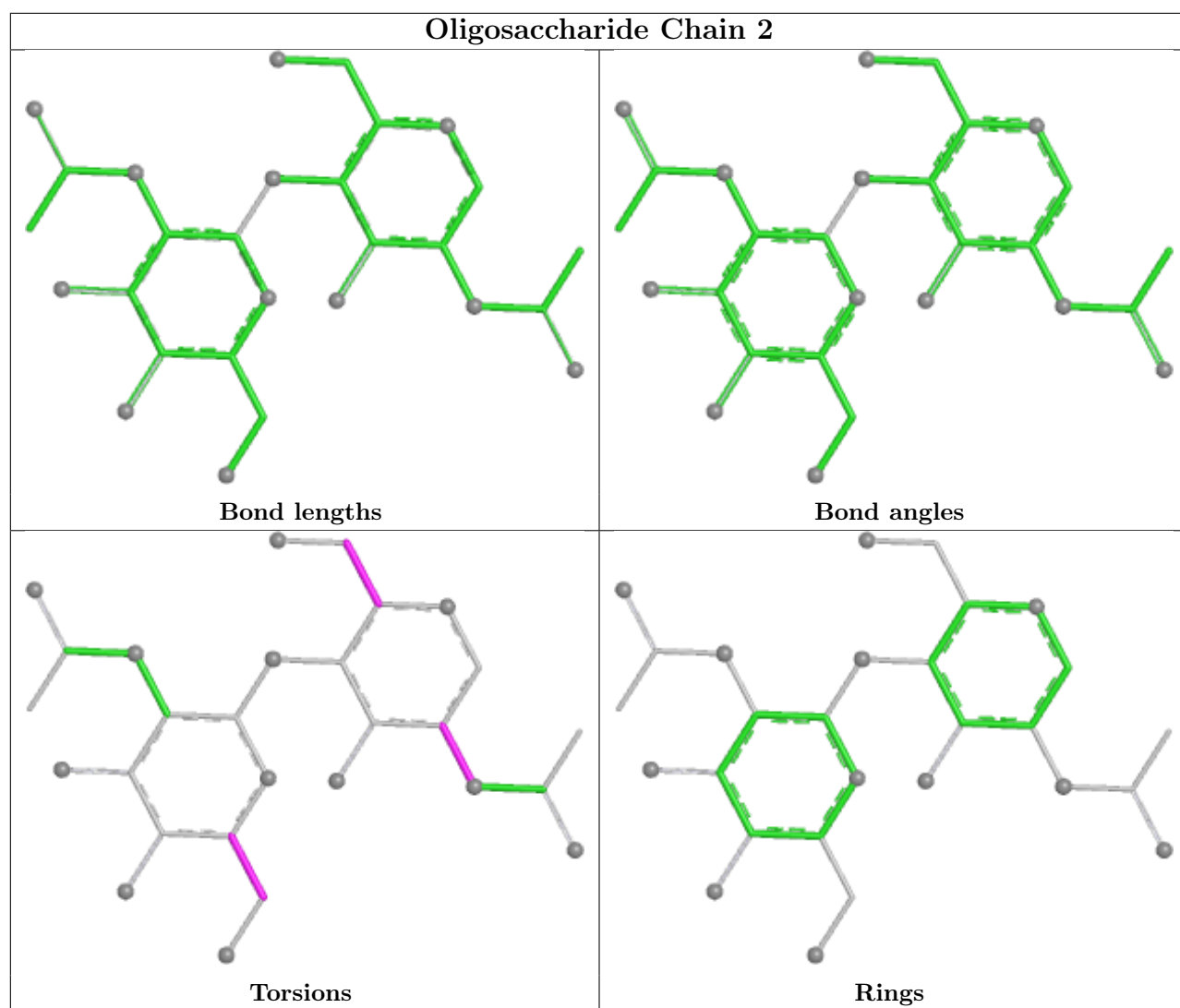


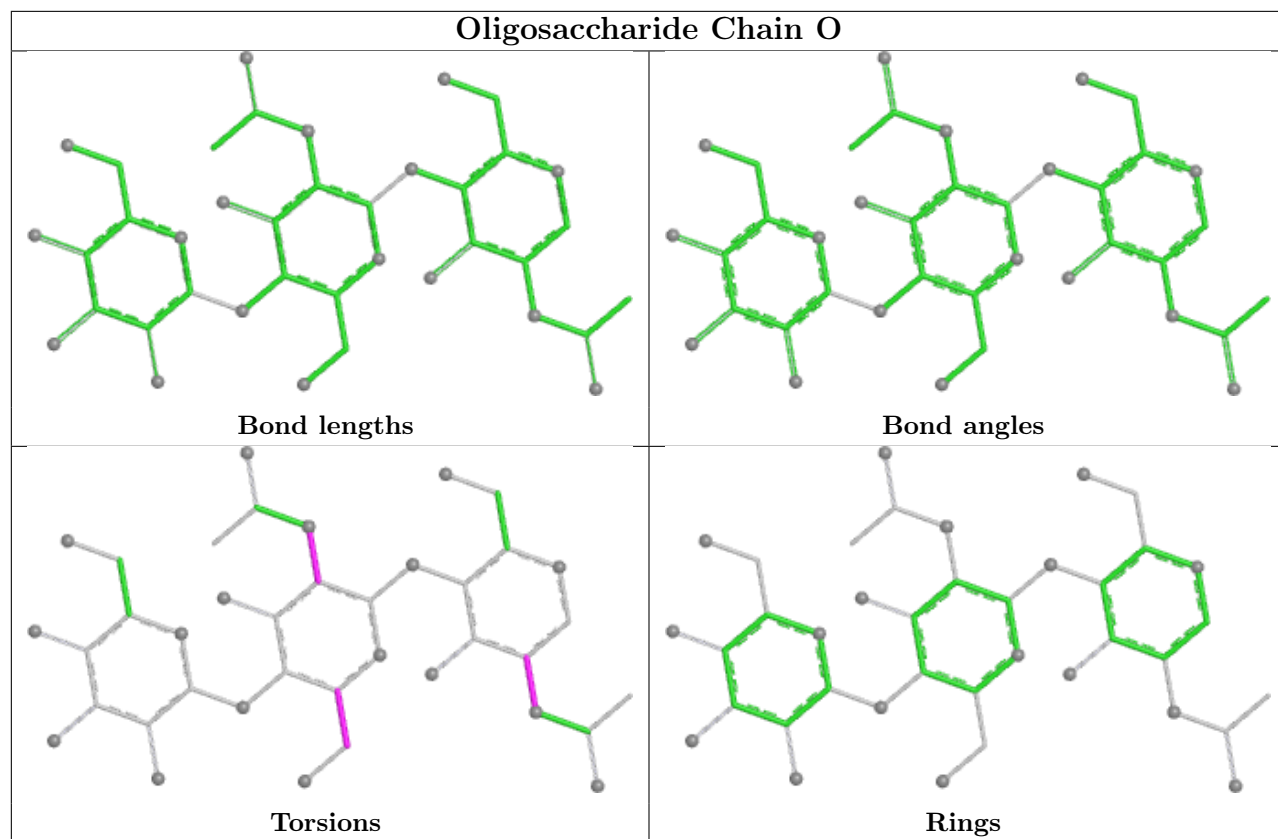


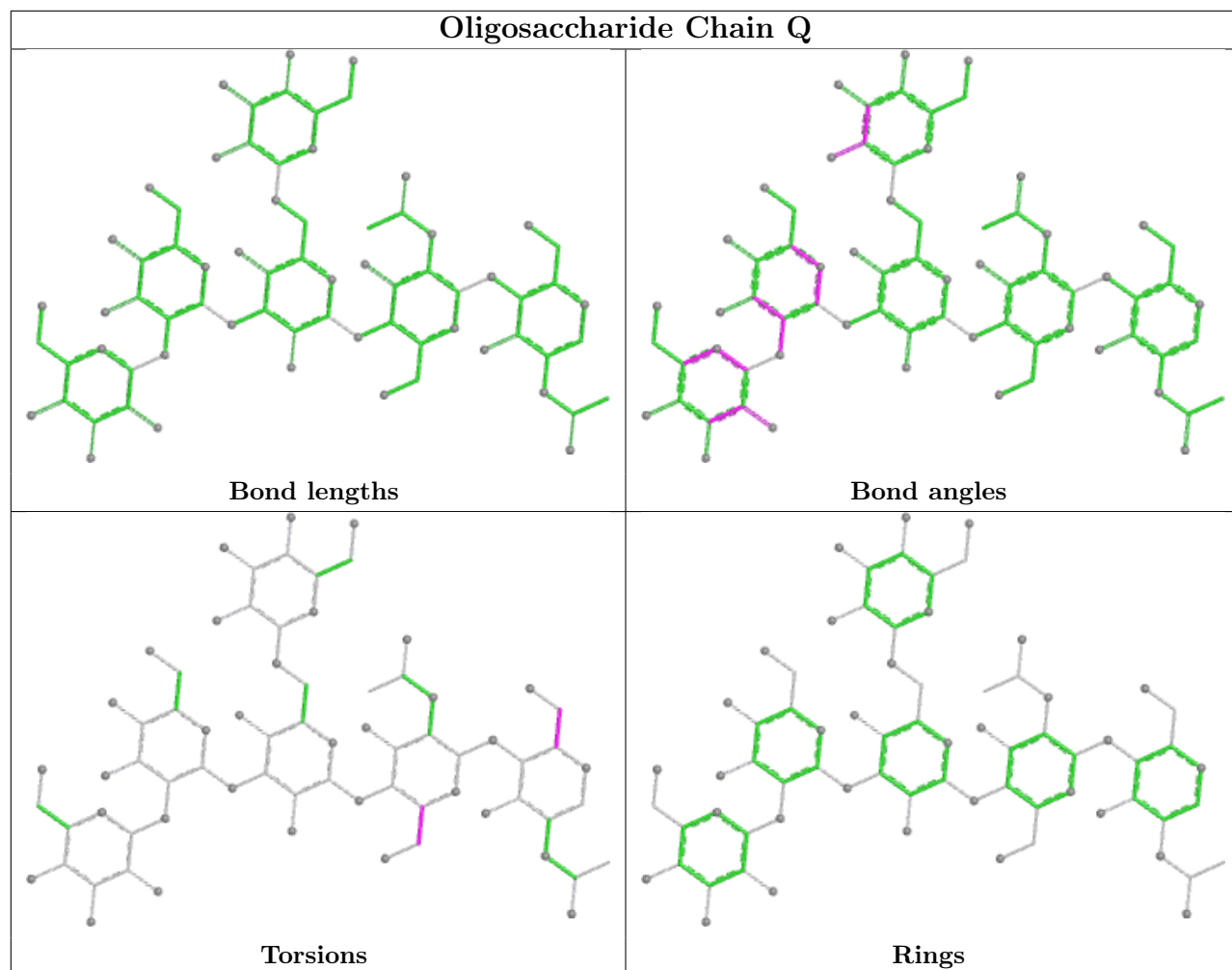


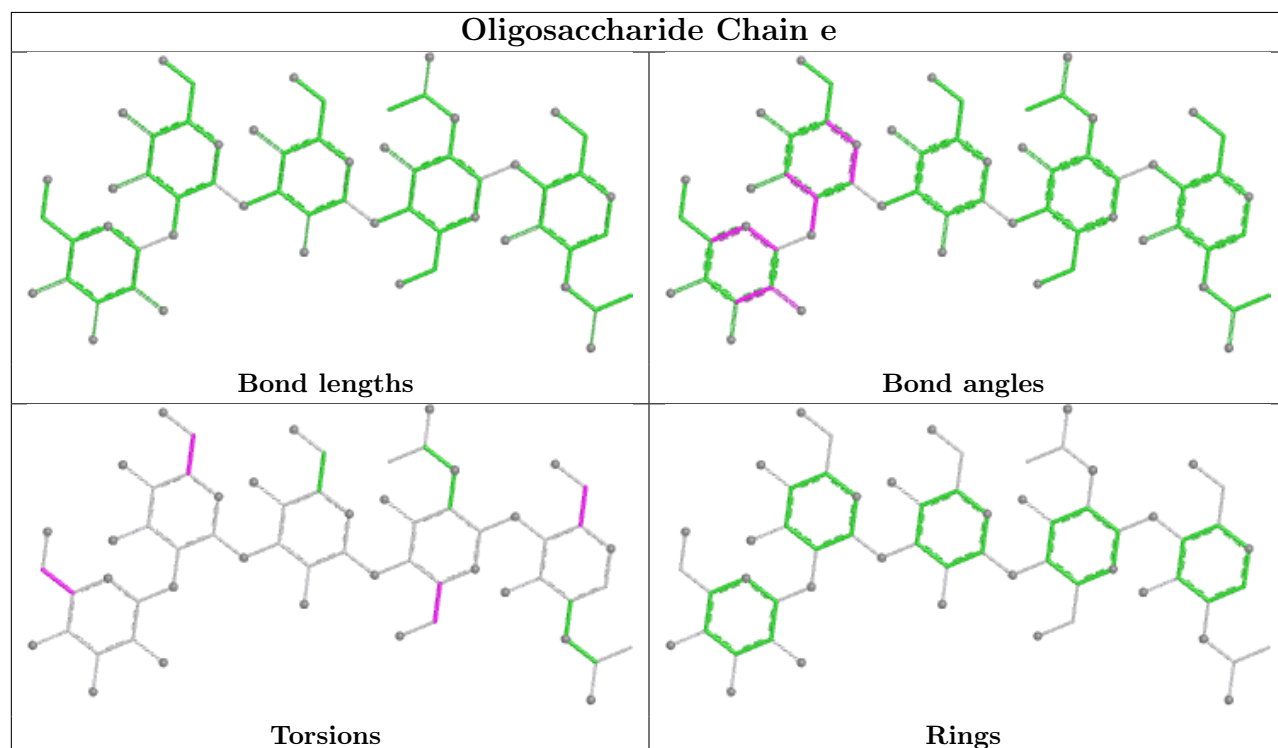
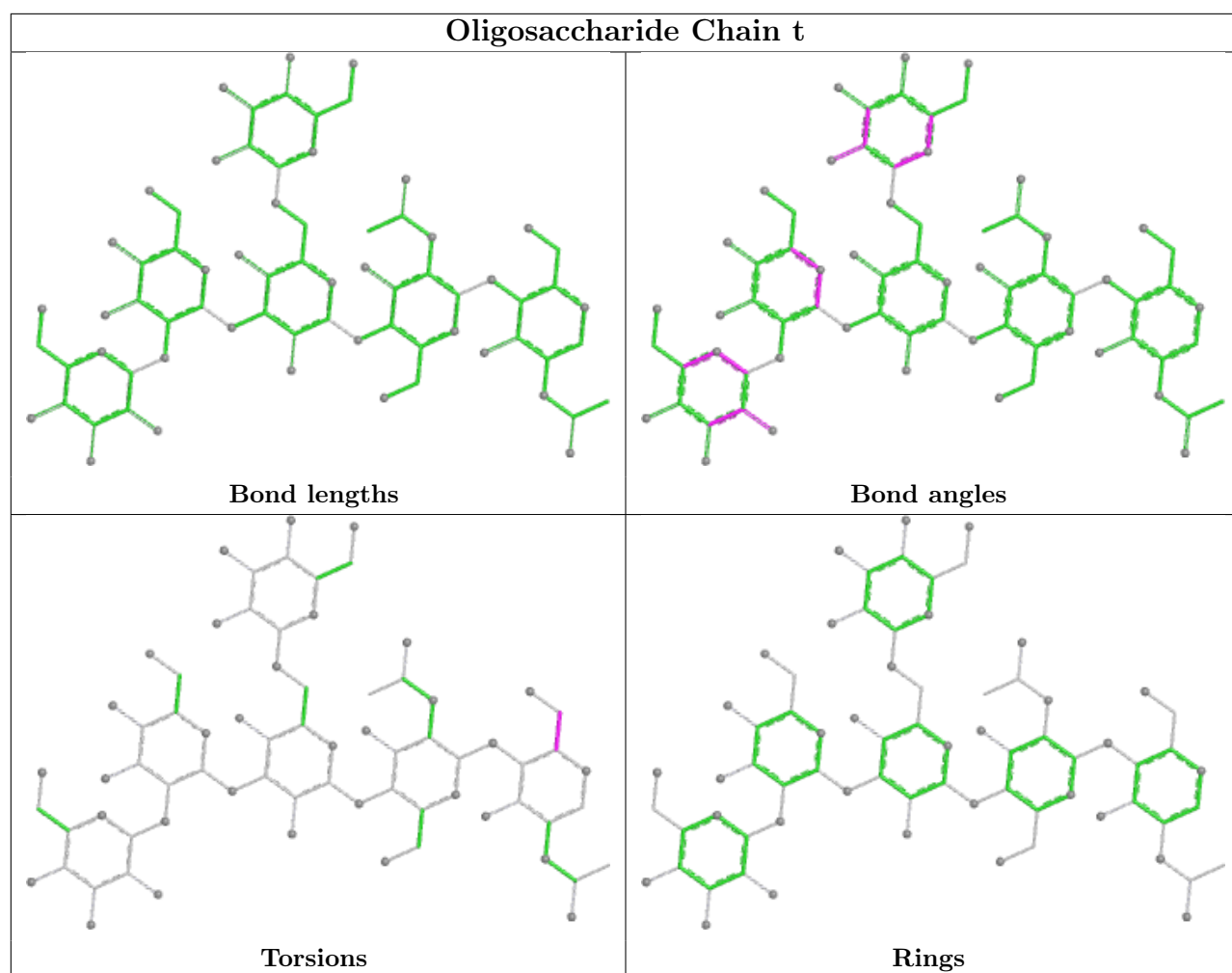












5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	G	601	1	14,14,15	0.17	0	17,19,21	0.53	0
10	NAG	C	601	1	14,14,15	0.19	0	17,19,21	0.53	0
10	NAG	G	602	1	14,14,15	0.18	0	17,19,21	0.48	0
10	NAG	B	701	2	14,14,15	0.32	0	17,19,21	0.48	0
10	NAG	A	701	2	14,14,15	0.23	0	17,19,21	0.43	0
10	NAG	G	603	1	14,14,15	0.18	0	17,19,21	0.52	0
10	NAG	I	601	1	14,14,15	0.20	0	17,19,21	0.51	0
10	NAG	F	701	2	14,14,15	0.23	0	17,19,21	0.42	0
10	NAG	I	602	1	14,14,15	0.20	0	17,19,21	0.42	0
10	NAG	F	702	2	14,14,15	0.21	0	17,19,21	0.55	0
10	NAG	C	602	1	14,14,15	0.20	0	17,19,21	0.49	0
10	NAG	C	603	1	14,14,15	0.23	0	17,19,21	0.45	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	G	601	1	-	2/6/23/26	0/1/1/1
10	NAG	C	601	1	-	4/6/23/26	0/1/1/1
10	NAG	G	602	1	-	2/6/23/26	0/1/1/1
10	NAG	B	701	2	-	2/6/23/26	0/1/1/1
10	NAG	A	701	2	-	0/6/23/26	0/1/1/1
10	NAG	G	603	1	-	3/6/23/26	0/1/1/1
10	NAG	I	601	1	-	2/6/23/26	0/1/1/1
10	NAG	F	701	2	-	0/6/23/26	0/1/1/1
10	NAG	I	602	1	-	1/6/23/26	0/1/1/1
10	NAG	F	702	2	-	2/6/23/26	0/1/1/1
10	NAG	C	602	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	603	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

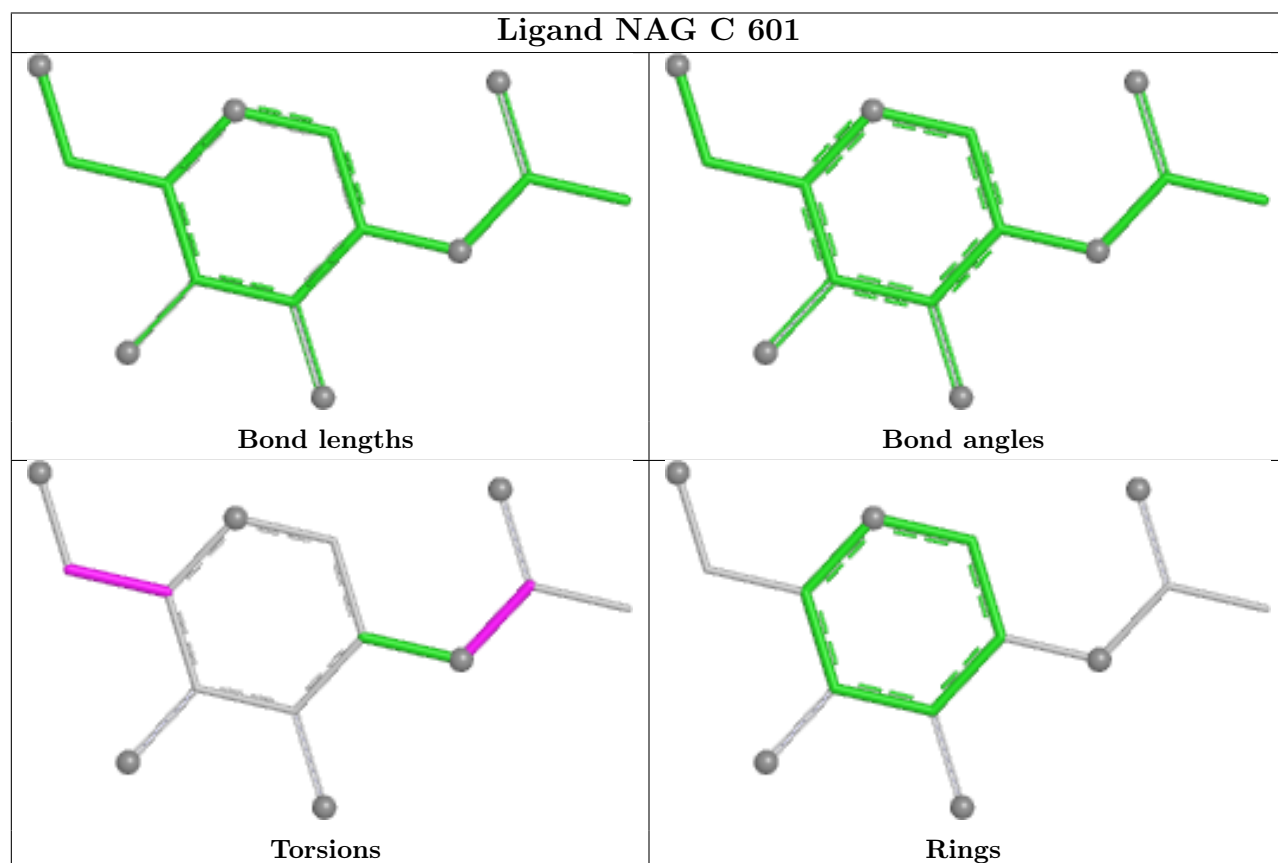
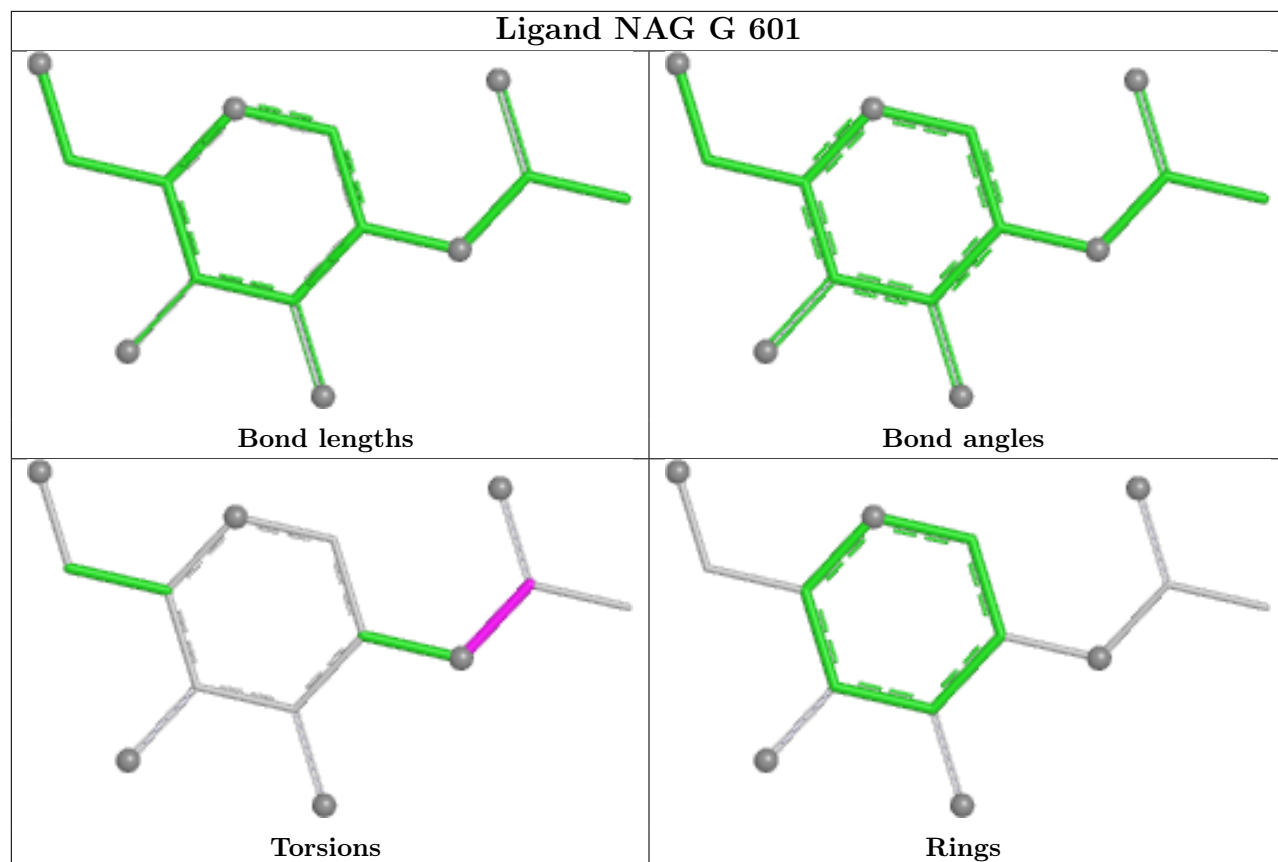
5 of 21 torsion outliers are listed below:

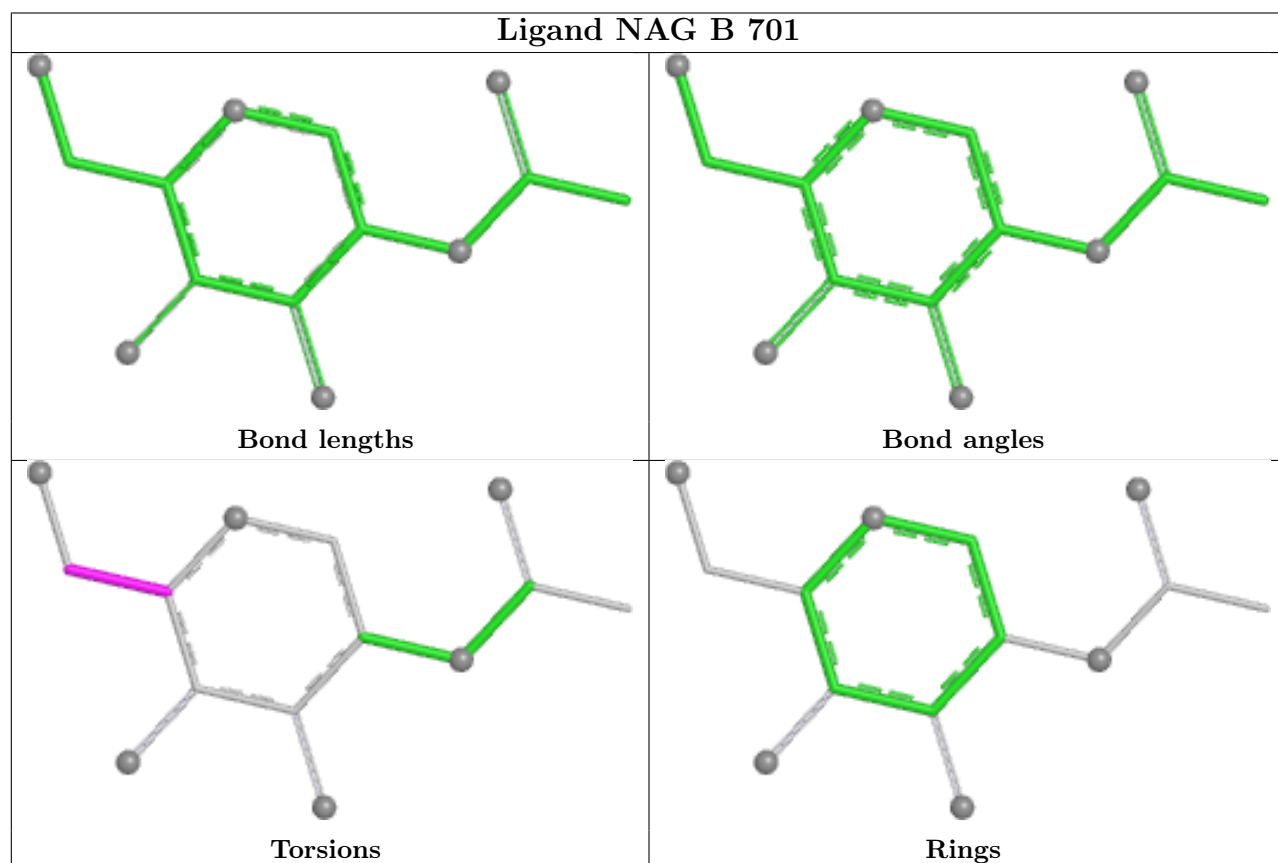
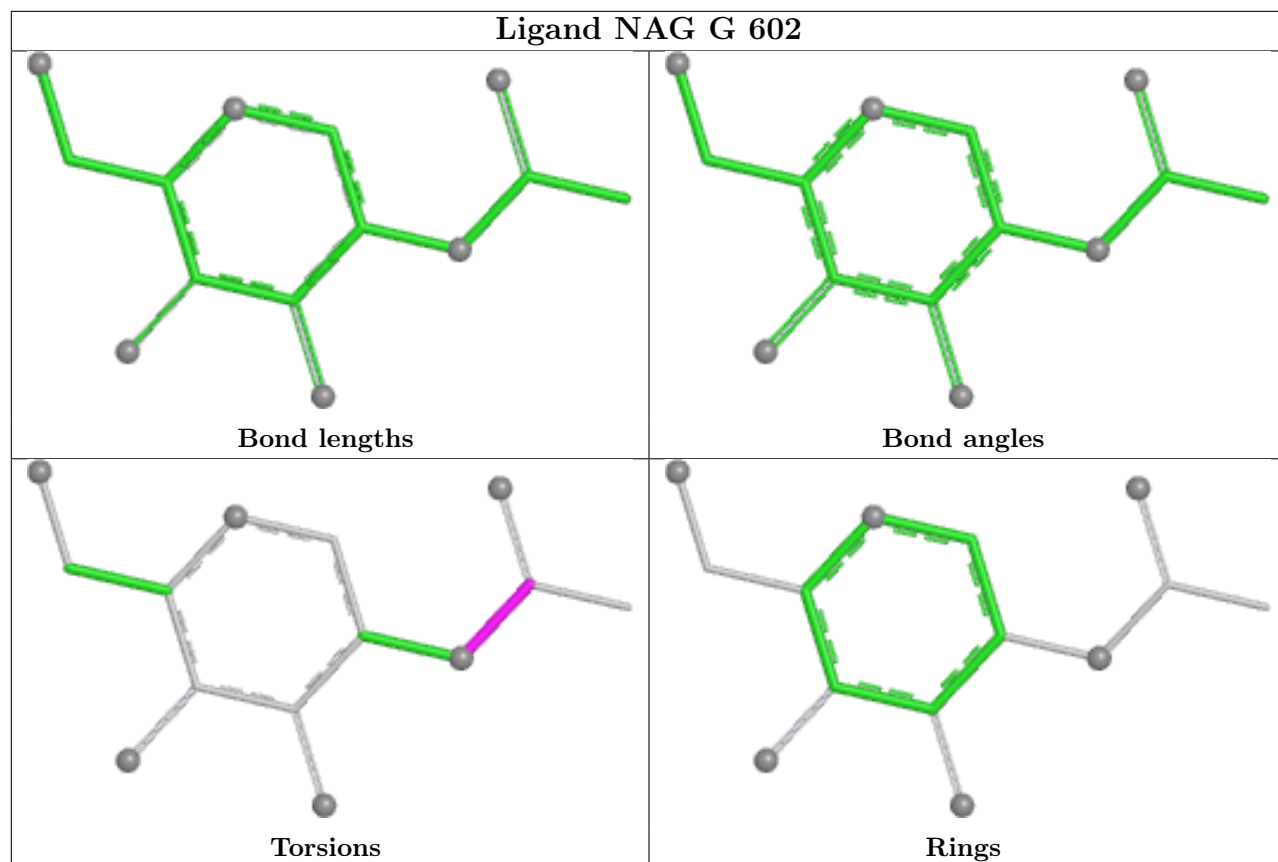
Mol	Chain	Res	Type	Atoms
10	C	601	NAG	C8-C7-N2-C2
10	C	601	NAG	O7-C7-N2-C2
10	C	602	NAG	C8-C7-N2-C2
10	C	602	NAG	O7-C7-N2-C2
10	G	601	NAG	C8-C7-N2-C2

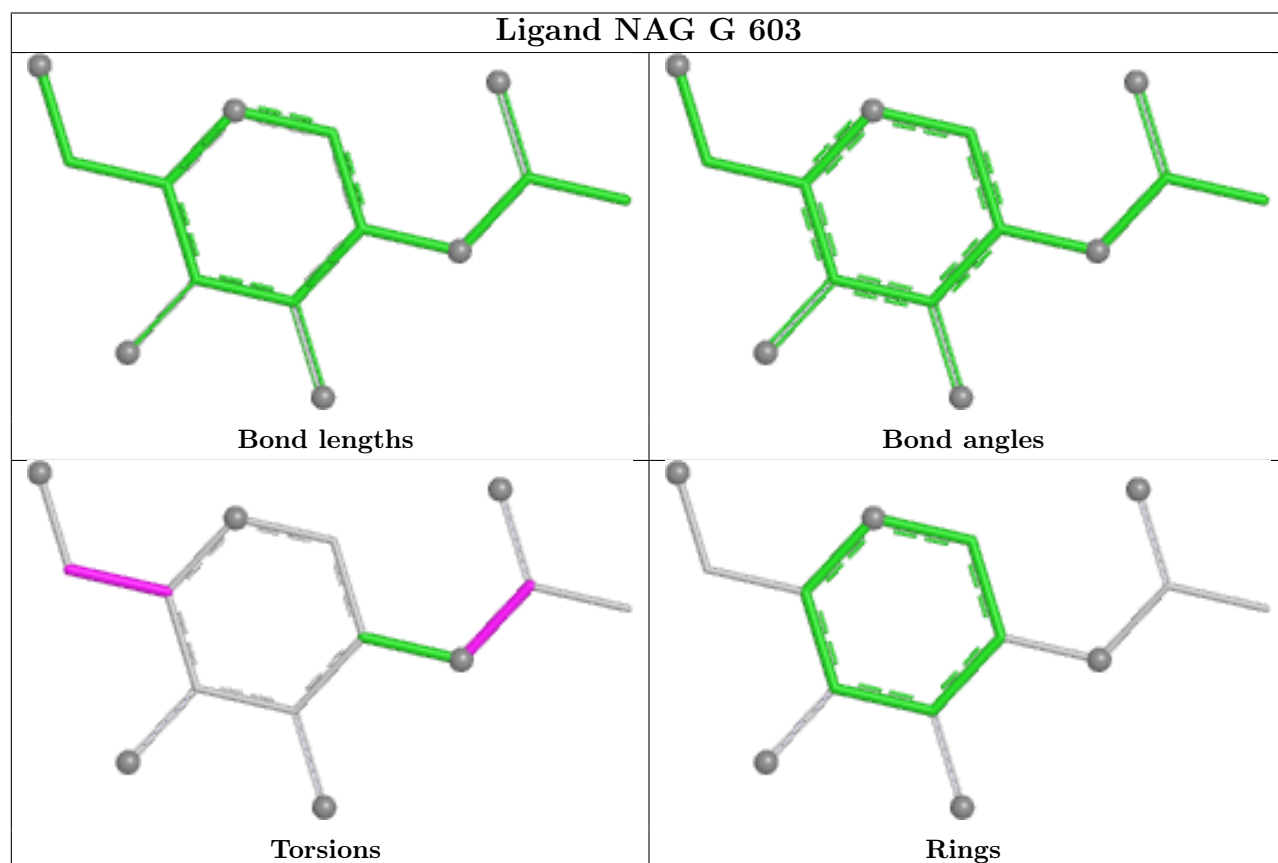
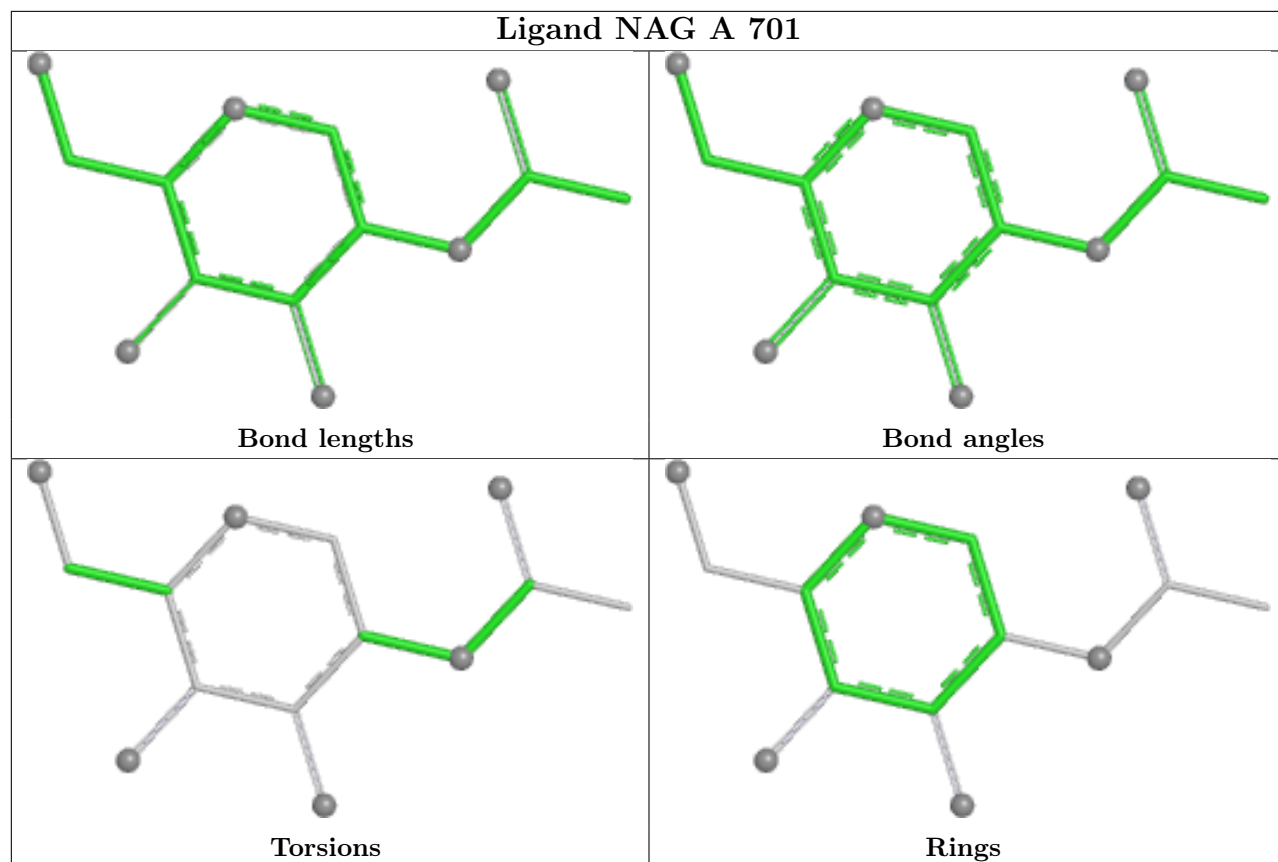
There are no ring outliers.

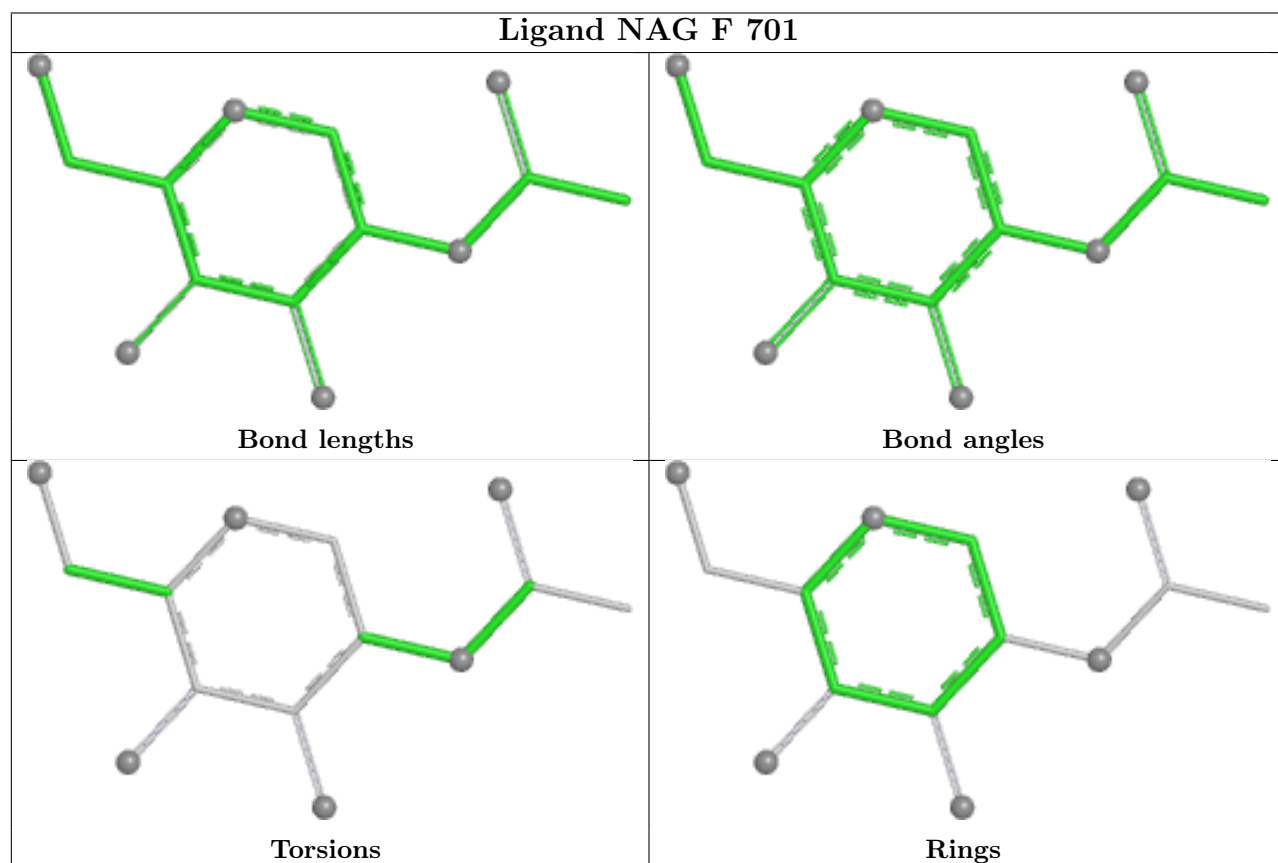
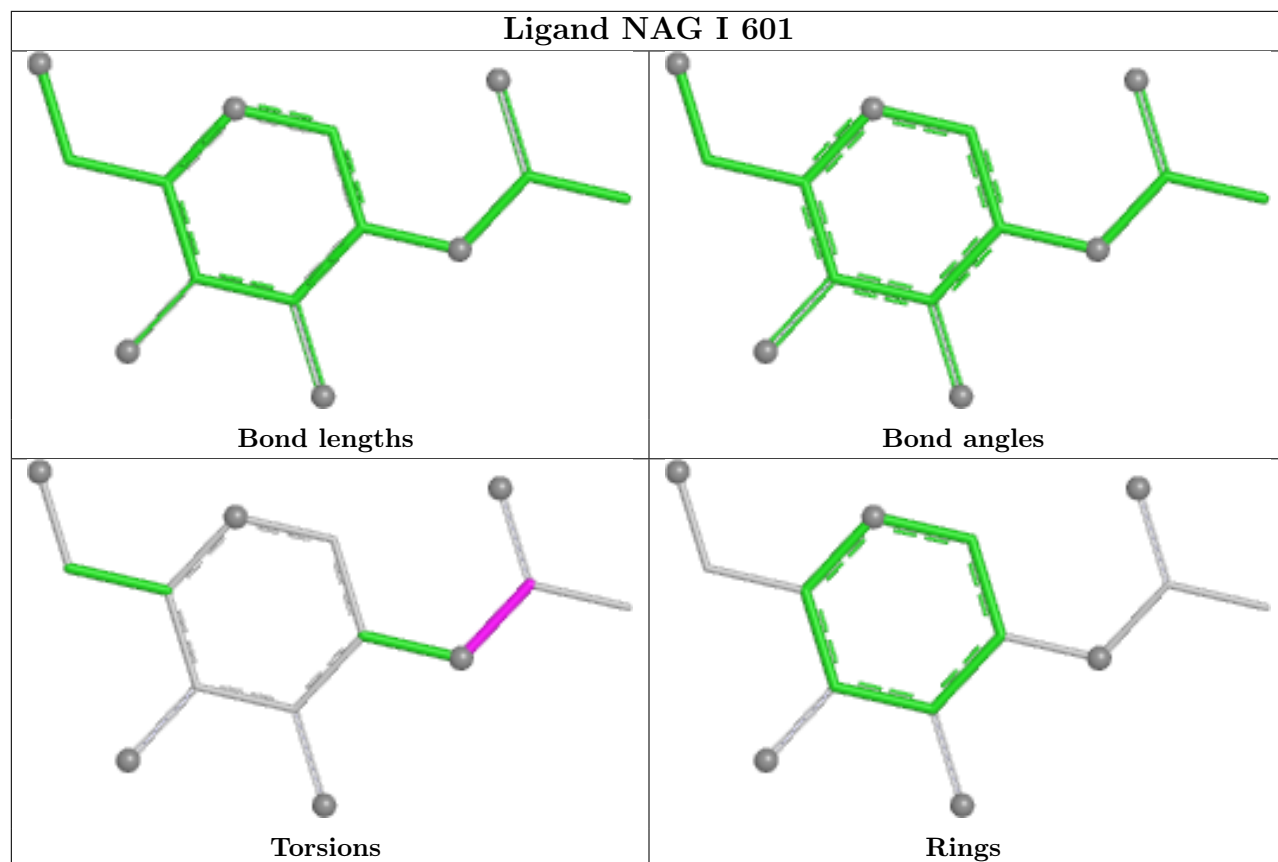
No monomer is involved in short contacts.

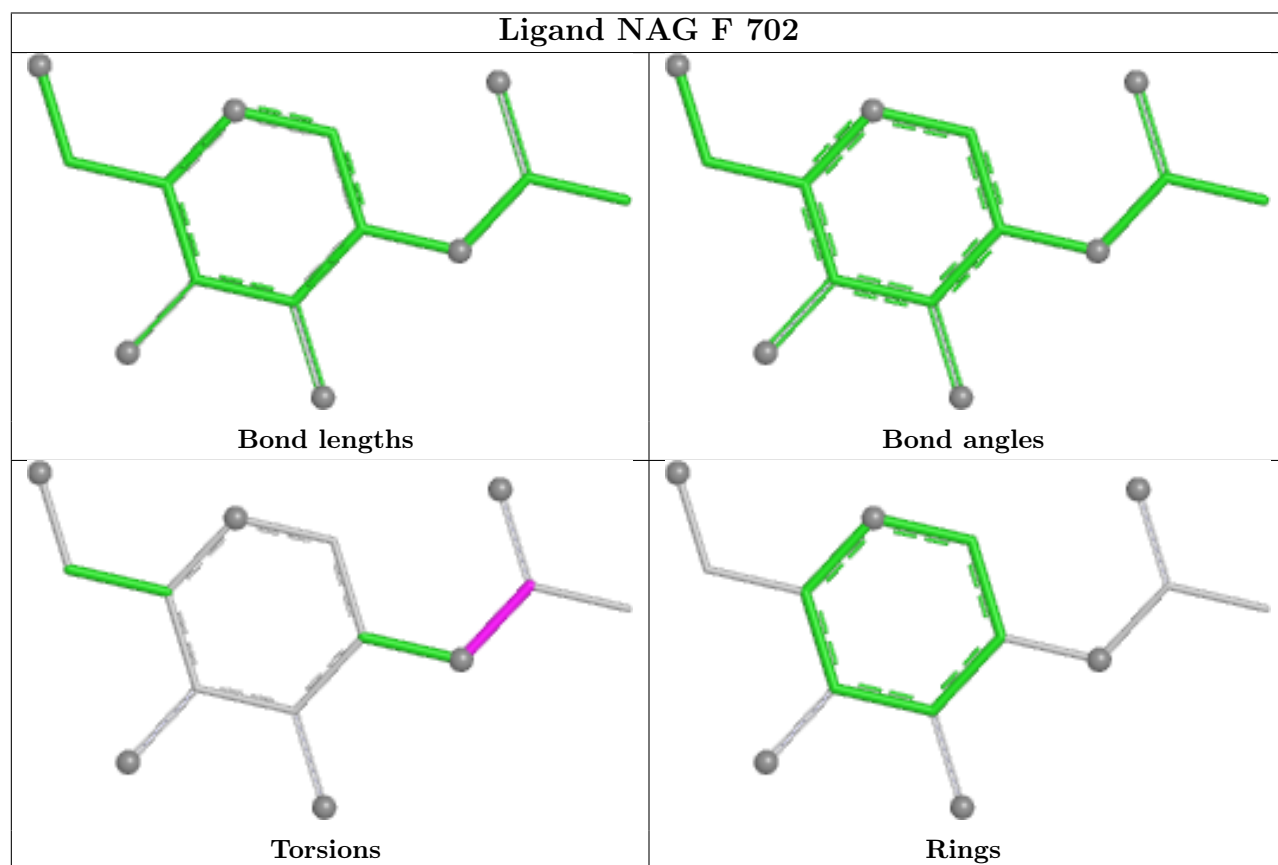
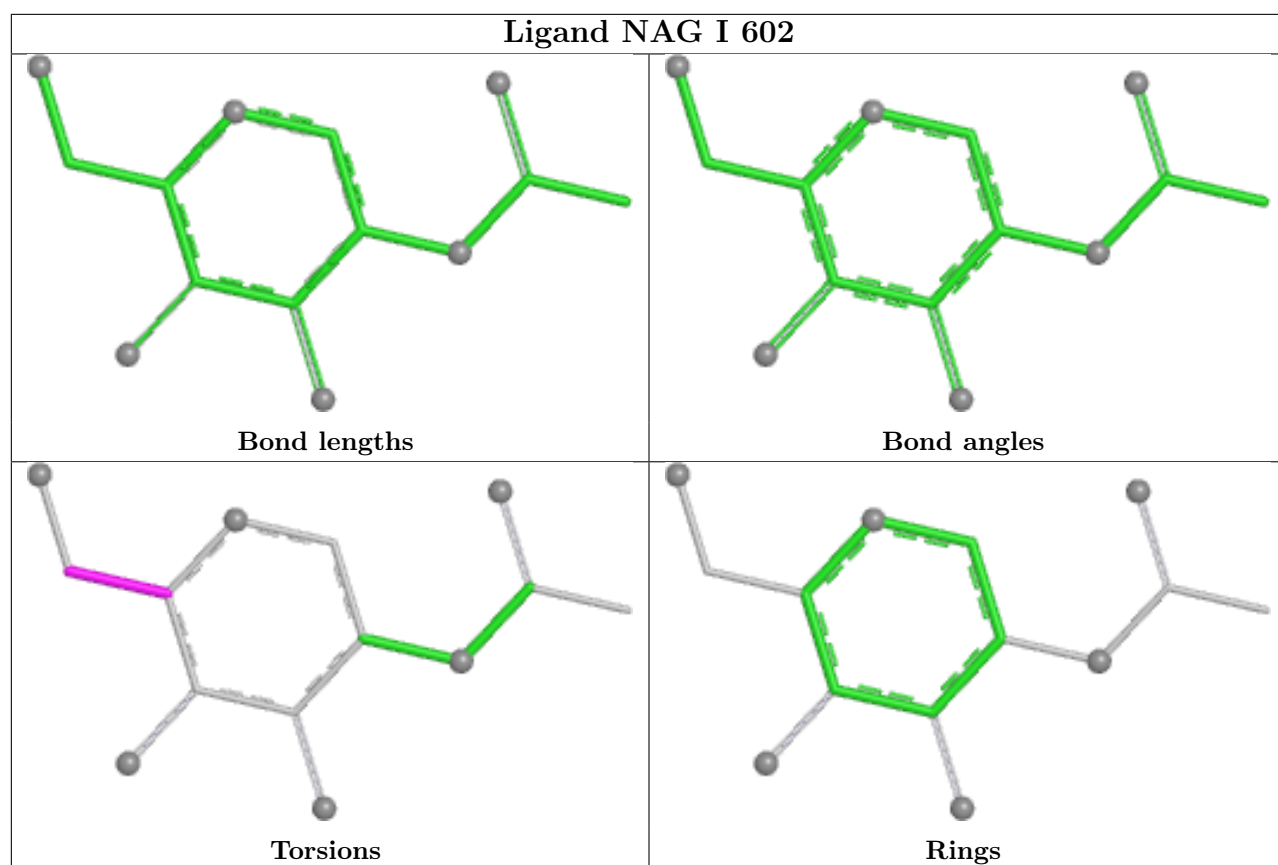
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

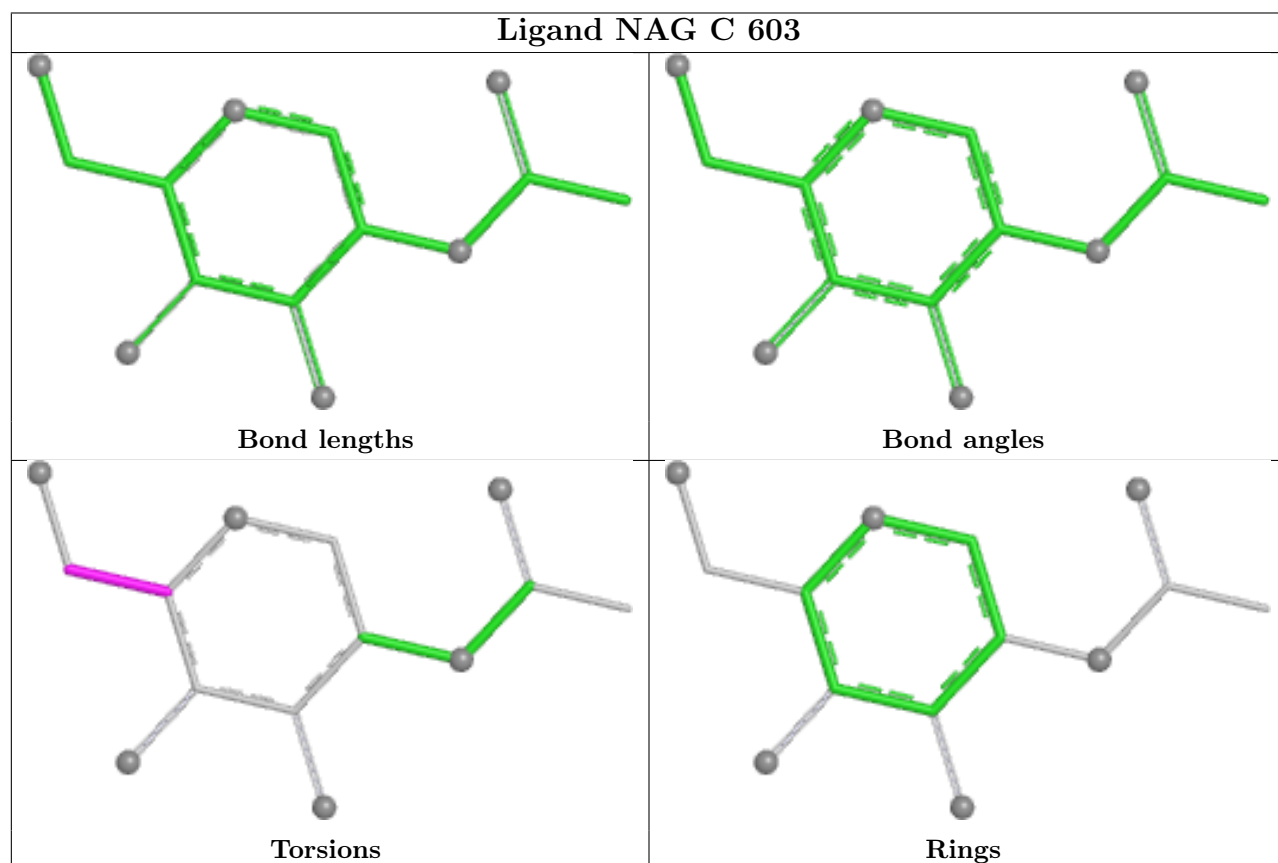
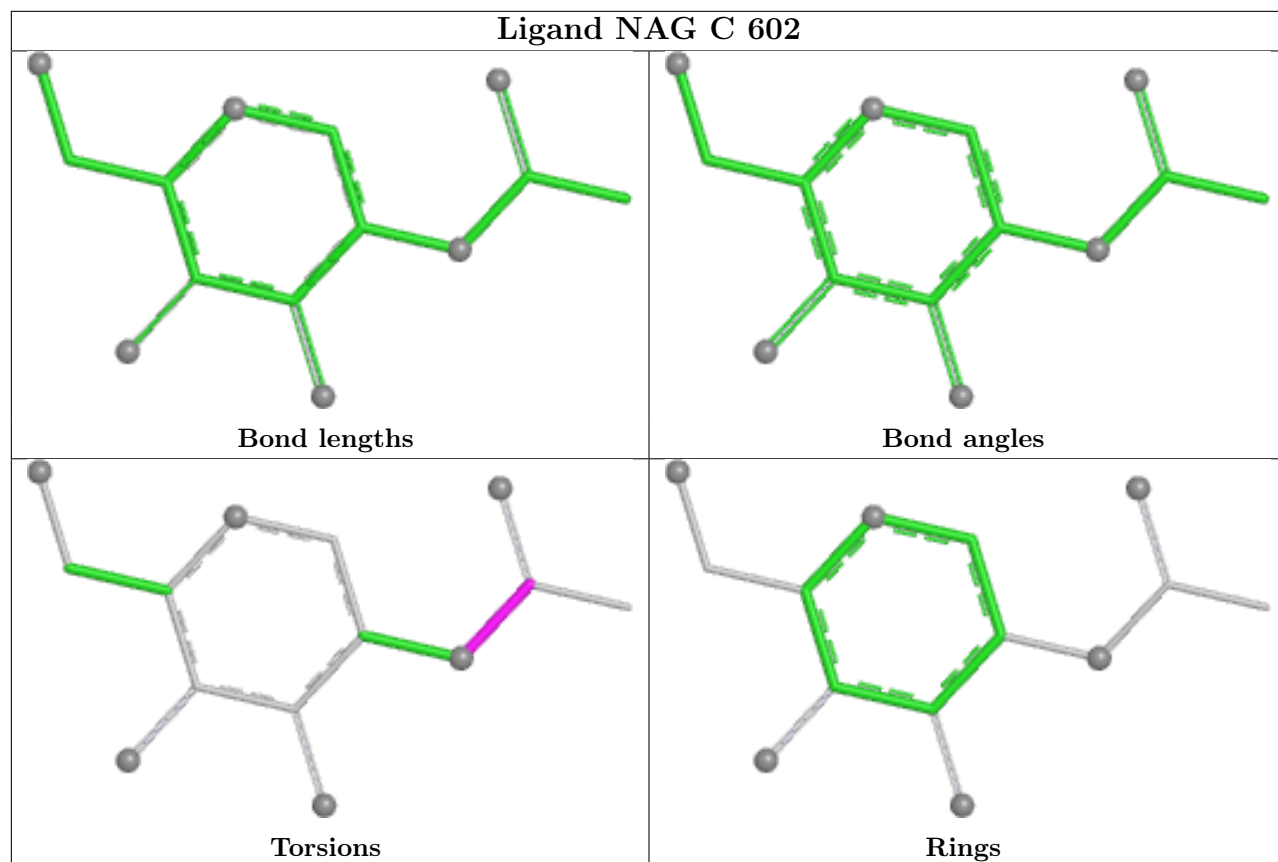












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

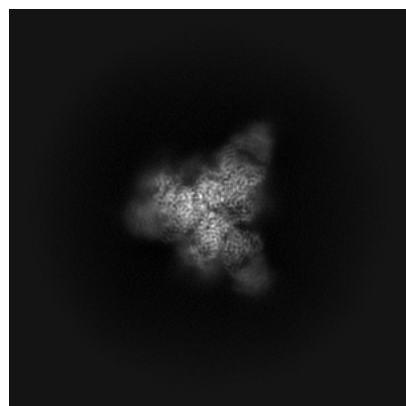
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29725. These allow visual inspection of the internal detail of the map and identification of artifacts.

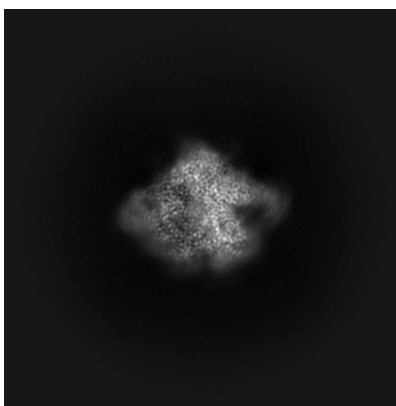
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

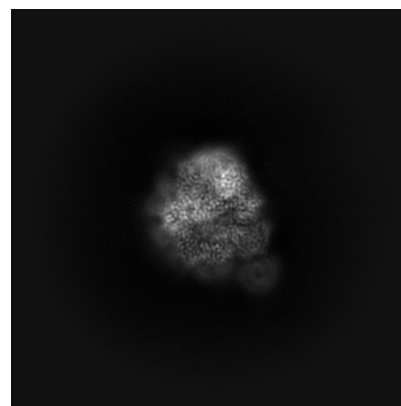
6.1.1 Primary map



X

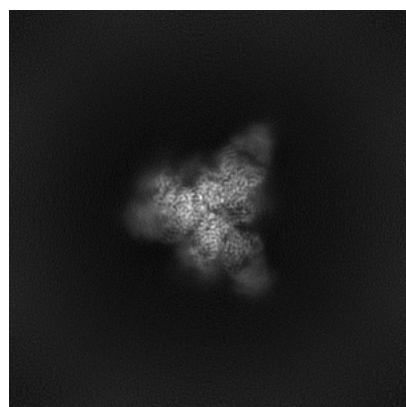


Y

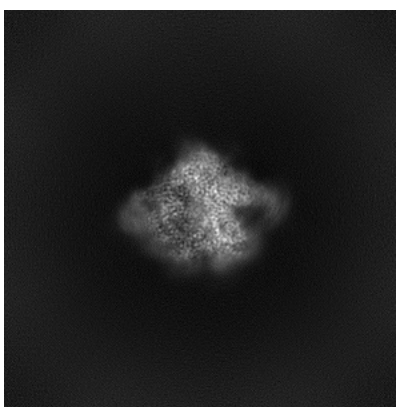


Z

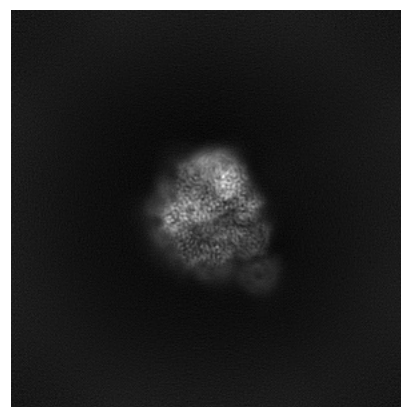
6.1.2 Raw map



X



Y

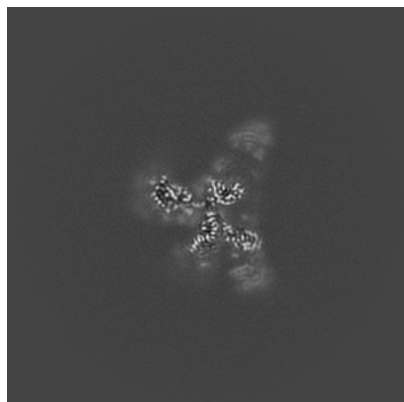


Z

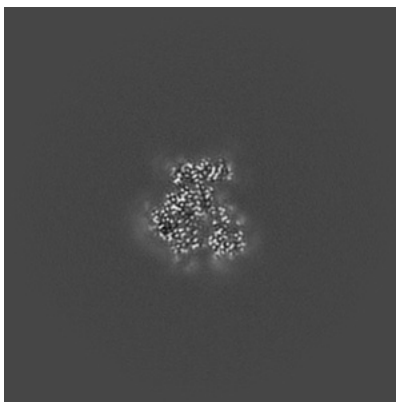
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

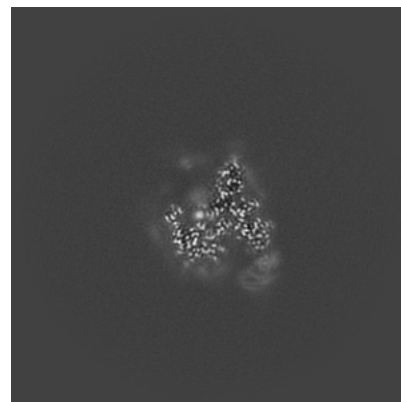
6.2.1 Primary map



X Index: 240

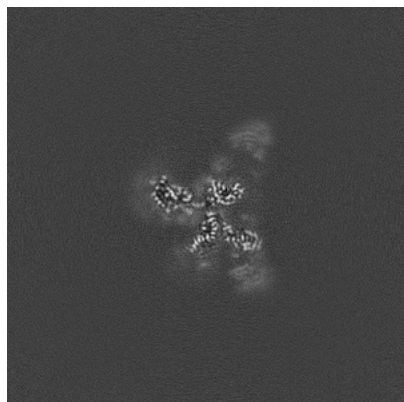


Y Index: 240

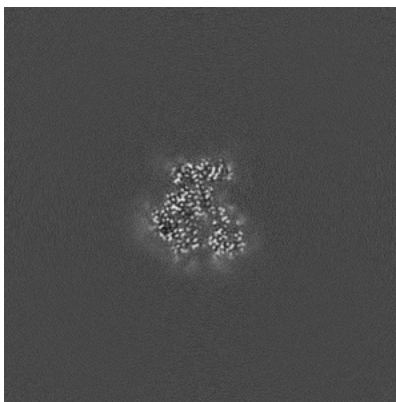


Z Index: 240

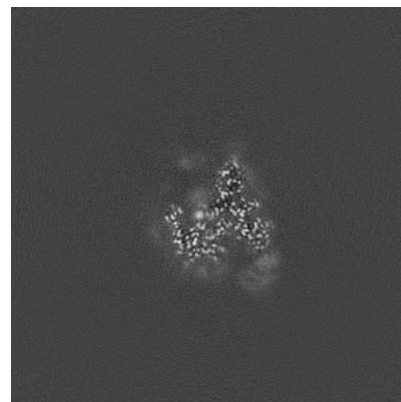
6.2.2 Raw map



X Index: 240



Y Index: 240

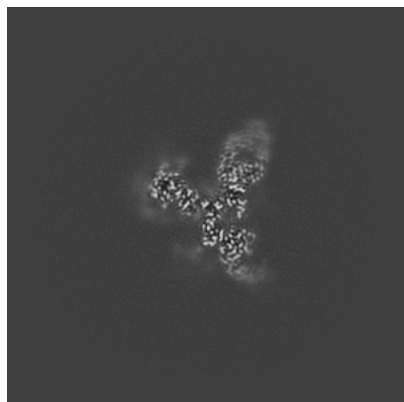


Z Index: 240

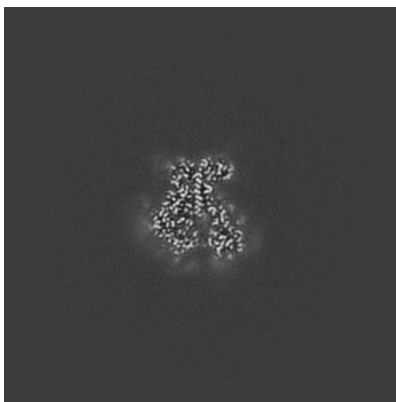
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

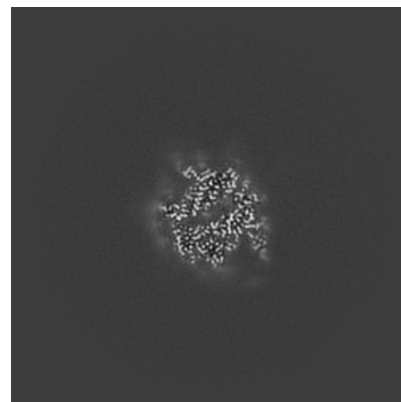
6.3.1 Primary map



X Index: 253

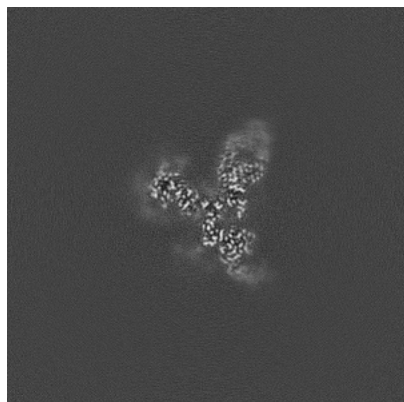


Y Index: 242

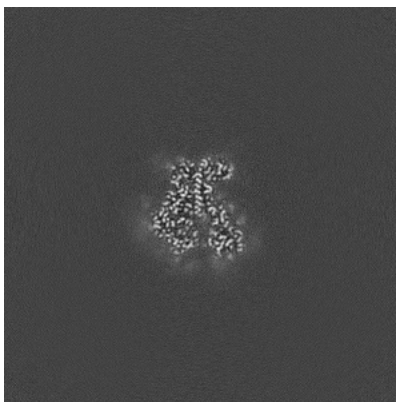


Z Index: 253

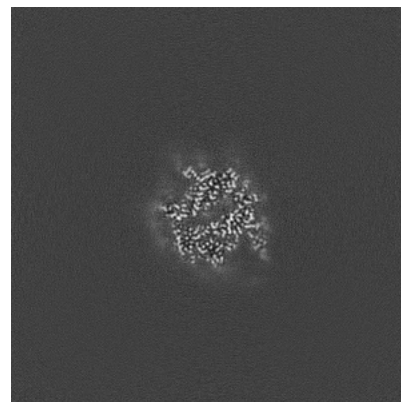
6.3.2 Raw map



X Index: 253



Y Index: 242

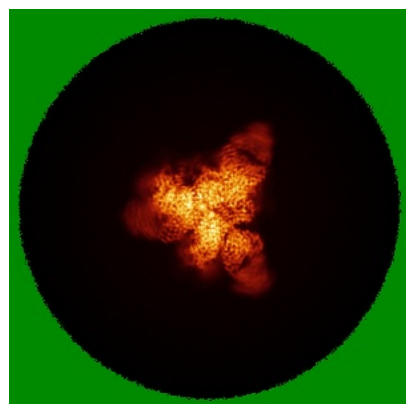


Z Index: 253

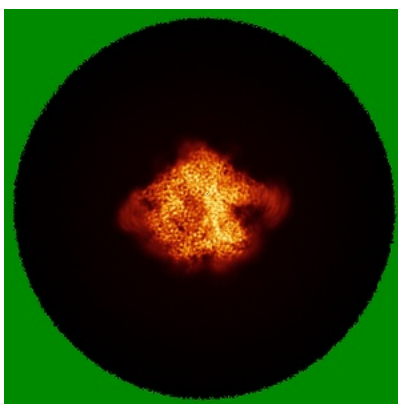
The images above show the largest variance slices of the map in three orthogonal directions.

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

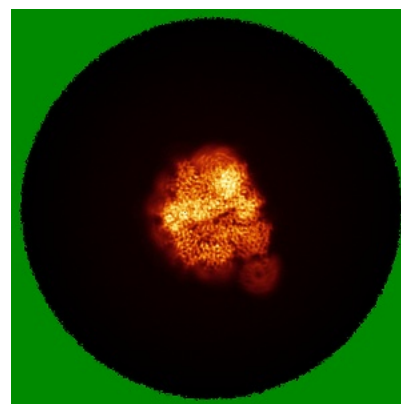
6.4.1 Primary map



X

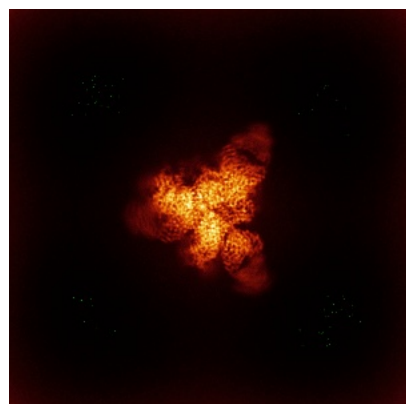


Y

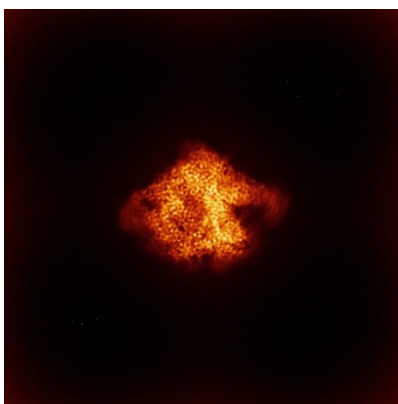


Z

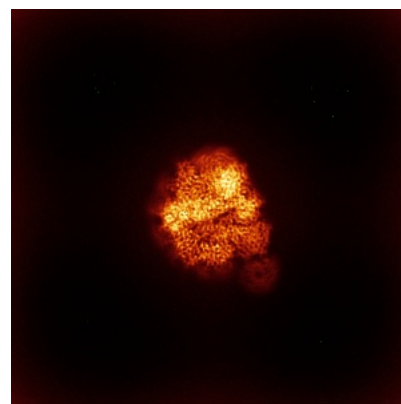
6.4.2 Raw map



X



Y

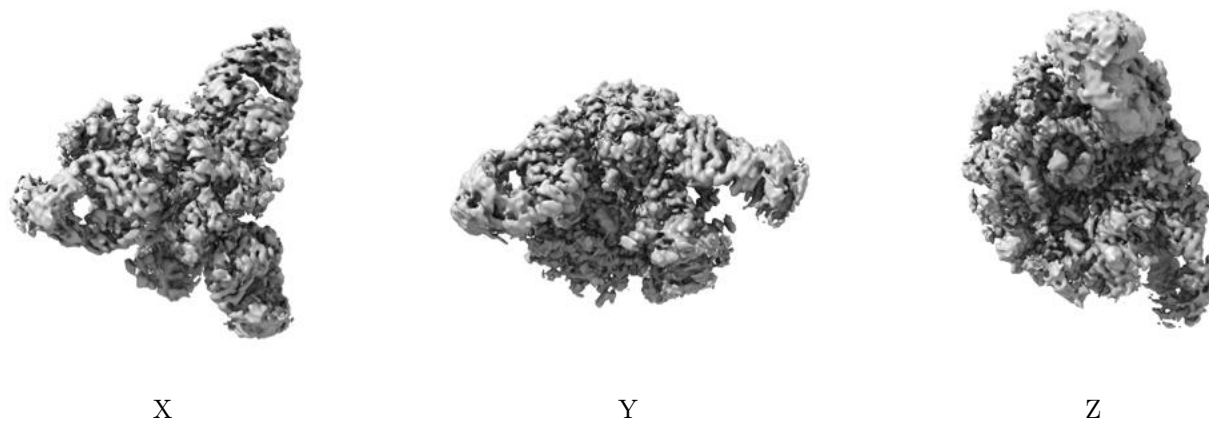


Z

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.

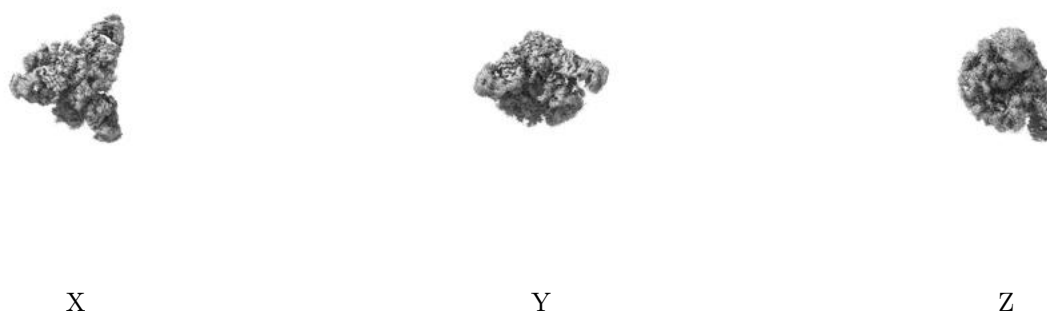
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

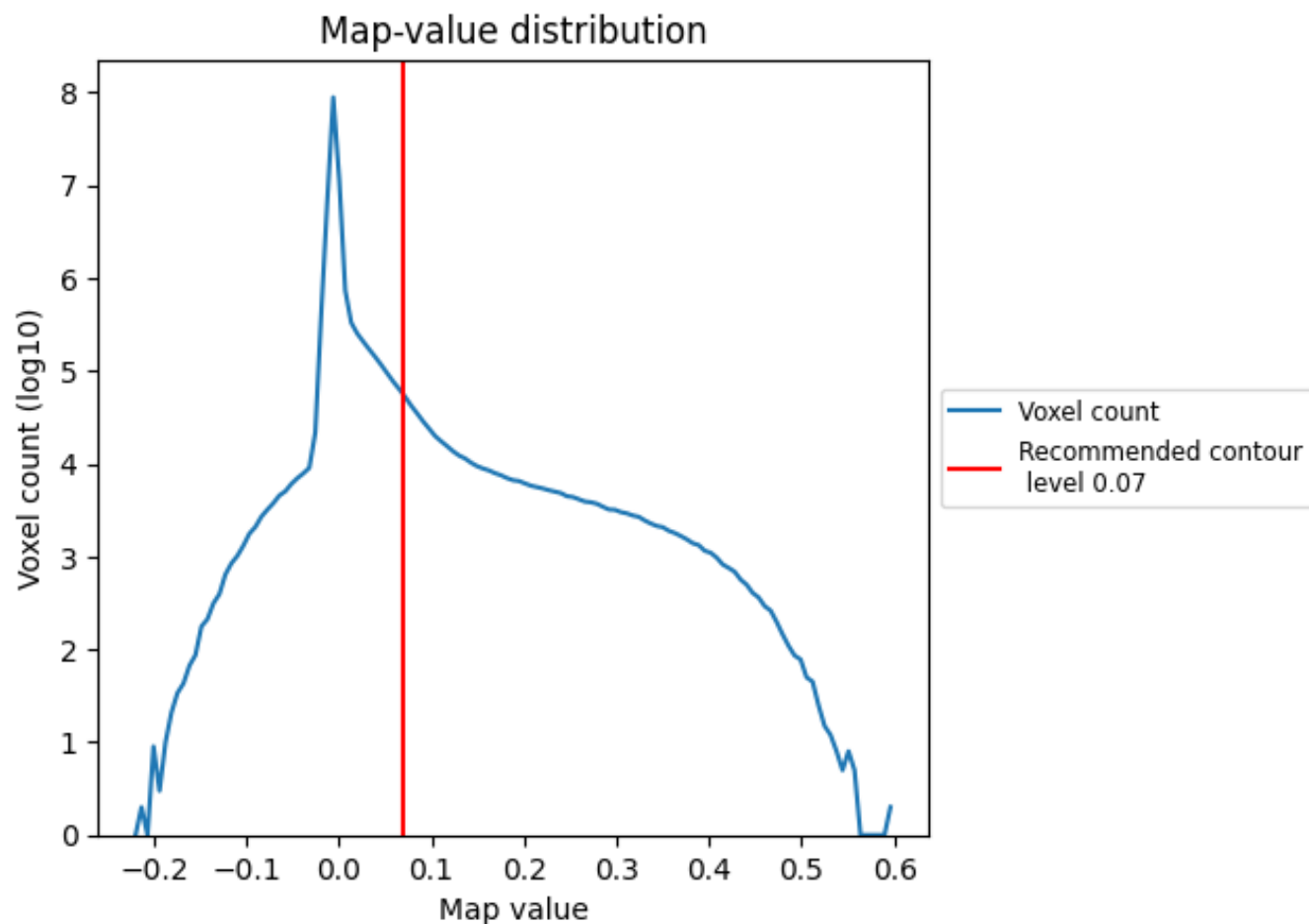
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

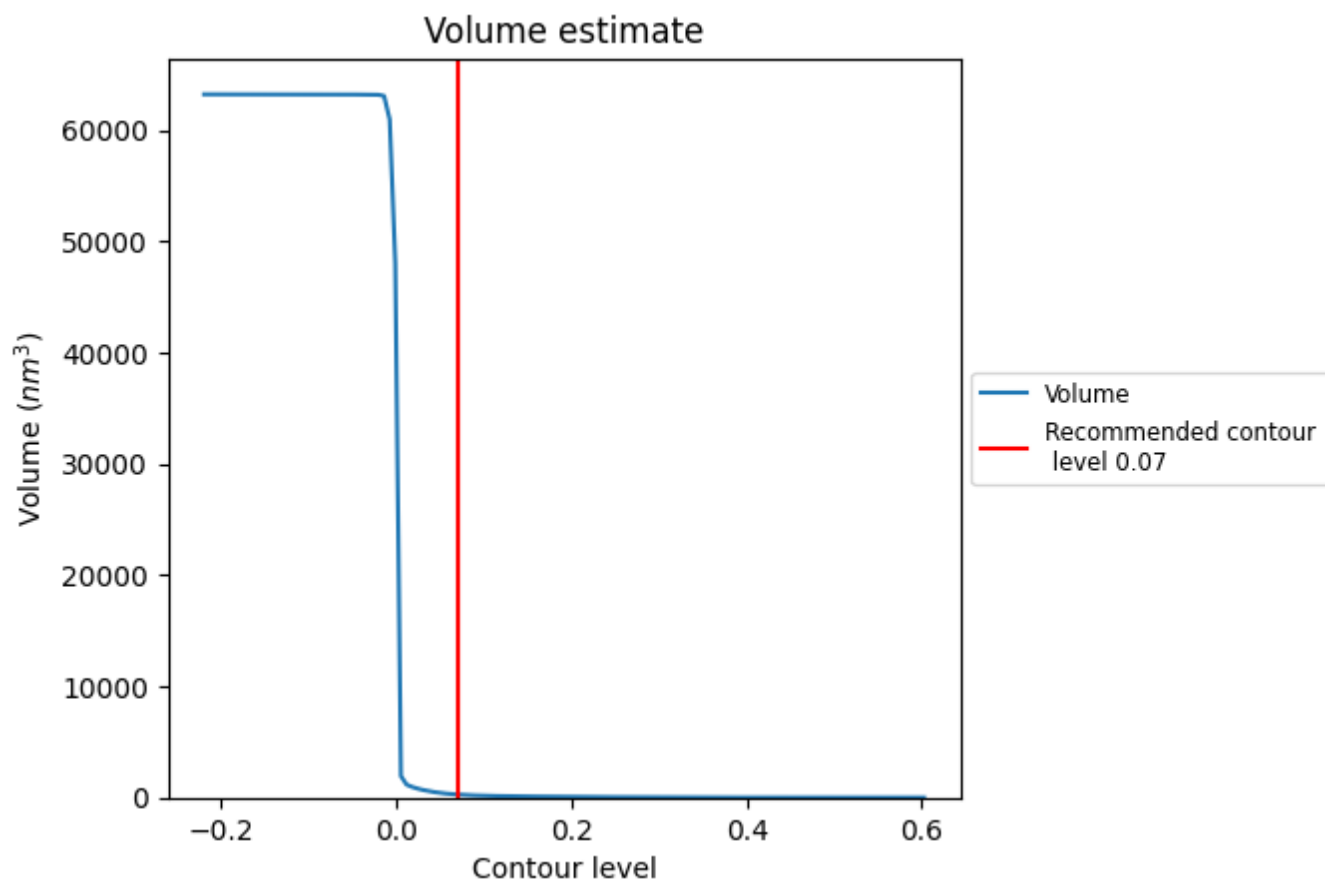
This section contains the results of statistical analysis of the map.

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.

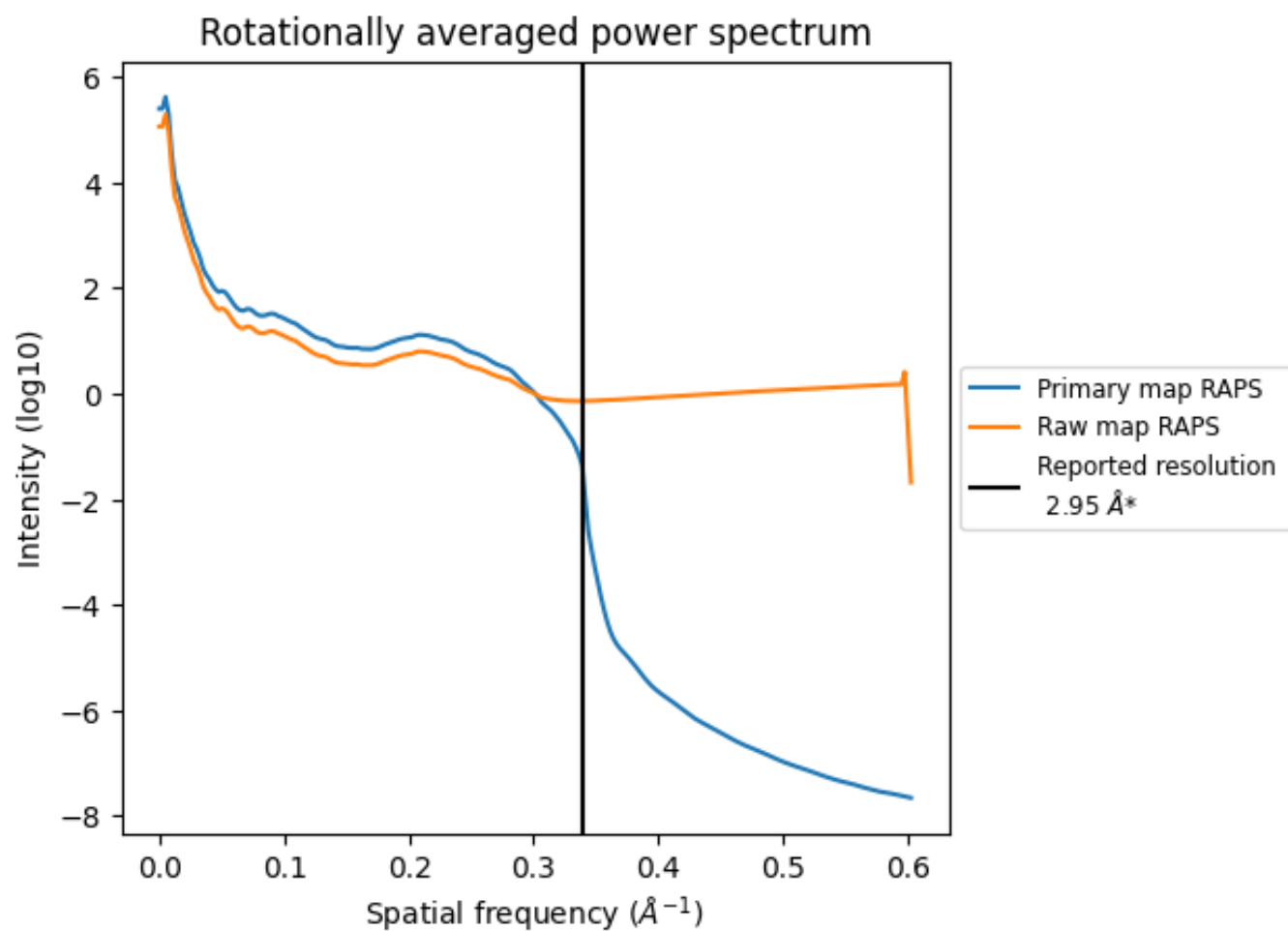
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

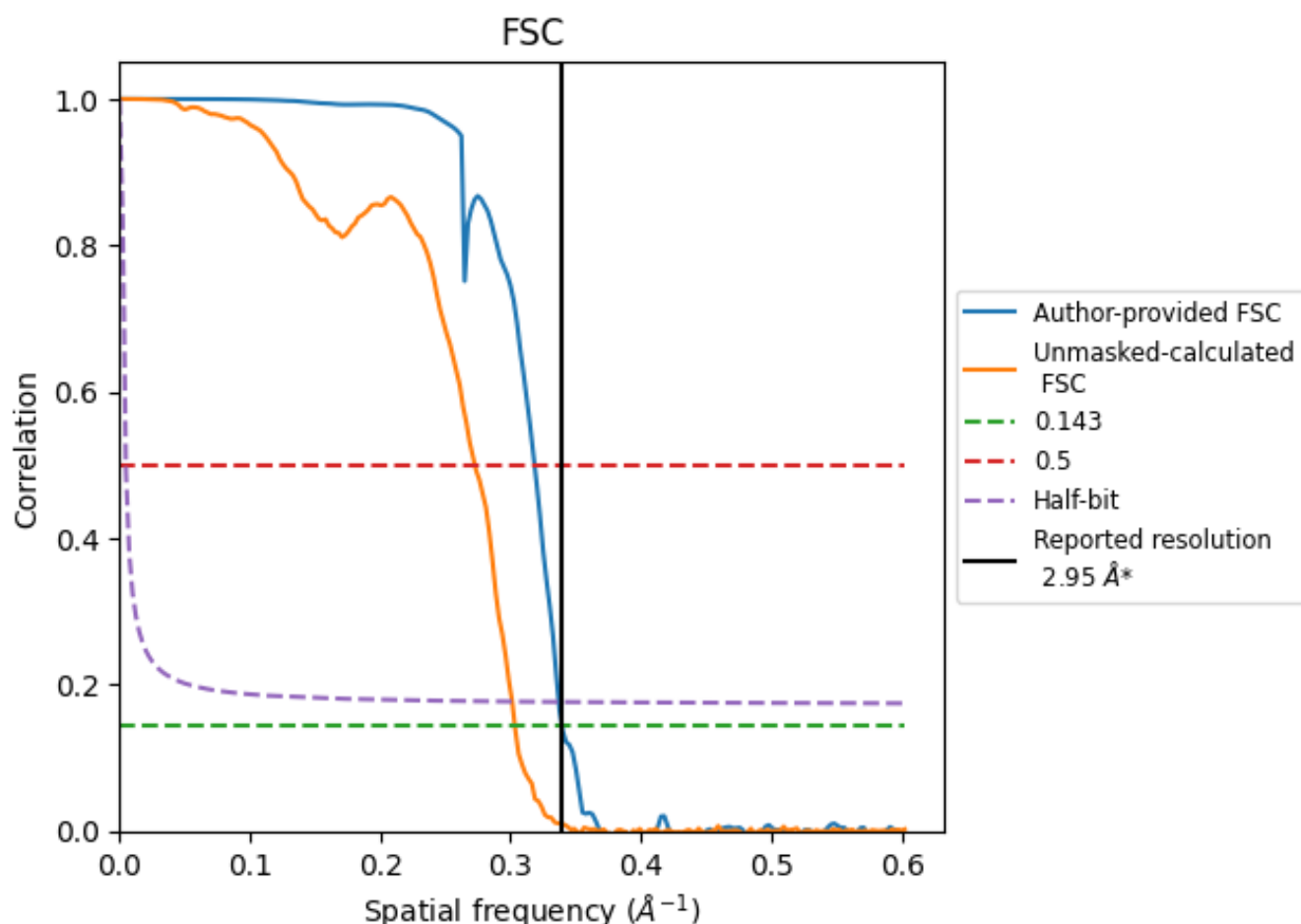


*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

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 0.339 Å⁻¹

8.2 Resolution estimates [i](#)

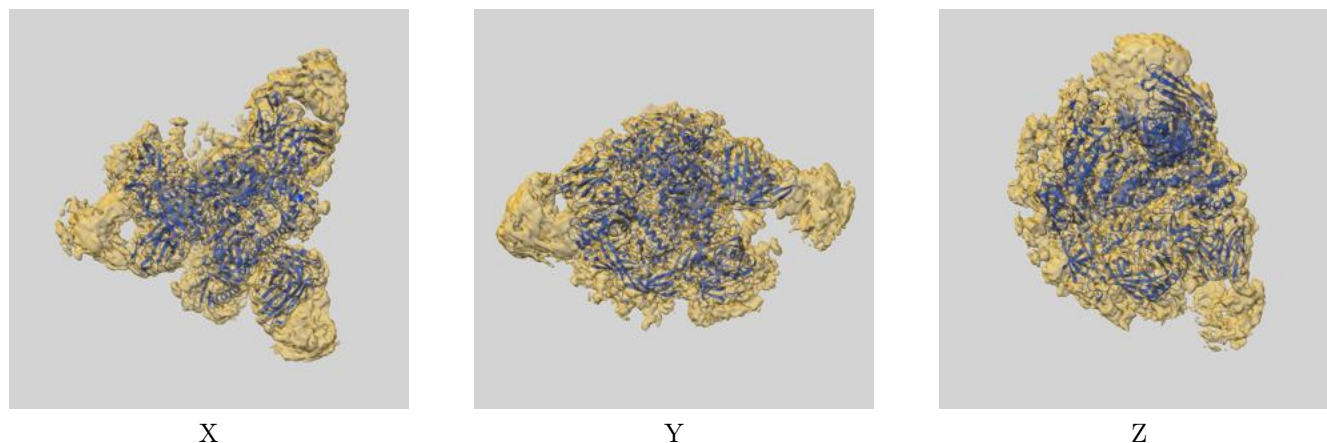
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.14	2.97
Unmasked-calculated*	3.30	3.67	3.32

*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 3.30 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

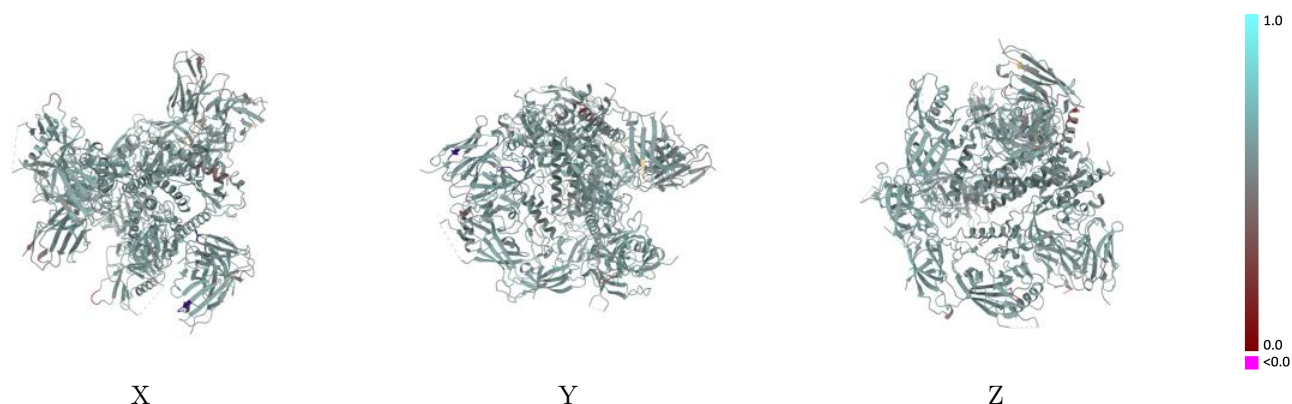
This section contains information regarding the fit between EMDB map EMD-29725 and PDB model 8G4M. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



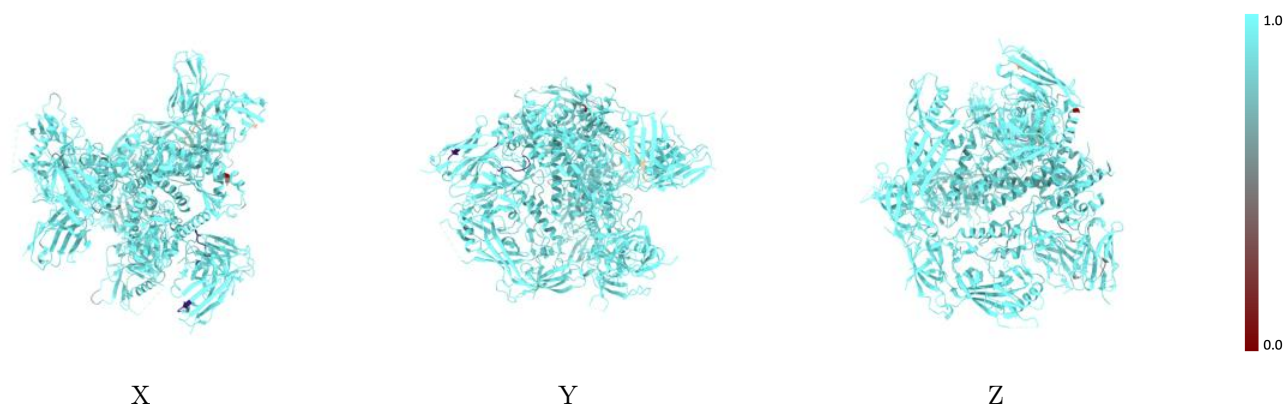
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



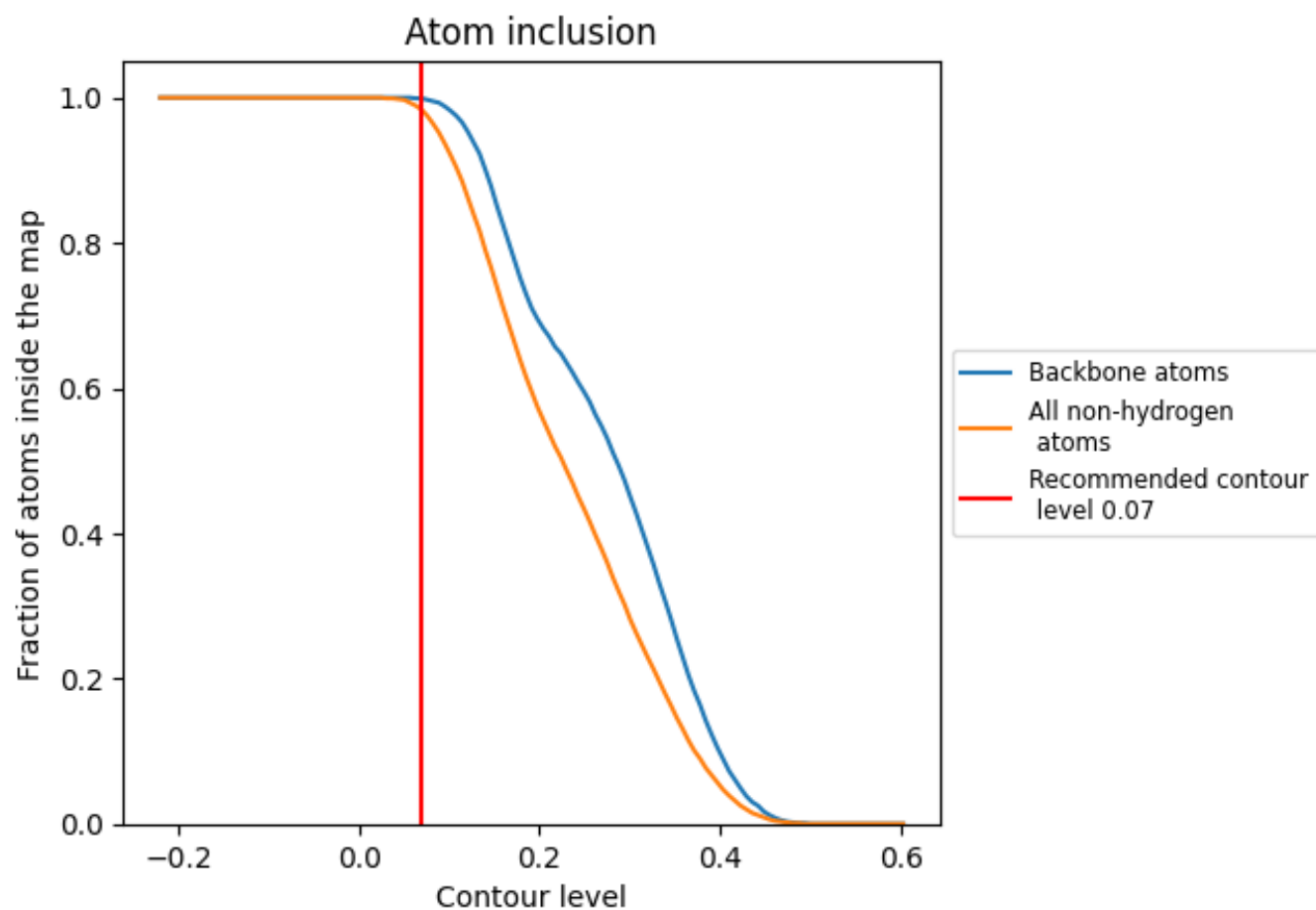
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9830	 0.5640
0	 0.9640	 0.4740
1	 0.8930	 0.4560
2	 0.9290	 0.5020
A	 0.9890	 0.5790
B	 0.9920	 0.5810
C	 0.9860	 0.5760
D	 0.9860	 0.5520
E	 0.9910	 0.5430
F	 0.9680	 0.5530
G	 0.9840	 0.5760
H	 0.9780	 0.5720
I	 0.9850	 0.5730
J	 0.9900	 0.5750
K	 0.9960	 0.5630
L	 0.9790	 0.5560
M	 1.0000	 0.5360
N	 1.0000	 0.4110
O	 1.0000	 0.5290
P	 0.8570	 0.5020
Q	 0.9580	 0.5120
R	 0.8930	 0.4670
S	 0.8930	 0.4810
T	 0.8930	 0.4660
U	 0.9290	 0.5140
V	 1.0000	 0.4950
W	 0.9640	 0.4600
X	 0.9290	 0.4820
Y	 0.9640	 0.4950
Z	 1.0000	 0.4840
a	 1.0000	 0.5330
b	 0.9290	 0.4020
c	 1.0000	 0.5290
d	 0.8210	 0.4960
e	 0.9670	 0.5060



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Chain	Atom inclusion	Q-score
f	 0.9640	 0.4590
g	 0.9640	 0.4910
h	 0.9640	 0.4640
i	 1.0000	 0.5300
j	 0.9640	 0.4720
k	 0.9290	 0.4830
l	 1.0000	 0.4570
m	 0.8930	 0.4000
n	 1.0000	 0.4840
o	 1.0000	 0.5240
p	 0.9290	 0.3750
q	 1.0000	 0.5480
r	 0.7860	 0.5010
s	 0.8930	 0.4700
t	 0.9440	 0.4640
u	 0.8930	 0.4580
v	 0.8930	 0.4450
w	 0.9290	 0.4690
x	 0.8930	 0.4620
y	 0.9640	 0.4640
z	 0.9640	 0.5030