



## Full wwPDB EM Validation Report ⓘ

Oct 30, 2023 – 04:49 PM EDT

PDB ID : 8TTW  
EMDB ID : EMD-41613  
Title : Cryo-EM structure of BG505 SOSIP.664 HIV-1 Env trimer in complex with temsavir, 8ANC195, and 10-1074  
Authors : Tolbert, W.D.; Pozharski, E.; Pazgier, M.  
Deposited on : 2023-08-15  
Resolution : 2.96 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

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

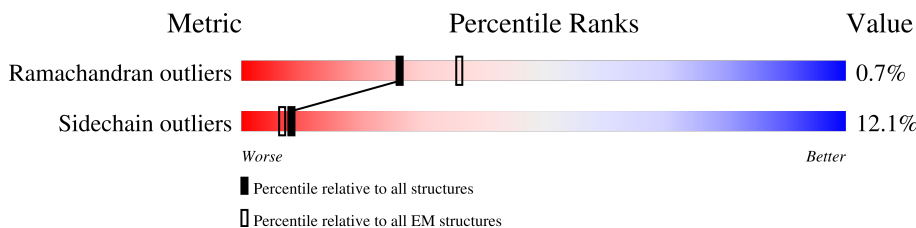
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



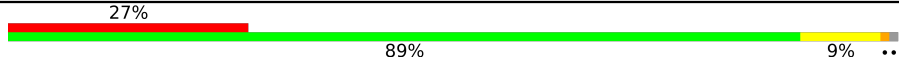
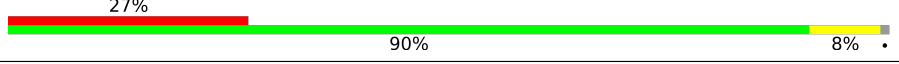
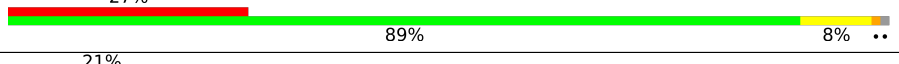
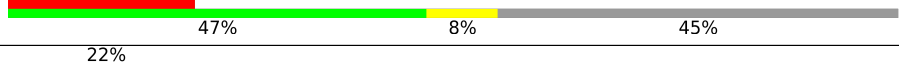
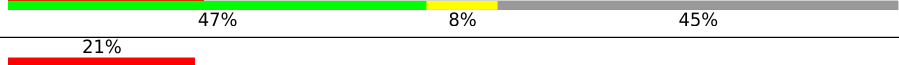
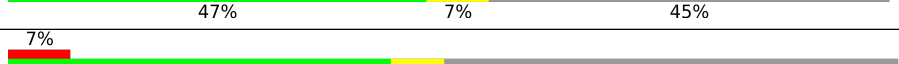
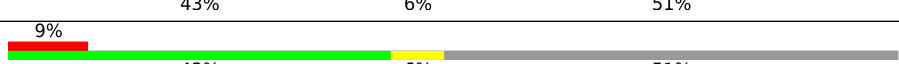
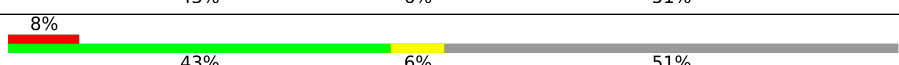
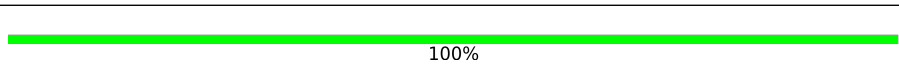
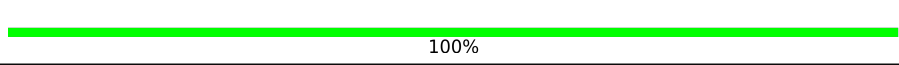
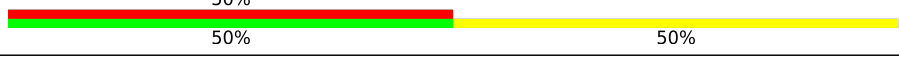
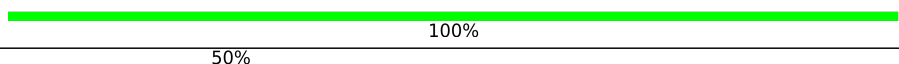
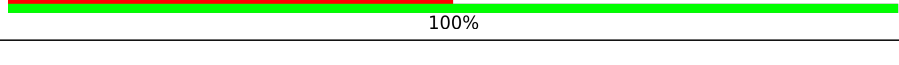
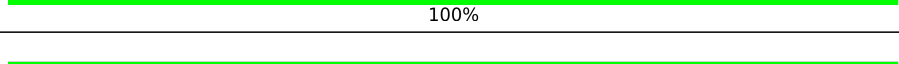
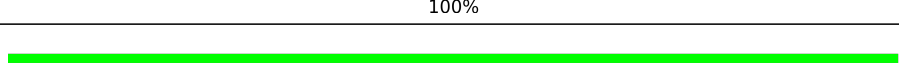
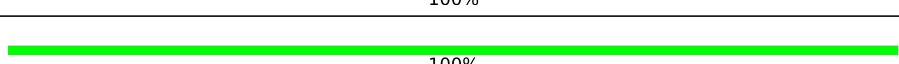
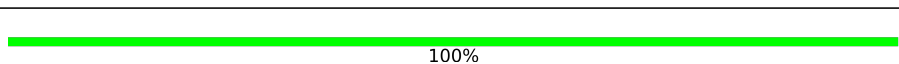
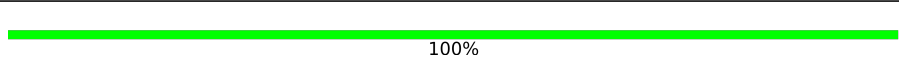
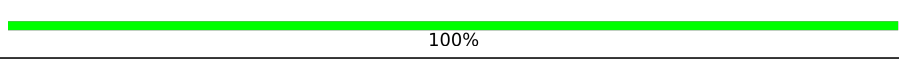
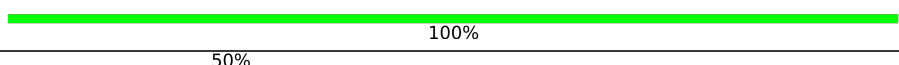
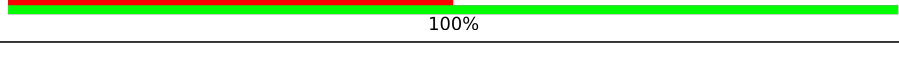
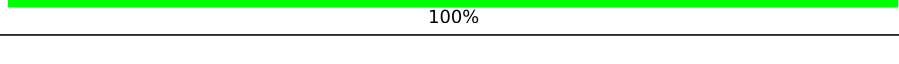
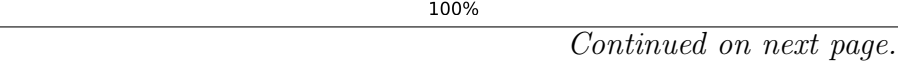


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	481	83% 10% 6%
1	E	481	85% 9% 6%
1	I	481	84% 9% 6%
2	B	153	71% 9% 20%
2	F	153	69% 11% 20%
2	J	153	73% 8% 20%
3	C	238	17% 84% 12% 5%
3	G	238	19% 85% 11% 5%
3	K	238	19% 85% 10% 5%

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Mol	Chain	Length	Quality of chain
4	D	215	
4	H	215	
4	L	215	
5	M	238	
5	O	238	
5	Q	238	
6	N	214	
6	P	214	
6	R	214	
7	1	2	
7	2	2	
7	4	2	
7	5	2	
7	6	2	
7	7	2	
7	S	2	
7	T	2	
7	U	2	
7	V	2	
7	W	2	
7	X	2	
7	Y	2	
7	Z	2	
7	a	2	
7	d	2	

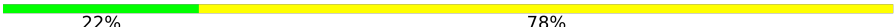
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Mol	Chain	Length	Quality of chain
7	e	2	100%
7	g	2	50% 50%
7	h	2	100%
7	i	2	50% 100%
7	j	2	100%
7	k	2	100%
7	l	2	50% 100%
7	m	2	100%
7	p	2	100%
7	q	2	100%
7	s	2	50% 50%
7	t	2	100%
7	u	2	50% 100%
7	v	2	100%
7	w	2	100%
7	x	2	50% 100%
7	y	2	100%
8	b	10	20% 80%
8	n	10	20% 80%
8	z	10	30% 70%
9	0	5	60% 40%
9	c	5	60% 40%
9	o	5	60% 40%
10	3	9	22% 78%
10	f	9	22% 78%

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Mol	Chain	Length	Quality of chain
10	r	9	 22% 78%

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 31275 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 gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	451	3554	2230	628	668	28	0	0
1	E	451	3554	2230	628	668	28	0	0
1	I	451	3554	2230	628	668	28	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	GLU	engineered mutation	UNP Q2N0S6
A	510	ARG	LYS	engineered mutation	UNP Q2N0S6
A	512	ARG	ALA	engineered mutation	UNP Q2N0S6
A	513	ARG	VAL	engineered mutation	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	GLU	engineered mutation	UNP Q2N0S6
E	510	ARG	LYS	engineered mutation	UNP Q2N0S6
E	512	ARG	ALA	engineered mutation	UNP Q2N0S6
E	513	ARG	VAL	engineered mutation	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	509	ARG	GLU	engineered mutation	UNP Q2N0S6
I	510	ARG	LYS	engineered mutation	UNP Q2N0S6
I	512	ARG	ALA	engineered mutation	UNP Q2N0S6
I	513	ARG	VAL	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP.664 transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	123	Total	C	N	O	S	0	0
			979	619	169	185	6		
2	F	123	Total	C	N	O	S	0	0
			979	619	169	185	6		
2	J	123	Total	C	N	O	S	0	0
			979	619	169	185	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
F	559	PRO	ILE	engineered mutation	UNP Q2N0S5
F	605	CYS	THR	engineered mutation	UNP Q2N0S5
J	559	PRO	ILE	engineered mutation	UNP Q2N0S5
J	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 3 is a protein called Antibody 8anc195 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	227	Total	C	N	O	S	0	0
			1710	1084	291	330	5		
3	G	227	Total	C	N	O	S	0	0
			1710	1084	291	330	5		
3	K	227	Total	C	N	O	S	0	0
			1710	1084	291	330	5		

- Molecule 4 is a protein called Antibody 8anc195 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	212	Total	C	N	O	S	0	0
			1626	1017	282	322	5		
4	H	212	Total	C	N	O	S	0	0
			1626	1017	282	322	5		
4	L	212	Total	C	N	O	S	0	0
			1626	1017	282	322	5		

- Molecule 5 is a protein called Antibody 10-1074 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	130	Total	C	N	O	S	0	0
			1021	646	171	200	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	130	Total	C	N	O	S	0	0
			1021	646	171	200	4		
5	Q	130	Total	C	N	O	S	0	0
			1021	646	171	200	4		

- Molecule 6 is a protein called Antibody 10-1074 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	105	Total	C	N	O	S	0	0
			812	507	150	152	3		
6	P	105	Total	C	N	O	S	0	0
			812	507	150	152	3		
6	R	105	Total	C	N	O	S	0	0
			812	507	150	152	3		

- Molecule 7 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
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		

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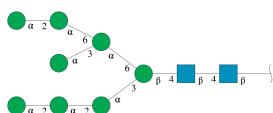
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	d	2	28	16	2	10	0	0
7	e	2	28	16	2	10	0	0
7	g	2	28	16	2	10	0	0
7	h	2	28	16	2	10	0	0
7	i	2	28	16	2	10	0	0
7	j	2	28	16	2	10	0	0
7	k	2	28	16	2	10	0	0
7	l	2	28	16	2	10	0	0
7	m	2	28	16	2	10	0	0
7	p	2	28	16	2	10	0	0
7	q	2	28	16	2	10	0	0
7	s	2	28	16	2	10	0	0
7	t	2	28	16	2	10	0	0
7	u	2	28	16	2	10	0	0
7	v	2	28	16	2	10	0	0
7	w	2	28	16	2	10	0	0
7	x	2	28	16	2	10	0	0
7	y	2	28	16	2	10	0	0
7	1	2	28	16	2	10	0	0
7	2	2	28	16	2	10	0	0
7	4	2	28	16	2	10	0	0

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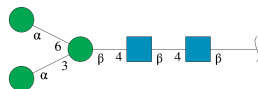
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	5	2	28	16	2	10	0	0
7	6	2	28	16	2	10	0	0
7	7	2	28	16	2	10	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	b	10	116	64	2	50	0	0
8	n	10	116	64	2	50	0	0
8	z	10	116	64	2	50	0	0

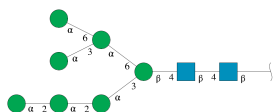
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

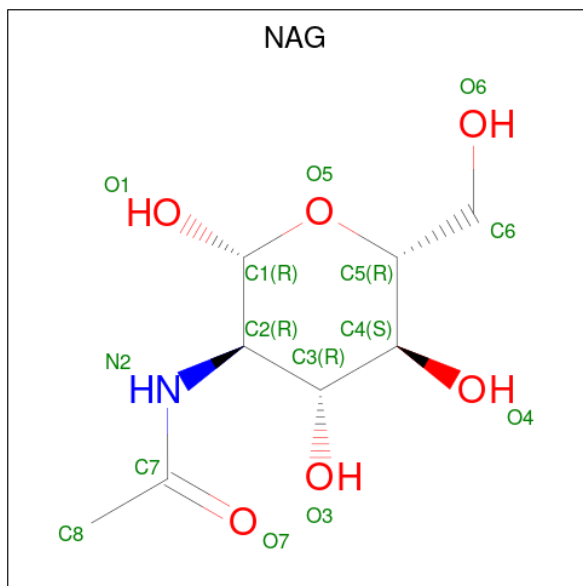
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra

nose-(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
			Total	C	N	O		
10	f	9	105	58	2	45	0	0
10	r	9	105	58	2	45	0	0
10	3	9	105	58	2	45	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



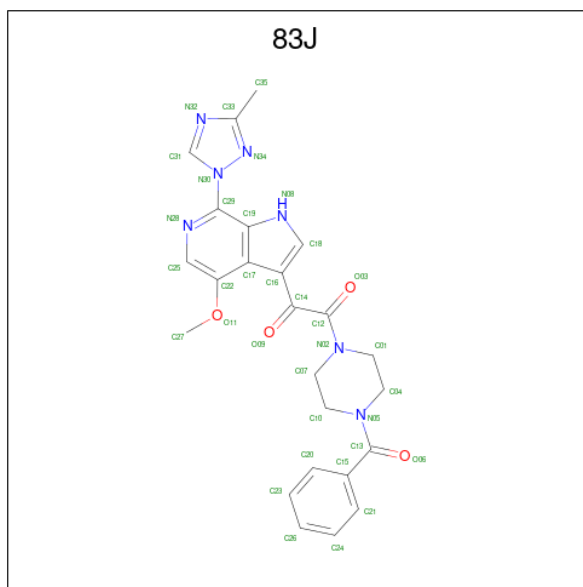
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	A	1	14	8	1	5	0
11	A	1	14	8	1	5	0
11	A	1	14	8	1	5	0
11	A	1	14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 14	C 8	N 1	O 5	0
11	F	1	Total 14	C 8	N 1	O 5	0
11	F	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	I	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0
11	J	1	Total 14	C 8	N 1	O 5	0
11	K	1	Total 14	C 8	N 1	O 5	0

- Molecule 12 is 1-[4-(benzenecarbonyl)piperazin-1-yl]-2-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]ethane-1,2-dione (three-letter code: 83J) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>7</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

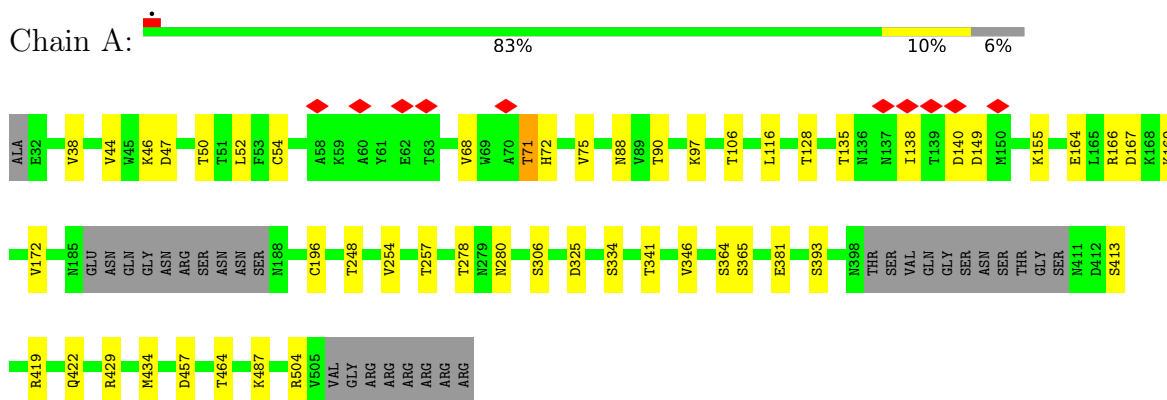


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	A	1	Total	C	N	O	0
			35	24	7	4	
12	E	1	Total	C	N	O	0
			35	24	7	4	
12	I	1	Total	C	N	O	0
			35	24	7	4	

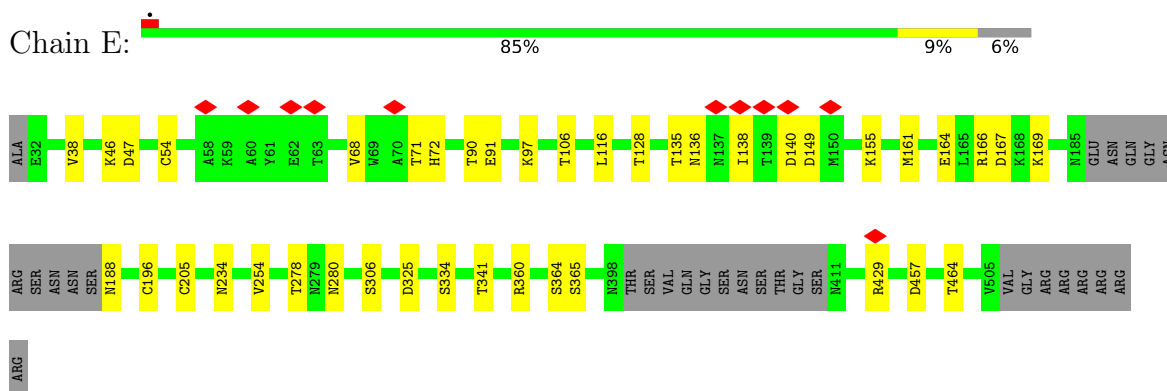
### 3 Residue-property plots [i](#)

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.

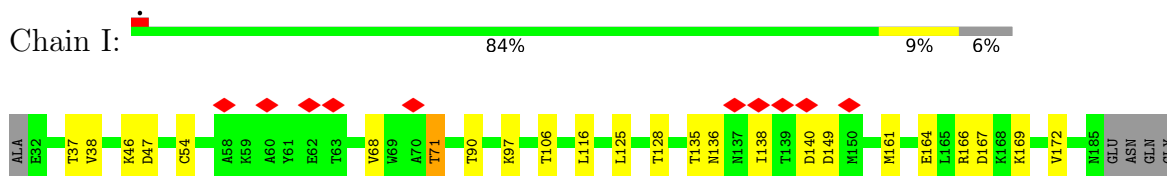
- Molecule 1: Envelope glycoprotein gp160

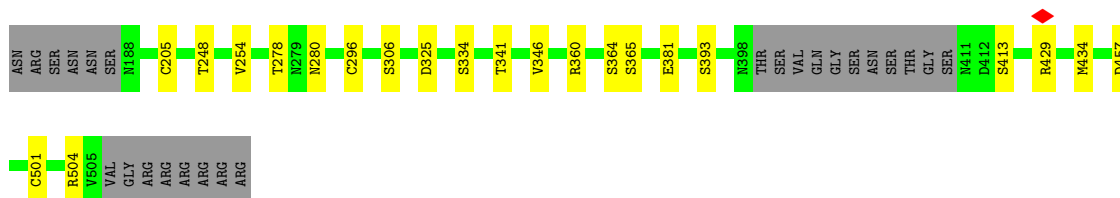


- Molecule 1: Envelope glycoprotein gp160

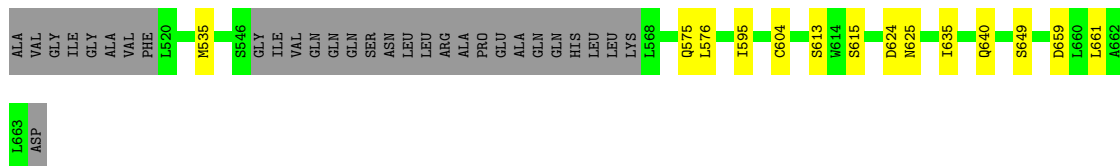


- Molecule 1: Envelope glycoprotein gp160

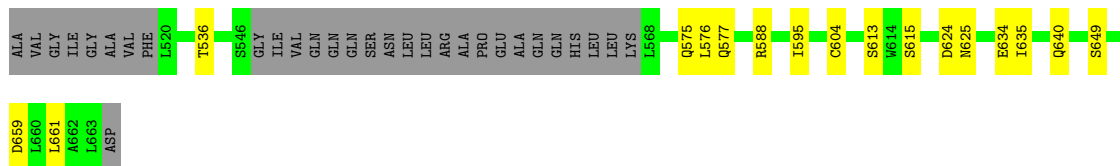




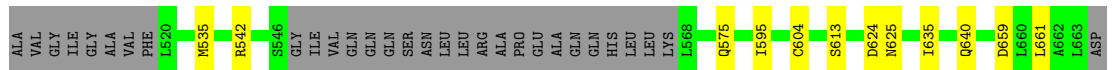
• Molecule 2: BG505 SOSIP.664 transmembrane protein gp41



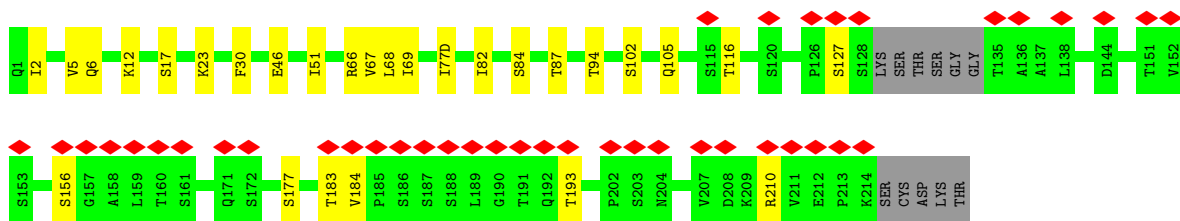
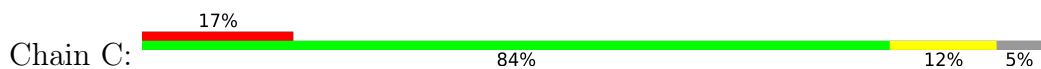
• Molecule 2: BG505 SOSIP.664 transmembrane protein gp41



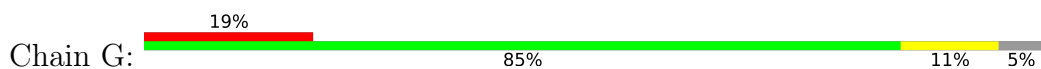
• Molecule 2: BG505 SOSIP.664 transmembrane protein gp41

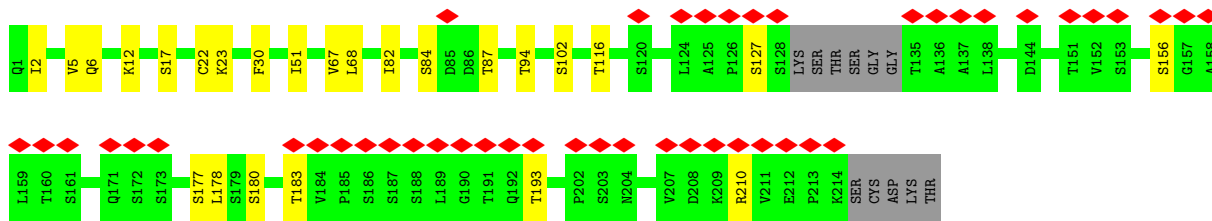


• Molecule 3: Antibody 8anc195 heavy chain

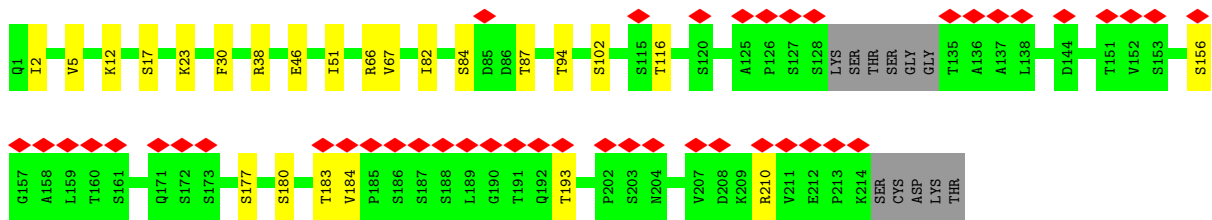
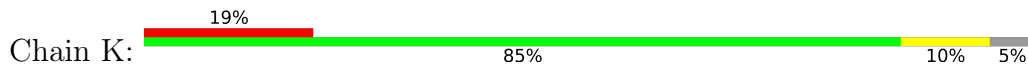


• Molecule 3: Antibody 8anc195 heavy chain

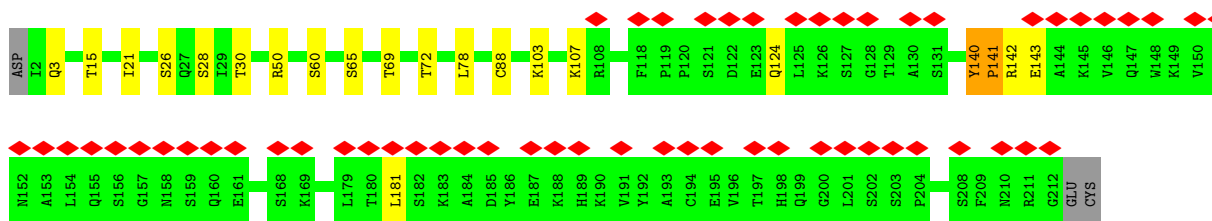
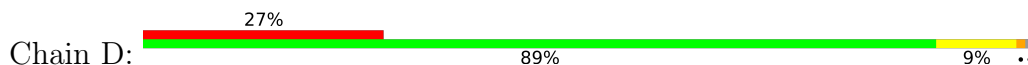




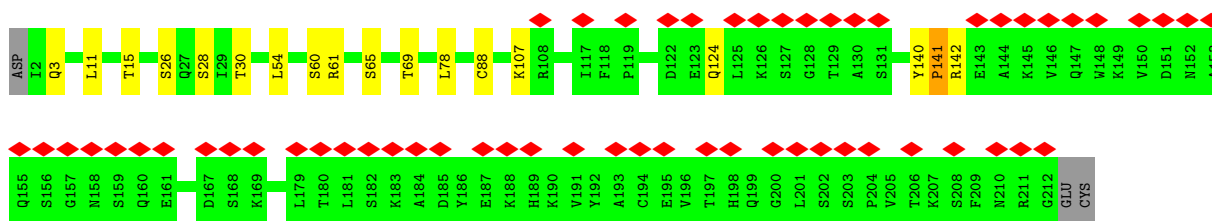
• Molecule 3: Antibody 8anc195 heavy chain



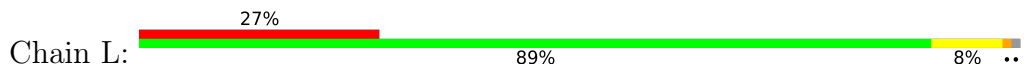
• Molecule 4: Antibody 8anc195 light chain



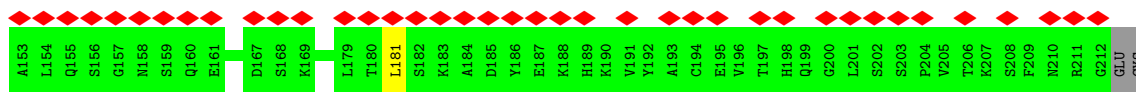
• Molecule 4: Antibody 8anc195 light chain



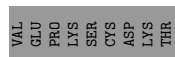
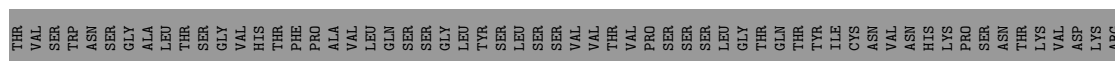
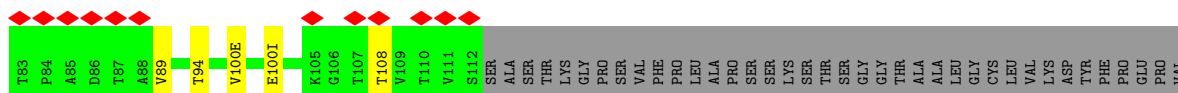
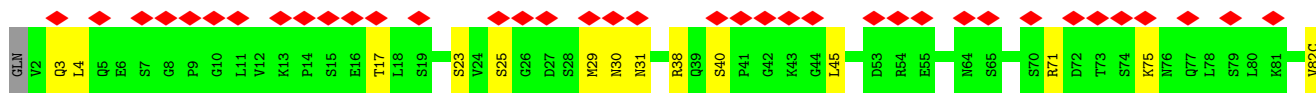
• Molecule 4: Antibody 8anc195 light chain



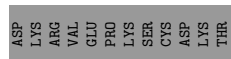
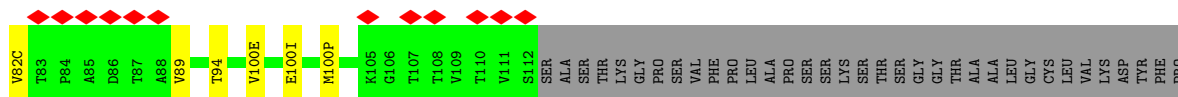
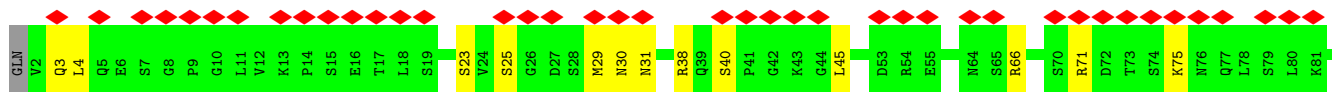




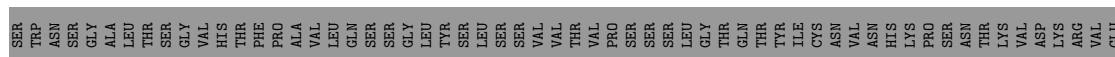
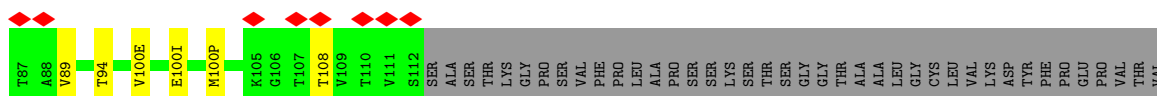
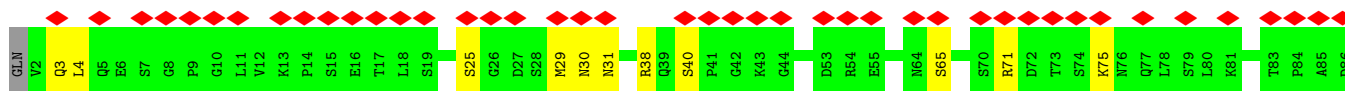
• Molecule 5: Antibody 10-1074 heavy chain



• Molecule 5: Antibody 10-1074 heavy chain

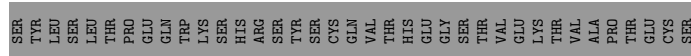
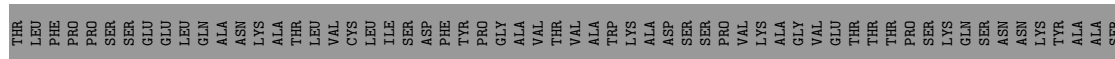
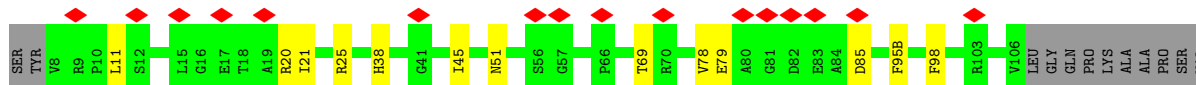


• Molecule 5: Antibody 10-1074 heavy chain

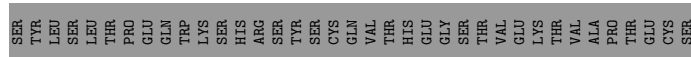
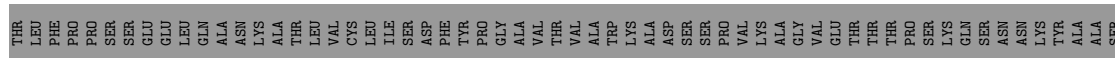
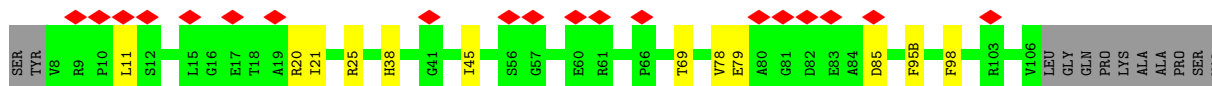
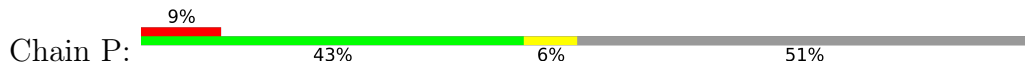


PRO  
LYS  
SER  
CYS  
ASP  
LYS  
THR

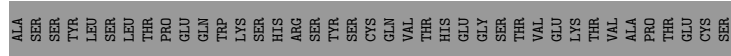
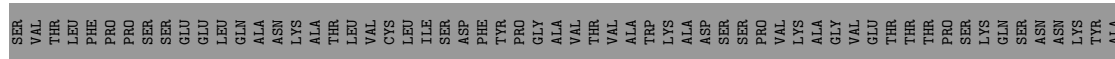
• Molecule 6: Antibody 10-1074 light chain



• Molecule 6: Antibody 10-1074 light chain



• Molecule 6: Antibody 10-1074 light chain



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



MAG1  
MAG2

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

Chain T:  100%

TRG1  
TRG2

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

Chain U:  100%

TRG1  
TRG2

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

Chain V:  100%

TRG1  
TRG2

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

Chain W:  100%

TRG1  
TRG2

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

Chain X:  100%

TRG1  
TRG2

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

Chain Y:  100%

TRG1  
TRG2

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

Chain Z:  50%  
 100%



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

Chain a:  100%



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

Chain d:  100%



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

Chain e:  100%



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

Chain g:  50% 50%



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

Chain h:  100%



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

Chain i:  50% 100%



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

Chain j:  100%



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

Chain k:  100%



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

Chain l:  50%  
 100%



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

Chain m:  100%



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

Chain p:  100%



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

Chain q:  100%



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



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



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



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



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



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



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

Chain y:  100%



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

Chain 1:  100%



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

Chain 2:  100%



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

Chain 4:  50% 50%



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

Chain 5:  100%



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

Chain 6:  50% 100%





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

Chain 7:  100%



MAG1  
MAG2

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

Chain b:  20%  80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

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

Chain n:  20%  80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

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

Chain z:  30%  70%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 9: 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 c:  60%  40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 9: 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%





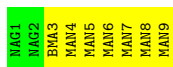
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0: 60% 40%



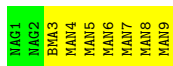
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 22% 78%



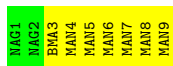
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r: 22% 78%



- Molecule 10: 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 3: 22% 78%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	319575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.007	Depositor
Minimum map value	-1.362	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.1151	Depositor
Map size (Å)	319.68, 319.68, 319.68	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88799995, 0.88799995, 0.88799995	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 83J, MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	0/3628	0.54	0/4926
1	E	0.29	0/3628	0.53	0/4926
1	I	0.30	0/3628	0.54	0/4926
2	B	0.24	0/996	0.46	0/1351
2	F	0.24	0/996	0.46	0/1351
2	J	0.24	0/996	0.46	0/1351
3	C	0.26	0/1755	0.47	0/2397
3	G	0.26	0/1755	0.47	0/2397
3	K	0.26	0/1755	0.47	0/2397
4	D	0.27	0/1661	0.51	0/2255
4	H	0.27	0/1661	0.51	0/2255
4	L	0.27	0/1661	0.52	0/2255
5	M	0.25	0/1046	0.48	0/1424
5	O	0.25	0/1046	0.48	0/1424
5	Q	0.25	0/1046	0.48	0/1424
6	N	0.24	0/833	0.53	0/1132
6	P	0.26	0/833	0.54	0/1132
6	R	0.25	0/833	0.53	0/1132
All	All	0.27	0/29757	0.51	0/40455

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

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/481 (92%)	401 (90%)	41 (9%)	3 (1%)	22	56
1	E	445/481 (92%)	401 (90%)	40 (9%)	4 (1%)	17	51
1	I	445/481 (92%)	399 (90%)	43 (10%)	3 (1%)	22	56
2	B	119/153 (78%)	105 (88%)	13 (11%)	1 (1%)	19	53
2	F	119/153 (78%)	106 (89%)	12 (10%)	1 (1%)	19	53
2	J	119/153 (78%)	106 (89%)	12 (10%)	1 (1%)	19	53
3	C	223/238 (94%)	209 (94%)	14 (6%)	0	100	100
3	G	223/238 (94%)	209 (94%)	14 (6%)	0	100	100
3	K	223/238 (94%)	209 (94%)	14 (6%)	0	100	100
4	D	210/215 (98%)	196 (93%)	11 (5%)	3 (1%)	11	39
4	H	210/215 (98%)	197 (94%)	10 (5%)	3 (1%)	11	39
4	L	210/215 (98%)	196 (93%)	11 (5%)	3 (1%)	11	39
5	M	128/238 (54%)	124 (97%)	3 (2%)	1 (1%)	19	53
5	O	128/238 (54%)	122 (95%)	5 (4%)	1 (1%)	19	53
5	Q	128/238 (54%)	122 (95%)	5 (4%)	1 (1%)	19	53
6	N	103/214 (48%)	95 (92%)	8 (8%)	0	100	100
6	P	103/214 (48%)	93 (90%)	10 (10%)	0	100	100
6	R	103/214 (48%)	92 (89%)	11 (11%)	0	100	100
All	All	3684/4617 (80%)	3382 (92%)	277 (8%)	25 (1%)	26	56

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	625	ASN
4	D	140	TYR
4	D	141	PRO
1	E	196	CYS

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Mol	Chain	Res	Type
2	F	625	ASN
4	H	141	PRO
2	J	625	ASN
4	L	140	TYR
4	L	141	PRO
4	D	142	ARG
4	H	142	ARG
1	A	71	THR
1	E	71	THR
4	H	140	TYR
4	L	142	ARG
1	A	429	ARG
1	I	71	THR
1	I	429	ARG
5	M	25	SER
5	O	25	SER
5	Q	25	SER
1	E	429	ARG
1	A	164	GLU
1	E	164	GLU
1	I	164	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/428 (94%)	354 (88%)	49 (12%)	5	19
1	E	403/428 (94%)	366 (91%)	37 (9%)	9	30
1	I	403/428 (94%)	359 (89%)	44 (11%)	6	23
2	B	106/129 (82%)	93 (88%)	13 (12%)	4	18
2	F	106/129 (82%)	90 (85%)	16 (15%)	3	12
2	J	106/129 (82%)	95 (90%)	11 (10%)	7	24
3	C	195/204 (96%)	167 (86%)	28 (14%)	3	13
3	G	195/204 (96%)	170 (87%)	25 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	195/204 (96%)	171 (88%)	24 (12%)	4	18
4	D	179/182 (98%)	159 (89%)	20 (11%)	6	22
4	H	179/182 (98%)	163 (91%)	16 (9%)	9	32
4	L	179/182 (98%)	160 (89%)	19 (11%)	6	24
5	M	114/208 (55%)	96 (84%)	18 (16%)	2	10
5	O	114/208 (55%)	96 (84%)	18 (16%)	2	10
5	Q	114/208 (55%)	98 (86%)	16 (14%)	3	14
6	N	84/178 (47%)	71 (84%)	13 (16%)	2	11
6	P	84/178 (47%)	72 (86%)	12 (14%)	3	13
6	R	84/178 (47%)	72 (86%)	12 (14%)	3	13
All	All	3243/3987 (81%)	2852 (88%)	391 (12%)	8	19

All (391) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	44	VAL
1	A	46	LYS
1	A	47	ASP
1	A	50	THR
1	A	52	LEU
1	A	54	CYS
1	A	68	VAL
1	A	71	THR
1	A	72	HIS
1	A	75	VAL
1	A	88	ASN
1	A	90	THR
1	A	97	LYS
1	A	106	THR
1	A	116	LEU
1	A	128	THR
1	A	135	THR
1	A	138	ILE
1	A	140	ASP
1	A	149	ASP
1	A	155	LYS
1	A	166	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	167	ASP
1	A	169	LYS
1	A	172	VAL
1	A	196	CYS
1	A	248	THR
1	A	254	VAL
1	A	257	THR
1	A	278	THR
1	A	280	ASN
1	A	306	SER
1	A	325	ASP
1	A	334	SER
1	A	341	THR
1	A	346	VAL
1	A	364	SER
1	A	365	SER
1	A	381	GLU
1	A	393	SER
1	A	413	SER
1	A	419	ARG
1	A	422	GLN
1	A	434	MET
1	A	457	ASP
1	A	464	THR
1	A	487	LYS
1	A	504	ARG
2	B	535	MET
2	B	575	GLN
2	B	576	LEU
2	B	595	ILE
2	B	604	CYS
2	B	613	SER
2	B	615	SER
2	B	624	ASP
2	B	635	ILE
2	B	640	GLN
2	B	649	SER
2	B	659	ASP
2	B	661	LEU
3	C	2	ILE
3	C	5	VAL
3	C	6	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	12	LYS
3	C	17	SER
3	C	23	LYS
3	C	30	PHE
3	C	46	GLU
3	C	51	ILE
3	C	66	ARG
3	C	67	VAL
3	C	68	LEU
3	C	69	ILE
3	C	77(D)	ILE
3	C	82	ILE
3	C	84	SER
3	C	87	THR
3	C	94	THR
3	C	102	SER
3	C	105	GLN
3	C	116	THR
3	C	127	SER
3	C	156	SER
3	C	177	SER
3	C	183	THR
3	C	184	VAL
3	C	193	THR
3	C	210	ARG
4	D	3	GLN
4	D	15	THR
4	D	21	ILE
4	D	26	SER
4	D	28	SER
4	D	30	THR
4	D	50	ARG
4	D	60	SER
4	D	65	SER
4	D	69	THR
4	D	72	THR
4	D	78	LEU
4	D	88	CYS
4	D	103	LYS
4	D	107	LYS
4	D	124	GLN
4	D	140	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	141	PRO
4	D	143	GLU
4	D	181	LEU
1	E	38	VAL
1	E	46	LYS
1	E	47	ASP
1	E	54	CYS
1	E	68	VAL
1	E	72	HIS
1	E	90	THR
1	E	91	GLU
1	E	97	LYS
1	E	106	THR
1	E	116	LEU
1	E	128	THR
1	E	135	THR
1	E	136	ASN
1	E	138	ILE
1	E	140	ASP
1	E	149	ASP
1	E	155	LYS
1	E	161	MET
1	E	166	ARG
1	E	167	ASP
1	E	169	LYS
1	E	188	ASN
1	E	205	CYS
1	E	234	ASN
1	E	254	VAL
1	E	278	THR
1	E	280	ASN
1	E	306	SER
1	E	325	ASP
1	E	334	SER
1	E	341	THR
1	E	360	ARG
1	E	364	SER
1	E	365	SER
1	E	457	ASP
1	E	464	THR
2	F	536	THR
2	F	575	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	576	LEU
2	F	577	GLN
2	F	588	ARG
2	F	595	ILE
2	F	604	CYS
2	F	613	SER
2	F	615	SER
2	F	624	ASP
2	F	634	GLU
2	F	635	ILE
2	F	640	GLN
2	F	649	SER
2	F	659	ASP
2	F	661	LEU
3	G	2	ILE
3	G	5	VAL
3	G	6	GLN
3	G	12	LYS
3	G	17	SER
3	G	22	CYS
3	G	23	LYS
3	G	30	PHE
3	G	51	ILE
3	G	67	VAL
3	G	68	LEU
3	G	82	ILE
3	G	84	SER
3	G	87	THR
3	G	94	THR
3	G	102	SER
3	G	116	THR
3	G	127	SER
3	G	156	SER
3	G	177	SER
3	G	178	LEU
3	G	180	SER
3	G	183	THR
3	G	193	THR
3	G	210	ARG
4	H	3	GLN
4	H	11	LEU
4	H	15	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	26	SER
4	H	28	SER
4	H	30	THR
4	H	54	LEU
4	H	60	SER
4	H	61	ARG
4	H	65	SER
4	H	69	THR
4	H	78	LEU
4	H	88	CYS
4	H	107	LYS
4	H	124	GLN
4	H	141	PRO
1	I	37	THR
1	I	38	VAL
1	I	46	LYS
1	I	47	ASP
1	I	54	CYS
1	I	68	VAL
1	I	71	THR
1	I	90	THR
1	I	97	LYS
1	I	106	THR
1	I	116	LEU
1	I	125	LEU
1	I	128	THR
1	I	135	THR
1	I	136	ASN
1	I	138	ILE
1	I	140	ASP
1	I	149	ASP
1	I	161	MET
1	I	166	ARG
1	I	167	ASP
1	I	169	LYS
1	I	172	VAL
1	I	205	CYS
1	I	248	THR
1	I	254	VAL
1	I	278	THR
1	I	280	ASN
1	I	296	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	306	SER
1	I	325	ASP
1	I	334	SER
1	I	341	THR
1	I	346	VAL
1	I	360	ARG
1	I	364	SER
1	I	365	SER
1	I	381	GLU
1	I	393	SER
1	I	413	SER
1	I	434	MET
1	I	457	ASP
1	I	501	CYS
1	I	504	ARG
2	J	535	MET
2	J	542	ARG
2	J	575	GLN
2	J	595	ILE
2	J	604	CYS
2	J	613	SER
2	J	624	ASP
2	J	635	ILE
2	J	640	GLN
2	J	659	ASP
2	J	661	LEU
3	K	2	ILE
3	K	5	VAL
3	K	12	LYS
3	K	17	SER
3	K	23	LYS
3	K	30	PHE
3	K	38	ARG
3	K	46	GLU
3	K	51	ILE
3	K	66	ARG
3	K	67	VAL
3	K	82	ILE
3	K	84	SER
3	K	87	THR
3	K	94	THR
3	K	102	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	K	116	THR
3	K	156	SER
3	K	177	SER
3	K	180	SER
3	K	183	THR
3	K	184	VAL
3	K	193	THR
3	K	210	ARG
4	L	3	GLN
4	L	21	ILE
4	L	26	SER
4	L	28	SER
4	L	30	THR
4	L	50	ARG
4	L	60	SER
4	L	61	ARG
4	L	63	ARG
4	L	65	SER
4	L	69	THR
4	L	78	LEU
4	L	88	CYS
4	L	103	LYS
4	L	107	LYS
4	L	124	GLN
4	L	140	TYR
4	L	141	PRO
4	L	181	LEU
5	M	3	GLN
5	M	4	LEU
5	M	17	THR
5	M	23	SER
5	M	29	MET
5	M	30	ASN
5	M	31	ASN
5	M	38	ARG
5	M	40	SER
5	M	45	LEU
5	M	71	ARG
5	M	75	LYS
5	M	82(C)	VAL
5	M	89	VAL
5	M	94	THR

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Mol	Chain	Res	Type
5	M	100(E)	VAL
5	M	100(I)	GLU
5	M	108	THR
6	N	11	LEU
6	N	20	ARG
6	N	21	ILE
6	N	25	ARG
6	N	38	HIS
6	N	45	ILE
6	N	51	ASN
6	N	69	THR
6	N	78	VAL
6	N	79	GLU
6	N	85	ASP
6	N	95(B)	PHE
6	N	98	PHE
5	O	3	GLN
5	O	4	LEU
5	O	23	SER
5	O	29	MET
5	O	30	ASN
5	O	31	ASN
5	O	38	ARG
5	O	40	SER
5	O	45	LEU
5	O	66	ARG
5	O	71	ARG
5	O	75	LYS
5	O	82(C)	VAL
5	O	89	VAL
5	O	94	THR
5	O	100(E)	VAL
5	O	100(I)	GLU
5	O	100(P)	MET
6	P	11	LEU
6	P	20	ARG
6	P	21	ILE
6	P	25	ARG
6	P	38	HIS
6	P	45	ILE
6	P	69	THR
6	P	78	VAL

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Mol	Chain	Res	Type
6	P	79	GLU
6	P	85	ASP
6	P	95(B)	PHE
6	P	98	PHE
5	Q	3	GLN
5	Q	4	LEU
5	Q	29	MET
5	Q	30	ASN
5	Q	31	ASN
5	Q	38	ARG
5	Q	40	SER
5	Q	65	SER
5	Q	71	ARG
5	Q	75	LYS
5	Q	89	VAL
5	Q	94	THR
5	Q	100(E)	VAL
5	Q	100(I)	GLU
5	Q	100(P)	MET
5	Q	108	THR
6	R	11	LEU
6	R	20	ARG
6	R	25	ARG
6	R	38	HIS
6	R	45	ILE
6	R	51	ASN
6	R	69	THR
6	R	78	VAL
6	R	85	ASP
6	R	87	TYR
6	R	95(B)	PHE
6	R	98	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	607	ASN
2	B	630	GLN
2	B	651	ASN
4	D	166	GLN
4	D	199	GLN
2	F	630	GLN

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Mol	Chain	Res	Type
4	H	137	ASN
4	H	199	GLN
2	J	630	GLN
2	J	651	ASN
3	K	6	GLN
4	L	199	GLN
5	M	77	GLN
6	N	37	GLN
6	N	50	ASN
5	O	77	GLN
6	P	51	ASN
5	Q	77	GLN
5	Q	99	GLN
6	R	51	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

138 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	$\# Z  > 2$
9	NAG	0	1	1,9	14,14,15	0.26	0	17,19,21	0.50	0
9	NAG	0	2	9	14,14,15	0.20	0	17,19,21	0.43	0
9	BMA	0	3	9	11,11,12	0.66	0	15,15,17	0.80	0
9	MAN	0	4	9	11,11,12	0.61	0	15,15,17	0.95	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	0	5	9	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
7	NAG	1	1	1,7	14,14,15	0.29	0	17,19,21	0.39	0
7	NAG	1	2	7	14,14,15	0.22	0	17,19,21	0.39	0
7	NAG	2	1	1,7	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	2	2	7	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	3	1	10,1	14,14,15	0.42	0	17,19,21	0.40	0
10	NAG	3	2	10	14,14,15	0.27	0	17,19,21	0.54	0
10	BMA	3	3	10	11,11,12	0.75	0	15,15,17	1.20	1 (6%)
10	MAN	3	4	10	11,11,12	0.57	0	15,15,17	1.06	2 (13%)
10	MAN	3	5	10	11,11,12	0.57	0	15,15,17	0.95	1 (6%)
10	MAN	3	6	10	11,11,12	0.55	0	15,15,17	1.05	2 (13%)
10	MAN	3	7	10	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
10	MAN	3	8	10	11,11,12	0.60	0	15,15,17	1.13	2 (13%)
10	MAN	3	9	10	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
7	NAG	4	1	1,7	14,14,15	0.60	1 (7%)	17,19,21	0.54	0
7	NAG	4	2	7	14,14,15	0.24	0	17,19,21	0.47	0
7	NAG	5	1	1,7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	5	2	7	14,14,15	0.21	0	17,19,21	0.53	0
7	NAG	6	1	1,7	14,14,15	0.28	0	17,19,21	0.40	0
7	NAG	6	2	7	14,14,15	0.23	0	17,19,21	0.50	0
7	NAG	7	1	1,7	14,14,15	0.24	0	17,19,21	0.52	0
7	NAG	7	2	7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	S	1	1,7	14,14,15	0.51	0	17,19,21	0.47	0
7	NAG	S	2	7	14,14,15	0.25	0	17,19,21	0.48	0
7	NAG	T	1	2,7	14,14,15	0.35	0	17,19,21	0.55	0
7	NAG	T	2	7	14,14,15	0.31	0	17,19,21	0.47	0
7	NAG	U	1	1,7	14,14,15	0.51	0	17,19,21	0.46	0
7	NAG	U	2	7	14,14,15	0.26	0	17,19,21	0.48	0
7	NAG	V	1	2,7	14,14,15	0.34	0	17,19,21	0.53	0
7	NAG	V	2	7	14,14,15	0.31	0	17,19,21	0.46	0
7	NAG	W	1	1,7	14,14,15	0.51	0	17,19,21	0.47	0
7	NAG	W	2	7	14,14,15	0.27	0	17,19,21	0.47	0
7	NAG	X	1	2,7	14,14,15	0.39	0	17,19,21	0.54	0
7	NAG	X	2	7	14,14,15	0.30	0	17,19,21	0.47	0
7	NAG	Y	1	1,7	14,14,15	0.27	0	17,19,21	0.35	0
7	NAG	Y	2	7	14,14,15	0.17	0	17,19,21	0.46	0
7	NAG	Z	1	1,7	14,14,15	0.30	0	17,19,21	0.36	0
7	NAG	Z	2	7	14,14,15	0.20	0	17,19,21	0.39	0
7	NAG	a	1	1,7	14,14,15	0.27	0	17,19,21	0.38	0
7	NAG	a	2	7	14,14,15	0.19	0	17,19,21	0.43	0
8	NAG	b	1	1,8	14,14,15	0.29	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	b	10	8	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
8	NAG	b	2	8	14,14,15	0.42	0	17,19,21	0.61	1 (5%)
8	BMA	b	3	8	11,11,12	0.54	0	15,15,17	0.93	0
8	MAN	b	4	8	11,11,12	0.82	1 (9%)	15,15,17	1.05	2 (13%)
8	MAN	b	5	8	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
8	MAN	b	6	8	11,11,12	0.68	1 (9%)	15,15,17	1.19	2 (13%)
8	MAN	b	7	8	11,11,12	0.72	0	15,15,17	1.02	2 (13%)
8	MAN	b	8	8	11,11,12	0.77	0	15,15,17	1.28	2 (13%)
8	MAN	b	9	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
9	NAG	c	1	1,9	14,14,15	0.22	0	17,19,21	0.52	0
9	NAG	c	2	9	14,14,15	0.18	0	17,19,21	0.42	0
9	BMA	c	3	9	11,11,12	0.67	0	15,15,17	0.81	0
9	MAN	c	4	9	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
9	MAN	c	5	9	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
7	NAG	d	1	1,7	14,14,15	0.33	0	17,19,21	0.39	0
7	NAG	d	2	7	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	e	1	1,7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	e	2	7	14,14,15	0.24	0	17,19,21	0.42	0
10	NAG	f	1	10,1	14,14,15	0.43	0	17,19,21	0.39	0
10	NAG	f	2	10	14,14,15	0.29	0	17,19,21	0.55	0
10	BMA	f	3	10	11,11,12	0.74	0	15,15,17	1.20	1 (6%)
10	MAN	f	4	10	11,11,12	0.54	0	15,15,17	1.07	2 (13%)
10	MAN	f	5	10	11,11,12	0.58	0	15,15,17	0.95	1 (6%)
10	MAN	f	6	10	11,11,12	0.54	0	15,15,17	1.04	2 (13%)
10	MAN	f	7	10	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
10	MAN	f	8	10	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
10	MAN	f	9	10	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
7	NAG	g	1	1,7	14,14,15	0.58	1 (7%)	17,19,21	0.55	0
7	NAG	g	2	7	14,14,15	0.25	0	17,19,21	0.47	0
7	NAG	h	1	1,7	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	h	2	7	14,14,15	0.20	0	17,19,21	0.53	0
7	NAG	i	1	1,7	14,14,15	0.31	0	17,19,21	0.39	0
7	NAG	i	2	7	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	j	1	1,7	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	j	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	k	1	1,7	14,14,15	0.29	0	17,19,21	0.36	0
7	NAG	k	2	7	14,14,15	0.18	0	17,19,21	0.46	0
7	NAG	l	1	1,7	14,14,15	0.29	0	17,19,21	0.37	0
7	NAG	l	2	7	14,14,15	0.20	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	m	1	1,7	14,14,15	0.29	0	17,19,21	0.39	0
7	NAG	m	2	7	14,14,15	0.17	0	17,19,21	0.43	0
8	NAG	n	1	1,8	14,14,15	0.36	0	17,19,21	0.44	0
8	MAN	n	10	8	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
8	NAG	n	2	8	14,14,15	0.40	0	17,19,21	0.54	0
8	BMA	n	3	8	11,11,12	0.55	0	15,15,17	0.93	1 (6%)
8	MAN	n	4	8	11,11,12	0.79	1 (9%)	15,15,17	1.04	2 (13%)
8	MAN	n	5	8	11,11,12	0.68	0	15,15,17	1.12	2 (13%)
8	MAN	n	6	8	11,11,12	0.68	1 (9%)	15,15,17	1.18	2 (13%)
8	MAN	n	7	8	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
8	MAN	n	8	8	11,11,12	0.76	0	15,15,17	1.28	2 (13%)
8	MAN	n	9	8	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
9	NAG	o	1	1,9	14,14,15	0.23	0	17,19,21	0.54	0
9	NAG	o	2	9	14,14,15	0.19	0	17,19,21	0.43	0
9	BMA	o	3	9	11,11,12	0.67	0	15,15,17	0.80	0
9	MAN	o	4	9	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
9	MAN	o	5	9	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
7	NAG	p	1	1,7	14,14,15	0.32	0	17,19,21	0.38	0
7	NAG	p	2	7	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	q	1	1,7	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	q	2	7	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	r	1	10,1	14,14,15	0.43	0	17,19,21	0.38	0
10	NAG	r	2	10	14,14,15	0.27	0	17,19,21	0.54	0
10	BMA	r	3	10	11,11,12	0.73	0	15,15,17	1.23	1 (6%)
10	MAN	r	4	10	11,11,12	0.53	0	15,15,17	1.09	2 (13%)
10	MAN	r	5	10	11,11,12	0.58	0	15,15,17	0.94	1 (6%)
10	MAN	r	6	10	11,11,12	0.50	0	15,15,17	1.07	2 (13%)
10	MAN	r	7	10	11,11,12	0.56	0	15,15,17	1.02	2 (13%)
10	MAN	r	8	10	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
10	MAN	r	9	10	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
7	NAG	s	1	1,7	14,14,15	0.61	1 (7%)	17,19,21	0.55	0
7	NAG	s	2	7	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	t	1	1,7	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	t	2	7	14,14,15	0.21	0	17,19,21	0.54	0
7	NAG	u	1	1,7	14,14,15	0.26	0	17,19,21	0.38	0
7	NAG	u	2	7	14,14,15	0.23	0	17,19,21	0.48	0
7	NAG	v	1	1,7	14,14,15	0.24	0	17,19,21	0.52	0
7	NAG	v	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	w	1	1,7	14,14,15	0.27	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	w	2	7	14,14,15	0.19	0	17,19,21	0.47	0
7	NAG	x	1	1,7	14,14,15	0.31	0	17,19,21	0.36	0
7	NAG	x	2	7	14,14,15	0.20	0	17,19,21	0.39	0
7	NAG	y	1	1,7	14,14,15	0.39	0	17,19,21	0.36	0
7	NAG	y	2	7	14,14,15	0.21	0	17,19,21	0.40	0
8	NAG	z	1	1,8	14,14,15	0.28	0	17,19,21	0.61	0
8	MAN	z	10	8	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
8	NAG	z	2	8	14,14,15	0.46	0	17,19,21	0.60	0
8	BMA	z	3	8	11,11,12	0.54	0	15,15,17	0.97	1 (6%)
8	MAN	z	4	8	11,11,12	0.81	1 (9%)	15,15,17	1.06	2 (13%)
8	MAN	z	5	8	11,11,12	0.75	0	15,15,17	1.10	0
8	MAN	z	6	8	11,11,12	0.68	1 (9%)	15,15,17	1.19	2 (13%)
8	MAN	z	7	8	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
8	MAN	z	8	8	11,11,12	0.77	0	15,15,17	1.28	2 (13%)
8	MAN	z	9	8	11,11,12	0.62	0	15,15,17	0.97	2 (13%)

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
9	NAG	0	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	0	2	9	-	0/6/23/26	0/1/1/1
9	BMA	0	3	9	-	2/2/19/22	0/1/1/1
9	MAN	0	4	9	-	2/2/19/22	0/1/1/1
9	MAN	0	5	9	-	0/2/19/22	0/1/1/1
7	NAG	1	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	1	2	7	-	2/6/23/26	0/1/1/1
7	NAG	2	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	2	2	7	-	2/6/23/26	0/1/1/1
10	NAG	3	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	3	2	10	-	1/6/23/26	0/1/1/1
10	BMA	3	3	10	-	0/2/19/22	0/1/1/1
10	MAN	3	4	10	-	2/2/19/22	0/1/1/1
10	MAN	3	5	10	-	0/2/19/22	0/1/1/1
10	MAN	3	6	10	-	2/2/19/22	0/1/1/1
10	MAN	3	7	10	-	2/2/19/22	0/1/1/1
10	MAN	3	8	10	-	0/2/19/22	0/1/1/1

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	z	1	1,8	-	0/6/23/26	0/1/1/1
8	MAN	z	10	8	-	2/2/19/22	0/1/1/1
8	NAG	z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	z	3	8	-	2/2/19/22	0/1/1/1
8	MAN	z	4	8	-	1/2/19/22	0/1/1/1
8	MAN	z	5	8	-	0/2/19/22	0/1/1/1
8	MAN	z	6	8	-	1/2/19/22	0/1/1/1
8	MAN	z	7	8	-	0/2/19/22	0/1/1/1
8	MAN	z	8	8	-	0/2/19/22	0/1/1/1
8	MAN	z	9	8	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	s	1	NAG	O5-C1	-2.20	1.40	1.43
8	b	4	MAN	O5-C1	-2.16	1.40	1.43
7	4	1	NAG	O5-C1	-2.14	1.40	1.43
8	z	6	MAN	C1-C2	2.13	1.57	1.52
8	b	6	MAN	C1-C2	2.13	1.57	1.52
8	n	6	MAN	C1-C2	2.12	1.57	1.52
8	z	4	MAN	O5-C1	-2.11	1.40	1.43
7	g	1	NAG	O5-C1	-2.09	1.40	1.43
8	n	4	MAN	O5-C1	-2.04	1.40	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	8	MAN	O2-C2-C3	-3.23	103.67	110.14
8	z	8	MAN	O2-C2-C3	-3.23	103.67	110.14
8	n	8	MAN	O2-C2-C3	-3.18	103.77	110.14
10	r	8	MAN	C1-O5-C5	2.95	116.19	112.19
10	f	8	MAN	C1-O5-C5	2.94	116.17	112.19
10	3	8	MAN	C1-O5-C5	2.91	116.13	112.19
10	r	6	MAN	C1-O5-C5	2.88	116.09	112.19
10	3	6	MAN	C1-O5-C5	2.77	115.94	112.19
10	r	3	BMA	C1-C2-C3	2.73	113.02	109.67
10	f	6	MAN	C1-O5-C5	2.72	115.87	112.19
8	z	4	MAN	O2-C2-C3	-2.70	104.74	110.14
10	3	3	BMA	C1-C2-C3	2.69	112.97	109.67
10	f	3	BMA	C1-C2-C3	2.62	112.88	109.67
8	b	4	MAN	O2-C2-C3	-2.60	104.93	110.14
8	z	6	MAN	C1-O5-C5	2.60	115.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	4	MAN	O2-C2-C3	-2.60	104.93	110.14
8	n	4	MAN	O2-C2-C3	-2.59	104.95	110.14
10	r	4	MAN	C1-O5-C5	2.59	115.70	112.19
10	r	4	MAN	O2-C2-C3	-2.58	104.96	110.14
10	f	4	MAN	O2-C2-C3	-2.55	105.02	110.14
8	b	6	MAN	C1-O5-C5	2.54	115.63	112.19
8	n	6	MAN	C1-O5-C5	2.54	115.63	112.19
10	f	4	MAN	C1-O5-C5	2.47	115.53	112.19
8	n	8	MAN	C1-O5-C5	2.42	115.47	112.19
10	3	4	MAN	C1-O5-C5	2.38	115.42	112.19
8	b	10	MAN	O2-C2-C3	-2.38	105.37	110.14
9	c	5	MAN	C1-O5-C5	2.37	115.40	112.19
8	n	10	MAN	O2-C2-C3	-2.37	105.40	110.14
8	z	10	MAN	O2-C2-C3	-2.34	105.45	110.14
10	f	8	MAN	O2-C2-C3	-2.34	105.46	110.14
8	z	8	MAN	C1-O5-C5	2.33	115.35	112.19
10	r	8	MAN	O2-C2-C3	-2.33	105.47	110.14
9	0	5	MAN	O2-C2-C3	-2.33	105.47	110.14
10	3	8	MAN	O2-C2-C3	-2.31	105.50	110.14
8	b	8	MAN	C1-O5-C5	2.31	115.33	112.19
9	o	5	MAN	O2-C2-C3	-2.31	105.52	110.14
9	0	5	MAN	C1-O5-C5	2.30	115.31	112.19
9	c	5	MAN	O2-C2-C3	-2.30	105.54	110.14
9	o	5	MAN	C1-O5-C5	2.29	115.30	112.19
8	b	5	MAN	C1-O5-C5	2.29	115.29	112.19
10	3	9	MAN	O2-C2-C3	-2.28	105.58	110.14
10	r	9	MAN	O2-C2-C3	-2.27	105.59	110.14
10	f	9	MAN	O2-C2-C3	-2.26	105.60	110.14
8	b	9	MAN	O2-C2-C3	-2.25	105.63	110.14
10	r	5	MAN	O2-C2-C3	-2.24	105.64	110.14
8	z	9	MAN	O2-C2-C3	-2.23	105.67	110.14
10	f	9	MAN	C1-O5-C5	2.21	115.19	112.19
9	c	4	MAN	O2-C2-C3	-2.21	105.71	110.14
8	b	6	MAN	O2-C2-C3	-2.20	105.72	110.14
10	f	6	MAN	O2-C2-C3	-2.20	105.72	110.14
10	r	9	MAN	C1-O5-C5	2.20	115.18	112.19
10	3	7	MAN	O2-C2-C3	-2.20	105.73	110.14
10	f	7	MAN	O2-C2-C3	-2.19	105.74	110.14
9	0	4	MAN	O2-C2-C3	-2.19	105.74	110.14
8	n	9	MAN	O2-C2-C3	-2.19	105.74	110.14
10	3	5	MAN	O2-C2-C3	-2.19	105.75	110.14
8	z	6	MAN	O2-C2-C3	-2.19	105.75	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	r	7	MAN	O2-C2-C3	-2.19	105.76	110.14
8	n	6	MAN	O2-C2-C3	-2.18	105.77	110.14
9	o	4	MAN	O2-C2-C3	-2.18	105.78	110.14
8	n	5	MAN	C1-O5-C5	2.17	115.14	112.19
10	f	5	MAN	O2-C2-C3	-2.17	105.79	110.14
8	n	7	MAN	C1-O5-C5	2.17	115.13	112.19
8	z	7	MAN	C1-O5-C5	2.15	115.11	112.19
10	3	9	MAN	C1-O5-C5	2.14	115.09	112.19
10	r	7	MAN	C1-O5-C5	2.14	115.09	112.19
10	r	6	MAN	O2-C2-C3	-2.14	105.86	110.14
10	3	6	MAN	O2-C2-C3	-2.14	105.86	110.14
8	n	4	MAN	C1-O5-C5	2.13	115.08	112.19
8	b	7	MAN	O2-C2-C3	-2.13	105.86	110.14
8	b	9	MAN	C1-O5-C5	2.13	115.08	112.19
8	n	9	MAN	C1-O5-C5	2.13	115.08	112.19
8	z	7	MAN	O2-C2-C3	-2.13	105.87	110.14
8	n	7	MAN	O2-C2-C3	-2.11	105.92	110.14
8	b	5	MAN	O2-C2-C3	-2.10	105.94	110.14
10	3	7	MAN	C1-O5-C5	2.09	115.03	112.19
8	b	10	MAN	C1-O5-C5	2.09	115.03	112.19
8	b	7	MAN	C1-O5-C5	2.09	115.02	112.19
10	f	7	MAN	C1-O5-C5	2.06	114.98	112.19
8	z	10	MAN	C1-O5-C5	2.05	114.97	112.19
8	z	4	MAN	C1-O5-C5	2.05	114.97	112.19
9	o	4	MAN	C1-O5-C5	2.05	114.97	112.19
8	n	10	MAN	C1-O5-C5	2.05	114.96	112.19
8	b	4	MAN	C1-O5-C5	2.04	114.96	112.19
8	n	5	MAN	O2-C2-C3	-2.04	106.04	110.14
8	z	9	MAN	C1-O5-C5	2.04	114.95	112.19
8	z	3	BMA	O2-C2-C3	-2.02	106.09	110.14
9	0	4	MAN	C1-O5-C5	2.02	114.93	112.19
8	b	2	NAG	C1-O5-C5	2.02	114.92	112.19
9	c	4	MAN	C1-O5-C5	2.01	114.91	112.19
8	n	3	BMA	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	2	NAG	C3-C2-N2-C7
7	V	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
10	r	6	MAN	C4-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	4	1	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
7	i	1	NAG	O5-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
7	t	2	NAG	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
10	3	6	MAN	C4-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
7	q	2	NAG	O5-C5-C6-O6
7	u	1	NAG	O5-C5-C6-O6
7	2	2	NAG	O5-C5-C6-O6
7	5	2	NAG	O5-C5-C6-O6
7	6	1	NAG	O5-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
10	f	6	MAN	C4-C5-C6-O6
7	1	2	NAG	O5-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
10	r	6	MAN	O5-C5-C6-O6
10	f	4	MAN	C4-C5-C6-O6
10	r	4	MAN	C4-C5-C6-O6
10	3	4	MAN	C4-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
7	y	2	NAG	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	t	1	NAG	O5-C5-C6-O6
7	5	1	NAG	O5-C5-C6-O6
7	2	2	NAG	C4-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	V	1	NAG	C4-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
7	q	2	NAG	C4-C5-C6-O6
7	t	2	NAG	C4-C5-C6-O6
7	5	2	NAG	C4-C5-C6-O6
7	4	1	NAG	C4-C5-C6-O6
7	6	1	NAG	C4-C5-C6-O6
10	3	6	MAN	O5-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
7	u	1	NAG	C4-C5-C6-O6
10	f	4	MAN	O5-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
7	4	2	NAG	C4-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
10	f	6	MAN	O5-C5-C6-O6
10	r	4	MAN	O5-C5-C6-O6
10	3	4	MAN	O5-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
7	y	2	NAG	O5-C5-C6-O6
9	0	1	NAG	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
9	0	1	NAG	C4-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
7	t	1	NAG	C4-C5-C6-O6
7	5	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2
7	j	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	j	1	NAG	O7-C7-N2-C2
7	l	1	NAG	C8-C7-N2-C2
7	l	1	NAG	O7-C7-N2-C2
7	l	2	NAG	C8-C7-N2-C2
7	l	2	NAG	O7-C7-N2-C2
7	m	1	NAG	C8-C7-N2-C2
7	m	1	NAG	O7-C7-N2-C2
7	v	1	NAG	C8-C7-N2-C2
7	v	1	NAG	O7-C7-N2-C2
7	x	1	NAG	C8-C7-N2-C2
7	x	1	NAG	O7-C7-N2-C2
7	x	2	NAG	C8-C7-N2-C2
7	x	2	NAG	O7-C7-N2-C2
7	y	1	NAG	C8-C7-N2-C2
7	y	1	NAG	O7-C7-N2-C2
7	7	1	NAG	C8-C7-N2-C2
7	7	1	NAG	O7-C7-N2-C2
7	4	2	NAG	O5-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
9	o	1	NAG	O5-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
9	o	3	BMA	O5-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	2	1	NAG	C4-C5-C6-O6
9	0	3	BMA	O5-C5-C6-O6
9	c	3	BMA	O5-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
8	b	3	BMA	C4-C5-C6-O6
7	7	2	NAG	O5-C5-C6-O6
8	z	3	BMA	C4-C5-C6-O6
9	o	1	NAG	C4-C5-C6-O6
7	q	1	NAG	C4-C5-C6-O6
9	o	3	BMA	C4-C5-C6-O6
9	0	3	BMA	C4-C5-C6-O6
7	v	2	NAG	O5-C5-C6-O6
9	c	3	BMA	C4-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	y	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
7	2	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	n	3	BMA	C4-C5-C6-O6
7	y	1	NAG	C4-C5-C6-O6
10	r	7	MAN	C4-C5-C6-O6
7	6	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	q	1	NAG	O5-C5-C6-O6
10	r	7	MAN	O5-C5-C6-O6
7	k	1	NAG	C4-C5-C6-O6
7	u	2	NAG	O5-C5-C6-O6
10	f	7	MAN	C4-C5-C6-O6
7	w	1	NAG	C4-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
10	3	7	MAN	C4-C5-C6-O6
7	T	2	NAG	C1-C2-N2-C7
7	Z	2	NAG	O5-C5-C6-O6
7	x	2	NAG	O5-C5-C6-O6
9	o	4	MAN	O5-C5-C6-O6
10	f	7	MAN	O5-C5-C6-O6
10	3	7	MAN	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
9	o	4	MAN	C4-C5-C6-O6
7	h	1	NAG	C3-C2-N2-C7
9	0	4	MAN	O5-C5-C6-O6
8	b	4	MAN	O5-C5-C6-O6
9	0	4	MAN	C4-C5-C6-O6
7	v	1	NAG	C4-C5-C6-O6
7	7	2	NAG	C4-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
7	k	1	NAG	O5-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
7	w	1	NAG	O5-C5-C6-O6
8	z	3	BMA	O5-C5-C6-O6
7	V	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	m	1	NAG	C4-C5-C6-O6
9	c	4	MAN	C4-C5-C6-O6
9	c	4	MAN	O5-C5-C6-O6
8	z	4	MAN	O5-C5-C6-O6
7	t	1	NAG	C3-C2-N2-C7
7	5	1	NAG	C3-C2-N2-C7
10	f	2	NAG	C3-C2-N2-C7
10	r	2	NAG	C3-C2-N2-C7

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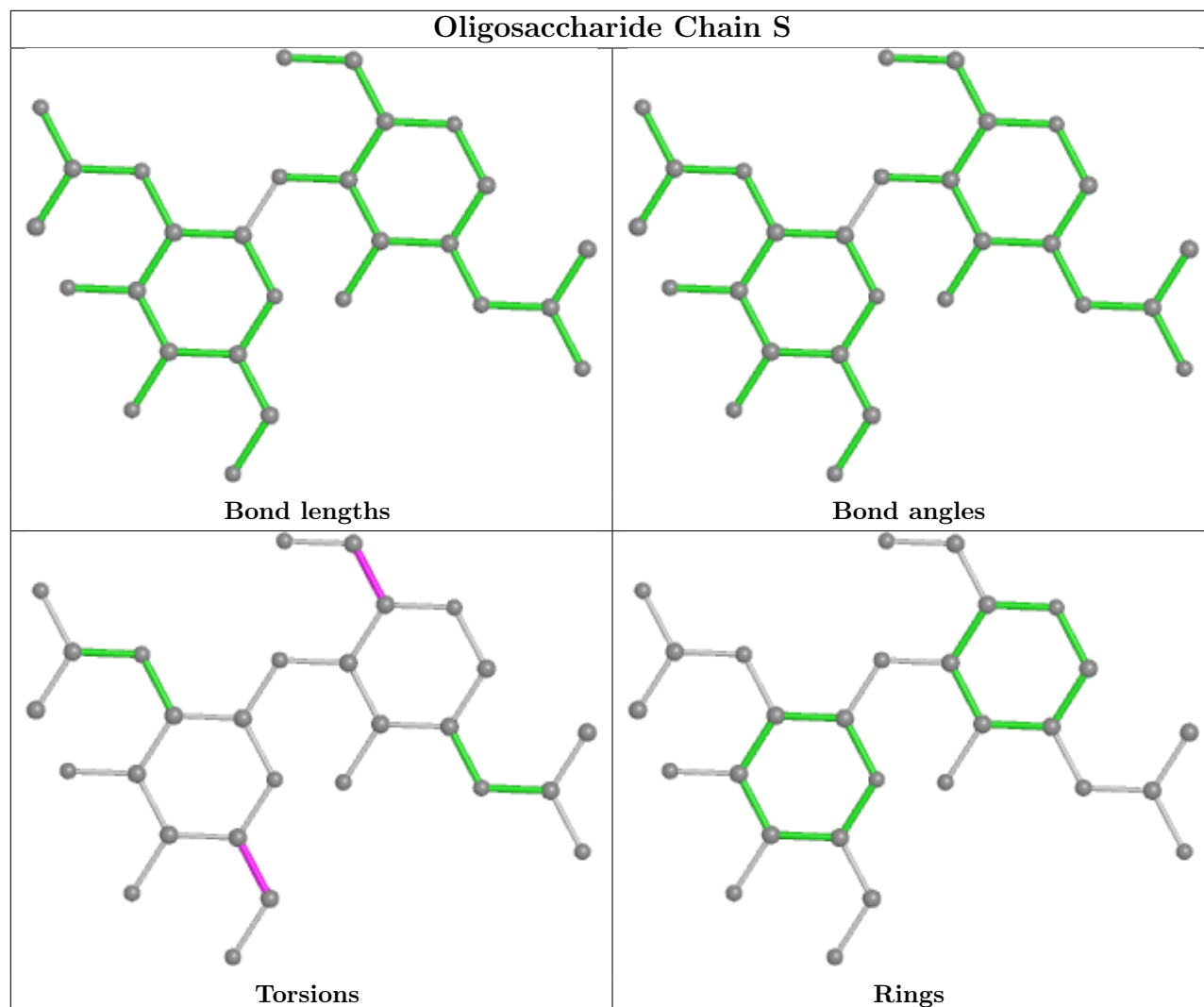
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Mol	Chain	Res	Type	Atoms
10	3	2	NAG	C3-C2-N2-C7
7	m	1	NAG	O5-C5-C6-O6
7	v	2	NAG	C4-C5-C6-O6
8	b	10	MAN	O5-C5-C6-O6
8	n	10	MAN	O5-C5-C6-O6
8	b	10	MAN	C4-C5-C6-O6
7	v	1	NAG	O5-C5-C6-O6
8	z	10	MAN	O5-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
8	z	6	MAN	C4-C5-C6-O6
8	n	6	MAN	C4-C5-C6-O6
8	n	10	MAN	C4-C5-C6-O6
8	n	3	BMA	O5-C5-C6-O6
8	b	6	MAN	C4-C5-C6-O6
8	z	10	MAN	C4-C5-C6-O6
8	n	4	MAN	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6

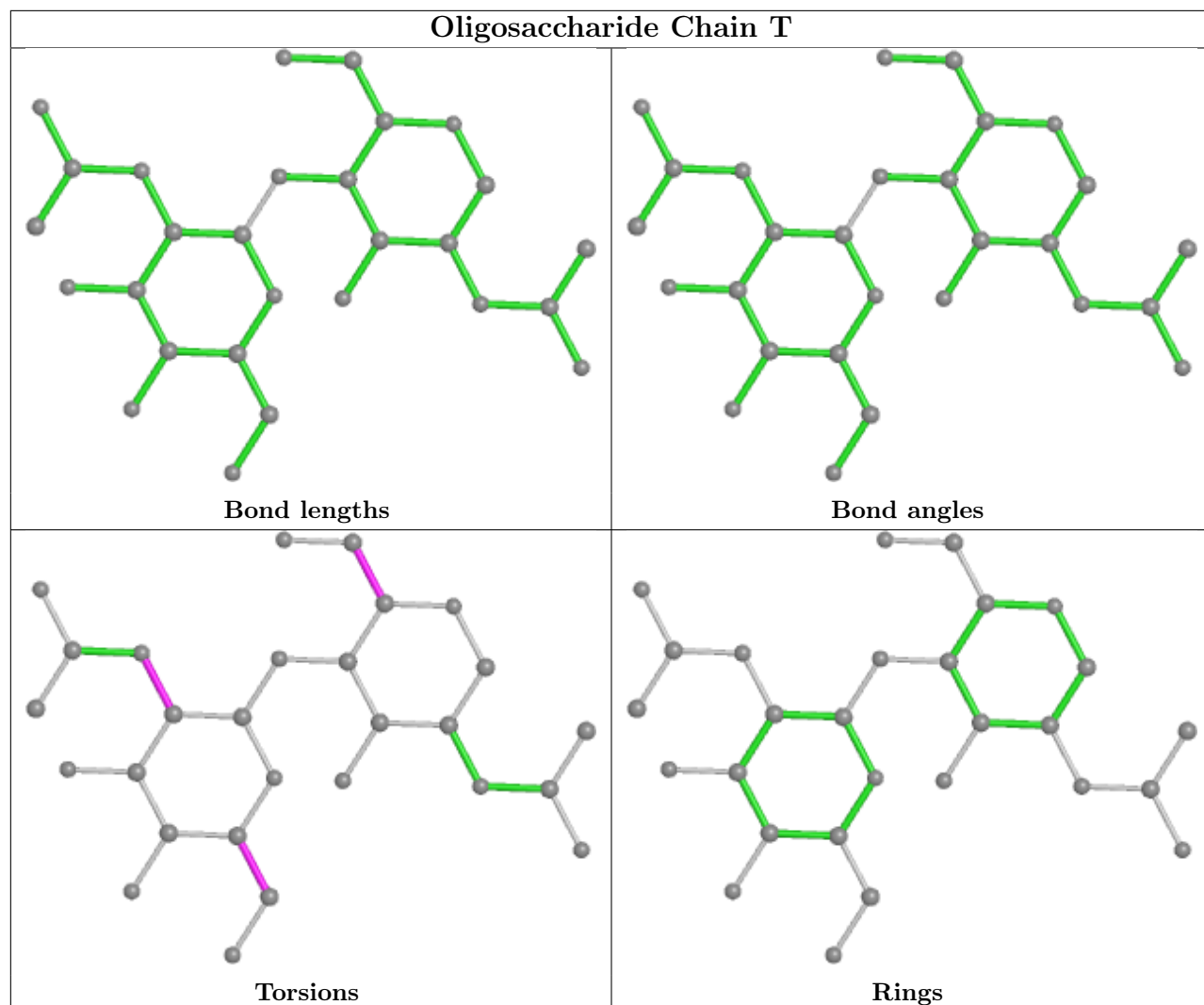
There are no ring outliers.

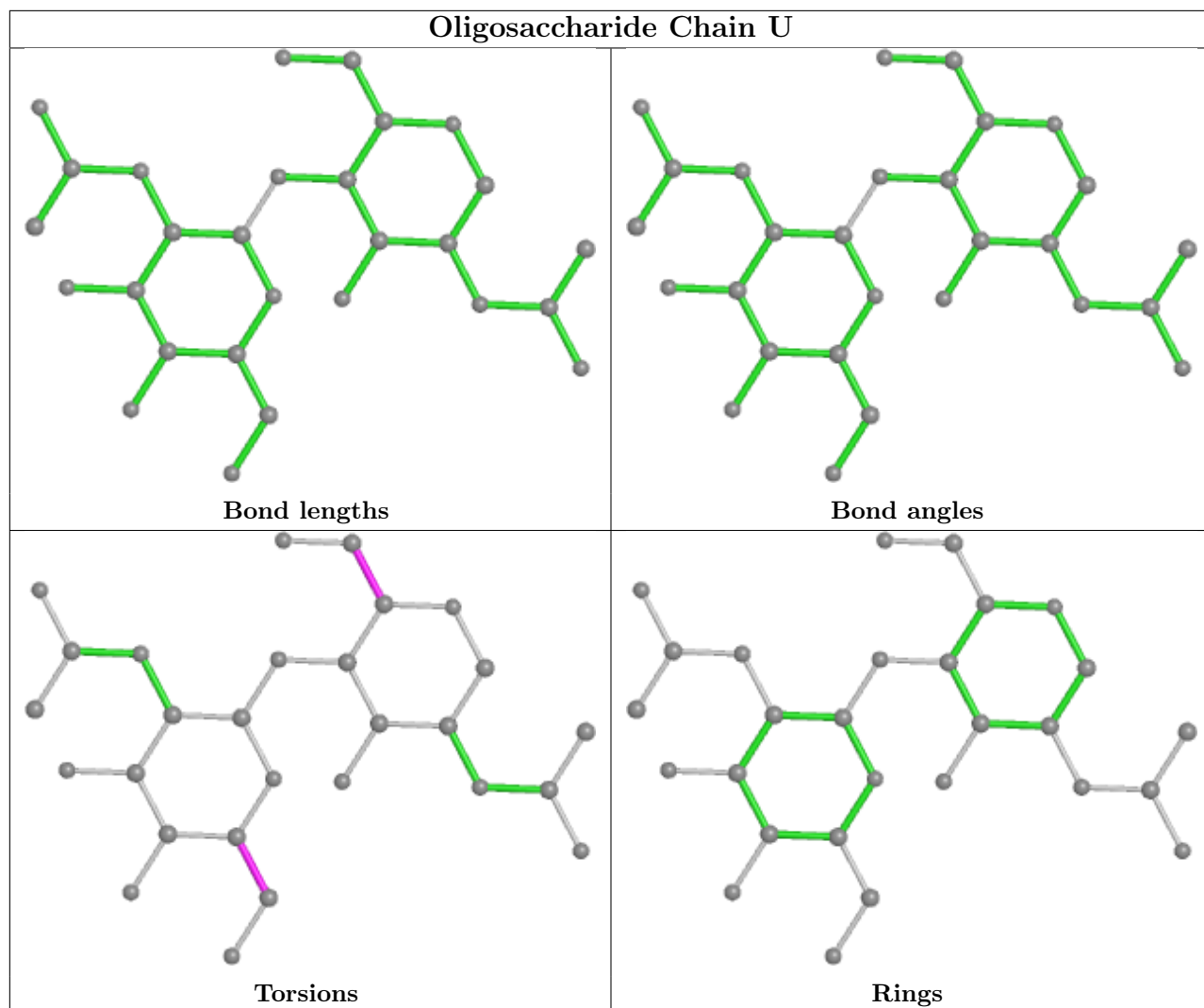
No monomer is involved in short contacts.

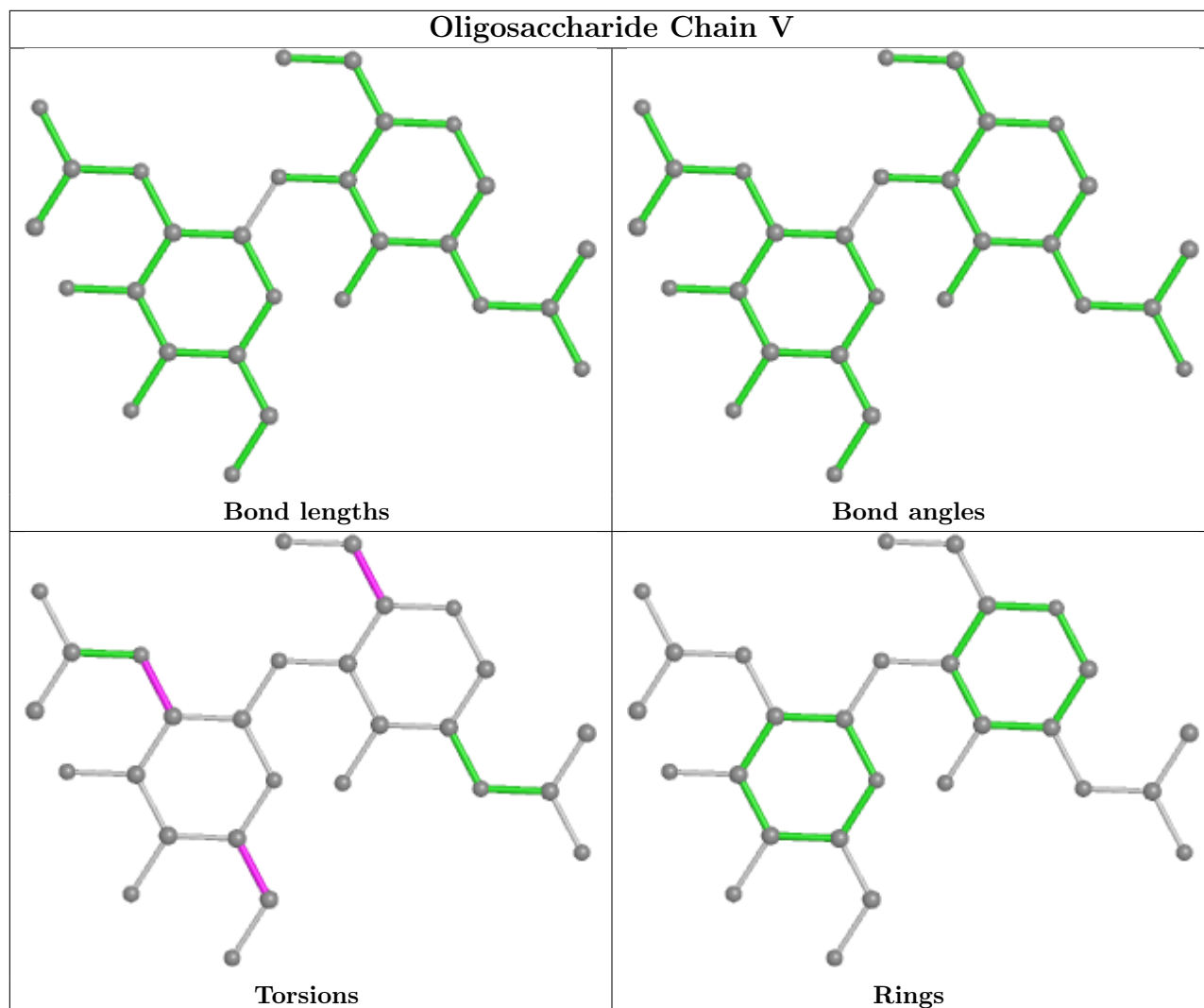
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

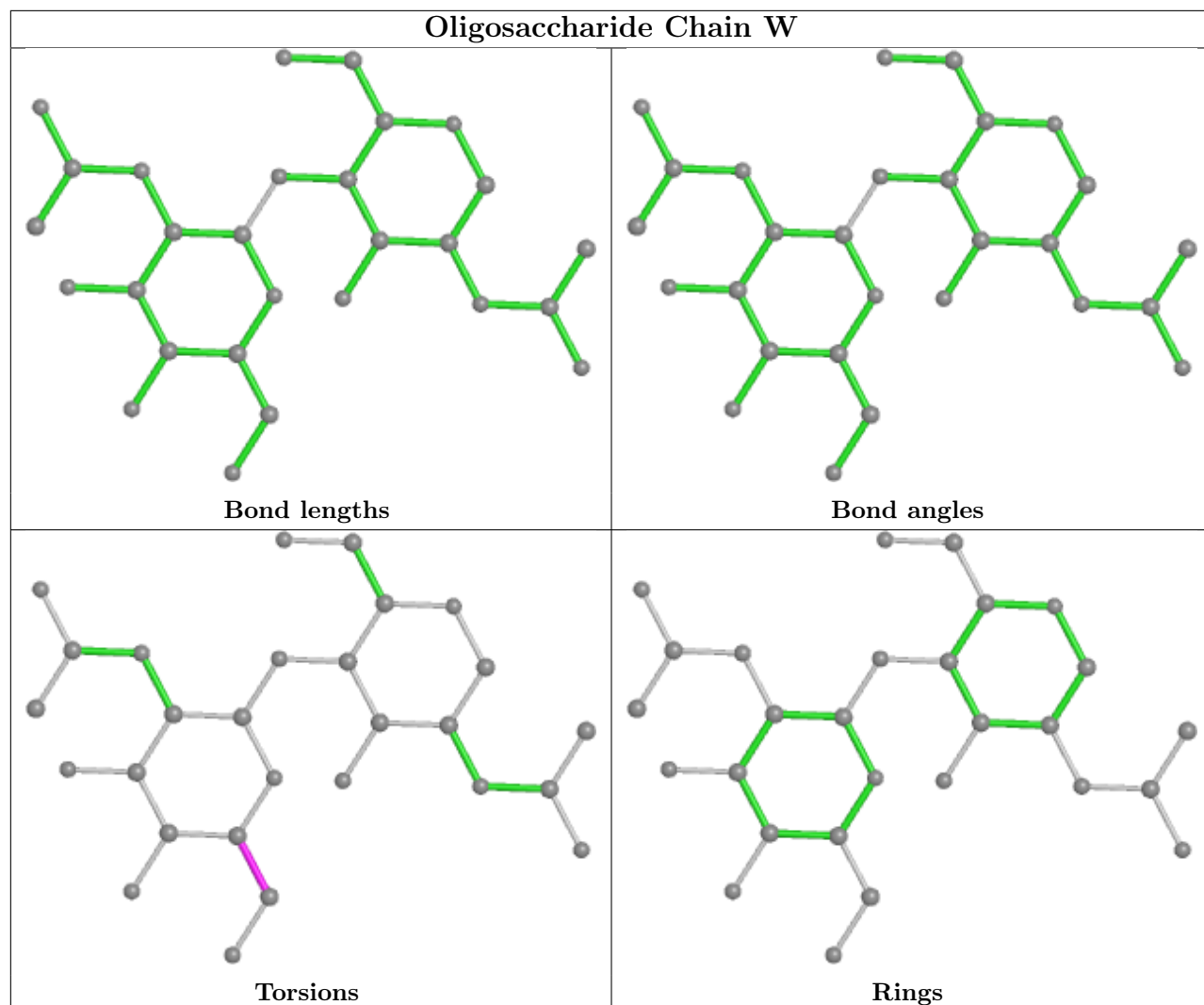


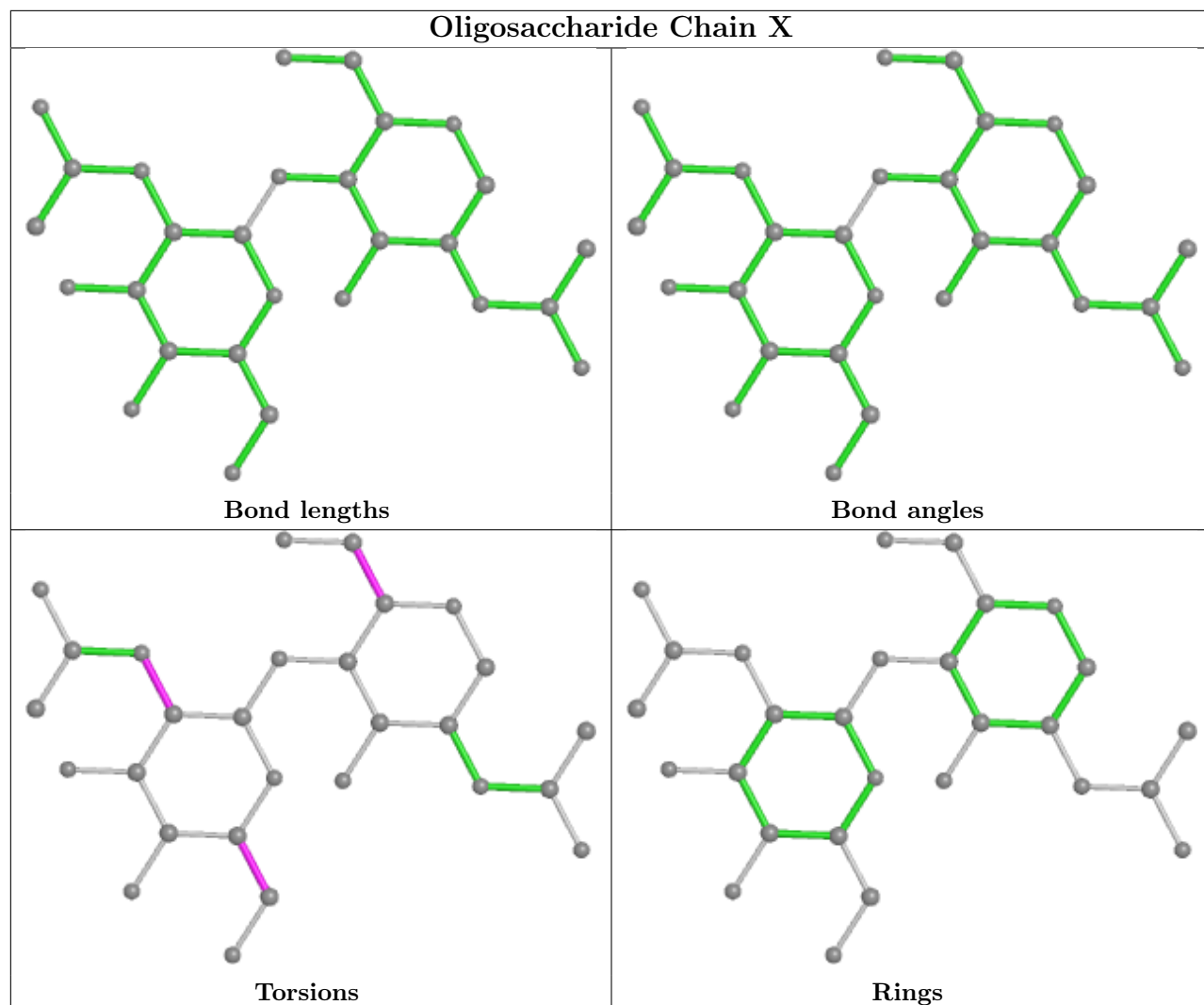


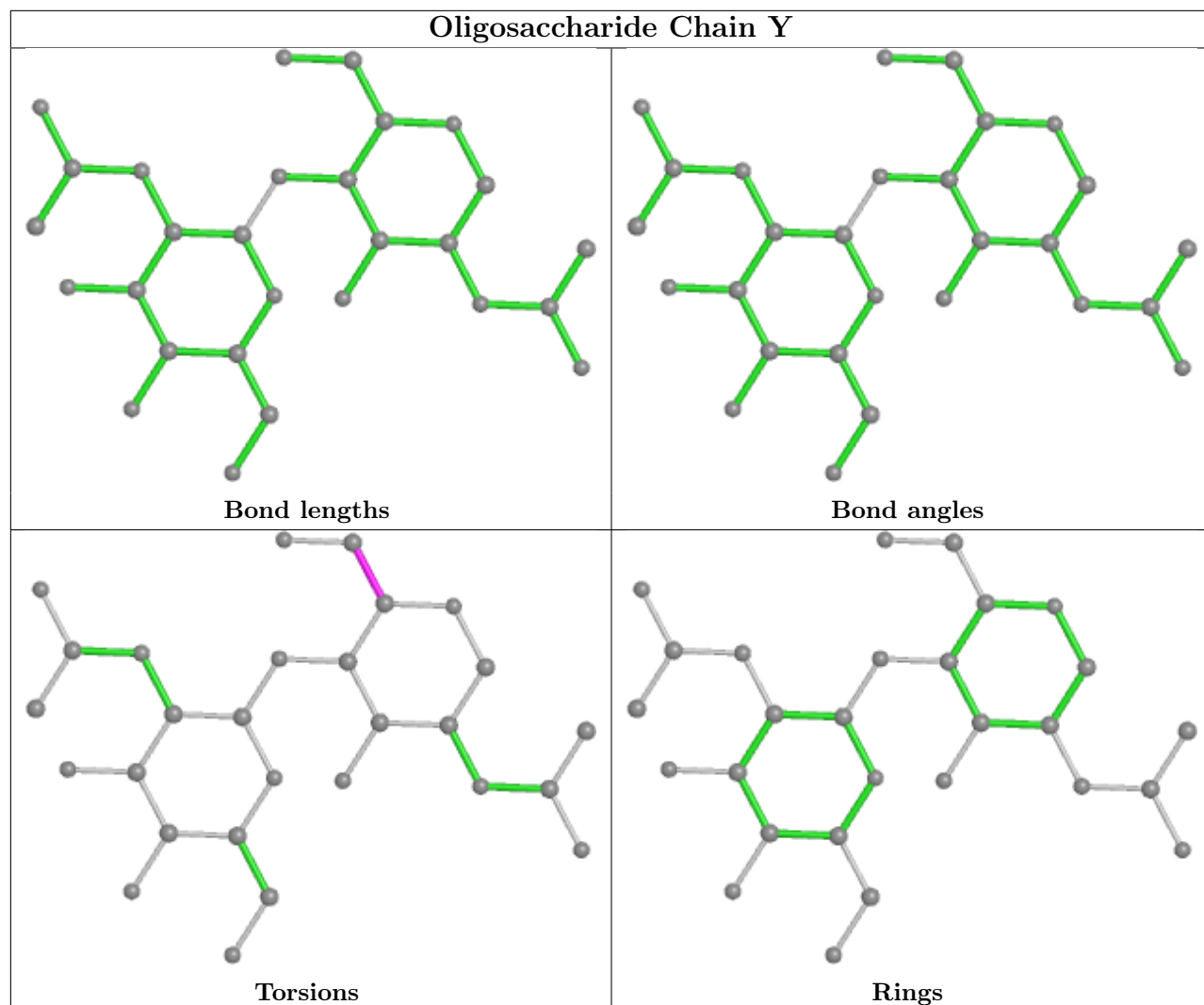


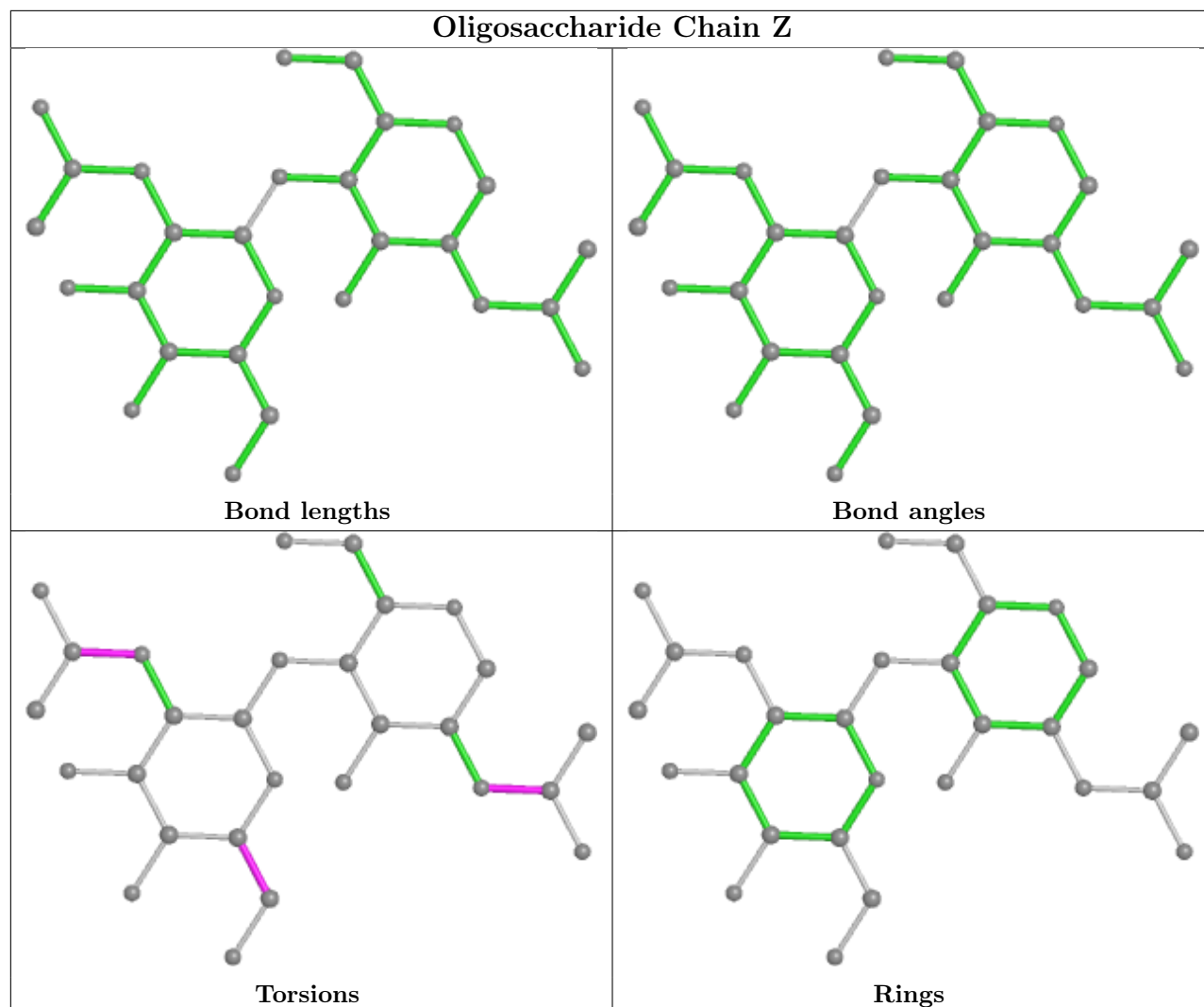


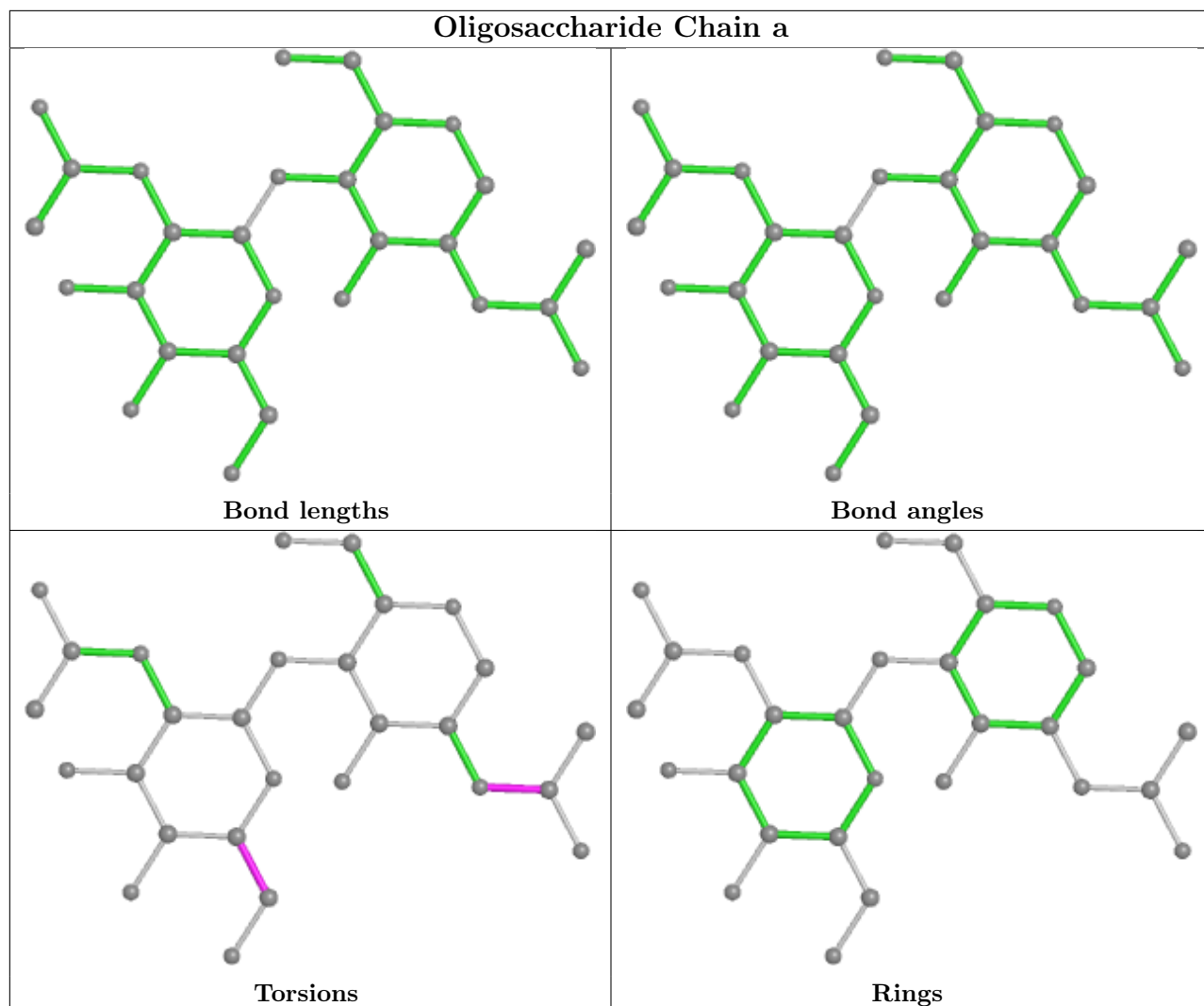




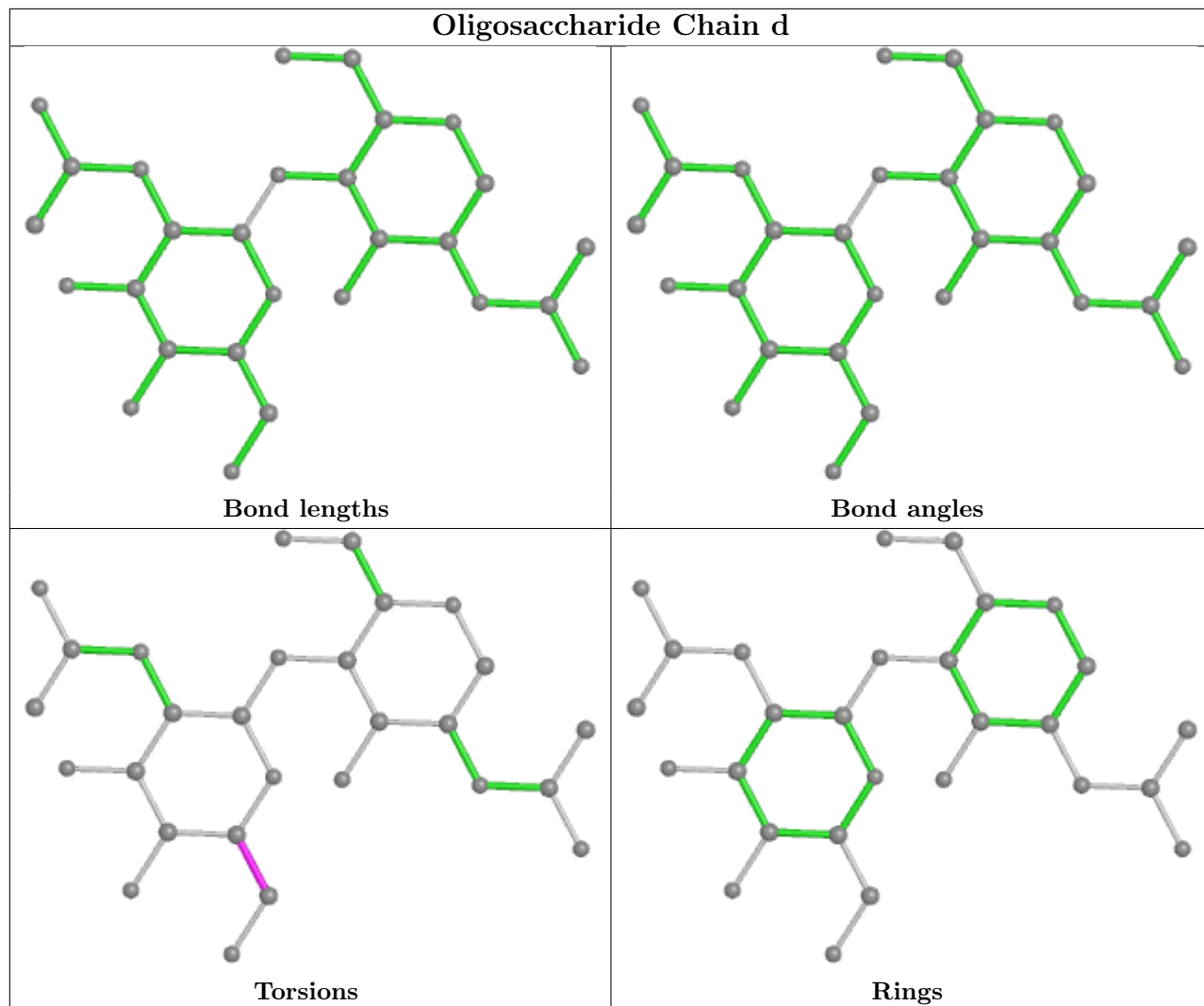


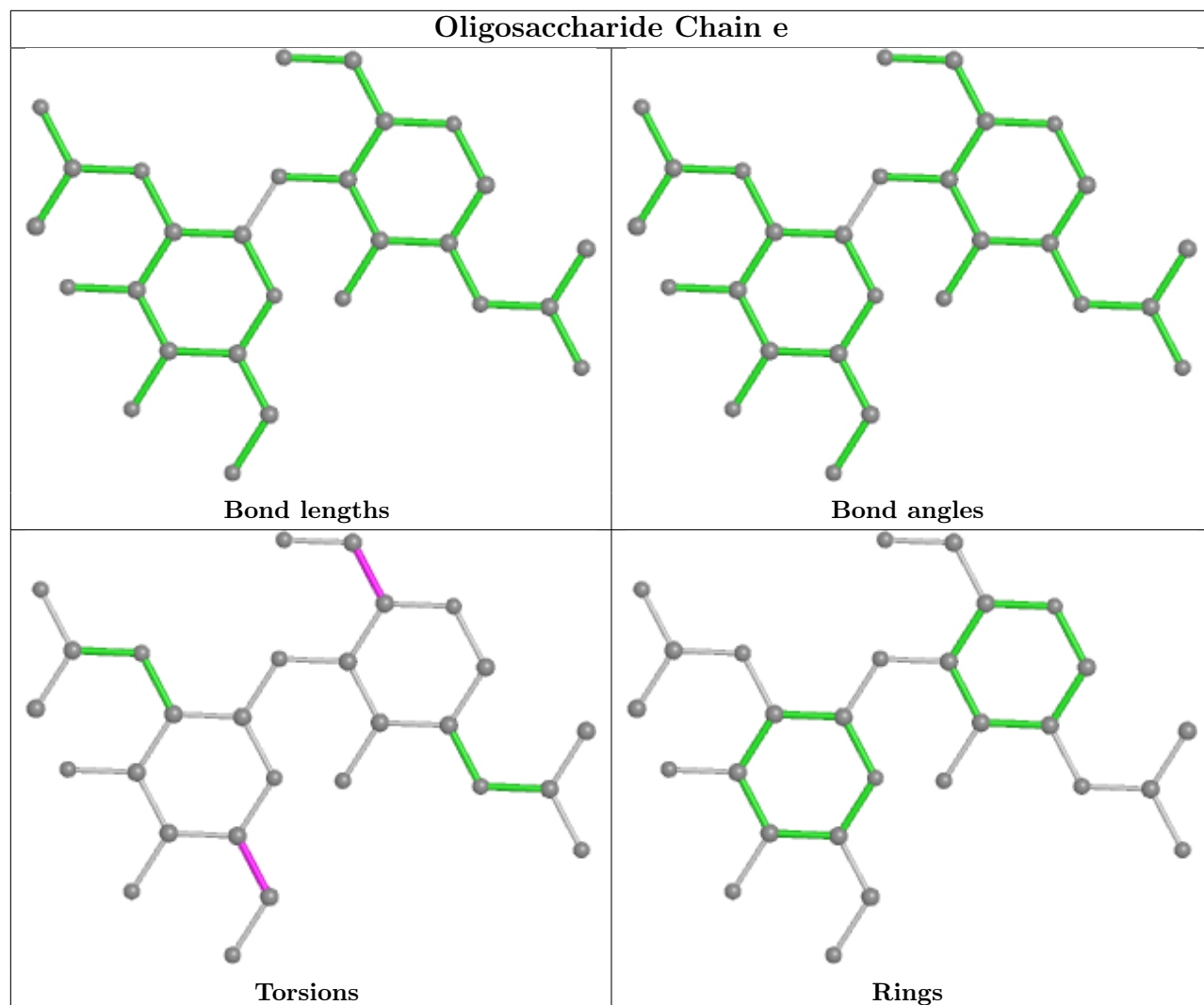


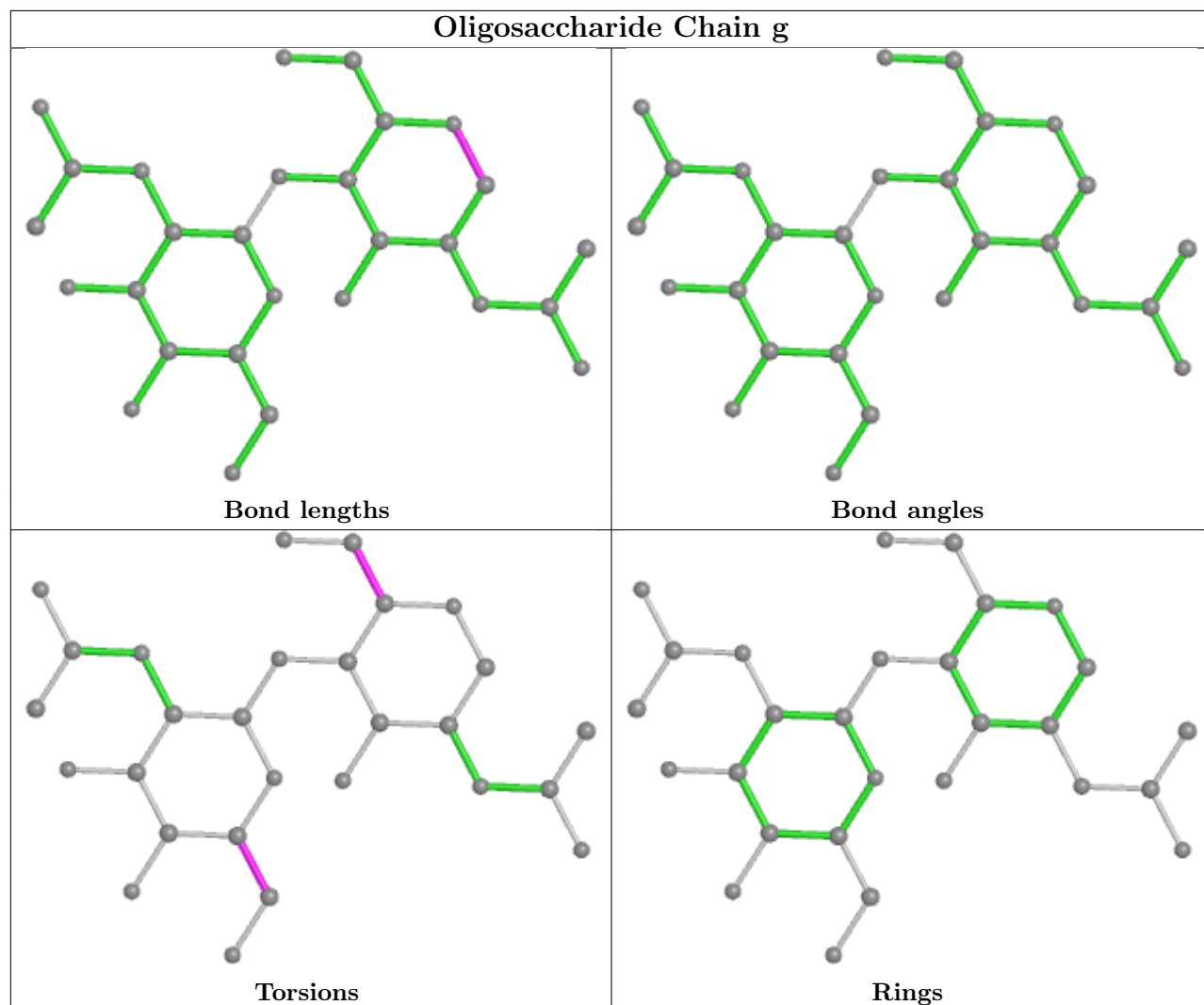


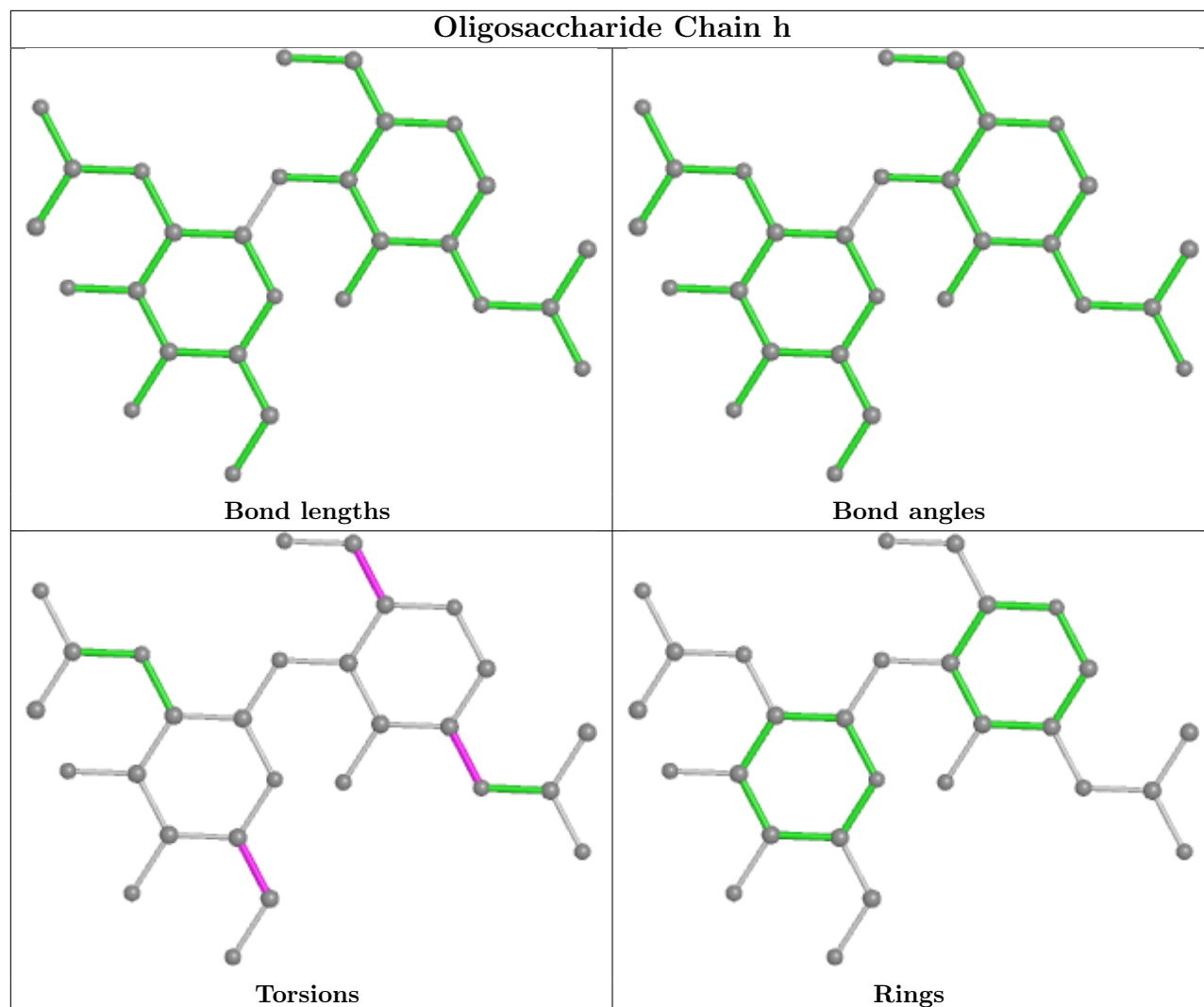


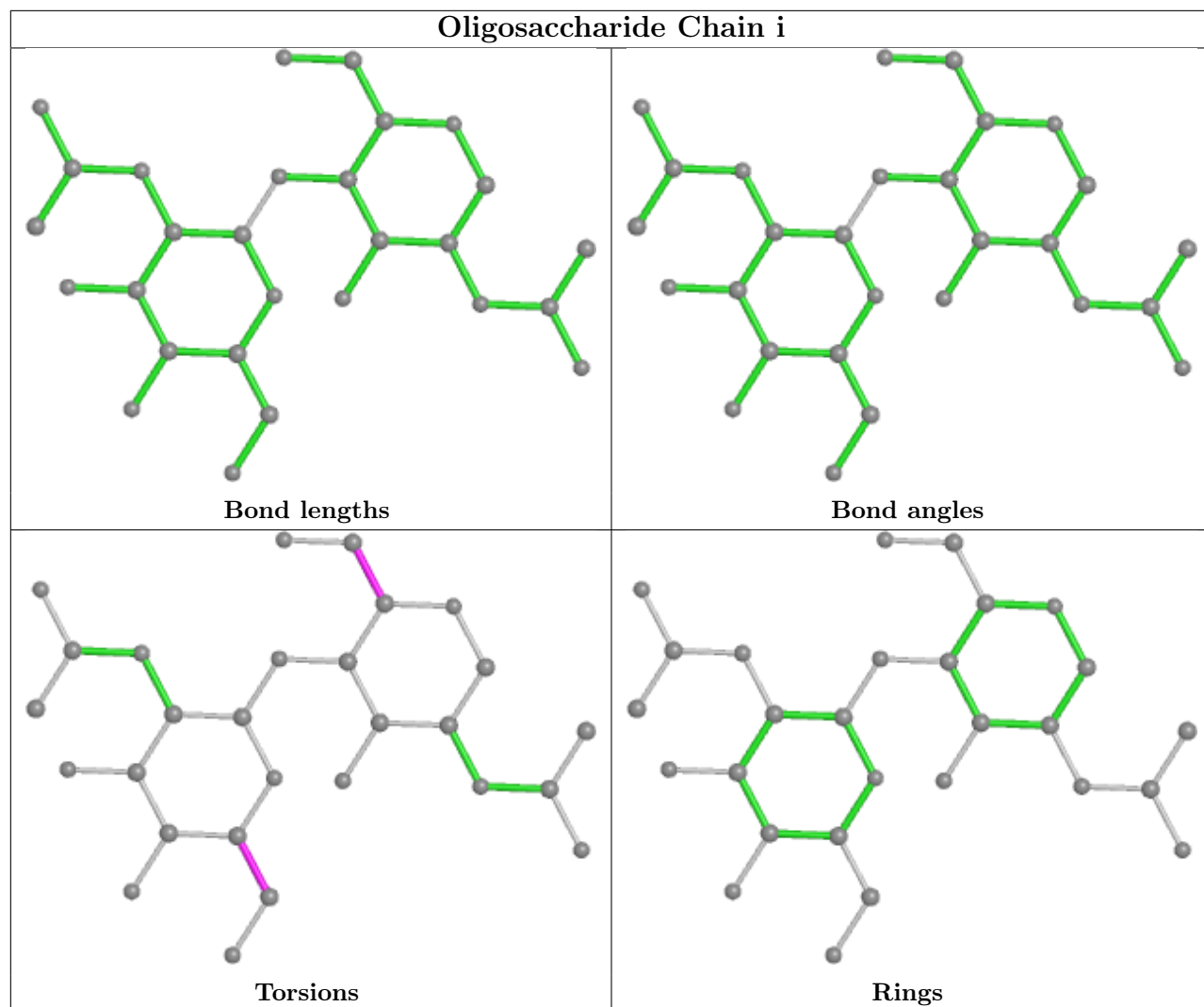


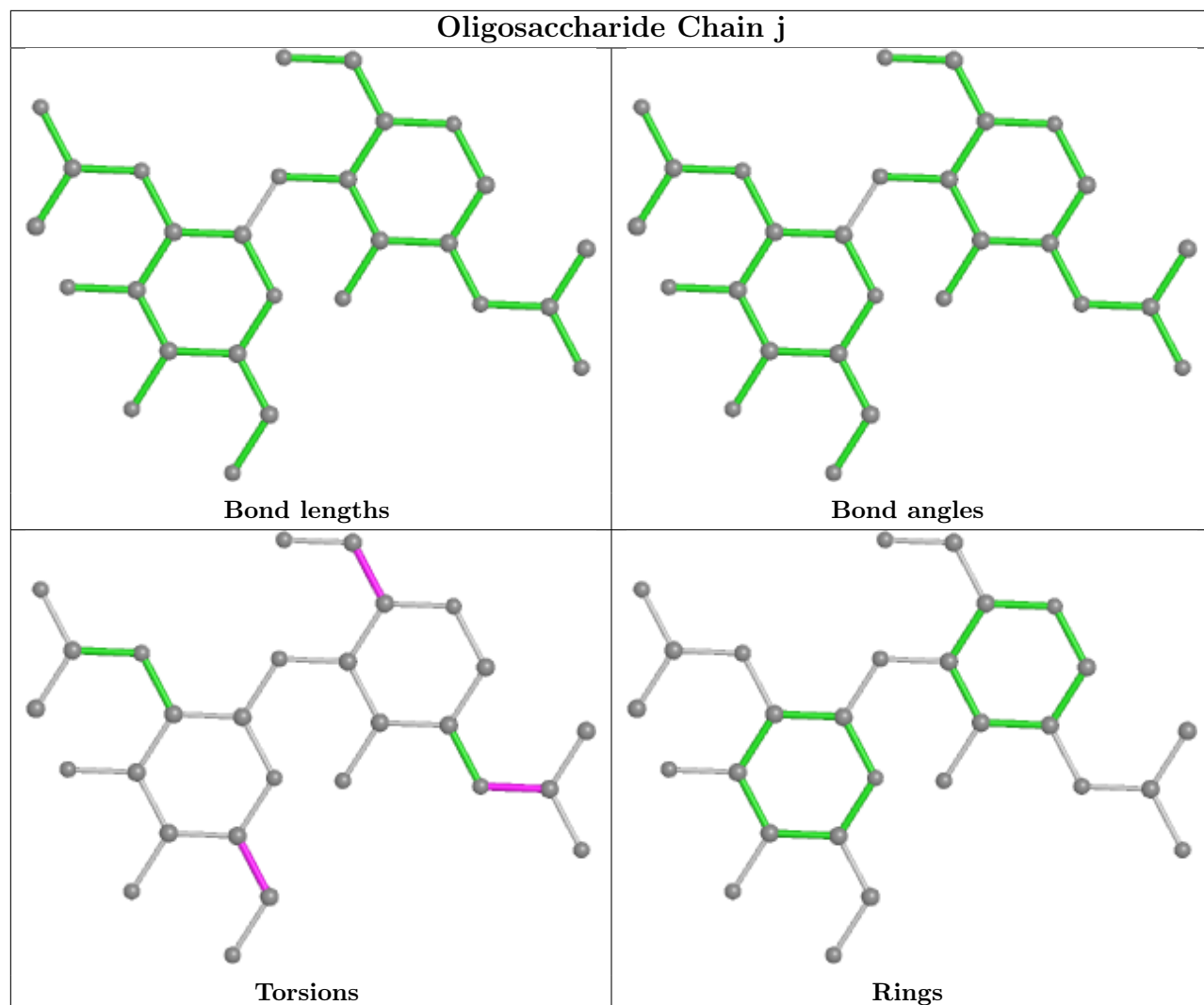


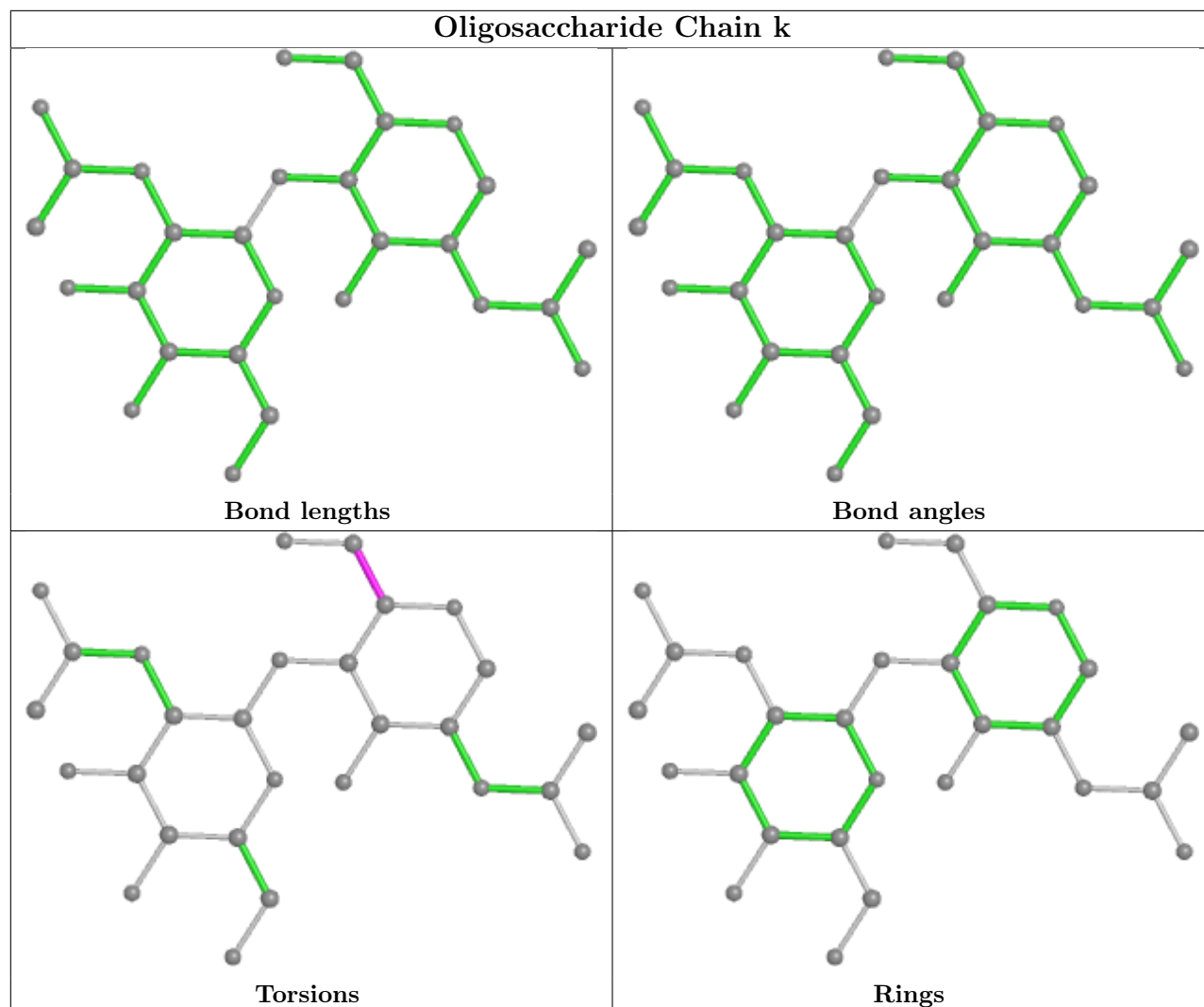


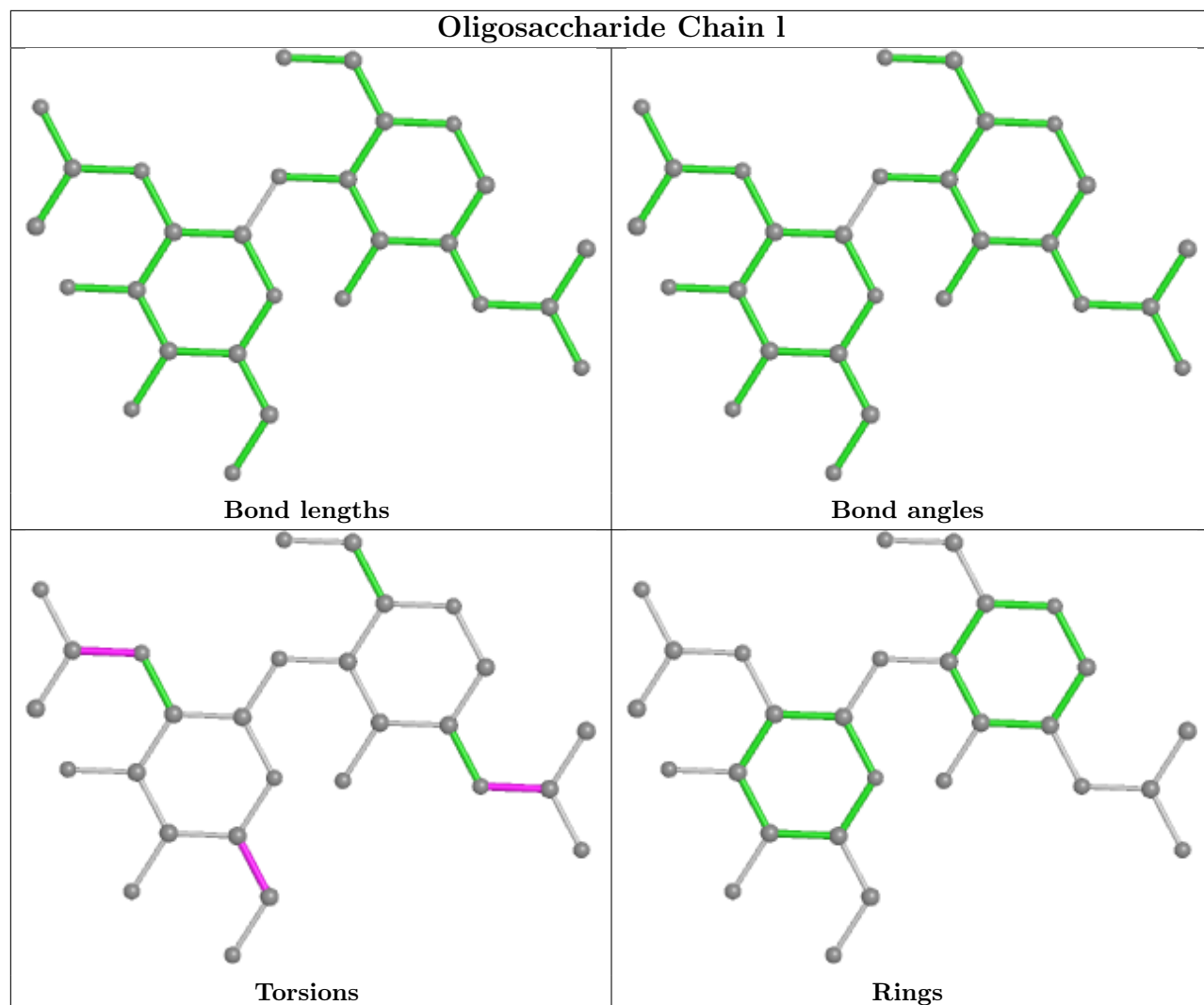




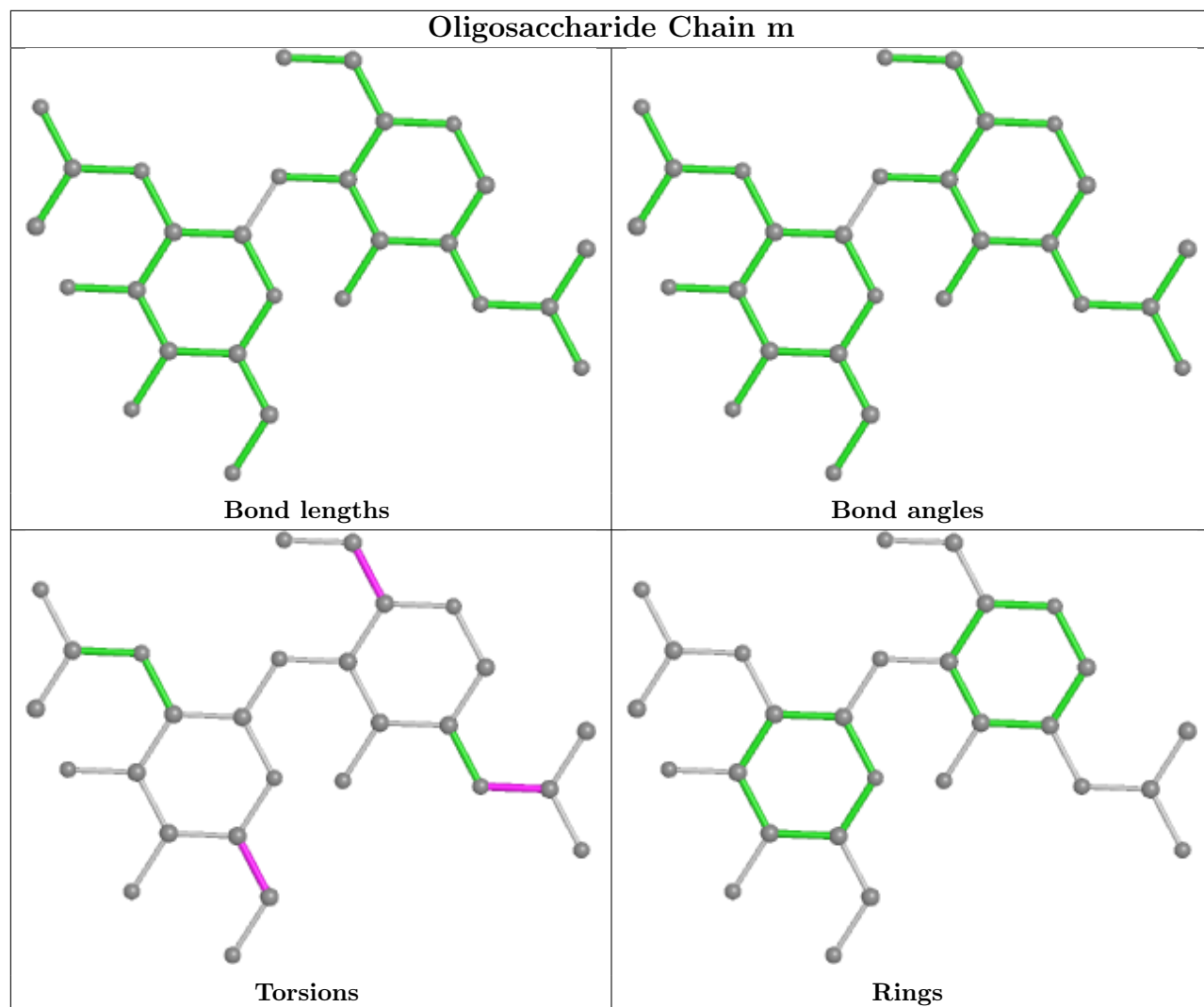


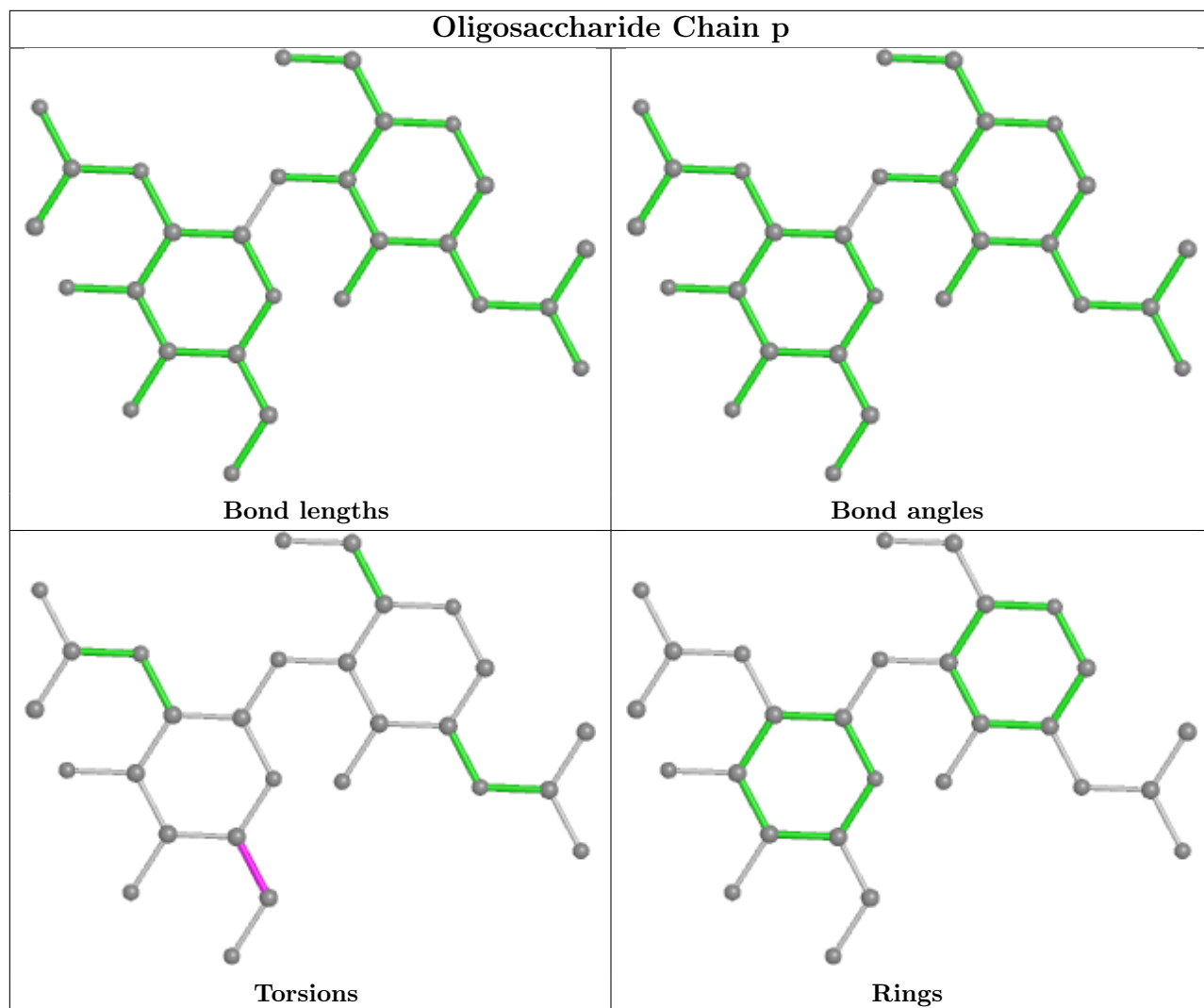


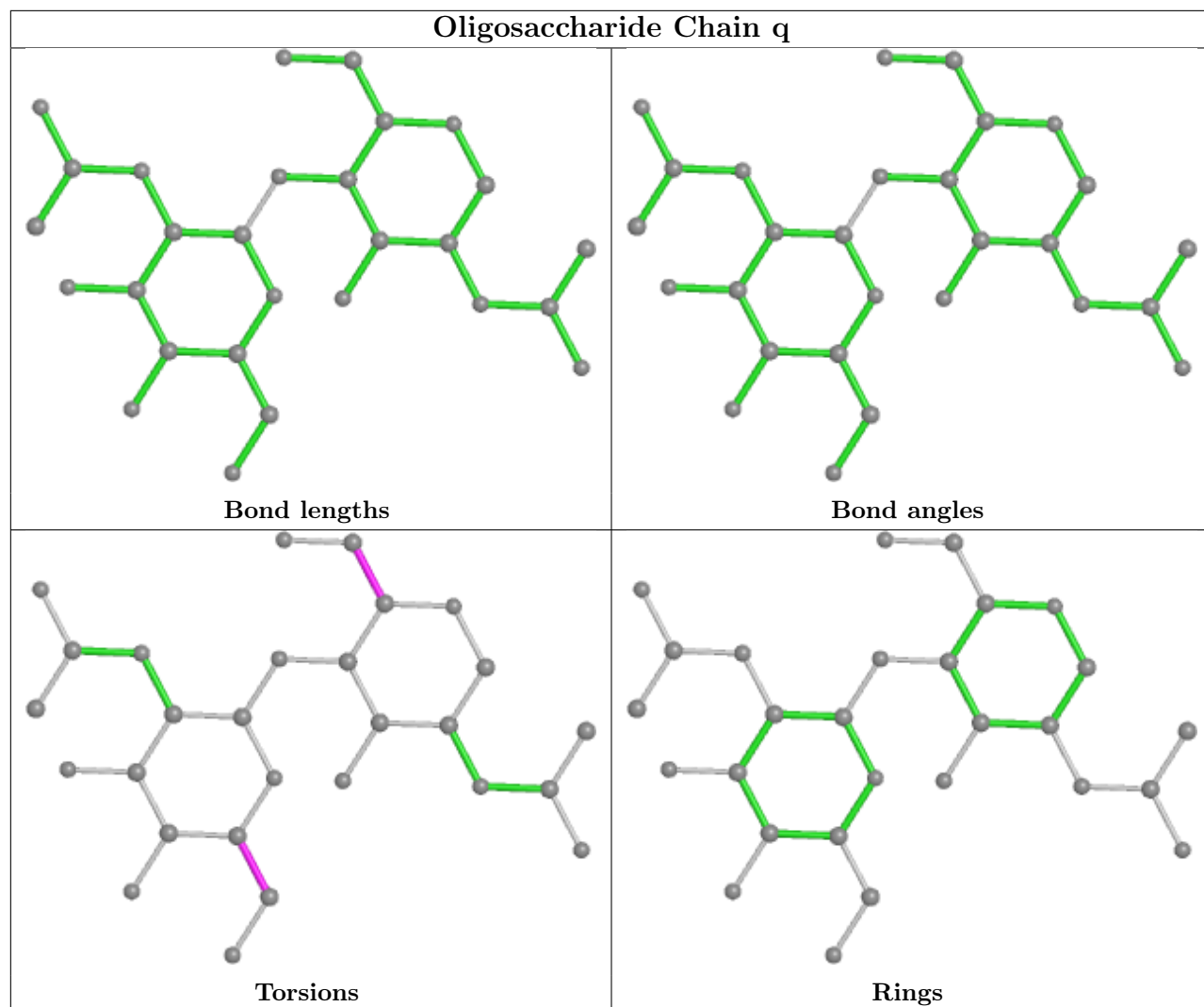


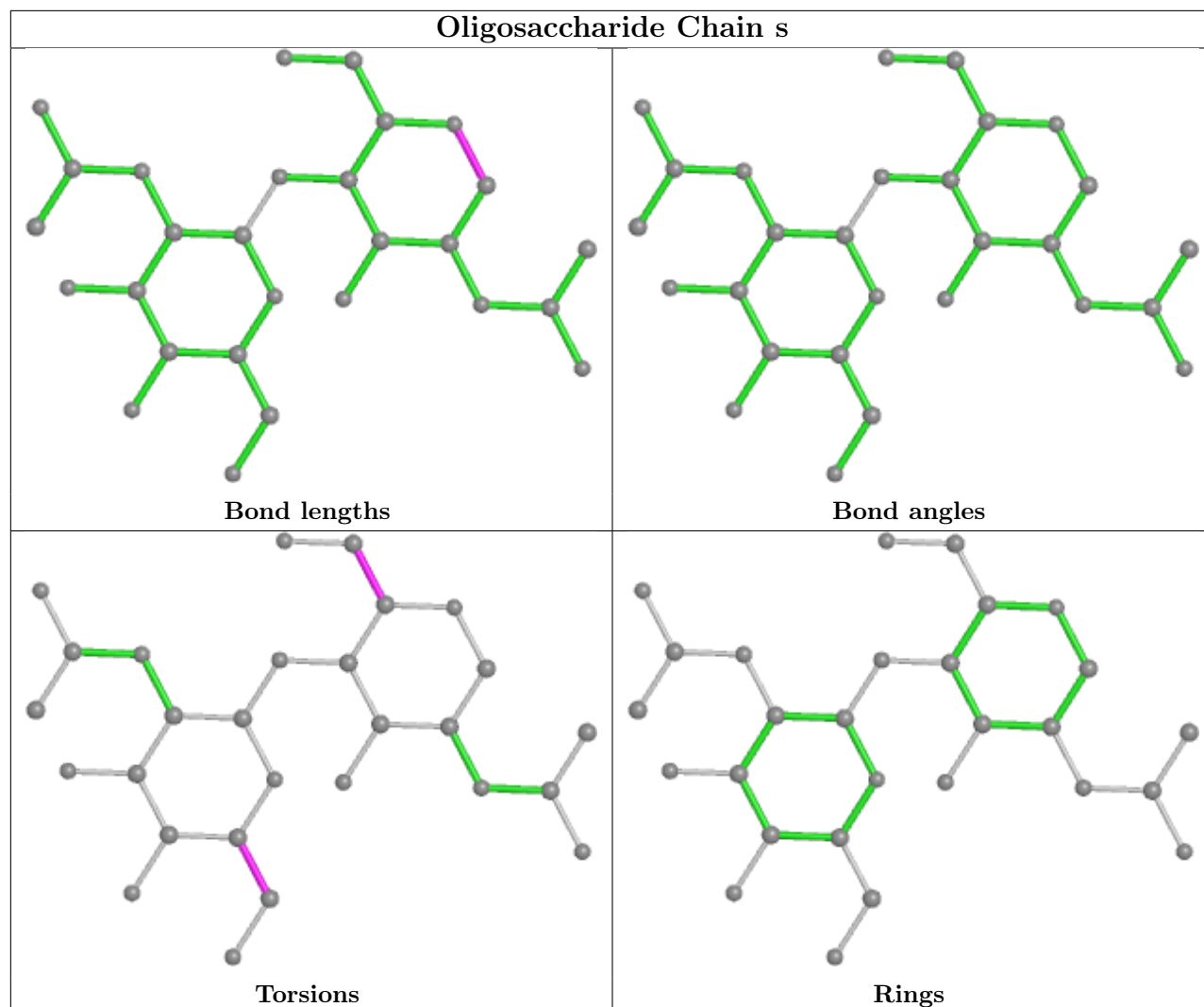


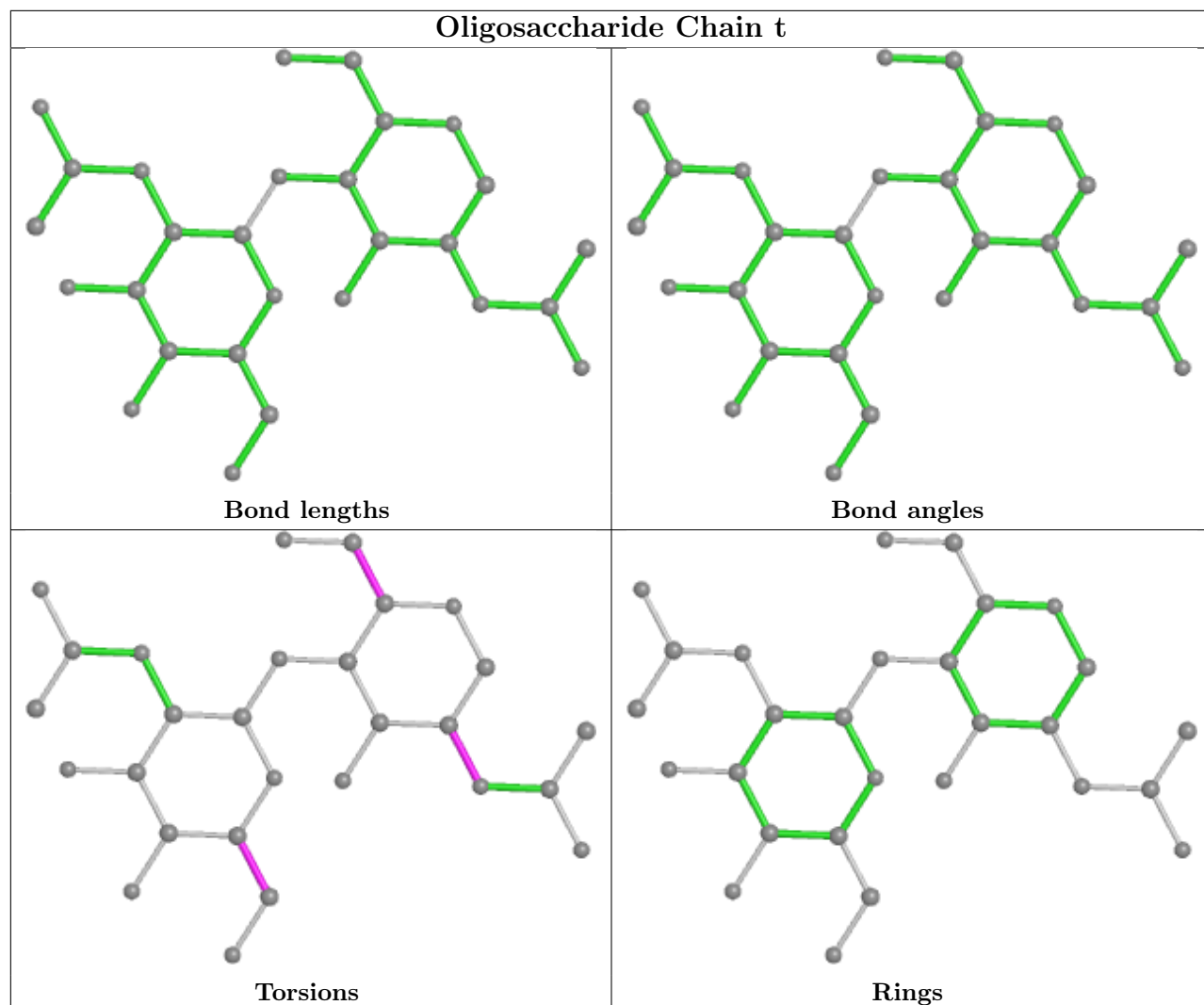


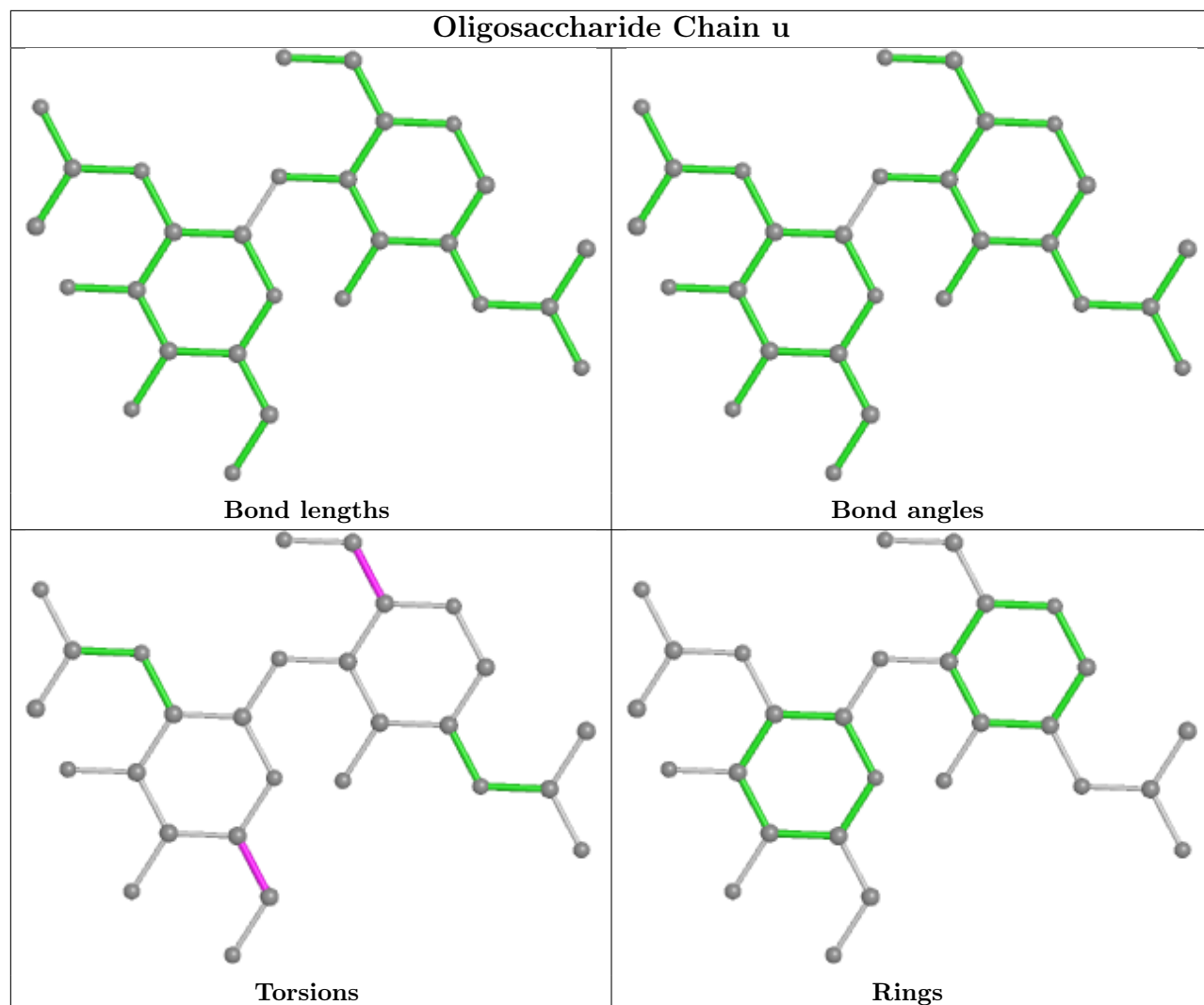


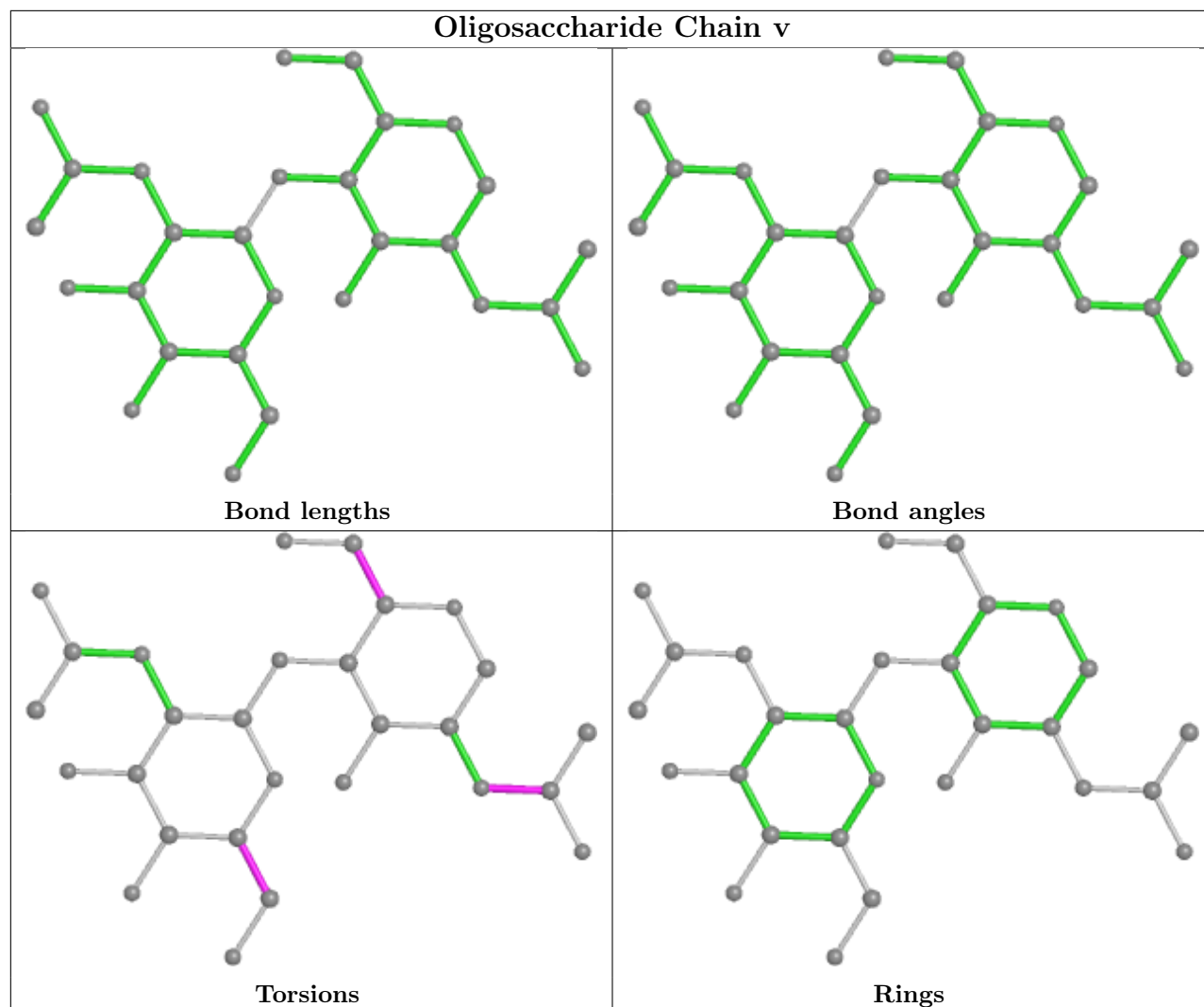


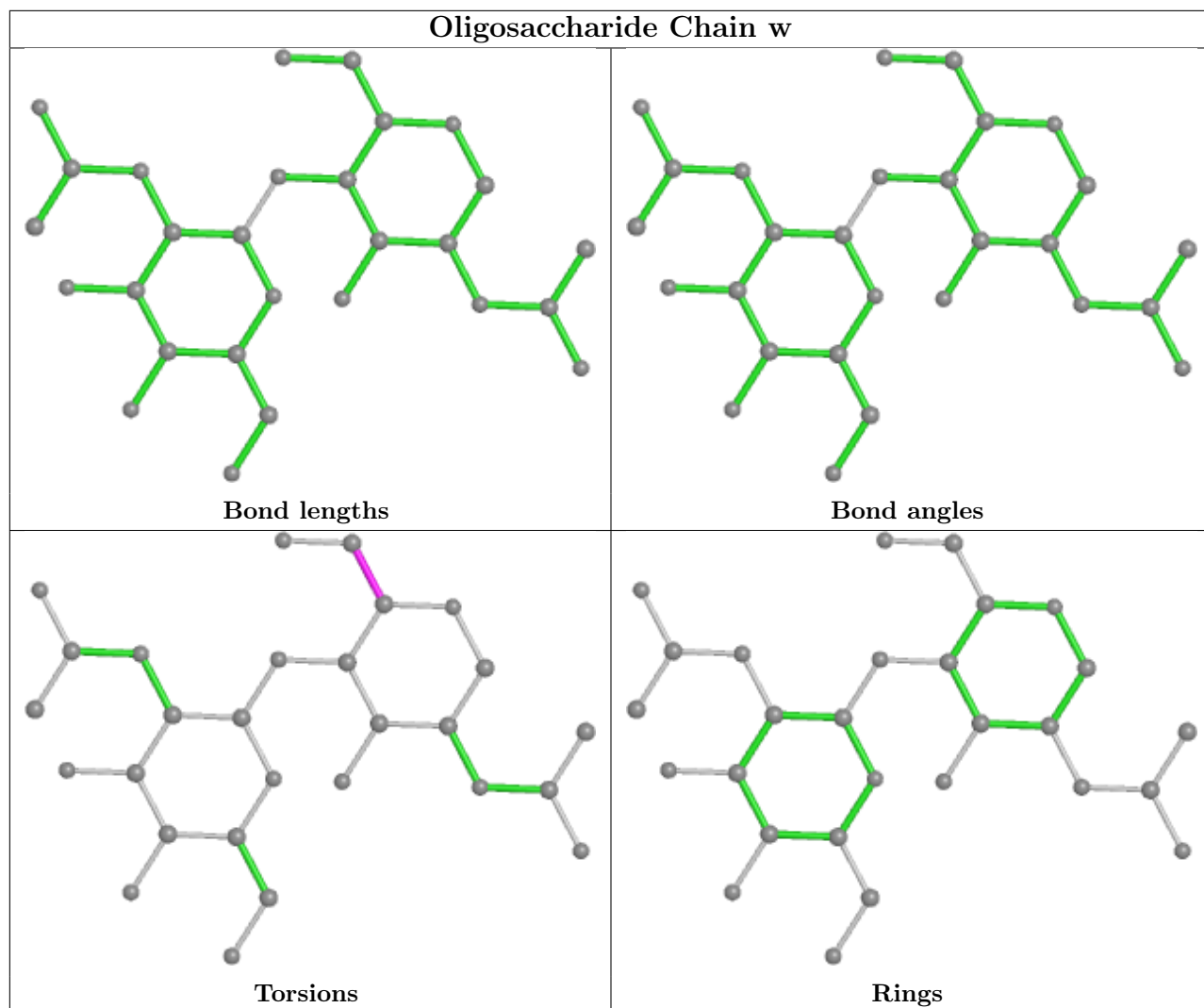




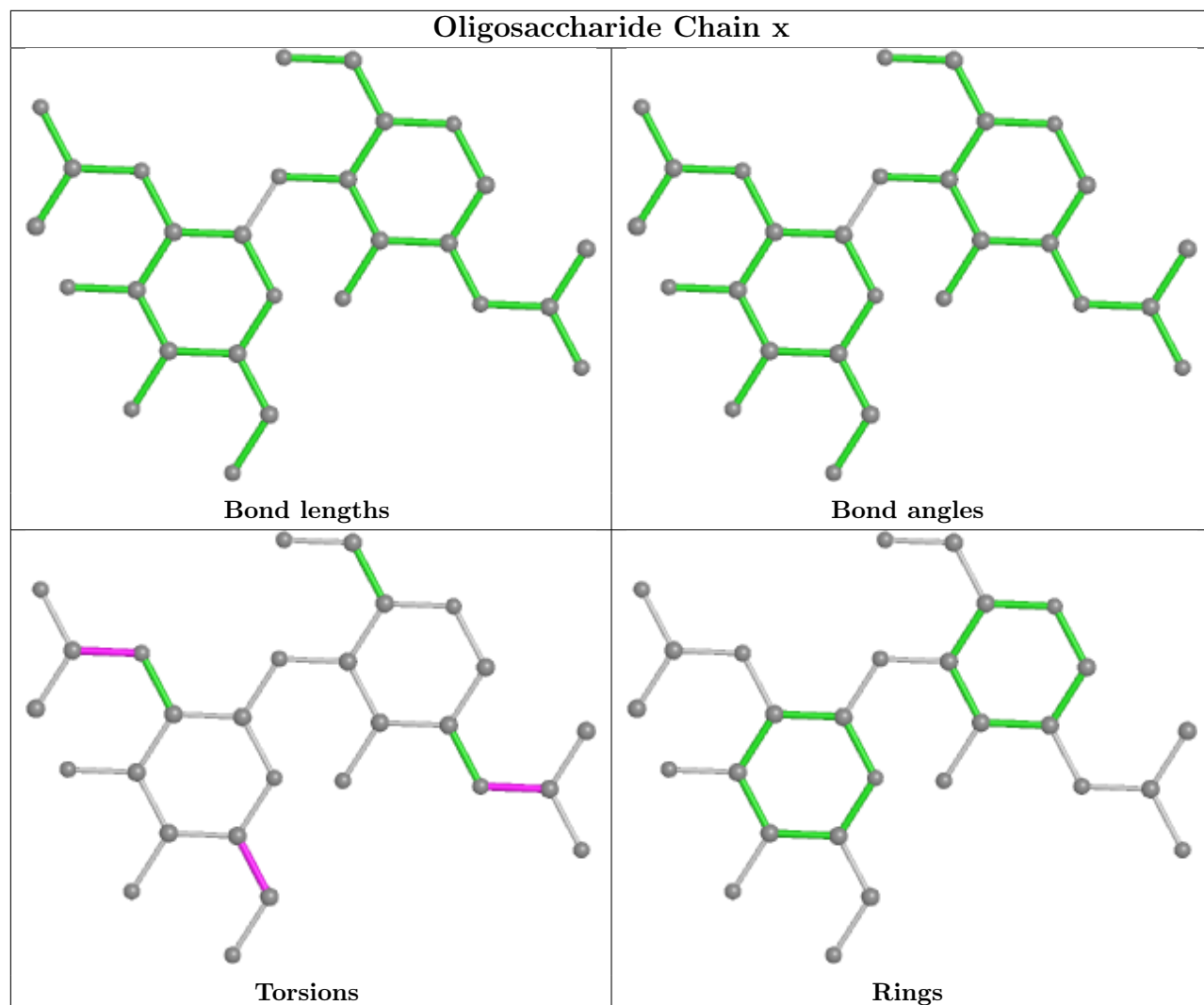


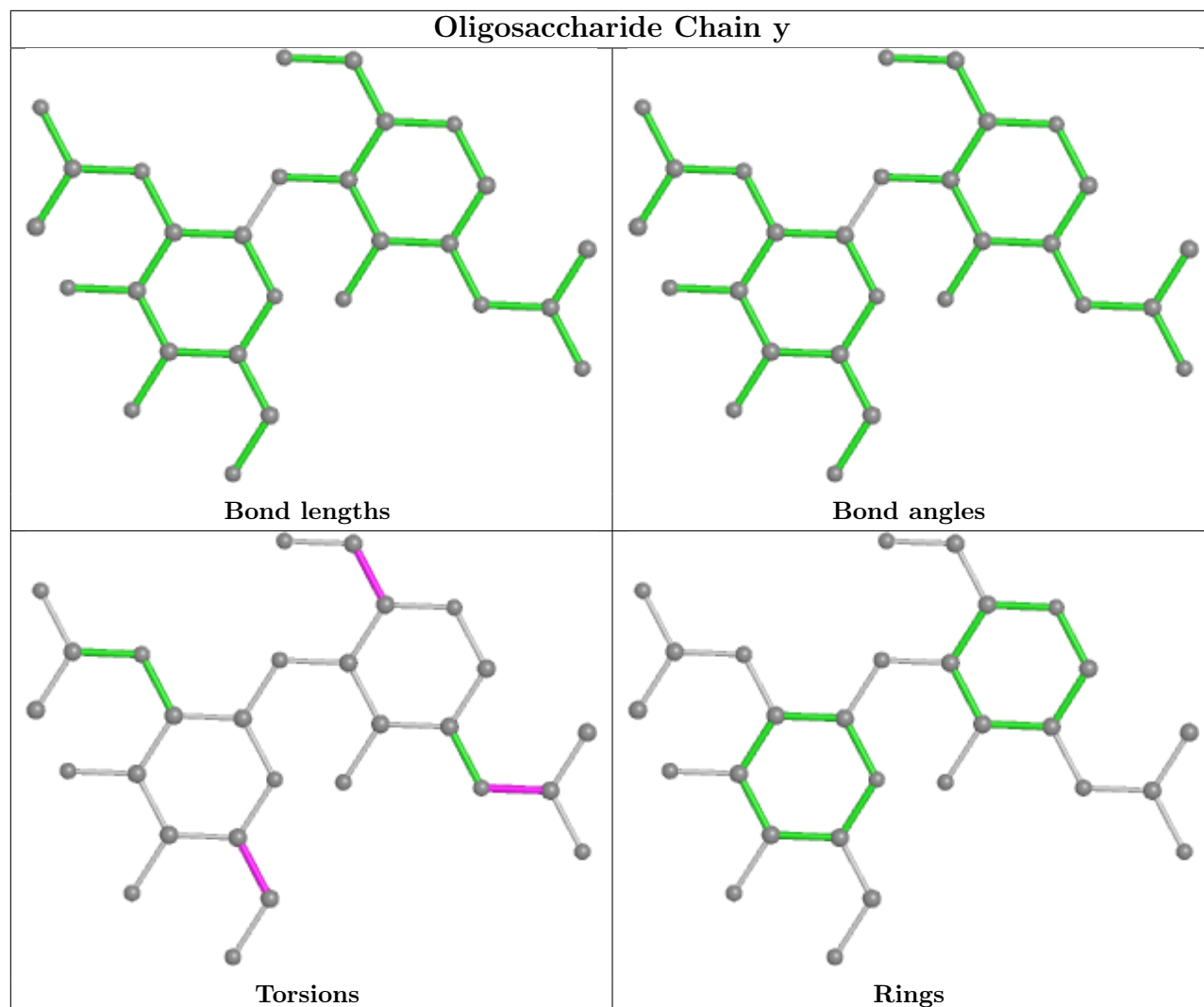


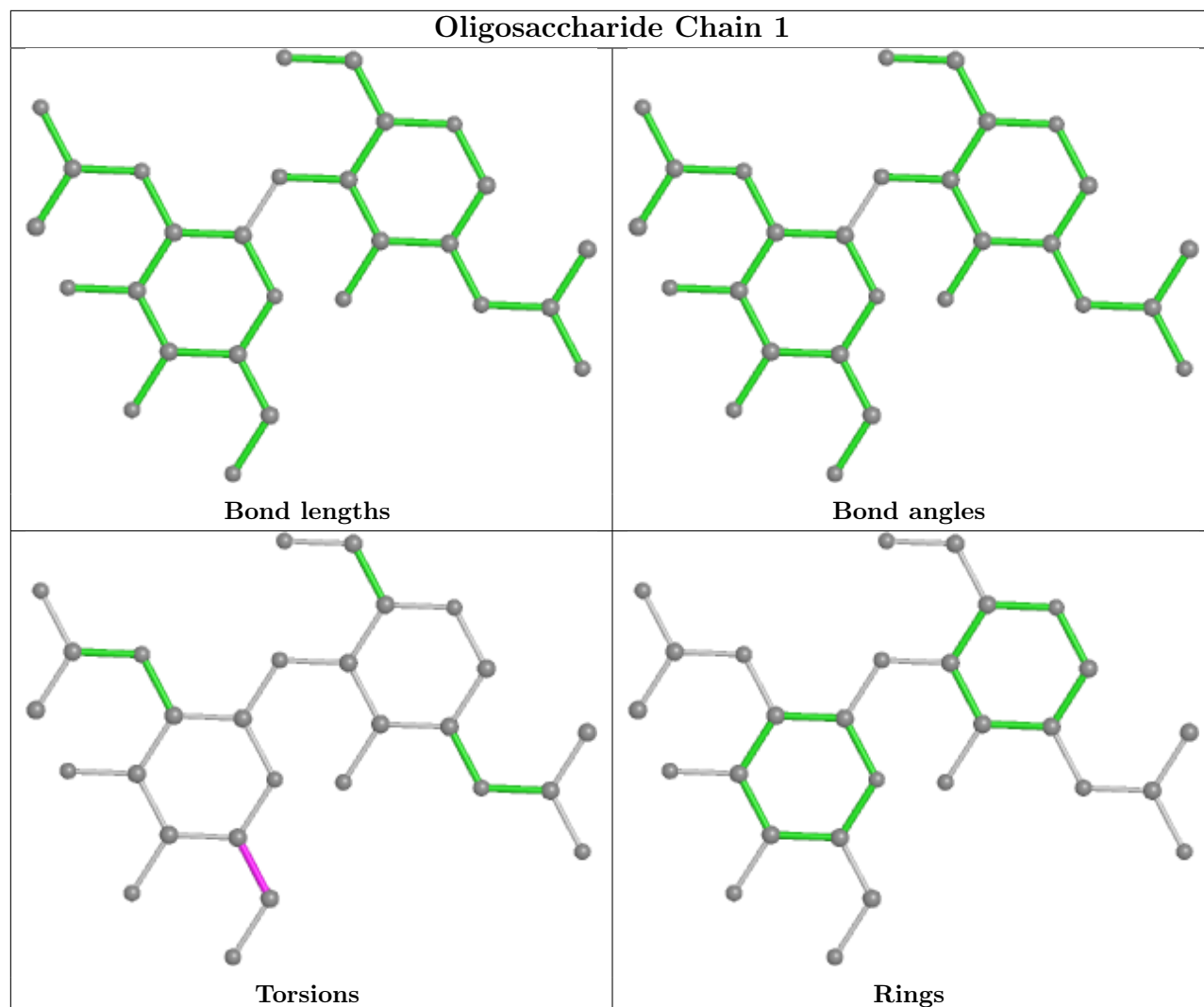


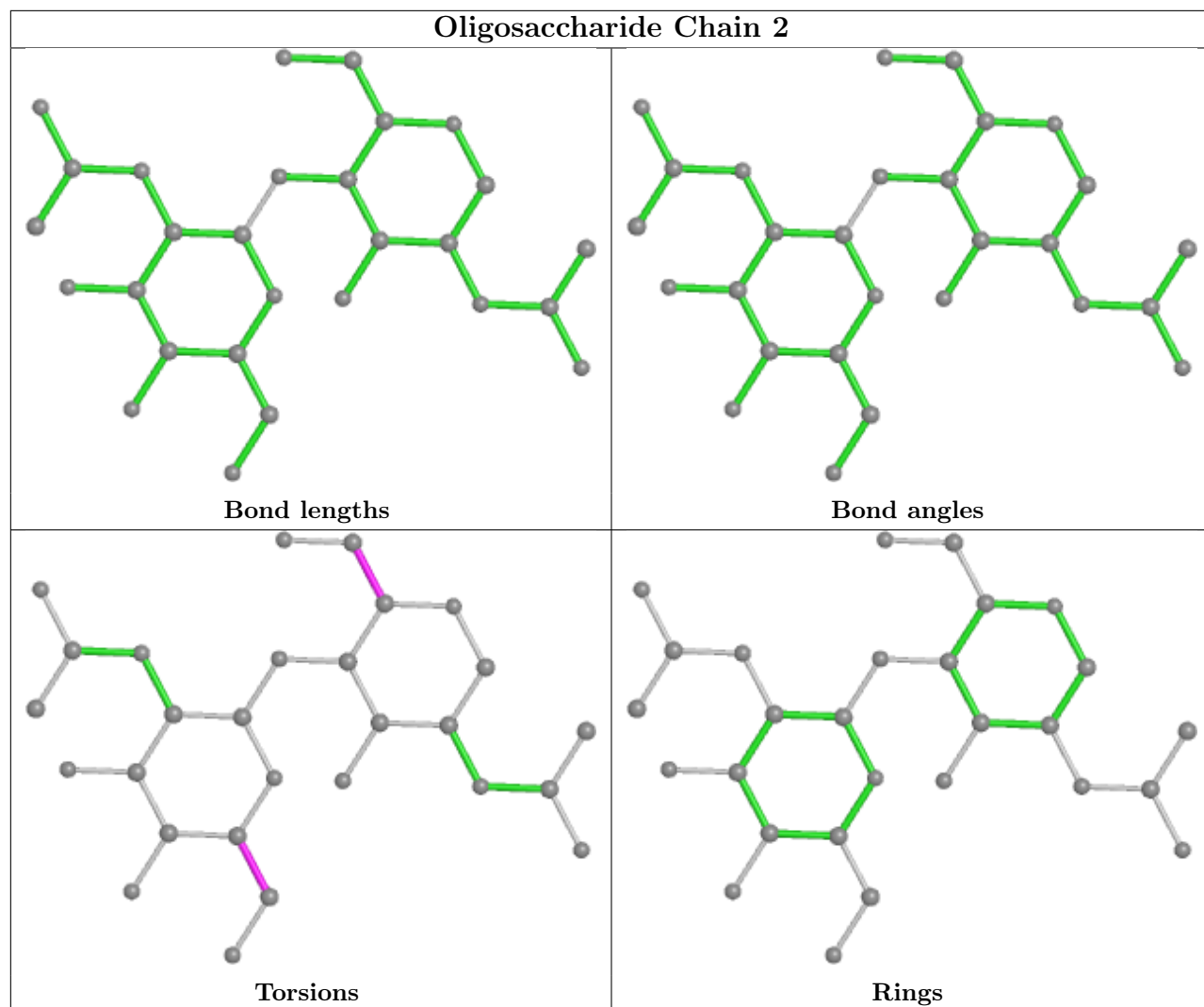


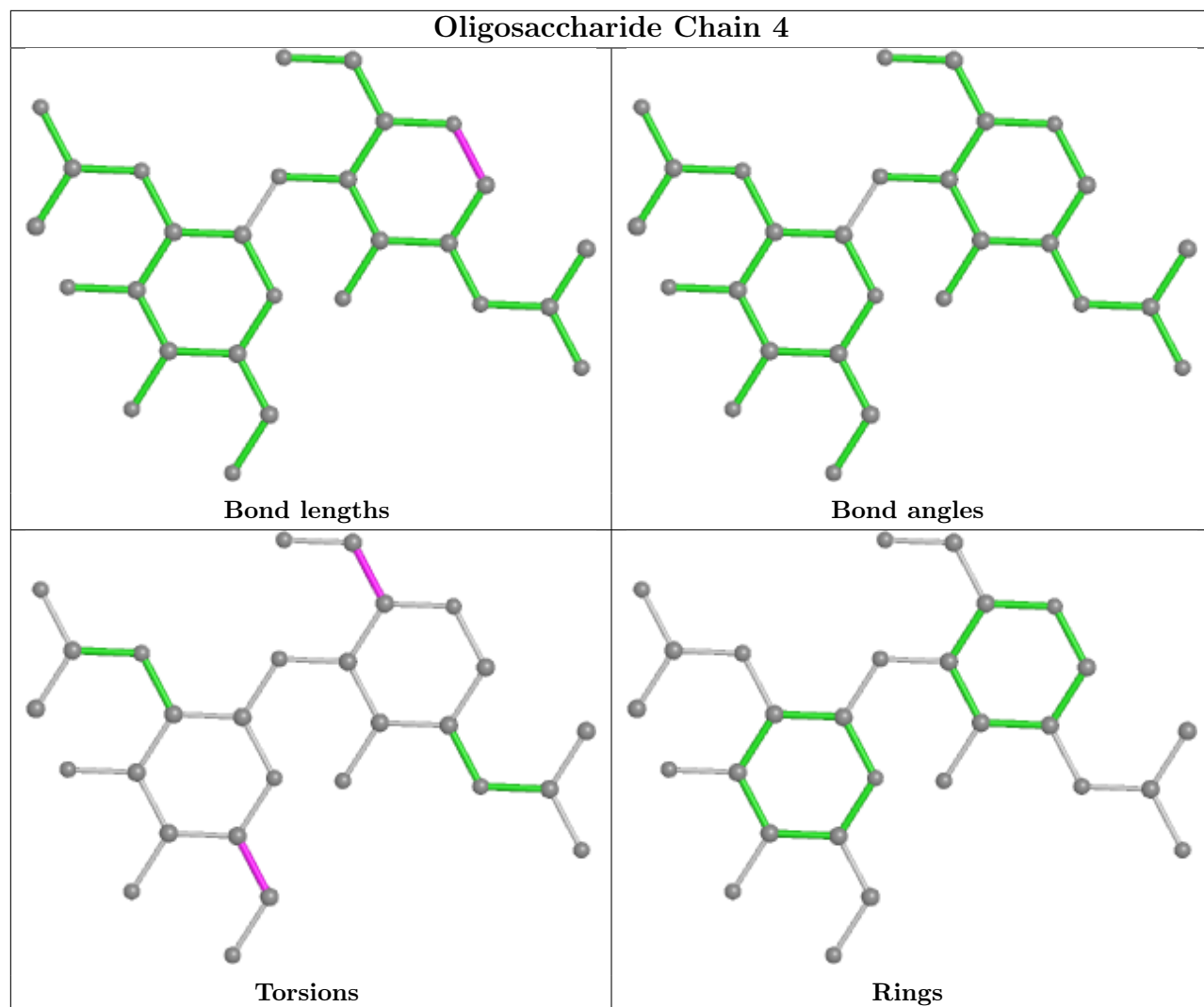


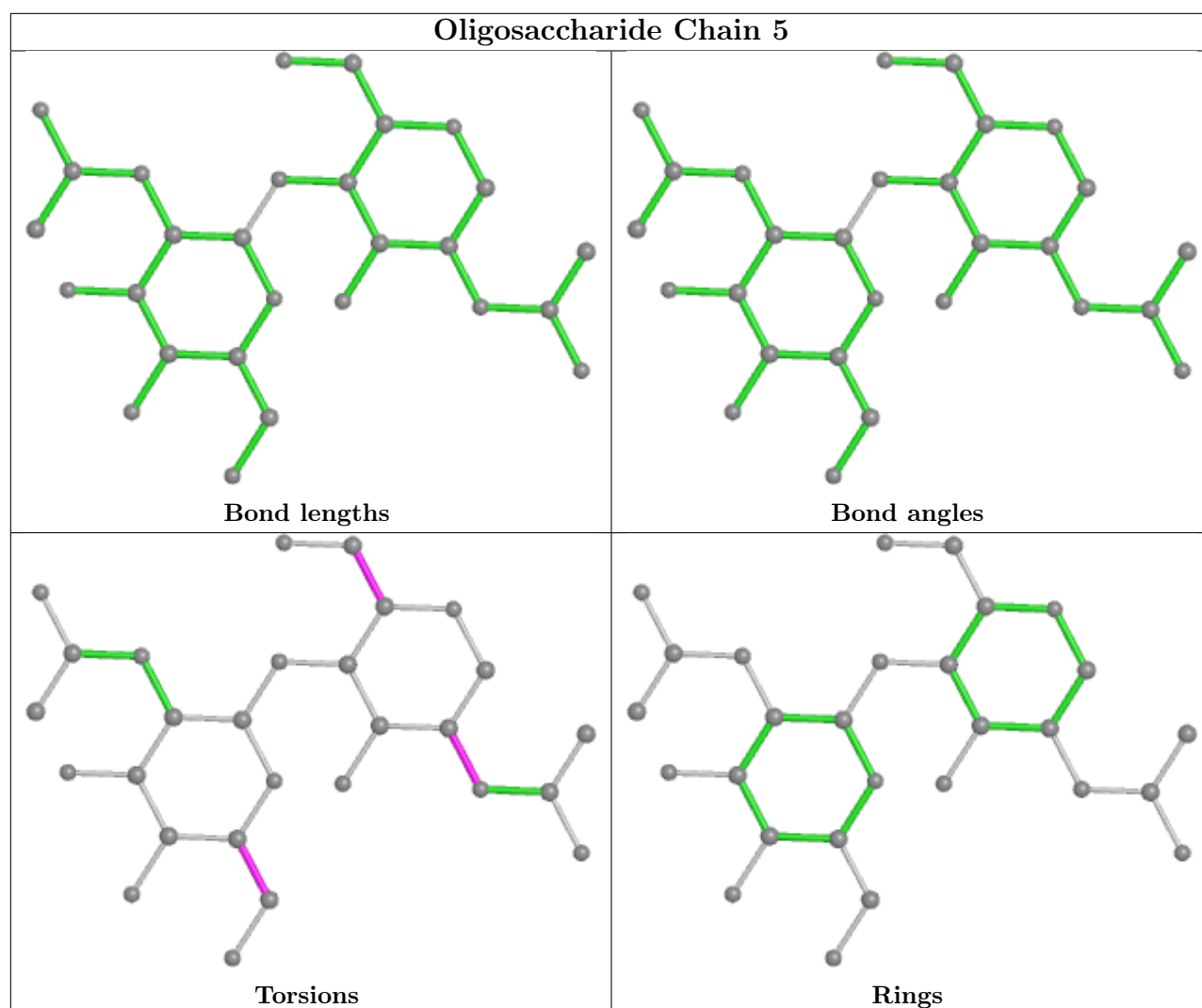


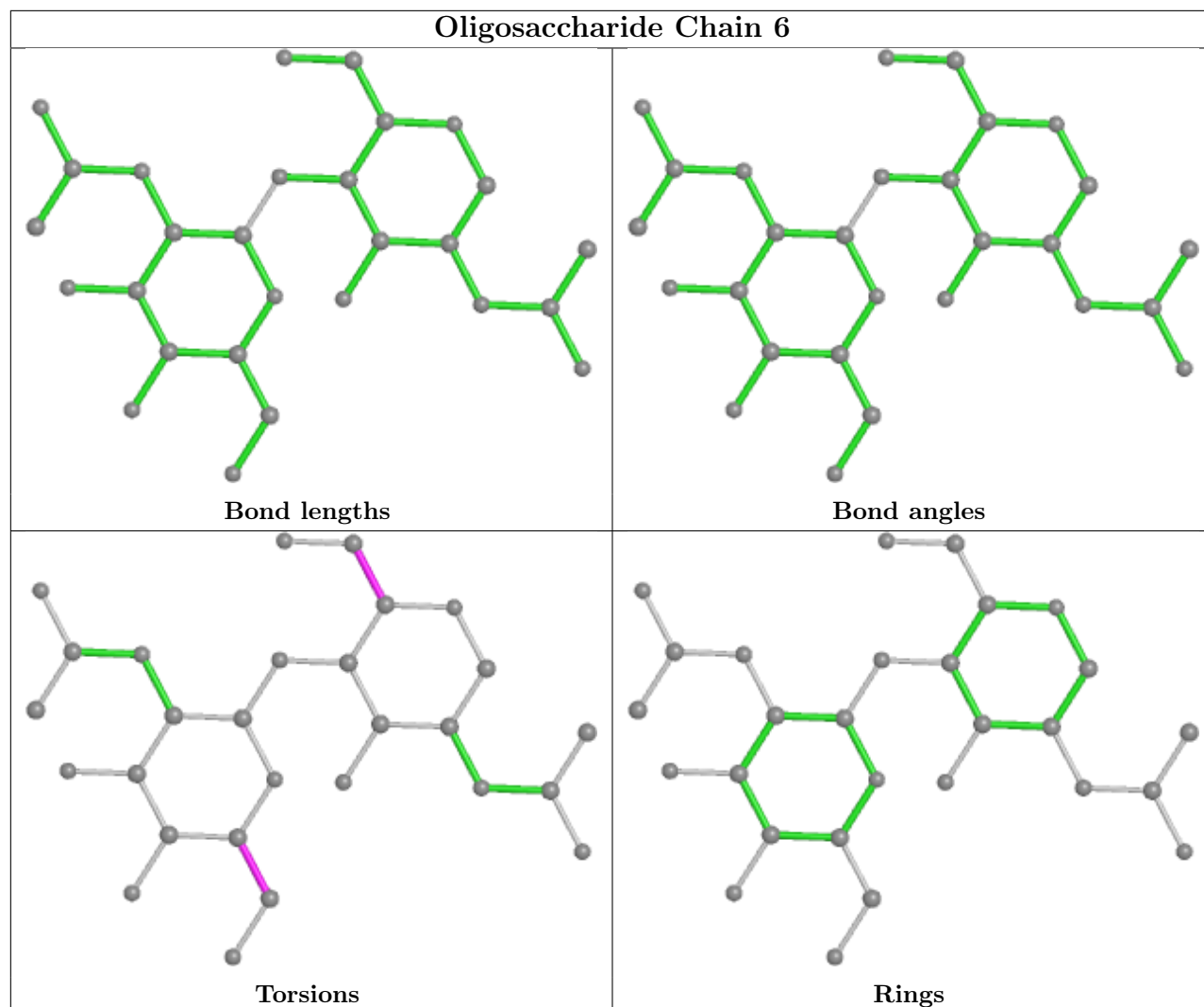


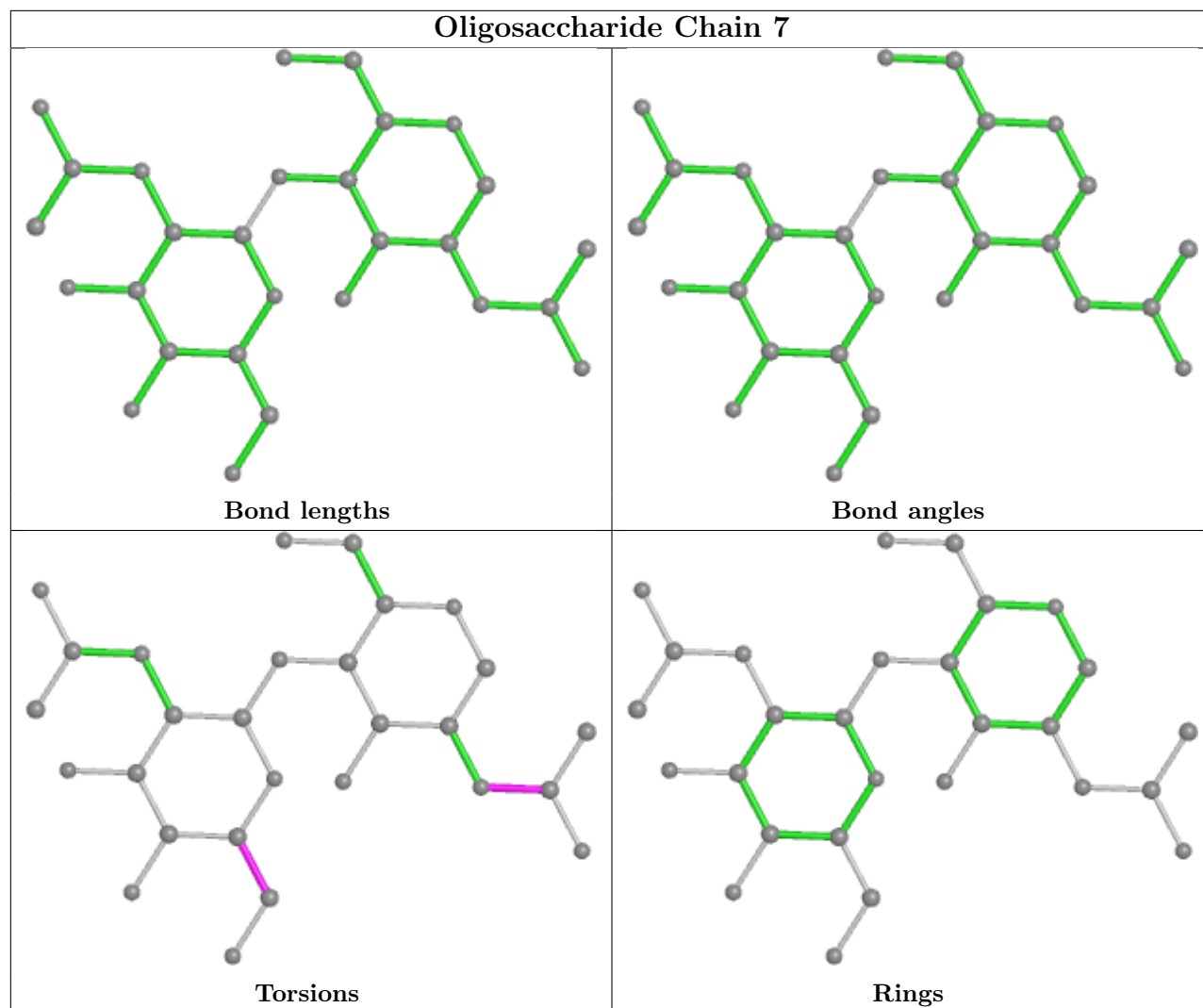




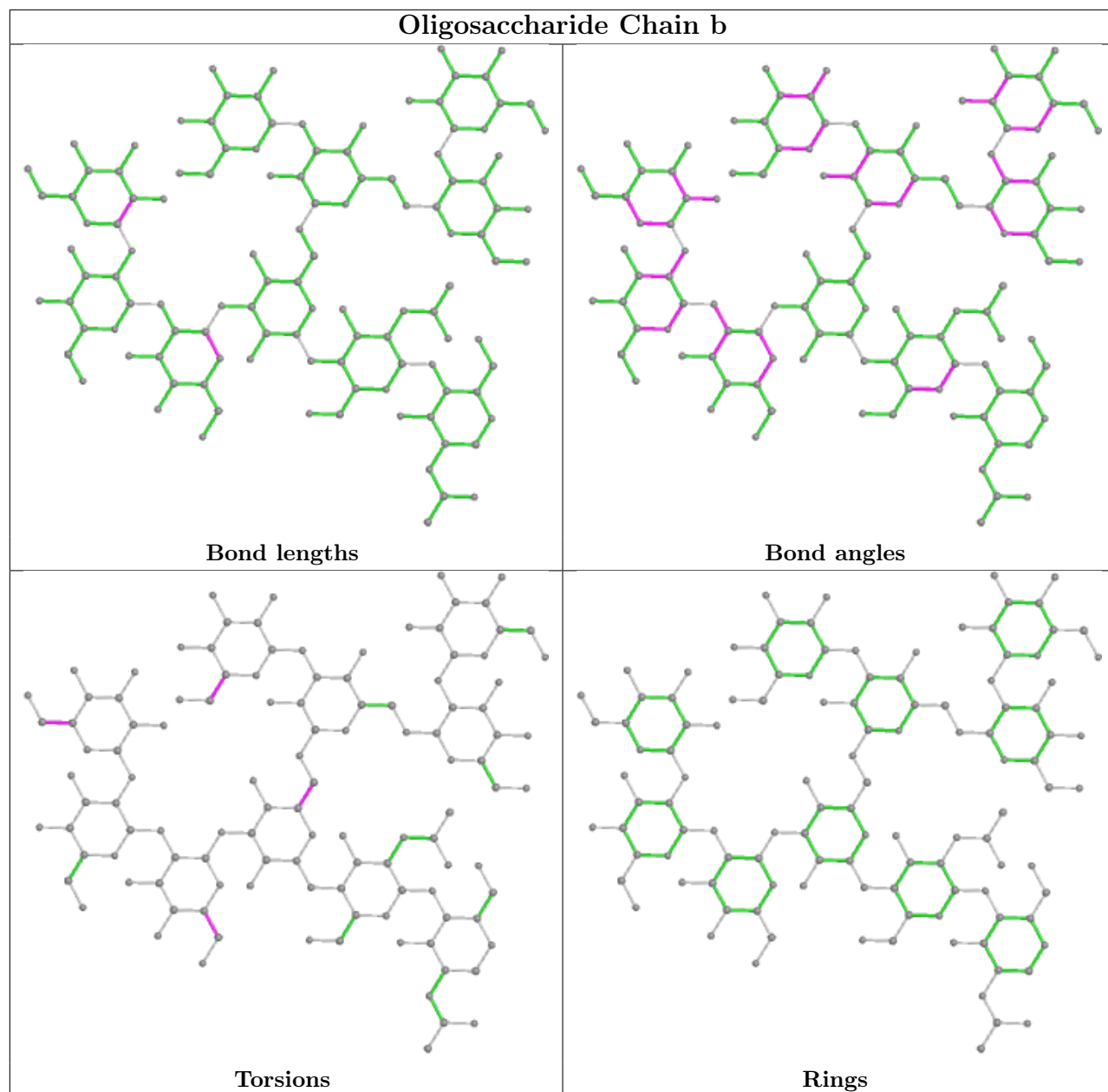


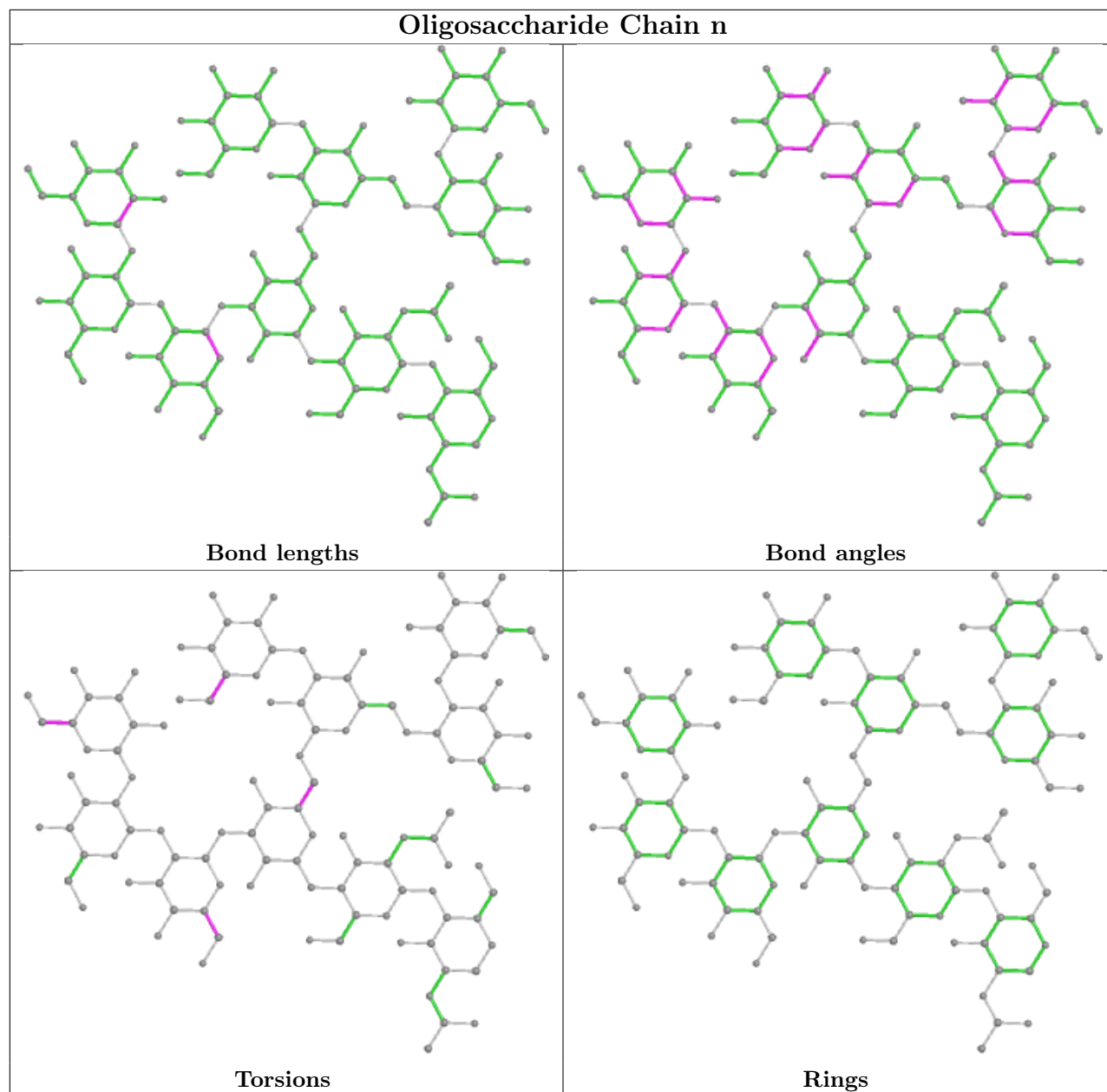


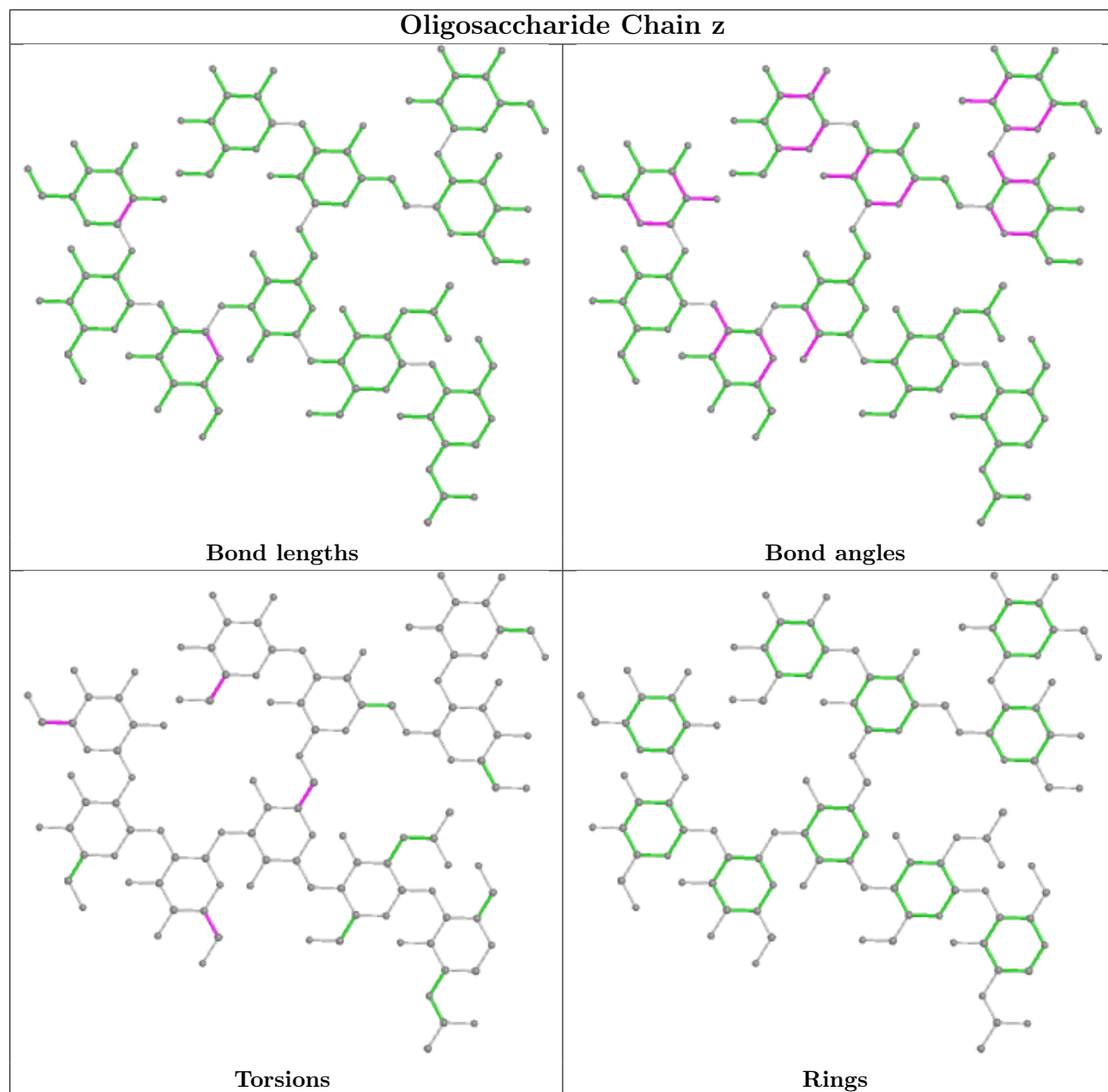


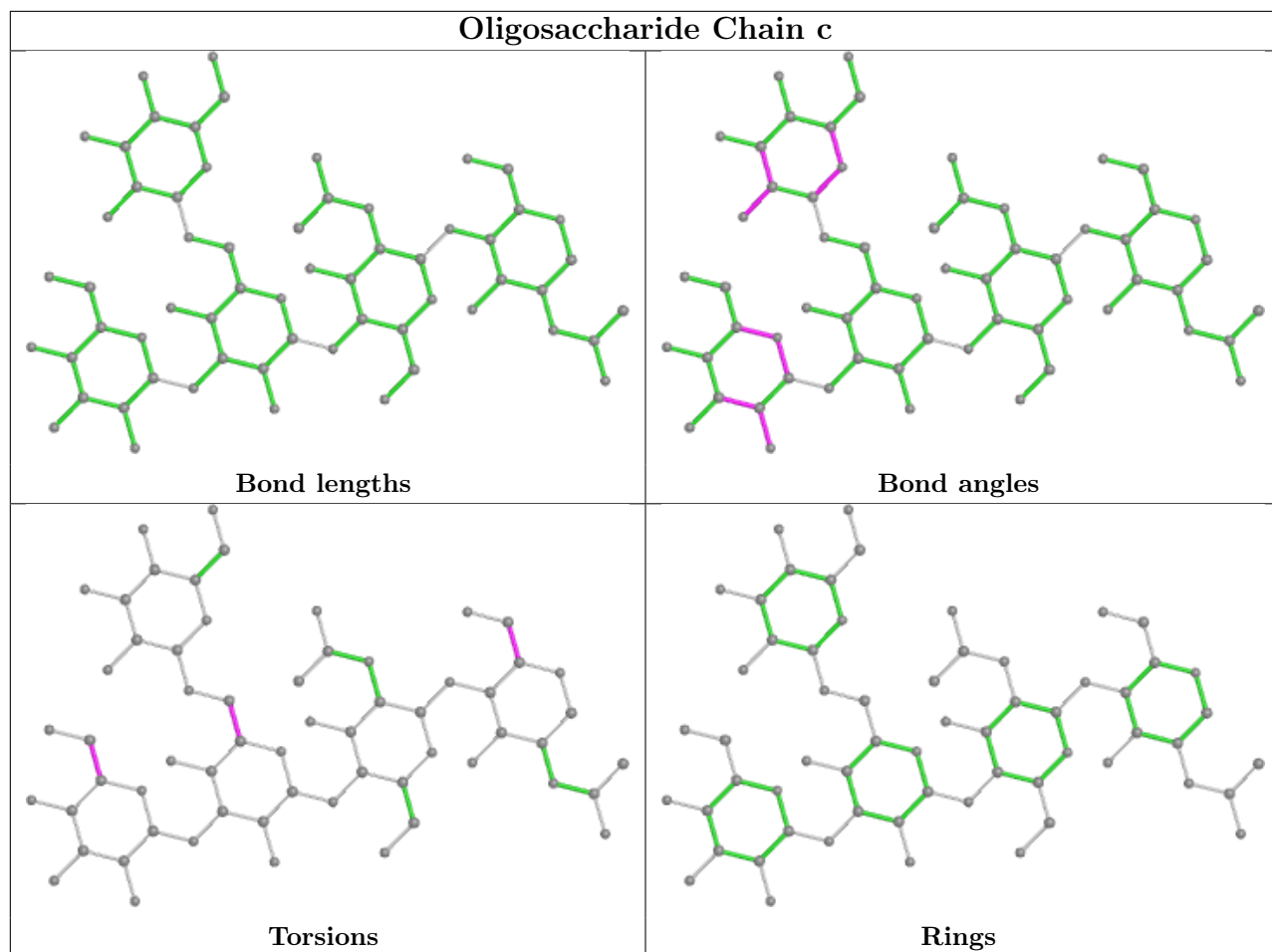


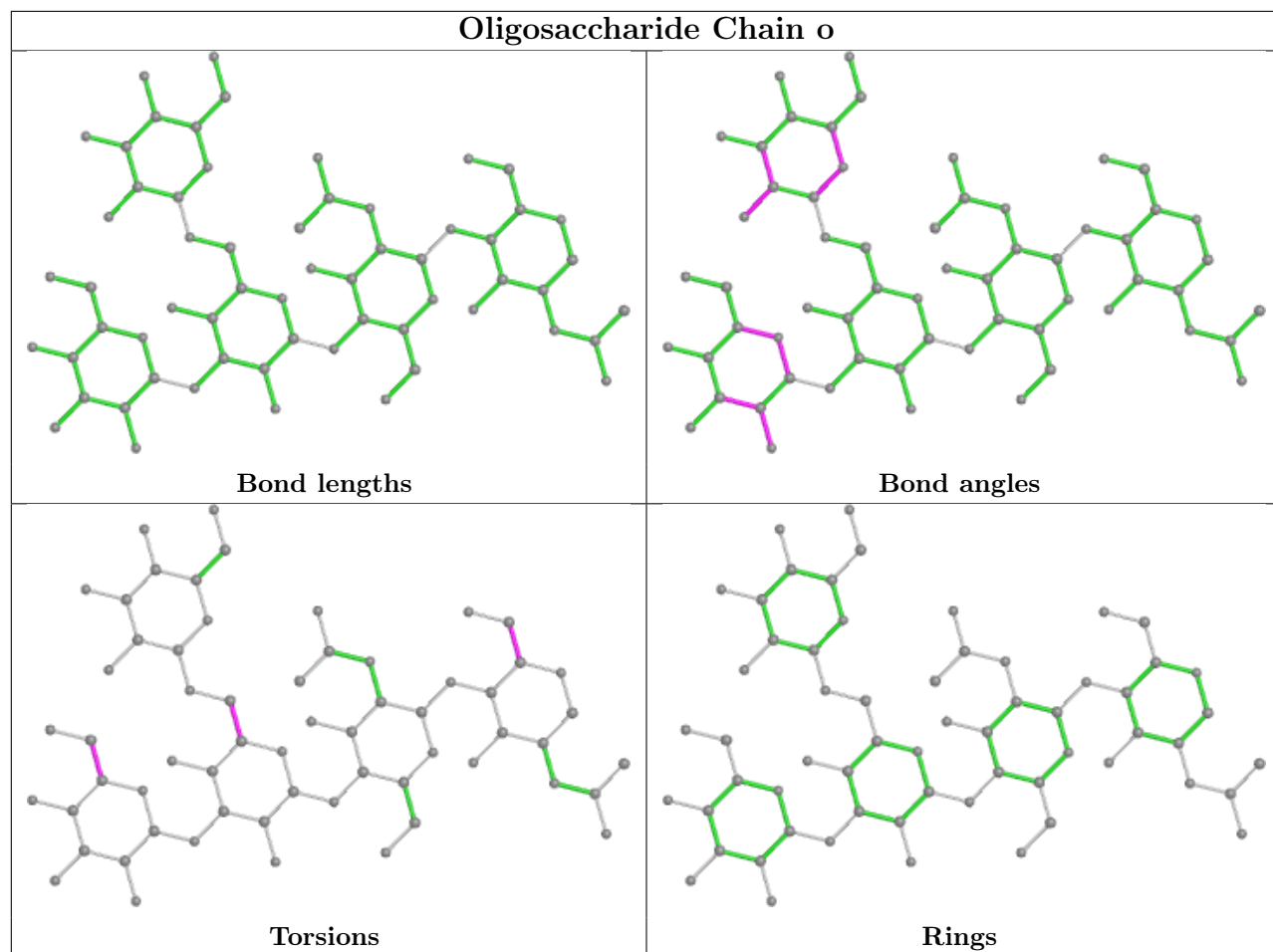


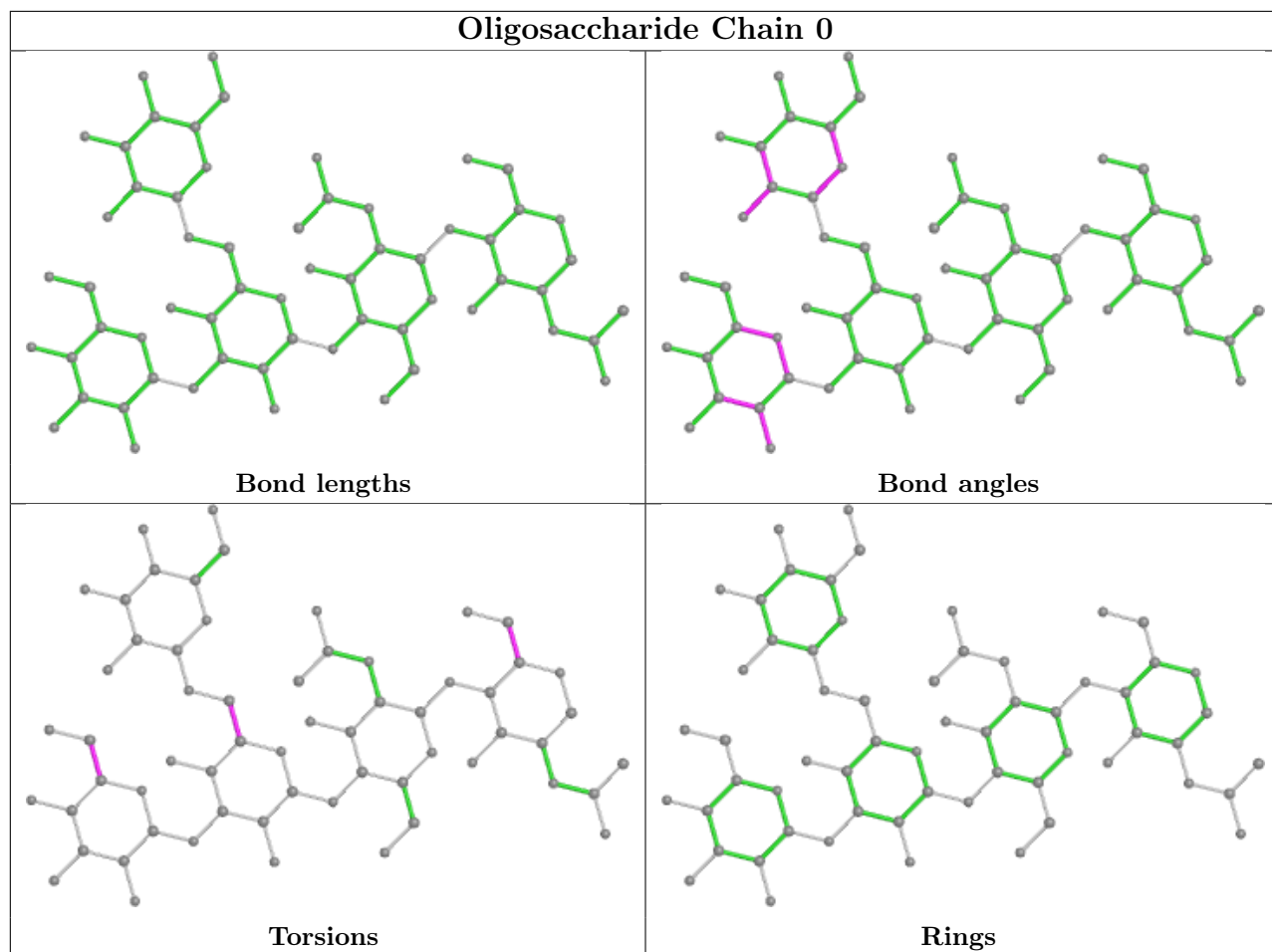


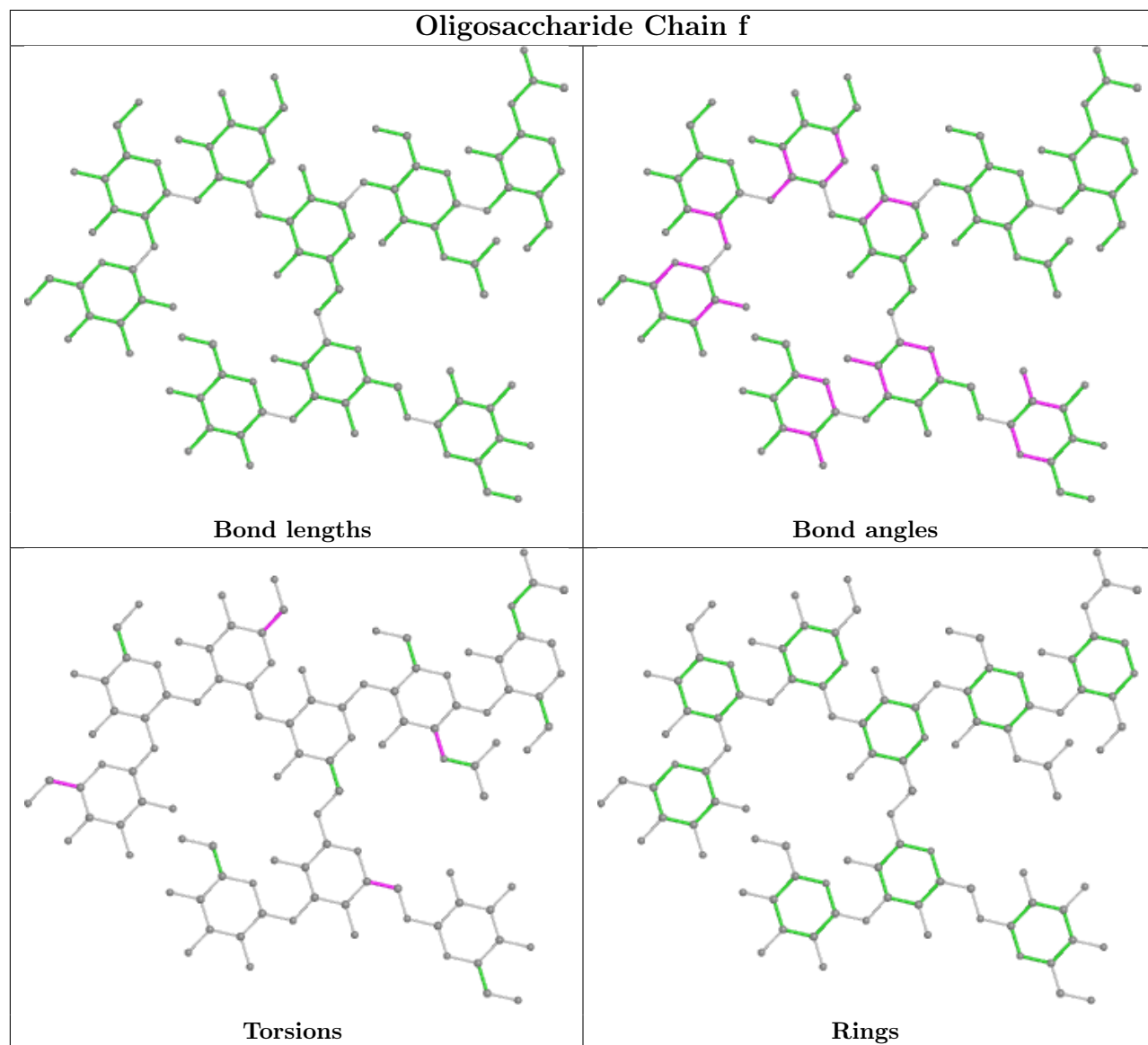


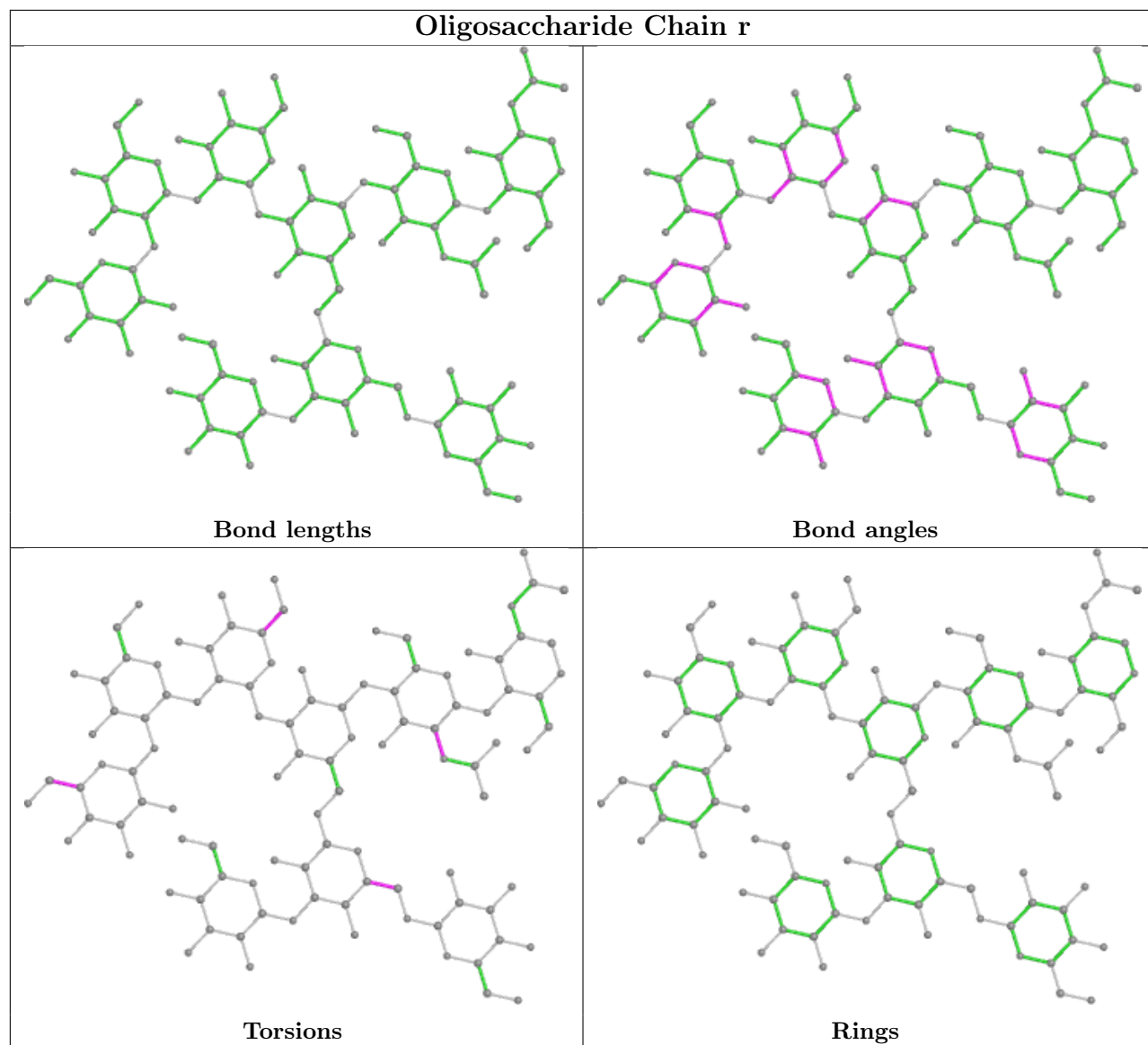




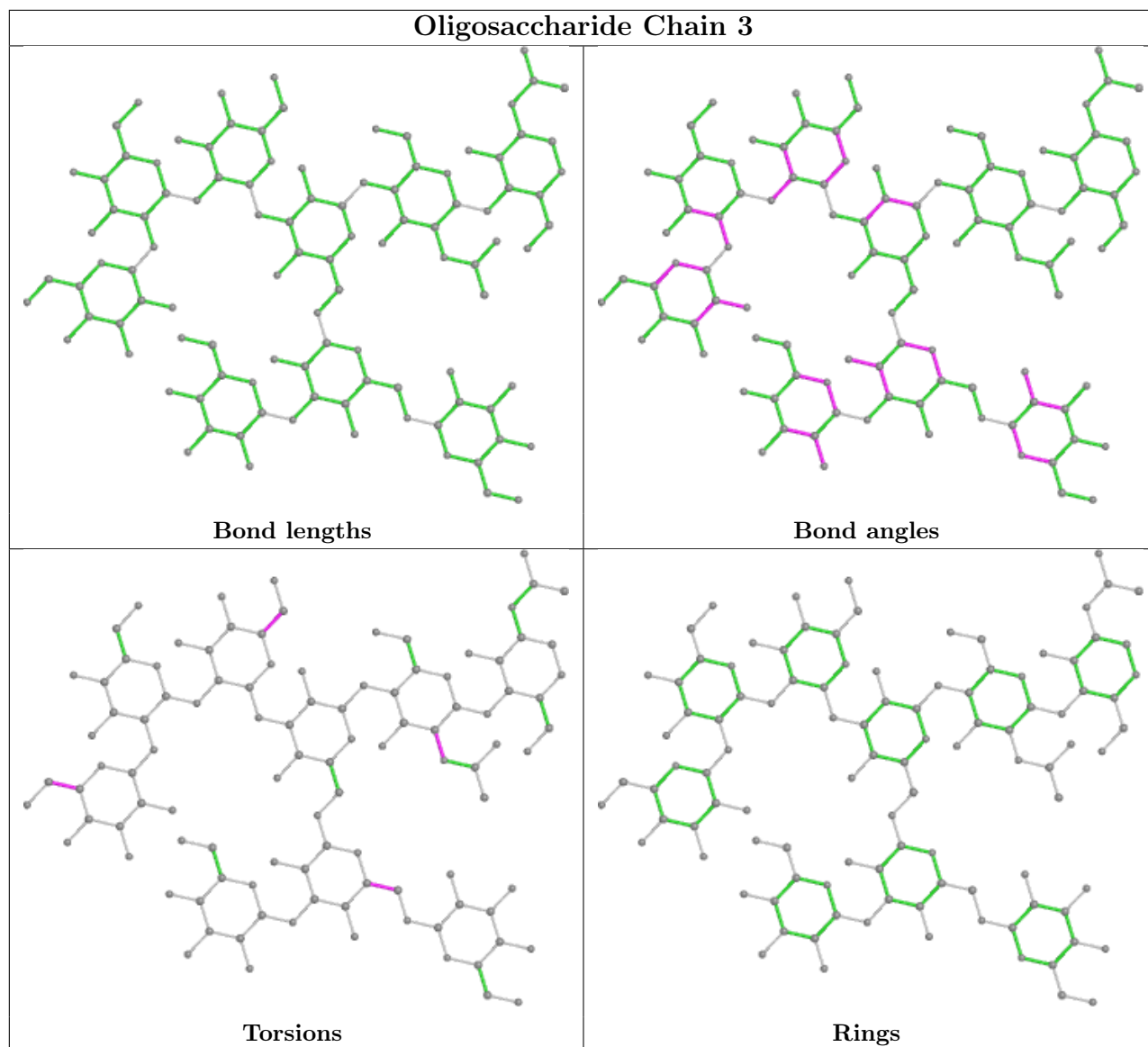












## 5.6 Ligand geometry [i](#)

24 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
11	NAG	G	301	3	14,14,15	0.21	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	J	702	2	14,14,15	0.19	0	17,19,21	0.49	0
11	NAG	A	602	1	14,14,15	0.26	0	17,19,21	0.50	0
11	NAG	B	702	2	14,14,15	0.20	0	17,19,21	0.50	0
12	83J	E	605	-	35,39,39	2.12	9 (25%)	43,56,56	3.78	16 (37%)
11	NAG	A	601	1	14,14,15	0.20	0	17,19,21	0.47	0
11	NAG	B	701	2	14,14,15	0.20	0	17,19,21	0.38	0
11	NAG	E	603	1	14,14,15	0.27	0	17,19,21	0.42	0
12	83J	A	605	-	35,39,39	2.13	9 (25%)	43,56,56	3.79	17 (39%)
11	NAG	I	603	1	14,14,15	0.26	0	17,19,21	0.42	0
11	NAG	J	701	2	14,14,15	0.21	0	17,19,21	0.38	0
11	NAG	A	603	1	14,14,15	0.26	0	17,19,21	0.44	0
11	NAG	C	301	3	14,14,15	0.20	0	17,19,21	0.41	0
11	NAG	A	604	1	14,14,15	0.26	0	17,19,21	0.39	0
11	NAG	I	604	1	14,14,15	0.47	0	17,19,21	0.61	0
11	NAG	E	602	1	14,14,15	0.28	0	17,19,21	0.51	0
11	NAG	I	601	1	14,14,15	0.19	0	17,19,21	0.46	0
11	NAG	K	301	3	14,14,15	0.21	0	17,19,21	0.41	0
11	NAG	F	702	2	14,14,15	0.20	0	17,19,21	0.50	0
11	NAG	E	601	1	14,14,15	0.20	0	17,19,21	0.47	0
11	NAG	F	701	2	14,14,15	0.21	0	17,19,21	0.37	0
11	NAG	I	602	1	14,14,15	0.26	0	17,19,21	0.51	0
11	NAG	E	604	1	14,14,15	0.47	0	17,19,21	0.60	0
12	83J	I	605	-	35,39,39	2.13	9 (25%)	43,56,56	3.77	17 (39%)

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
11	NAG	G	301	3	-	2/6/23/26	0/1/1/1
11	NAG	J	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	602	1	-	5/6/23/26	0/1/1/1
11	NAG	B	702	2	-	2/6/23/26	0/1/1/1
12	83J	E	605	-	-	2/18/36/36	0/5/5/5
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	3/6/23/26	0/1/1/1
11	NAG	E	603	1	-	2/6/23/26	0/1/1/1
12	83J	A	605	-	-	2/18/36/36	0/5/5/5
11	NAG	I	603	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	J	701	2	-	3/6/23/26	0/1/1/1
11	NAG	A	603	1	-	2/6/23/26	0/1/1/1
11	NAG	C	301	3	-	2/6/23/26	0/1/1/1
11	NAG	A	604	1	-	4/6/23/26	0/1/1/1
11	NAG	I	604	1	-	2/6/23/26	0/1/1/1
11	NAG	E	602	1	-	5/6/23/26	0/1/1/1
11	NAG	I	601	1	-	2/6/23/26	0/1/1/1
11	NAG	K	301	3	-	2/6/23/26	0/1/1/1
11	NAG	F	702	2	-	2/6/23/26	0/1/1/1
11	NAG	E	601	1	-	2/6/23/26	0/1/1/1
11	NAG	F	701	2	-	3/6/23/26	0/1/1/1
11	NAG	I	602	1	-	5/6/23/26	0/1/1/1
11	NAG	E	604	1	-	2/6/23/26	0/1/1/1
12	83J	I	605	-	-	2/18/36/36	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	605	83J	C12-N02	5.99	1.45	1.34
12	I	605	83J	C12-N02	5.99	1.45	1.34
12	E	605	83J	C12-N02	5.93	1.45	1.34
12	E	605	83J	C13-N05	5.18	1.46	1.34
12	I	605	83J	C13-N05	5.16	1.46	1.34
12	A	605	83J	C13-N05	5.16	1.46	1.34
12	A	605	83J	C29-N28	4.96	1.35	1.31
12	I	605	83J	C29-N28	4.90	1.35	1.31
12	E	605	83J	C29-N28	4.85	1.34	1.31
12	E	605	83J	C16-C17	-4.55	1.35	1.42
12	I	605	83J	C16-C17	-4.52	1.35	1.42
12	A	605	83J	C16-C17	-4.47	1.35	1.42
12	I	605	83J	C15-C13	2.60	1.54	1.50
12	E	605	83J	C15-C13	2.57	1.54	1.50
12	A	605	83J	C15-C13	2.56	1.54	1.50
12	I	605	83J	N34-N30	-2.53	1.34	1.39
12	E	605	83J	N34-N30	-2.51	1.34	1.39
12	A	605	83J	N34-N30	-2.47	1.34	1.39
12	A	605	83J	O09-C14	-2.36	1.18	1.23
12	E	605	83J	O09-C14	-2.33	1.18	1.23
12	I	605	83J	O09-C14	-2.33	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	605	83J	O03-C12	-2.14	1.18	1.23
12	A	605	83J	O03-C12	-2.13	1.18	1.23
12	I	605	83J	O03-C12	-2.07	1.18	1.23
12	I	605	83J	O11-C22	2.05	1.40	1.36
12	E	605	83J	O11-C22	2.03	1.40	1.36
12	A	605	83J	C22-C17	-2.01	1.38	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	605	83J	C18-C16-C14	-12.86	104.31	127.45
12	A	605	83J	C18-C16-C14	-12.81	104.39	127.45
12	I	605	83J	C18-C16-C14	-12.74	104.51	127.45
12	A	605	83J	O11-C22-C17	10.32	131.07	115.89
12	E	605	83J	O11-C22-C17	10.25	130.97	115.89
12	I	605	83J	O11-C22-C17	10.21	130.91	115.89
12	A	605	83J	O11-C22-C25	-8.22	105.98	125.08
12	E	605	83J	O11-C22-C25	-8.17	106.10	125.08
12	I	605	83J	O11-C22-C25	-8.12	106.21	125.08
12	A	605	83J	C20-C15-C13	-7.96	100.12	120.29
12	E	605	83J	C20-C15-C13	-7.93	100.18	120.29
12	I	605	83J	C20-C15-C13	-7.92	100.20	120.29
12	E	605	83J	C21-C15-C13	7.45	139.18	120.29
12	A	605	83J	C21-C15-C13	7.45	139.16	120.29
12	I	605	83J	C21-C15-C13	7.42	139.09	120.29
12	E	605	83J	N28-C29-N30	-6.00	108.90	114.33
12	A	605	83J	N28-C29-N30	-5.99	108.91	114.33
12	I	605	83J	N28-C29-N30	-5.69	109.18	114.33
12	I	605	83J	C16-C17-C19	-5.12	103.45	107.54
12	E	605	83J	C16-C17-C19	-5.08	103.48	107.54
12	A	605	83J	C16-C17-C19	-5.04	103.52	107.54
12	I	605	83J	C10-C07-N02	3.70	118.37	110.44
12	E	605	83J	C10-C07-N02	3.52	117.98	110.44
12	A	605	83J	C10-C07-N02	3.50	117.93	110.44
12	I	605	83J	C19-C29-N28	3.20	127.93	118.92
12	E	605	83J	C19-C29-N28	3.20	127.92	118.92
12	A	605	83J	C19-C29-N28	3.18	127.88	118.92
12	E	605	83J	C22-C25-N28	-2.90	118.37	122.73
12	A	605	83J	C22-C25-N28	-2.90	118.38	122.73
12	I	605	83J	C22-C25-N28	-2.88	118.40	122.73
12	I	605	83J	O09-C14-C12	2.83	121.86	117.74
12	E	605	83J	O09-C14-C12	2.78	121.79	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	605	83J	C14-C12-N02	2.71	121.19	118.52
12	I	605	83J	C16-C18-N08	-2.71	103.67	108.91
12	E	605	83J	C16-C18-N08	-2.70	103.69	108.91
12	A	605	83J	O09-C14-C12	2.68	121.64	117.74
12	A	605	83J	C16-C18-N08	-2.66	103.77	108.91
12	E	605	83J	C04-C01-N02	2.52	115.83	110.44
12	A	605	83J	C14-C12-N02	2.48	120.96	118.52
12	A	605	83J	C04-C01-N02	2.47	115.74	110.44
12	I	605	83J	C35-C33-N32	2.40	126.50	120.49
12	I	605	83J	C04-C01-N02	2.39	115.56	110.44
12	E	605	83J	C35-C33-N32	2.38	126.45	120.49
12	A	605	83J	C35-C33-N32	2.36	126.41	120.49
12	E	605	83J	C14-C12-N02	2.35	120.83	118.52
12	I	605	83J	O03-C12-N02	-2.13	119.27	122.67
12	A	605	83J	C07-N02-C01	2.11	116.69	112.62
12	A	605	83J	O03-C12-N02	-2.10	119.32	122.67
12	I	605	83J	C07-C10-N05	2.10	114.94	110.44
12	E	605	83J	C07-N02-C01	2.00	116.48	112.62

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	604	NAG	C3-C2-N2-C7
11	I	604	NAG	C3-C2-N2-C7
12	I	605	83J	C17-C22-O11-C27
11	J	701	NAG	C4-C5-C6-O6
11	B	701	NAG	C4-C5-C6-O6
12	A	605	83J	C17-C22-O11-C27
12	E	605	83J	C17-C22-O11-C27
11	J	701	NAG	O5-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	F	701	NAG	C4-C5-C6-O6
11	F	702	NAG	C4-C5-C6-O6
11	J	702	NAG	C4-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	A	604	NAG	O5-C5-C6-O6
11	A	601	NAG	O5-C5-C6-O6
11	E	601	NAG	O5-C5-C6-O6
11	I	601	NAG	O5-C5-C6-O6
11	C	301	NAG	C4-C5-C6-O6
11	K	301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	E	602	NAG	O5-C5-C6-O6
11	F	701	NAG	O5-C5-C6-O6
11	F	702	NAG	O5-C5-C6-O6
11	J	702	NAG	O5-C5-C6-O6
12	A	605	83J	C25-C22-O11-C27
11	A	602	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	I	602	NAG	O5-C5-C6-O6
12	E	605	83J	C25-C22-O11-C27
12	I	605	83J	C25-C22-O11-C27
11	A	604	NAG	C1-C2-N2-C7
11	K	301	NAG	O5-C5-C6-O6
11	G	301	NAG	C4-C5-C6-O6
11	A	602	NAG	C4-C5-C6-O6
11	E	602	NAG	C4-C5-C6-O6
11	I	602	NAG	C4-C5-C6-O6
11	A	602	NAG	C8-C7-N2-C2
11	A	602	NAG	O7-C7-N2-C2
11	E	602	NAG	C8-C7-N2-C2
11	E	602	NAG	O7-C7-N2-C2
11	I	602	NAG	C8-C7-N2-C2
11	I	602	NAG	O7-C7-N2-C2
11	C	301	NAG	O5-C5-C6-O6
11	A	603	NAG	O5-C5-C6-O6
11	I	603	NAG	O5-C5-C6-O6
11	G	301	NAG	O5-C5-C6-O6
11	E	603	NAG	O5-C5-C6-O6
11	A	604	NAG	C4-C5-C6-O6
11	B	701	NAG	C1-C2-N2-C7
11	J	701	NAG	C1-C2-N2-C7
11	F	701	NAG	C1-C2-N2-C7
11	E	604	NAG	C1-C2-N2-C7
11	I	603	NAG	C4-C5-C6-O6
11	A	603	NAG	C4-C5-C6-O6
11	I	601	NAG	C4-C5-C6-O6
11	I	604	NAG	C1-C2-N2-C7
11	A	601	NAG	C4-C5-C6-O6
11	E	601	NAG	C4-C5-C6-O6
11	E	603	NAG	C4-C5-C6-O6
11	A	602	NAG	C3-C2-N2-C7
11	A	604	NAG	C3-C2-N2-C7
11	E	602	NAG	C3-C2-N2-C7

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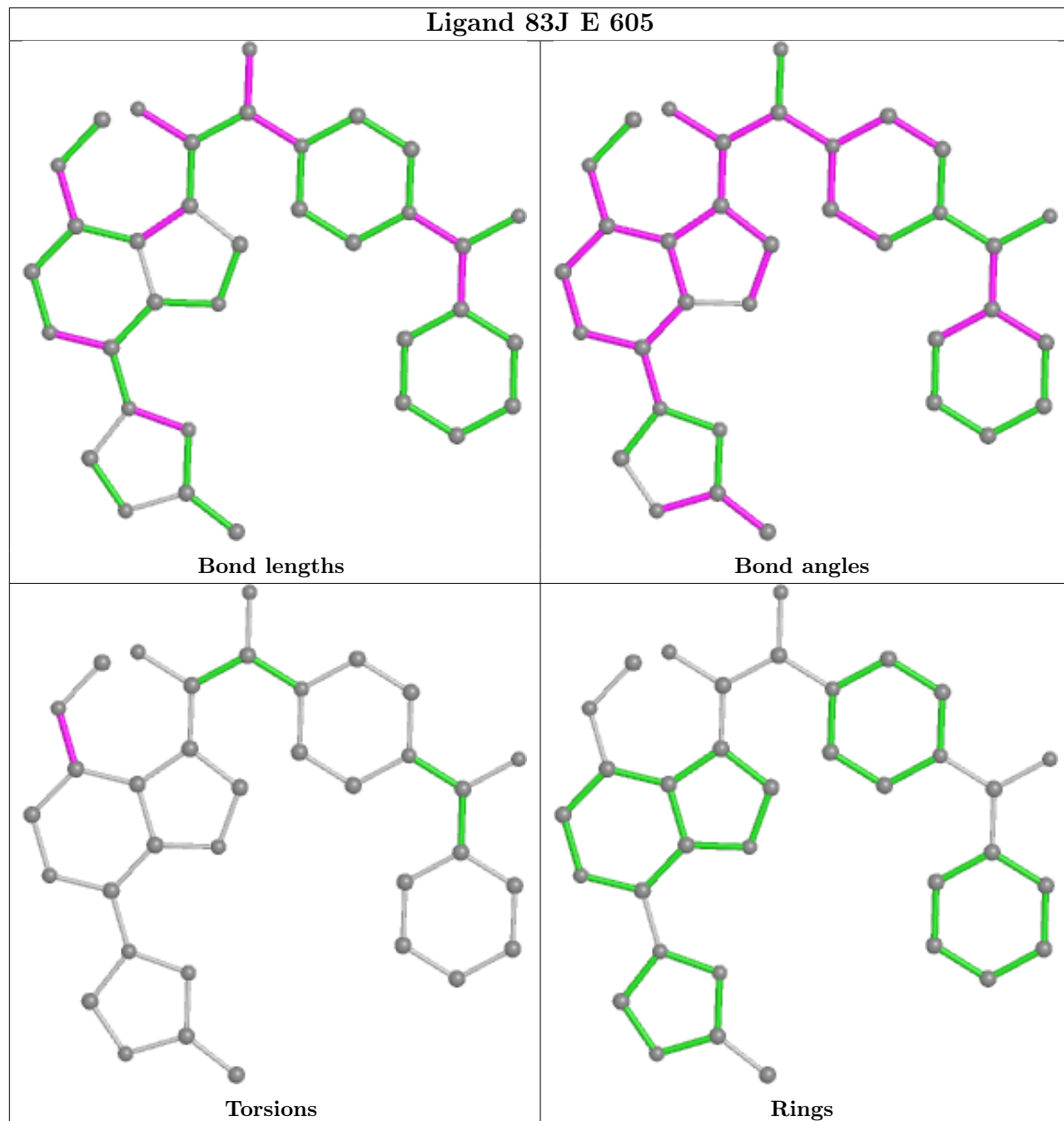
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
11	I	602	NAG	C3-C2-N2-C7

There are no ring outliers.

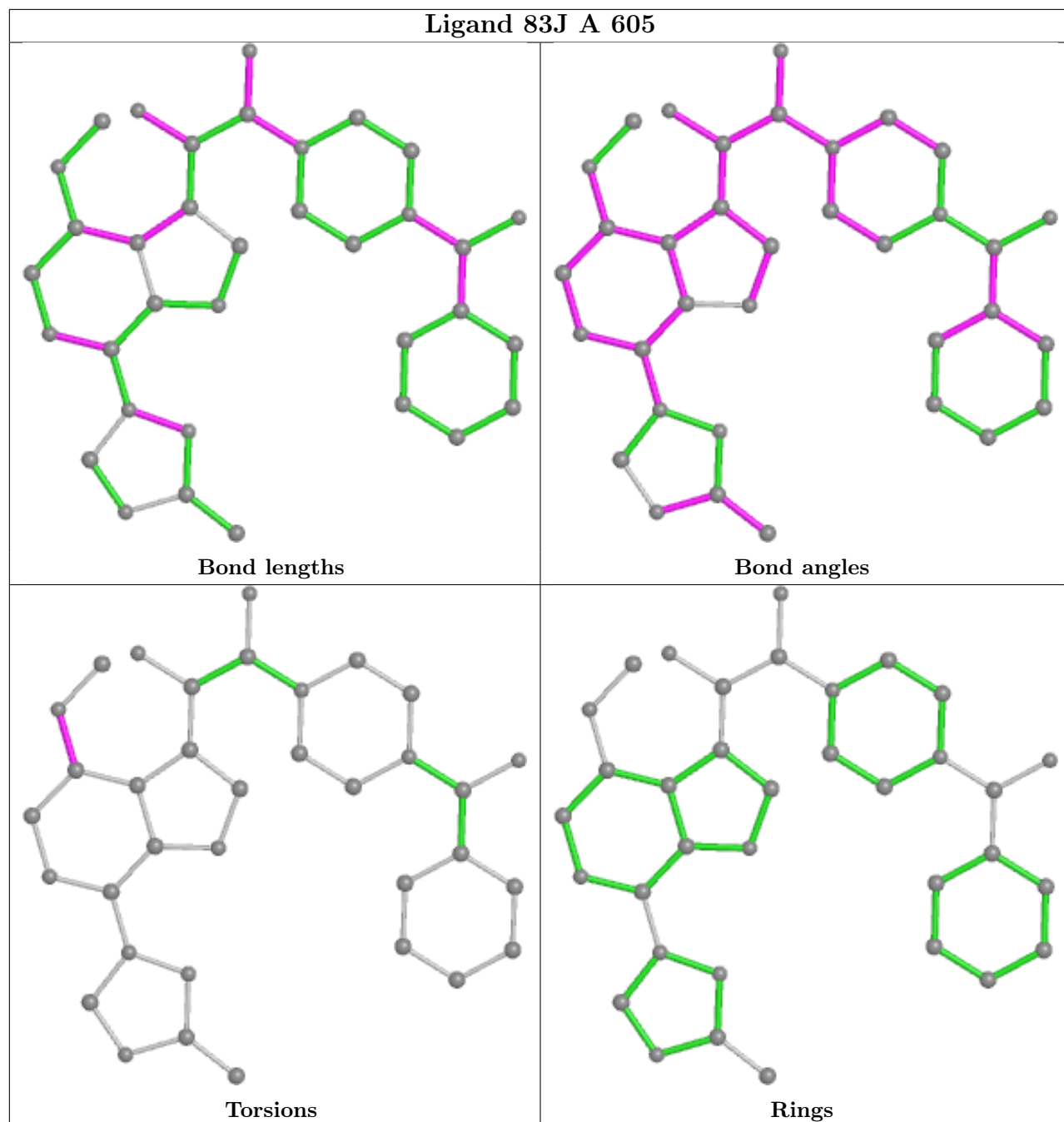
No monomer is involved in short contacts.

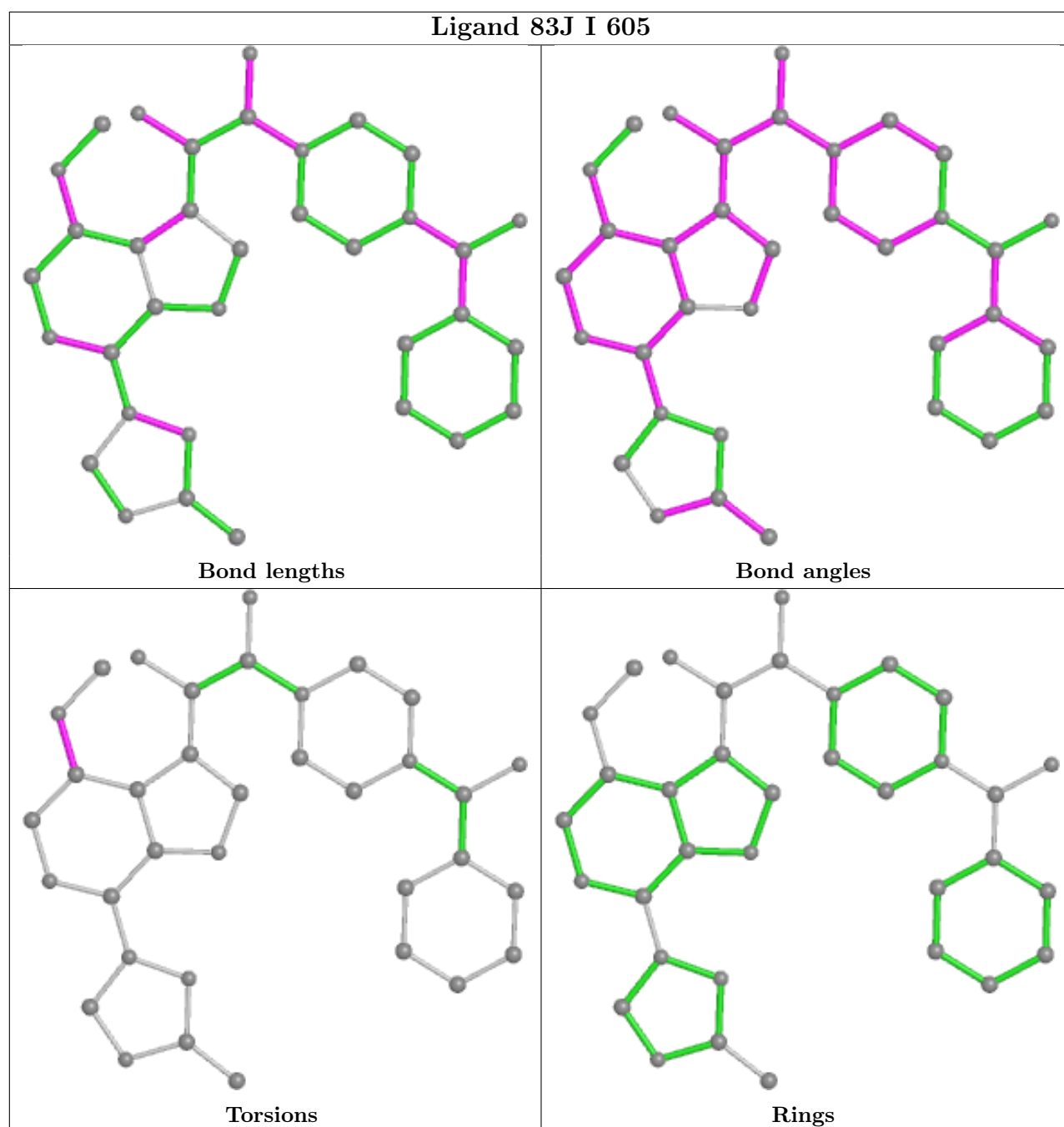
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand 83J E 605









## 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.

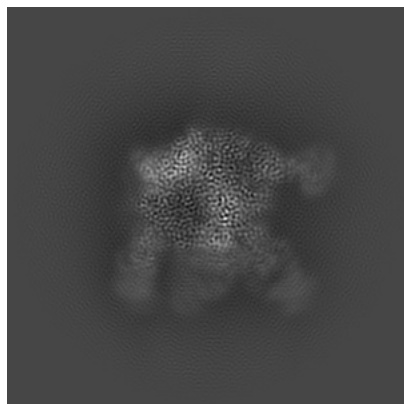
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41613. These allow visual inspection of the internal detail of the map and identification of artifacts.

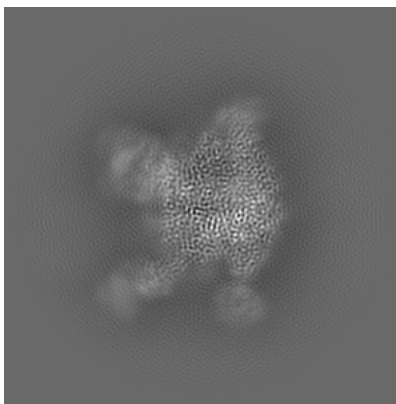
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

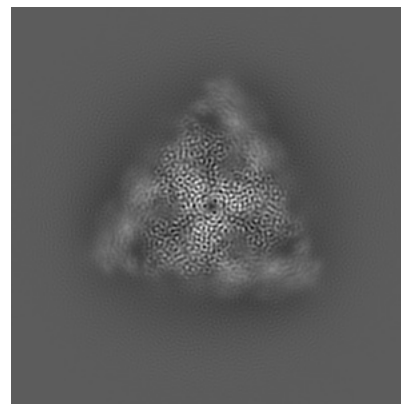
#### 6.1.1 Primary map



X

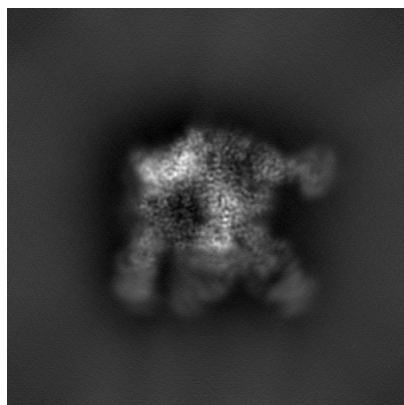


Y

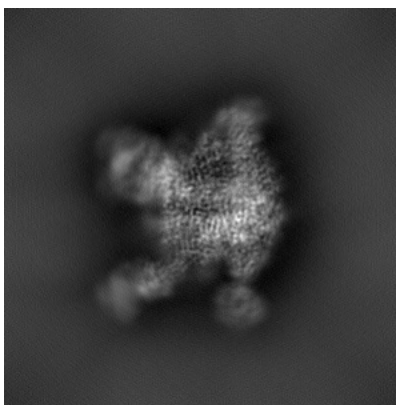


Z

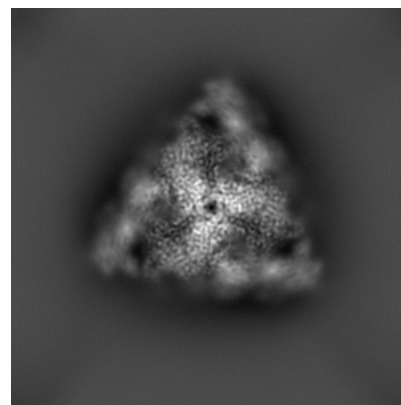
#### 6.1.2 Raw map



X



Y

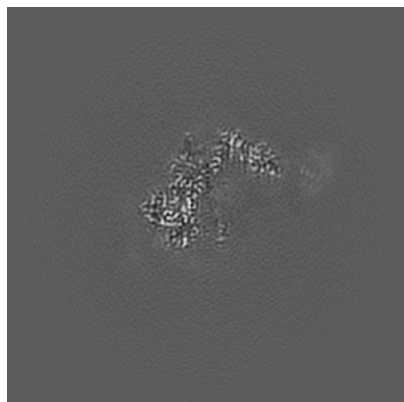


Z

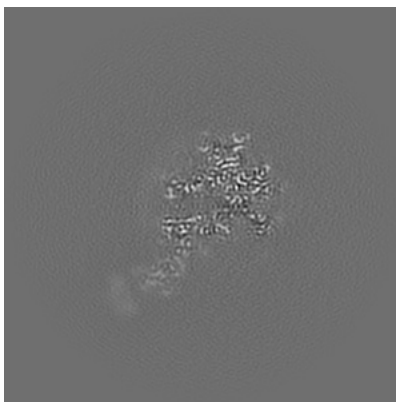
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

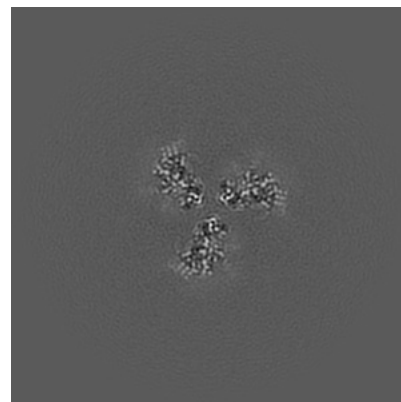
### 6.2.1 Primary map



X Index: 180

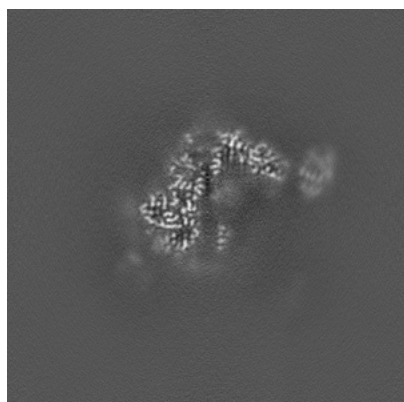


Y Index: 180

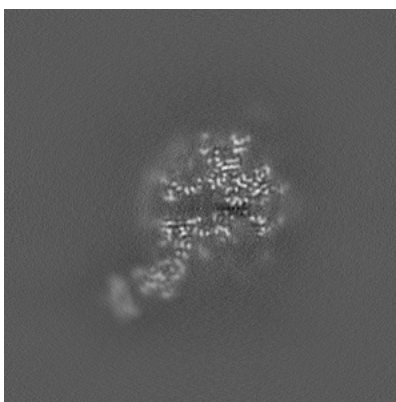


Z Index: 180

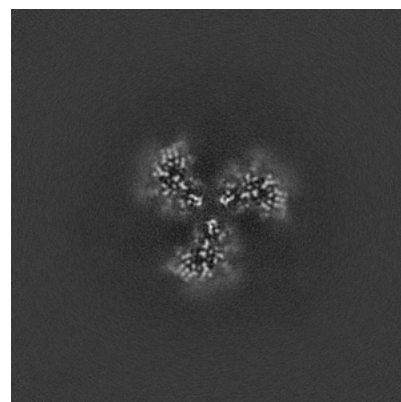
### 6.2.2 Raw map



X Index: 180



Y Index: 180

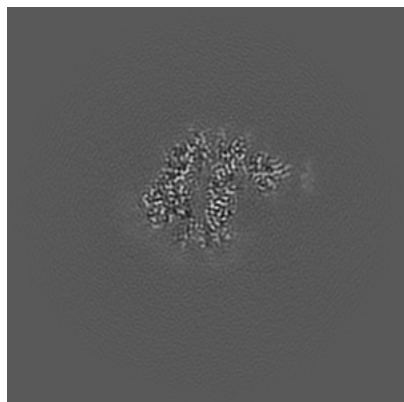


Z Index: 180

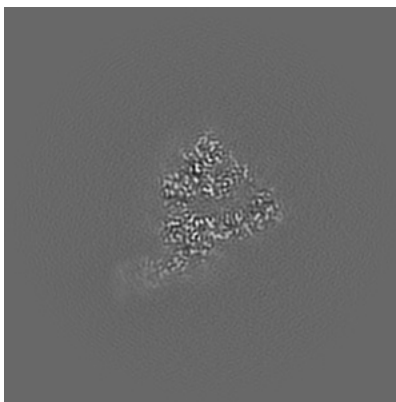
The images above show central slices of the map in three orthogonal directions.

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

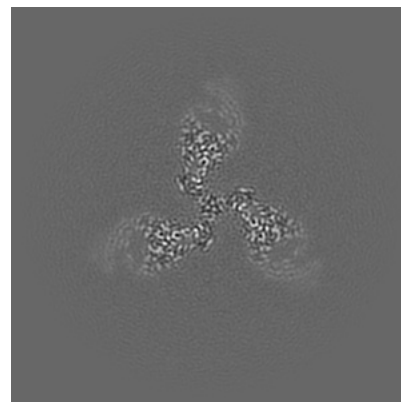
### 6.3.1 Primary map



X Index: 169

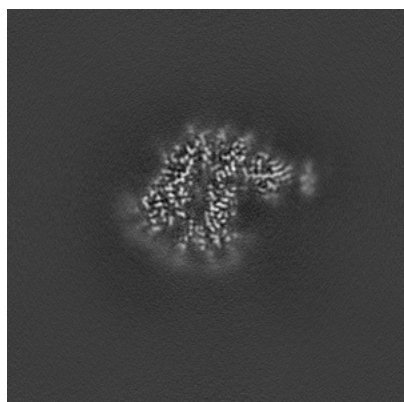


Y Index: 194

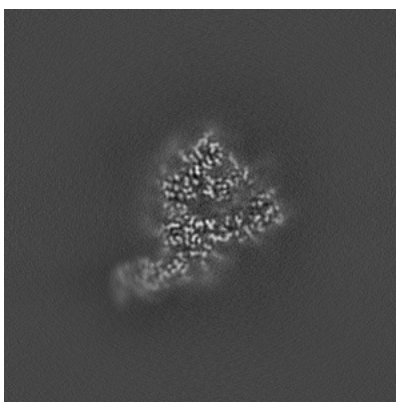


Z Index: 216

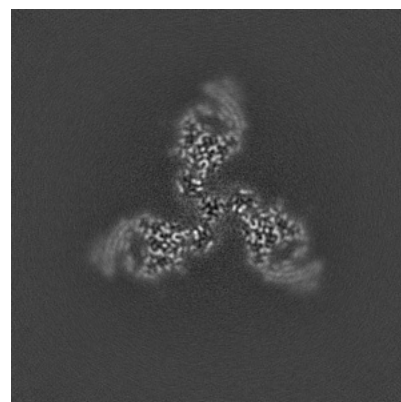
### 6.3.2 Raw map



X Index: 169



Y Index: 194

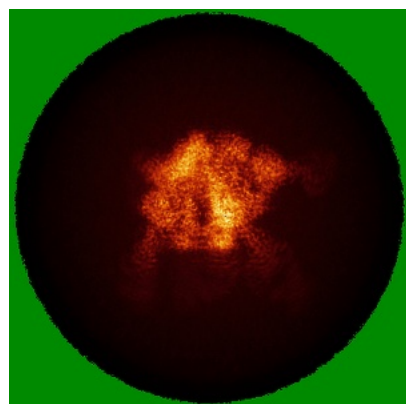


Z Index: 216

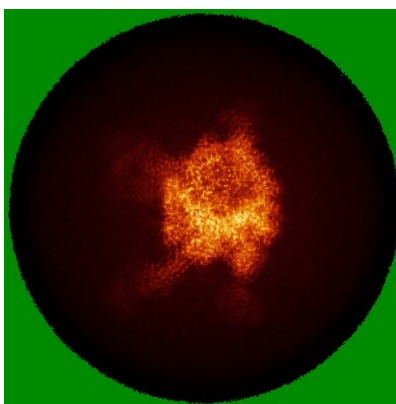
The images above show the largest variance slices of the map in three orthogonal directions.

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

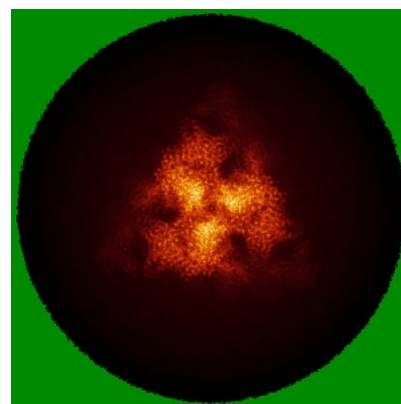
### 6.4.1 Primary map



X

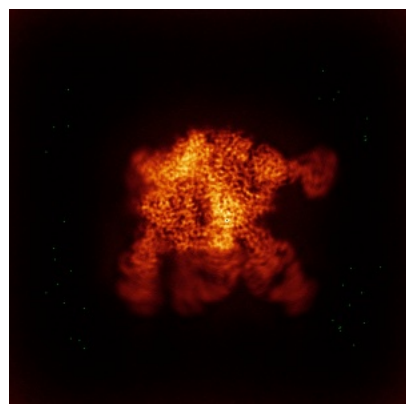


Y

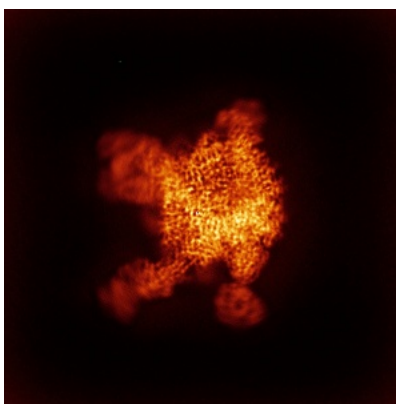


Z

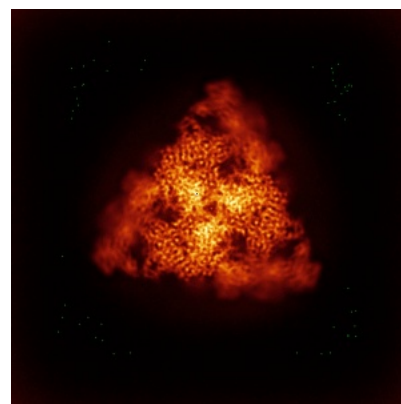
### 6.4.2 Raw map



X



Y



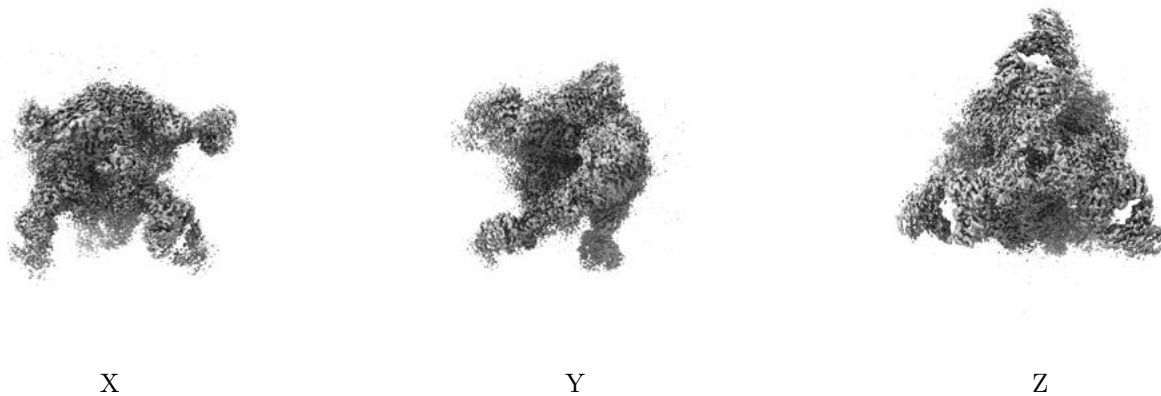
Z

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.



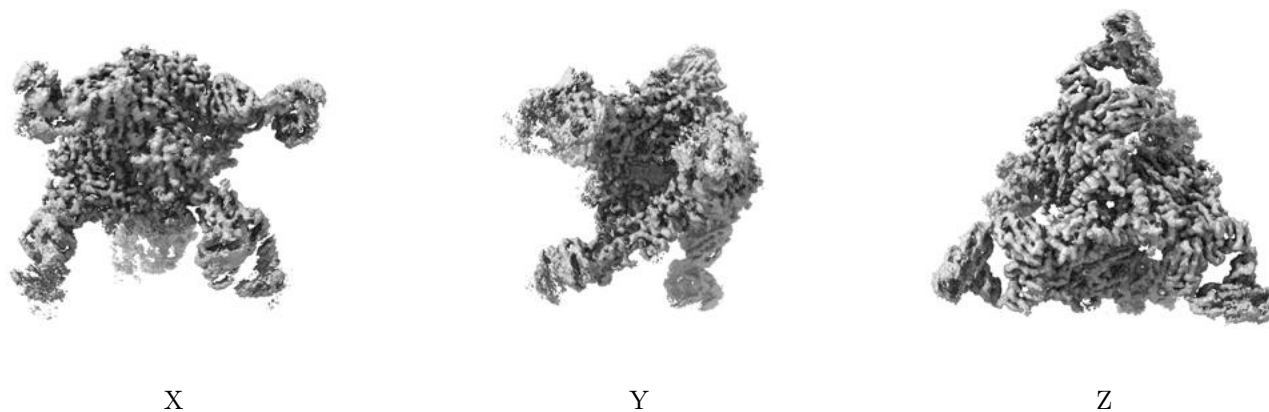
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1151. 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.

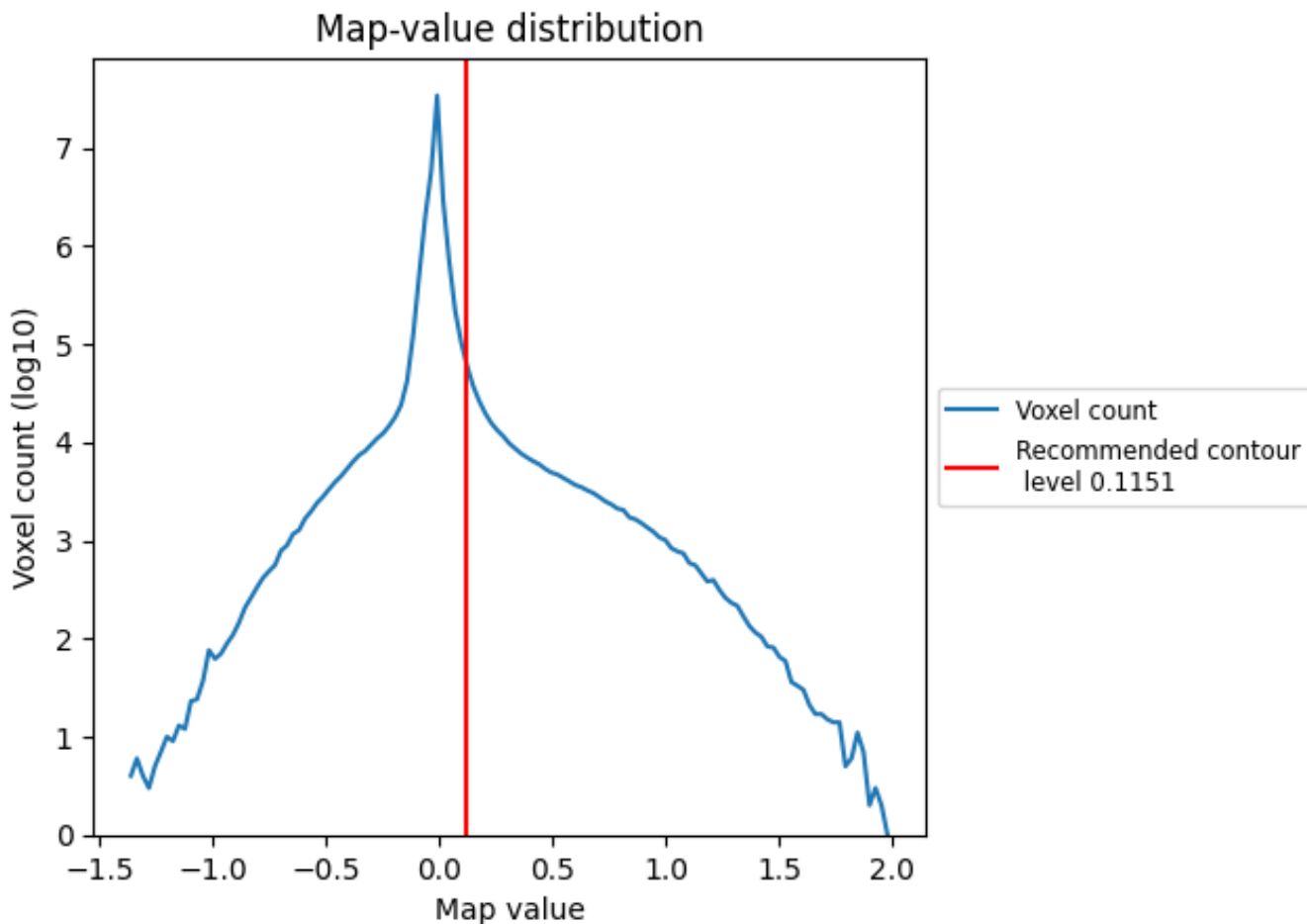
## 6.6 Mask visualisation [i](#)

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.

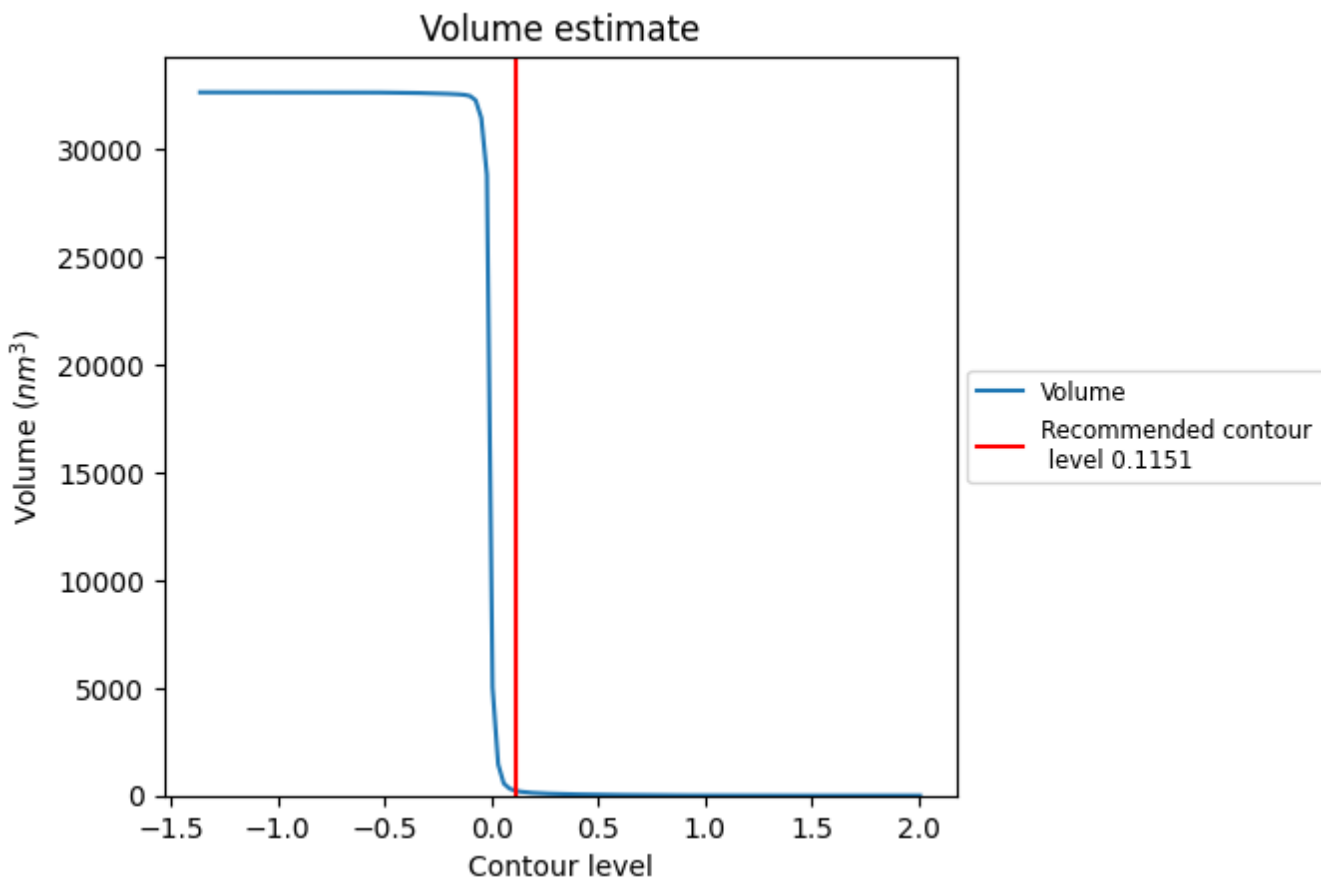
### 7.1 Map-value distribution [i](#)



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.



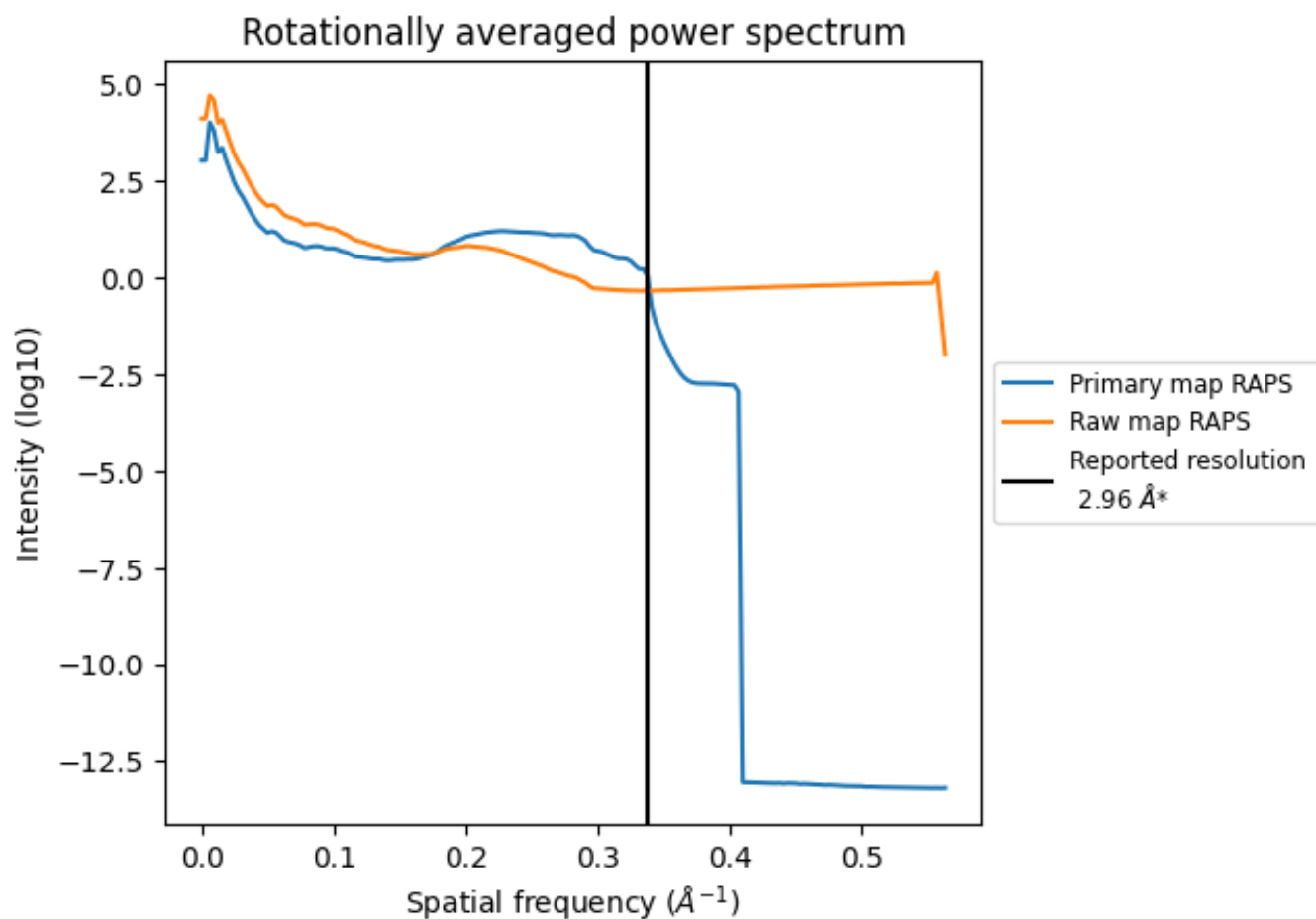
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226  $\text{nm}^3$ ; this corresponds to an approximate mass of 204 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

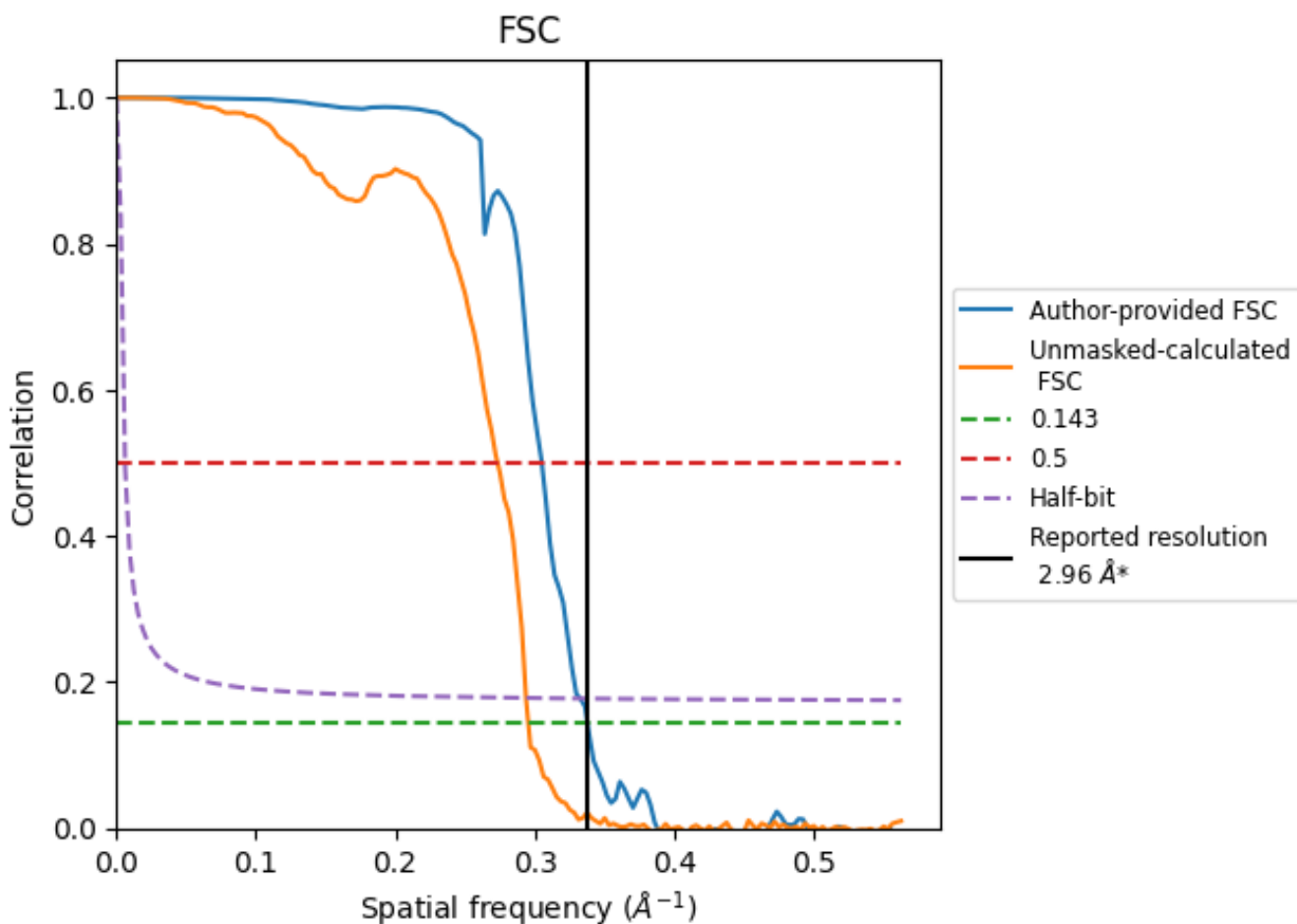


\*Reported resolution corresponds to spatial frequency of 0.338 Å<sup>-1</sup>

## 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 0.338 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

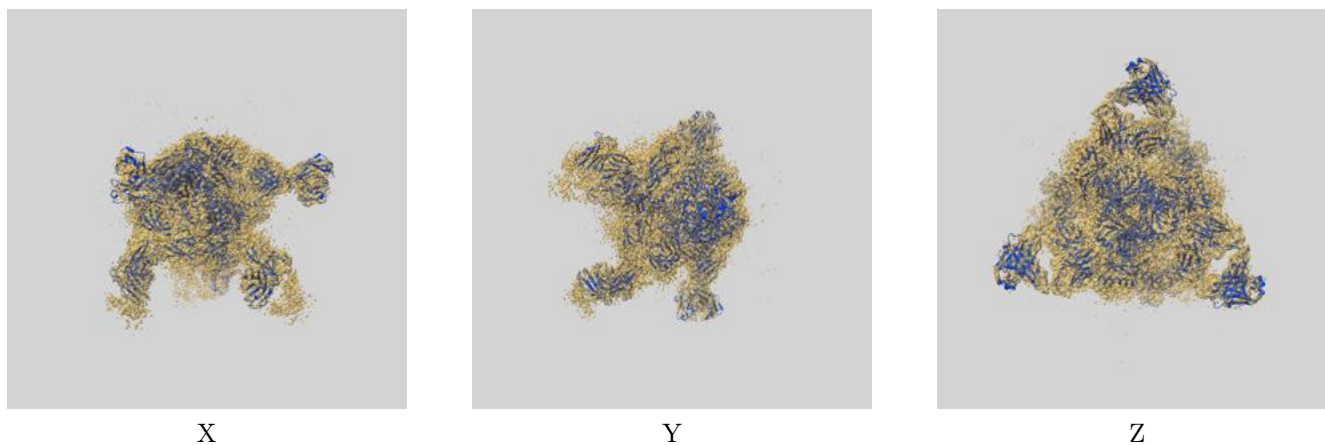
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.28	3.00
Unmasked-calculated*	3.38	3.66	3.40

\*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 3.38 differs from the reported value 2.96 by more than 10 %

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

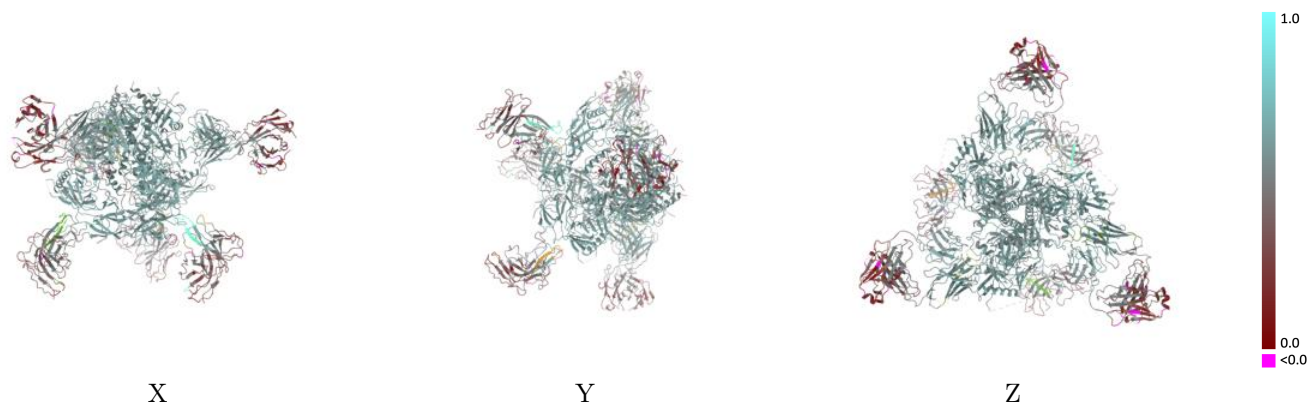
This section contains information regarding the fit between EMDB map EMD-41613 and PDB model 8TTW. Per-residue inclusion information can be found in section 3 on page 14.

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



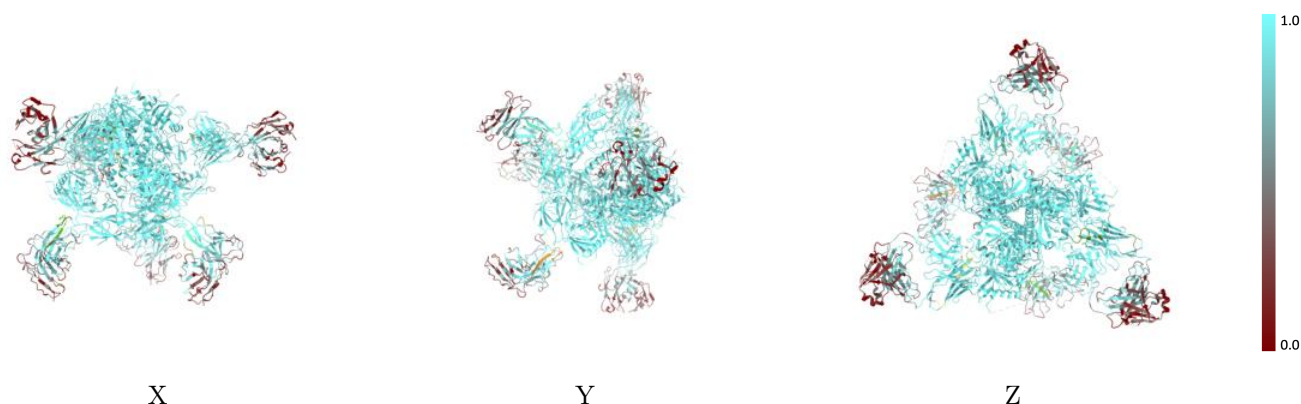
The images above show the 3D surface view of the map at the recommended contour level 0.1151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



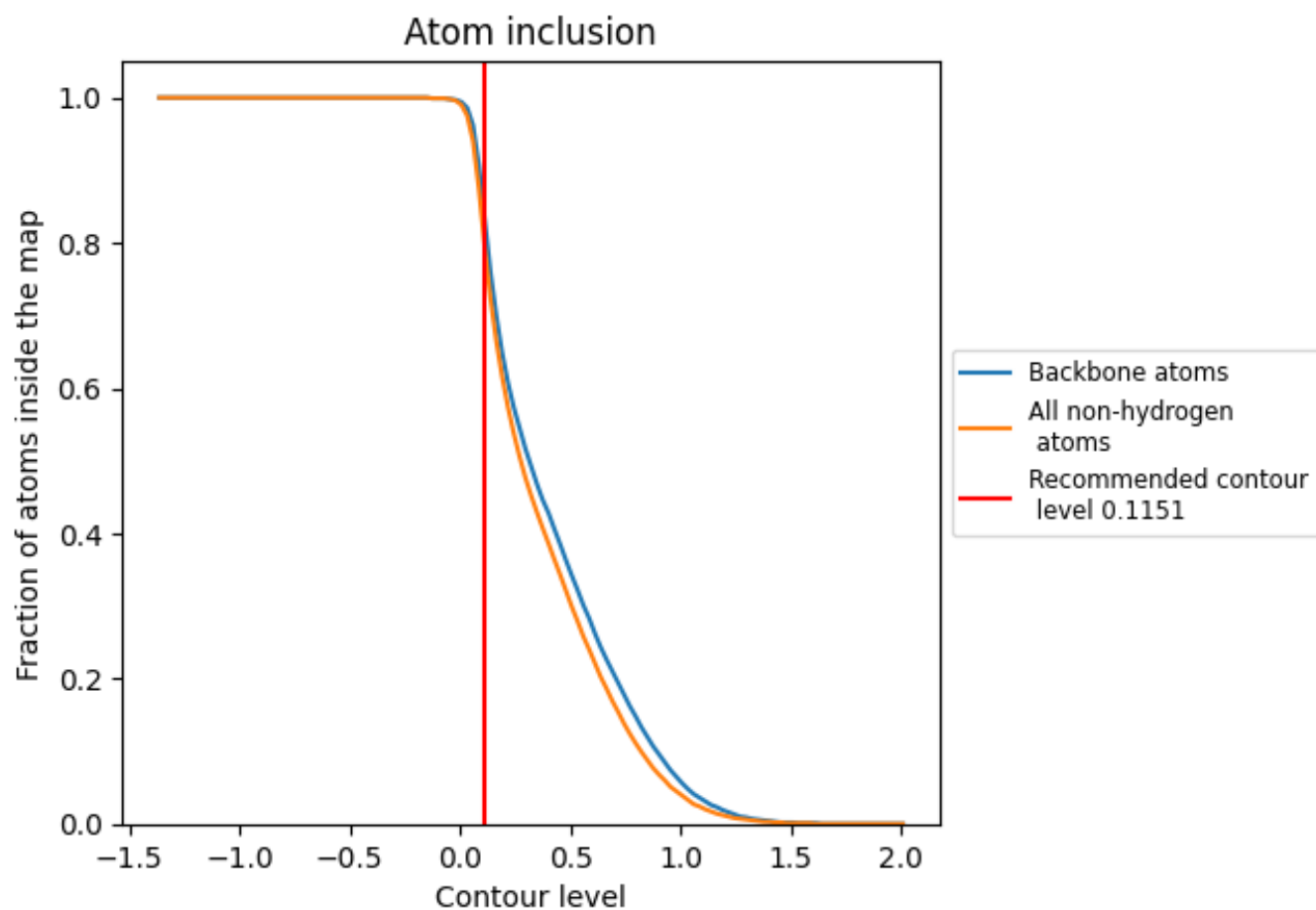
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1151).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.1151) and Q-score for the entire model and for each chain.





















































Chain	Atom inclusion	Q-score
All	 0.7850	 0.5070
0	 0.7210	 0.4540
1	 0.8210	 0.5260
2	 0.6070	 0.3570
3	 0.8190	 0.4920
4	 0.5360	 0.3220
5	 0.7140	 0.4270
6	 0.4640	 0.2650
7	 0.7140	 0.3720
A	 0.9260	 0.5830
B	 0.9370	 0.5820
C	 0.7320	 0.4800
D	 0.6400	 0.4460
E	 0.9290	 0.5830
F	 0.9320	 0.5800
G	 0.7240	 0.4760
H	 0.6320	 0.4430
I	 0.9230	 0.5820
J	 0.9320	 0.5800
K	 0.7300	 0.4770
L	 0.6370	 0.4420
M	 0.5510	 0.3950
N	 0.7150	 0.4390
O	 0.5410	 0.3930
P	 0.7100	 0.4410
Q	 0.5470	 0.3930
R	 0.7100	 0.4400
S	 0.8210	 0.5090
T	 0.8570	 0.5500
U	 0.8930	 0.5160
V	 0.8570	 0.5490
W	 0.8570	 0.5120
X	 0.8570	 0.5400
Y	 0.7140	 0.5210
Z	 0.5360	 0.2630



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Chain	Atom inclusion	Q-score
a	 0.6790	 0.4080
b	 0.8880	 0.5380
c	 0.7050	 0.4490
d	 0.8210	 0.5160
e	 0.6430	 0.3520
f	 0.8290	 0.4850
g	 0.5360	 0.3160
h	 0.7140	 0.4310
i	 0.4640	 0.2730
j	 0.7140	 0.3640
k	 0.7860	 0.5120
l	 0.5000	 0.2510
m	 0.6790	 0.4160
n	 0.8790	 0.5410
o	 0.7050	 0.4500
p	 0.8210	 0.5100
q	 0.6070	 0.3620
r	 0.8190	 0.4920
s	 0.5360	 0.3160
t	 0.7140	 0.4250
u	 0.4290	 0.2580
v	 0.6790	 0.3660
w	 0.7500	 0.5080
x	 0.5360	 0.2540
y	 0.7140	 0.4230
z	 0.8790	 0.5390