



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 05:38 AM EST

PDB ID : 6MN7
EMDB ID : EMD-9166
Title : Cryo-EM structure of BG505.SOSIP.664 in complex with BF520.1 antigen binding fragment
Authors : Williams, J.A.; Lee, K.K.; Overbaugh, J.
Deposited on : 2018-10-01
Resolution : 4.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

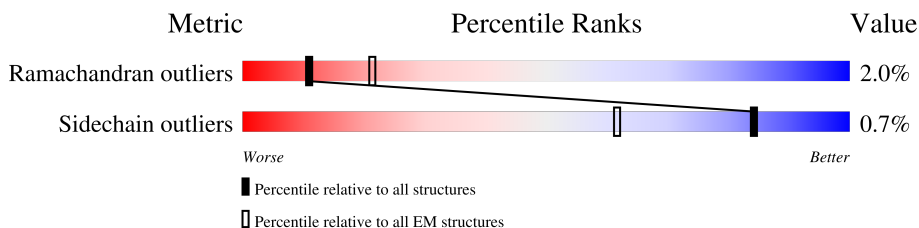
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.80 Å.

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




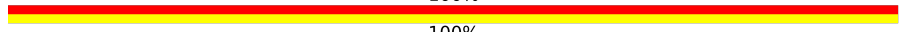
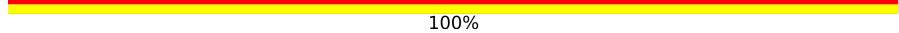
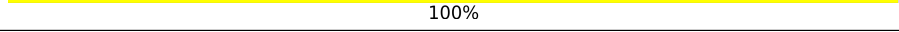
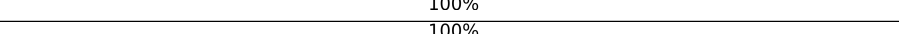


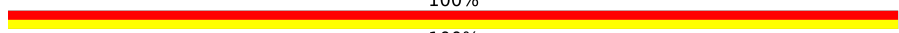

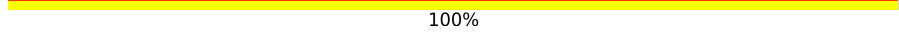
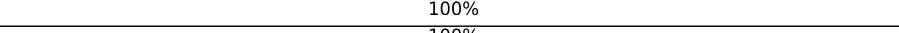
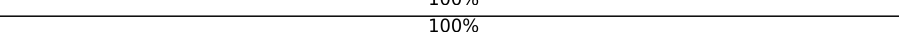
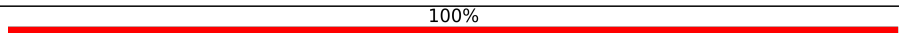

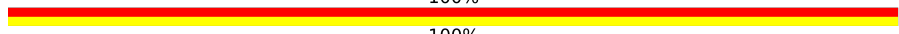
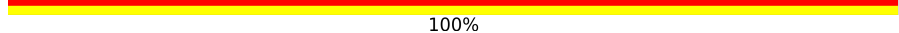
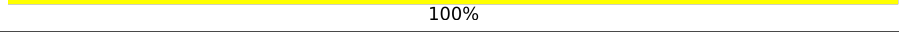
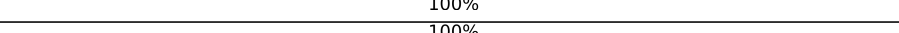
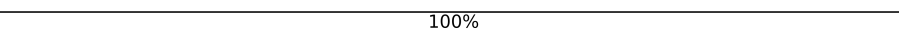

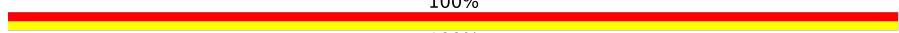




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	476	49% 89% 8%
1	C	476	49% 89% 8%
1	D	476	48% 89% 8%
2	B	153	57% 82% 5% 14%
2	E	153	58% 82% 5% 14%
2	F	153	59% 82% 5% 14%
3	G	236	76% 94% 5%
3	H	236	78% 94% 5%
3	I	236	75% 94% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	2	3	67% 
4	3	3	100% 
4	J	3	100% 
4	L	3	100% 
4	M	3	100% 
4	Q	3	100% 
4	V	3	67% 
4	W	3	100% 
4	a	3	100% 
4	c	3	100% 
4	d	3	100% 
4	h	3	100% 
4	m	3	100% 
4	n	3	100% 
4	q	3	100% 
4	s	3	100% 
4	t	3	100% 
4	x	3	100% 
5	1	2	100% 
5	4	2	100% 
5	5	2	100% 
5	6	2	100% 
5	7	2	100% 
5	K	2	100% 
5	N	2	100% 


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	O	2	100%
5	U	2	100%
5	X	2	100%
5	Y	2	100%
5	Z	2	100%
5	b	2	100%
5	e	2	100%
5	f	2	100%
5	l	2	50%
5	o	2	100%
5	p	2	100%
5	r	2	100%
5	u	2	100%
5	v	2	100%
6	P	7	86% 14%
6	g	7	86% 14%
6	w	7	86% 14%
7	R	5	80%
7	i	5	80%
7	y	5	80%
8	S	7	86% 14%
8	j	7	86% 14%
8	z	7	86% 14%
9	0	10	80% 20%
9	T	10	70% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	k	10	 A horizontal bar chart showing the quality of chain for Mol 9, Chain k, Length 10. The bar is divided into three segments: a green segment on the left labeled '20%', a red segment in the middle labeled '80%', and a yellow segment on the right labeled '80%'. The red segment is the largest, followed by the yellow segment, and the green segment is the smallest.

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 21447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope Glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	438	3453	2170	610	645	28	0	0
1	C	438	3453	2170	610	645	28	0	0
1	D	438	3453	2170	610	645	28	0	0

There are 6 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
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope Glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1051	667	180	198	6	0	0
2	E	132	1051	667	180	198	6	0	0
2	F	132	1051	667	180	198	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S7
B	605	CYS	THR	engineered mutation	UNP Q2N0S7
E	559	PRO	ILE	engineered mutation	UNP Q2N0S7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	605	CYS	THR	engineered mutation	UNP Q2N0S7
F	559	PRO	ILE	engineered mutation	UNP Q2N0S7
F	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 3 is a protein called BF520.1 Fab variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	236	Total	C	N	O	S	0	0
			1830	1160	310	349	11		
3	H	236	Total	C	N	O	S	0	0
			1830	1160	310	349	11		
3	I	236	Total	C	N	O	S	0	0
			1830	1160	310	349	11		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	L	3	Total	C	N	O	0	0
			39	22	2	15		
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	V	3	Total	C	N	O	0	0
			39	22	2	15		
4	W	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		
4	c	3	Total	C	N	O	0	0
			39	22	2	15		
4	d	3	Total	C	N	O	0	0
			39	22	2	15		
4	h	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	m	3	Total	C	N	O	0	0
			39	22	2	15		
4	n	3	Total	C	N	O	0	0
			39	22	2	15		
4	q	3	Total	C	N	O	0	0
			39	22	2	15		
4	s	3	Total	C	N	O	0	0
			39	22	2	15		
4	t	3	Total	C	N	O	0	0
			39	22	2	15		
4	x	3	Total	C	N	O	0	0
			39	22	2	15		
4	2	3	Total	C	N	O	0	0
			39	22	2	15		
4	3	3	Total	C	N	O	0	0
			39	22	2	15		

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



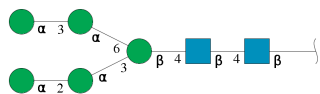
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	f	2	Total 28	C 16	N 2	O 10	0	0
5	l	2	Total 28	C 16	N 2	O 10	0	0
5	o	2	Total 28	C 16	N 2	O 10	0	0
5	p	2	Total 28	C 16	N 2	O 10	0	0
5	r	2	Total 28	C 16	N 2	O 10	0	0
5	u	2	Total 28	C 16	N 2	O 10	0	0
5	v	2	Total 28	C 16	N 2	O 10	0	0
5	1	2	Total 28	C 16	N 2	O 10	0	0
5	4	2	Total 28	C 16	N 2	O 10	0	0
5	5	2	Total 28	C 16	N 2	O 10	0	0
5	6	2	Total 28	C 16	N 2	O 10	0	0
5	7	2	Total 28	C 16	N 2	O 10	0	0

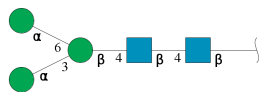
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	7	Total 83	C 46	N 2	O 35	0	0
6	g	7	Total 83	C 46	N 2	O 35	0	0
6	w	7	Total 83	C 46	N 2	O 35	0	0

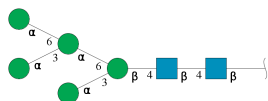
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



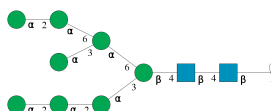
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	R	5	61	34	2	25	0	0
7	i	5	61	34	2	25	0	0
7	y	5	61	34	2	25	0	0

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



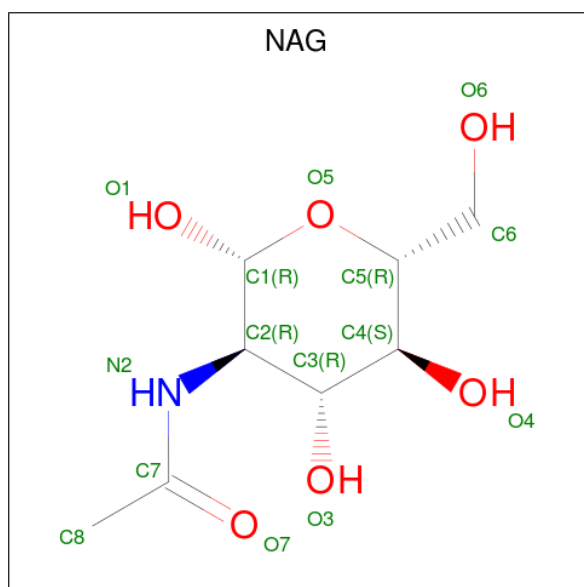
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	S	7	83	46	2	35	0	0
8	j	7	83	46	2	35	0	0
8	z	7	83	46	2	35	0	0

- Molecule 9 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
9	T	10	Total	C	N	O	0	0
			116	64	2	50		
9	k	10	Total	C	N	O	0	0
			116	64	2	50		
9	0	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

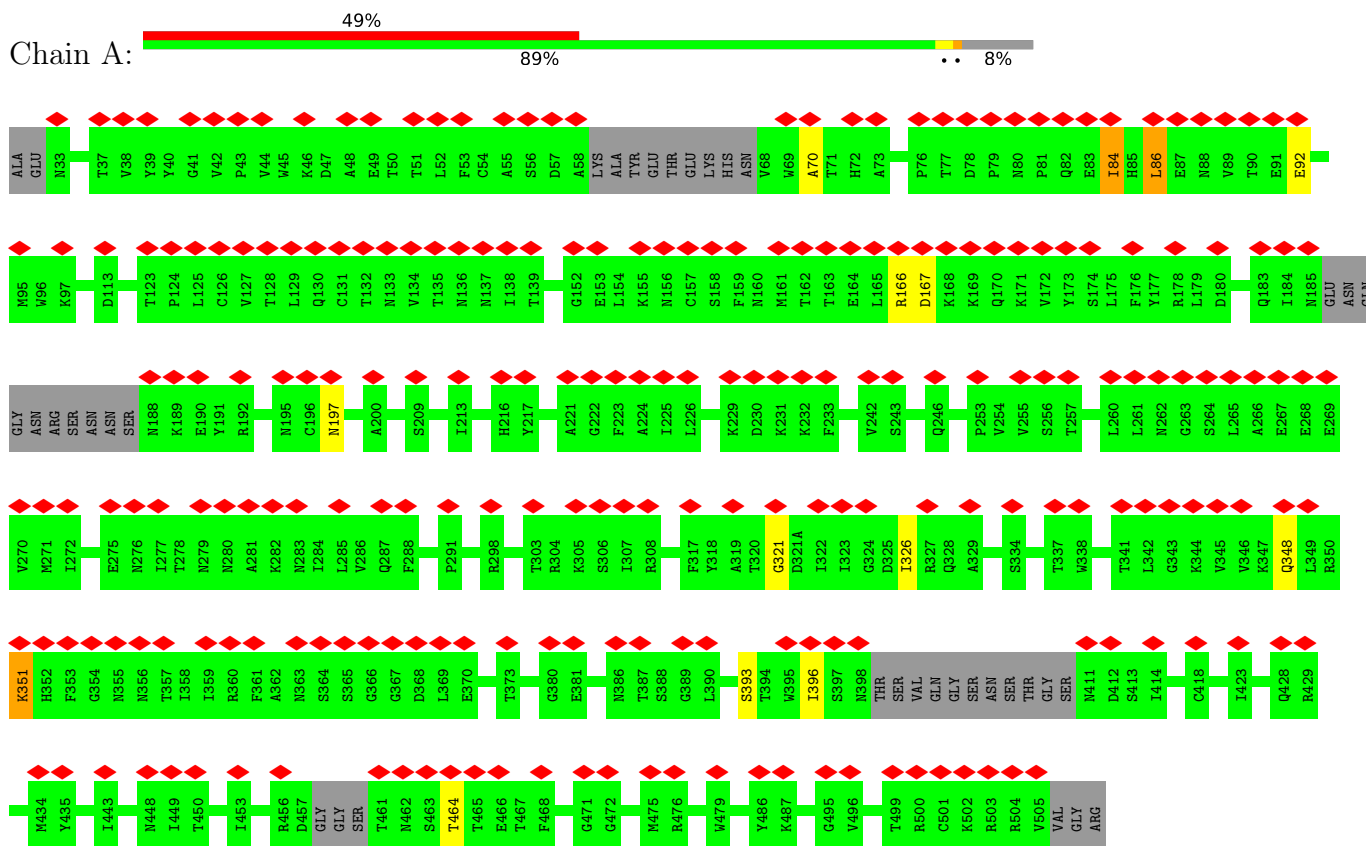
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	F	1	28	16	2	10	0

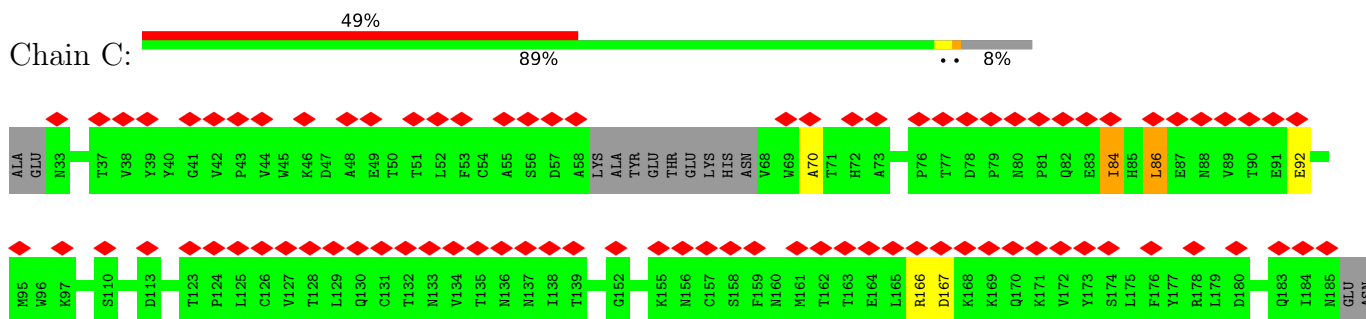
3 Residue-property plots

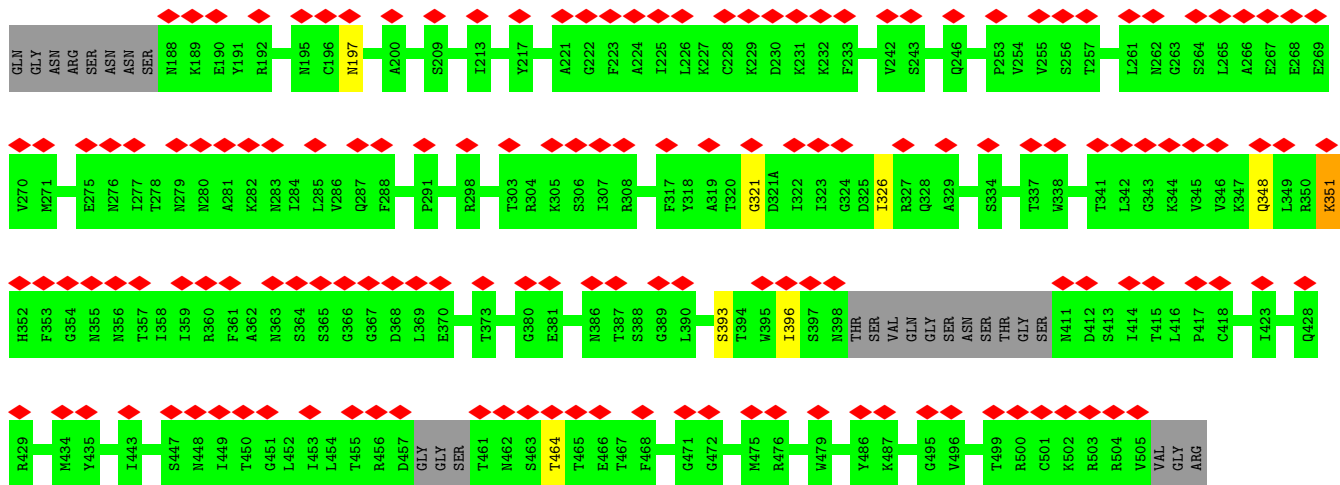
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Envelope Glycoprotein gp120

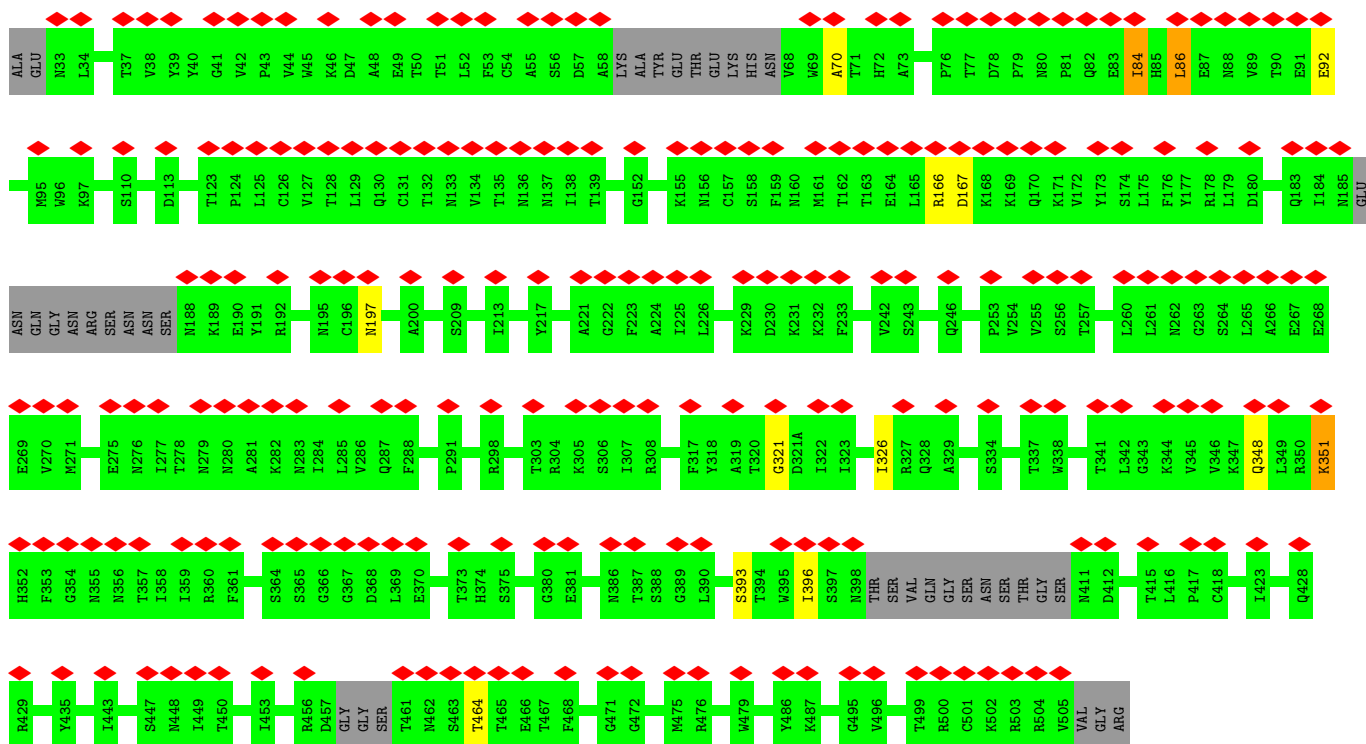
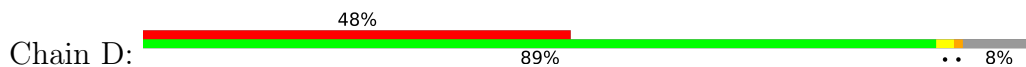


• Molecule 1: Envelope Glycoprotein gp120

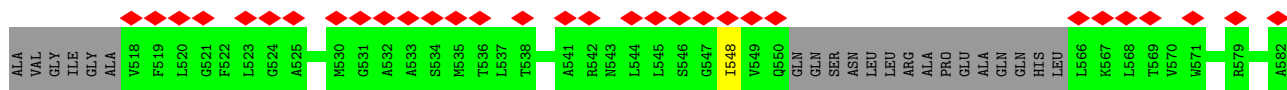
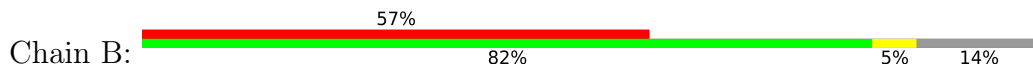


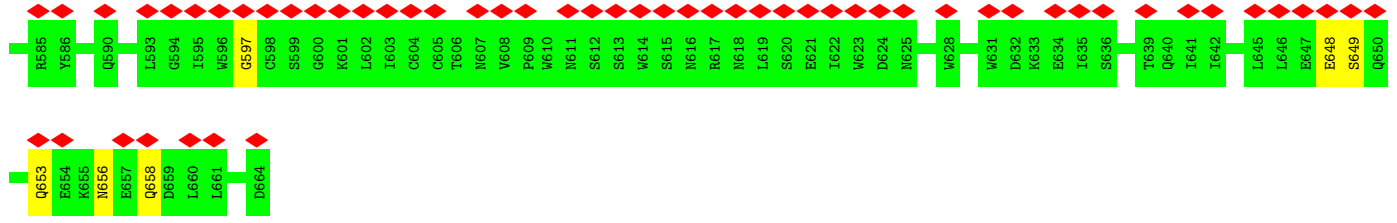


• Molecule 1: Envelope Glycoprotein gp120

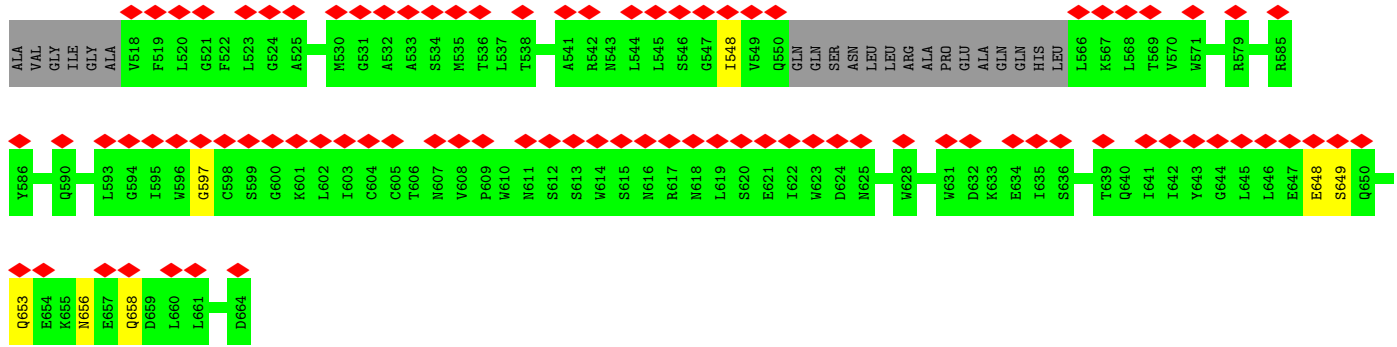
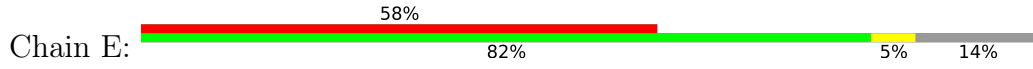


• Molecule 2: Envelope Glycoprotein gp41

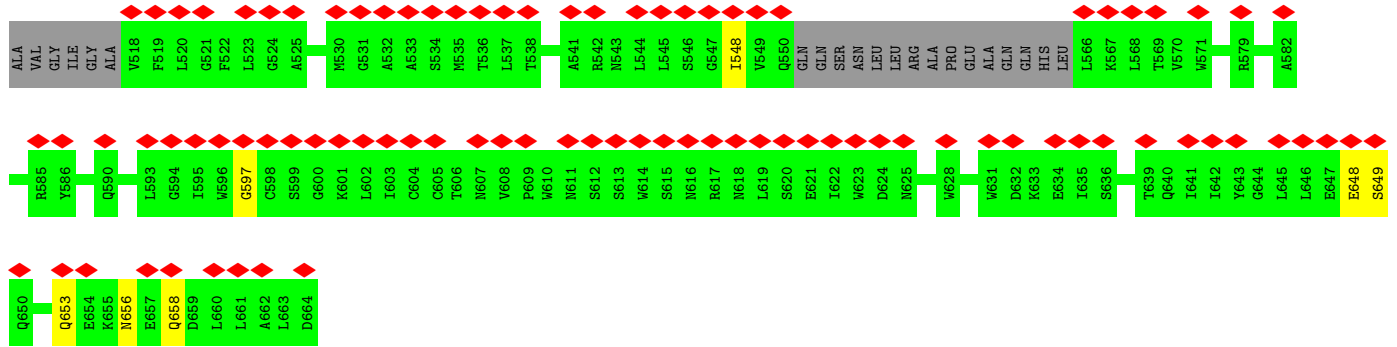
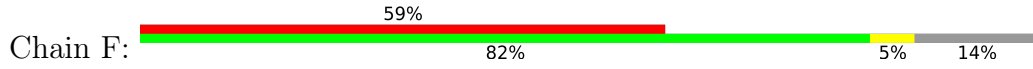




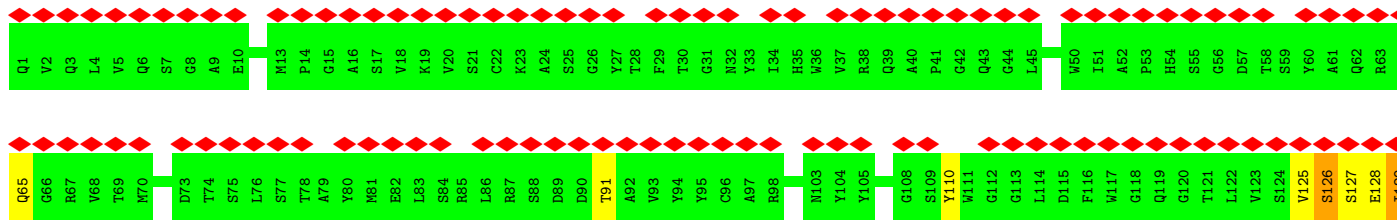
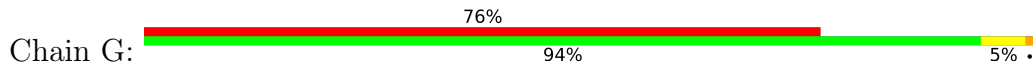
• Molecule 2: Envelope Glycoprotein gp41

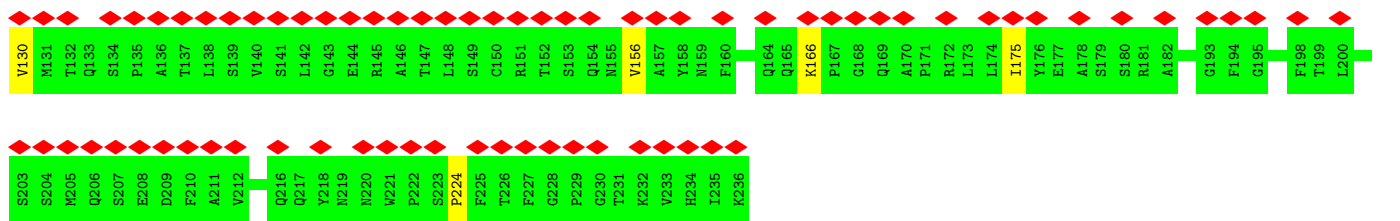


• Molecule 2: Envelope Glycoprotein gp41



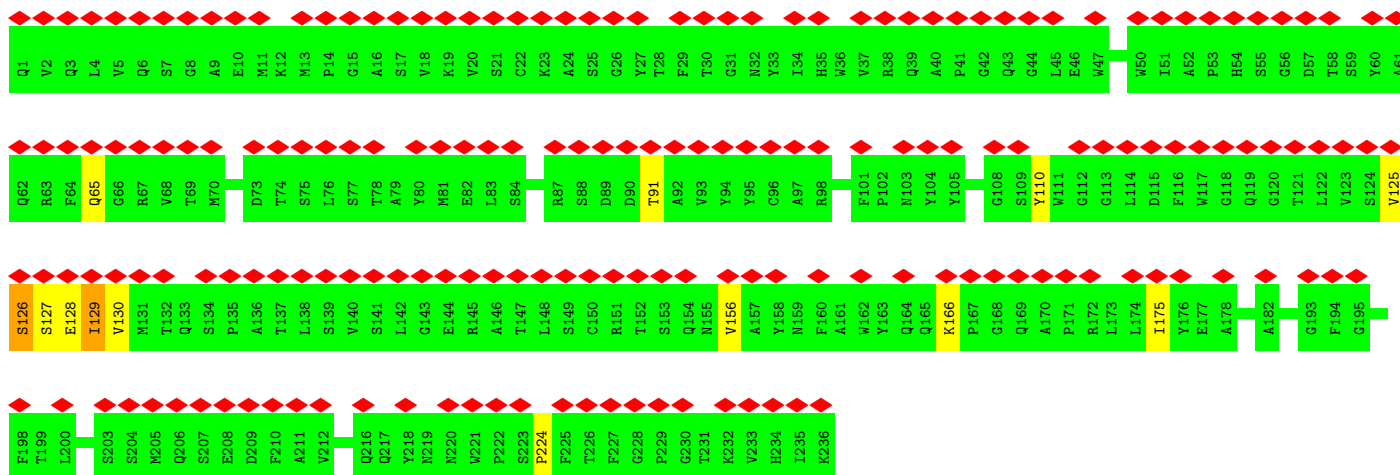
• Molecule 3: BF520.1 Fab variable region





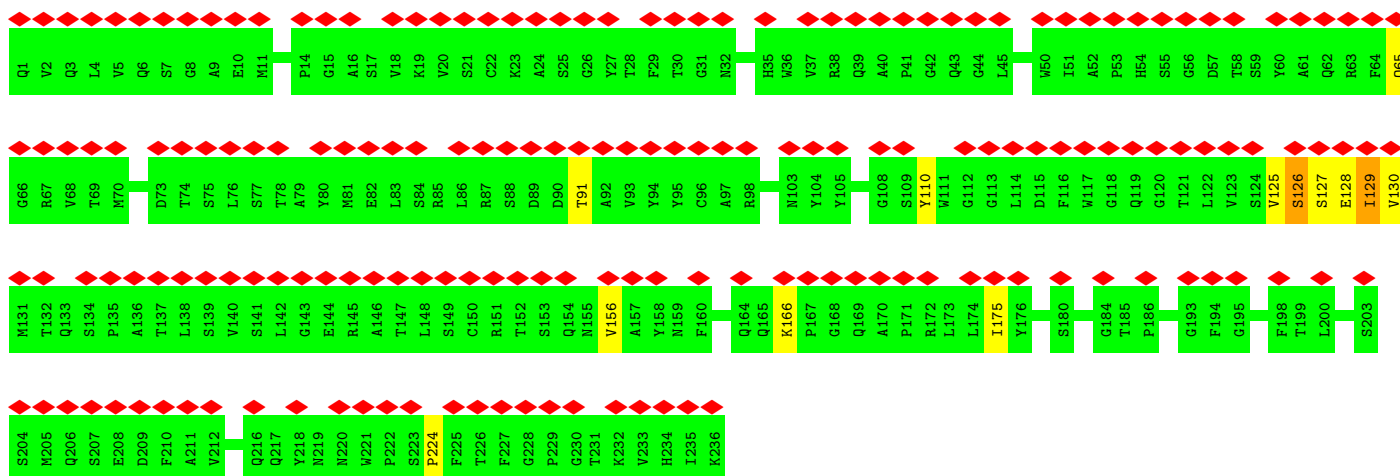
- Molecule 3: BF520.1 Fab variable region

Chain H: 78% 94% 5%



- Molecule 3: BF520.1 Fab variable region

Chain I: 75% 94% 5%



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

Chain J: 100% 100%



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



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



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



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



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



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



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



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



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



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



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



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

Chain q:  100%
100%



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

Chain s:  100%
100%



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

Chain t:  100%
100%



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

Chain x:  100%
100%



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

Chain 2:  67%
100%



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

Chain 3:  100%
100%



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



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



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



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



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



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



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



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



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



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



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



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

Chain o:  100%
100%



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

Chain p:  100%
100%



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

Chain r:  100%
100%



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

Chain u:  100%
100%



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

Chain v:  100%
100%



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

Chain 1:  100%
100%



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



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



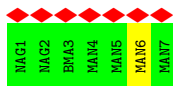
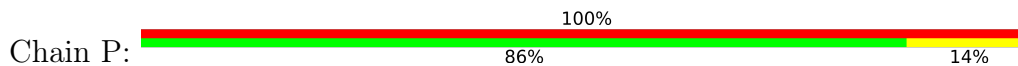
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

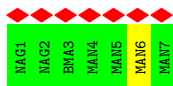
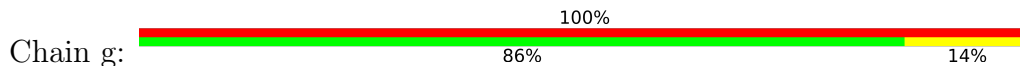


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

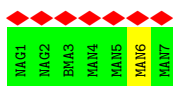
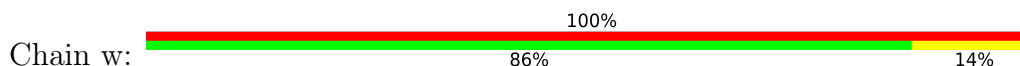


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

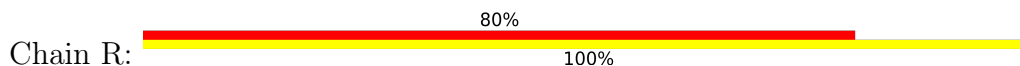
D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



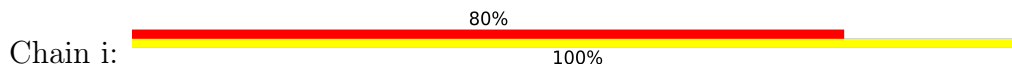
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



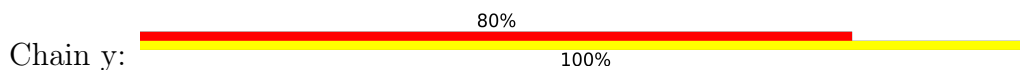
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



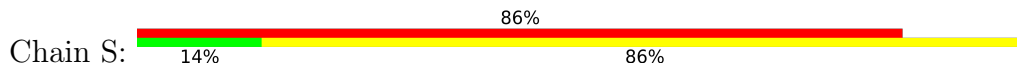
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



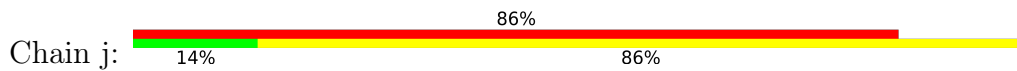
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



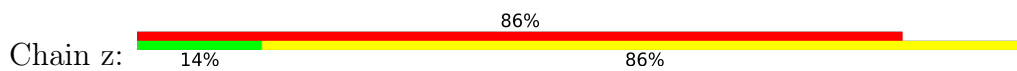
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



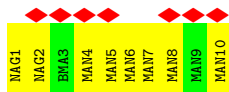
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



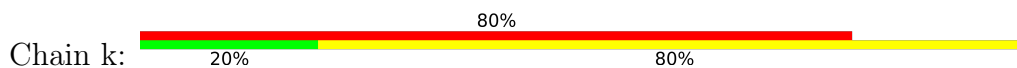
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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

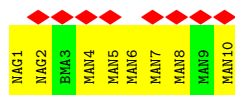
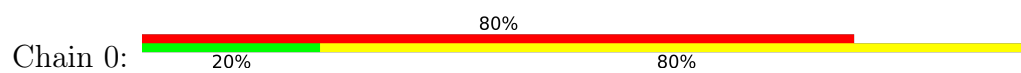


- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	67174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.335	Depositor
Minimum map value	-0.202	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.102	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2, 2.2, 2.2	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.64	3/3523 (0.1%)	0.73	15/4783 (0.3%)
1	C	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
1	D	0.64	2/3523 (0.1%)	0.73	15/4783 (0.3%)
2	B	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	E	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
2	F	0.72	1/1069 (0.1%)	0.81	5/1448 (0.3%)
3	G	1.21	10/1885 (0.5%)	1.33	15/2563 (0.6%)
3	H	1.21	10/1885 (0.5%)	1.33	15/2563 (0.6%)
3	I	1.21	10/1885 (0.5%)	1.33	15/2563 (0.6%)
All	All	0.85	40/19431 (0.2%)	0.96	105/26382 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	128	GLU	N-CA	13.71	1.73	1.46
3	G	128	GLU	N-CA	13.70	1.73	1.46
3	H	128	GLU	N-CA	13.69	1.73	1.46
3	I	127	SER	C-N	12.35	1.62	1.34
3	H	127	SER	C-N	12.31	1.62	1.34
3	G	127	SER	C-N	12.29	1.62	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	658	GLN	C-N	12.07	1.61	1.34
2	F	658	GLN	C-N	12.07	1.61	1.34
2	E	658	GLN	C-N	11.99	1.61	1.34
3	G	128	GLU	CA-C	11.81	1.83	1.52
3	H	128	GLU	CA-C	11.76	1.83	1.52
3	I	128	GLU	CA-C	11.73	1.83	1.52
3	G	129	ILE	N-CA	11.29	1.69	1.46
3	H	129	ILE	N-CA	11.27	1.68	1.46
3	I	129	ILE	N-CA	11.21	1.68	1.46
3	I	128	GLU	C-N	10.39	1.57	1.34
3	H	128	GLU	C-N	10.36	1.57	1.34
3	G	128	GLU	C-N	10.34	1.57	1.34
3	G	127	SER	CA-C	10.29	1.79	1.52
3	I	127	SER	CA-C	10.27	1.79	1.52
3	H	127	SER	CA-C	10.25	1.79	1.52
3	I	127	SER	N-CA	7.60	1.61	1.46
3	H	127	SER	N-CA	7.59	1.61	1.46
3	G	127	SER	N-CA	7.56	1.61	1.46
1	A	92	GLU	C-N	-6.46	1.19	1.34
1	C	92	GLU	C-N	-6.45	1.19	1.34
1	D	92	GLU	C-N	-6.45	1.19	1.34
3	H	129	ILE	C-N	6.12	1.48	1.34
3	G	129	ILE	C-N	6.10	1.48	1.34
3	I	129	ILE	C-N	6.07	1.48	1.34
1	D	84	ILE	C-N	6.00	1.47	1.34
1	A	84	ILE	C-N	5.99	1.47	1.34
1	C	84	ILE	C-N	5.98	1.47	1.34
3	I	129	ILE	CA-C	5.83	1.68	1.52
3	G	129	ILE	CA-C	5.82	1.68	1.52
3	G	126	SER	C-N	5.78	1.47	1.34
3	H	129	ILE	CA-C	5.77	1.68	1.52
3	H	126	SER	C-N	5.73	1.47	1.34
3	I	126	SER	C-N	5.71	1.47	1.34
1	A	393	SER	C-N	5.00	1.45	1.34

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	648	GLU	N-CA-C	14.18	149.29	111.00
2	E	648	GLU	N-CA-C	14.15	149.20	111.00
2	F	648	GLU	N-CA-C	14.15	149.19	111.00
1	A	84	ILE	O-C-N	12.71	143.03	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ILE	O-C-N	12.71	143.03	122.70
1	D	84	ILE	O-C-N	12.67	142.97	122.70
1	D	86	LEU	O-C-N	-12.64	102.47	122.70
1	A	86	LEU	O-C-N	-12.62	102.50	122.70
1	C	86	LEU	O-C-N	-12.58	102.58	122.70
1	D	393	SER	O-C-N	11.18	140.59	122.70
1	A	393	SER	O-C-N	11.17	140.57	122.70
1	C	393	SER	O-C-N	11.13	140.50	122.70
1	A	84	ILE	CA-C-N	-10.75	93.55	117.20
1	C	84	ILE	CA-C-N	-10.74	93.58	117.20
1	D	84	ILE	CA-C-N	-10.70	93.66	117.20
1	D	348	GLN	O-C-N	10.61	139.67	122.70
1	A	348	GLN	O-C-N	10.58	139.63	122.70
1	C	348	GLN	O-C-N	10.55	139.57	122.70
2	E	658	GLN	O-C-N	10.31	139.20	122.70
2	B	658	GLN	O-C-N	10.29	139.16	122.70
2	F	658	GLN	O-C-N	10.29	139.16	122.70
1	D	351	LYS	O-C-N	-10.15	106.46	122.70
1	C	351	LYS	O-C-N	-10.14	106.47	122.70
1	A	351	LYS	O-C-N	-10.08	106.57	122.70
3	G	127	SER	C-N-CA	9.35	145.07	121.70
3	H	127	SER	C-N-CA	9.34	145.04	121.70
3	I	127	SER	C-N-CA	9.34	145.04	121.70
1	C	84	ILE	C-N-CA	-8.88	99.50	121.70
1	A	84	ILE	C-N-CA	-8.88	99.51	121.70
1	D	84	ILE	C-N-CA	-8.86	99.56	121.70
3	G	128	GLU	N-CA-C	8.63	134.29	111.00
3	H	128	GLU	N-CA-C	8.62	134.26	111.00
3	I	128	GLU	N-CA-C	8.62	134.26	111.00
1	C	393	SER	CA-C-N	-8.38	98.77	117.20
1	D	393	SER	CA-C-N	-8.38	98.77	117.20
1	A	393	SER	CA-C-N	-8.38	98.77	117.20
1	A	348	GLN	CA-C-N	-8.03	99.53	117.20
1	D	348	GLN	CA-C-N	-8.02	99.57	117.20
1	C	348	GLN	CA-C-N	-8.01	99.58	117.20
2	B	658	GLN	CA-C-N	-7.98	99.65	117.20
2	F	658	GLN	CA-C-N	-7.97	99.67	117.20
2	E	658	GLN	CA-C-N	-7.95	99.71	117.20
3	G	91	THR	CA-CB-CG2	-7.70	101.61	112.40
3	H	91	THR	CA-CB-CG2	-7.67	101.67	112.40
3	I	91	THR	CA-CB-CG2	-7.63	101.71	112.40
3	I	156	VAL	C-N-CA	7.61	140.72	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	156	VAL	C-N-CA	7.58	140.64	121.70
3	H	156	VAL	C-N-CA	7.57	140.62	121.70
3	H	127	SER	N-CA-C	7.34	130.82	111.00
3	I	127	SER	N-CA-C	7.34	130.81	111.00
3	G	127	SER	N-CA-C	7.32	130.77	111.00
3	I	129	ILE	N-CA-C	7.32	130.75	111.00
3	G	129	ILE	N-CA-C	7.31	130.74	111.00
3	H	129	ILE	N-CA-C	7.31	130.74	111.00
3	H	128	GLU	CA-C-N	7.27	133.19	117.20
1	C	351	LYS	CA-C-N	7.25	133.15	117.20
3	I	128	GLU	CA-C-N	7.25	133.15	117.20
3	G	128	GLU	CA-C-N	7.24	133.12	117.20
1	D	351	LYS	CA-C-N	7.23	133.11	117.20
1	A	351	LYS	CA-C-N	7.20	133.05	117.20
2	F	648	GLU	N-CA-CB	-6.99	98.02	110.60
2	B	648	GLU	N-CA-CB	-6.98	98.04	110.60
2	E	648	GLU	N-CA-CB	-6.97	98.05	110.60
3	H	128	GLU	C-N-CA	6.95	139.08	121.70
3	I	128	GLU	C-N-CA	6.94	139.05	121.70
3	G	128	GLU	C-N-CA	6.92	139.01	121.70
3	H	127	SER	CA-C-O	-6.82	105.78	120.10
3	I	127	SER	CA-C-O	-6.81	105.79	120.10
3	G	127	SER	CA-C-O	-6.80	105.81	120.10
1	A	86	LEU	CA-C-N	6.77	132.10	117.20
1	C	86	LEU	CA-C-N	6.76	132.08	117.20
1	D	86	LEU	CA-C-N	6.76	132.08	117.20
1	A	348	GLN	C-N-CA	-6.73	104.86	121.70
1	D	348	GLN	C-N-CA	-6.73	104.88	121.70
1	C	348	GLN	C-N-CA	-6.72	104.89	121.70
1	D	86	LEU	C-N-CA	6.62	138.24	121.70
3	H	127	SER	CA-C-N	6.61	131.75	117.20
1	A	86	LEU	C-N-CA	6.60	138.20	121.70
3	I	127	SER	CA-C-N	6.59	131.71	117.20
3	G	127	SER	CA-C-N	6.59	131.69	117.20
1	C	86	LEU	C-N-CA	6.57	138.12	121.70
3	H	110	TYR	CA-CB-CG	-6.45	101.15	113.40
3	G	110	TYR	CA-CB-CG	-6.41	101.22	113.40
3	I	110	TYR	CA-CB-CG	-6.41	101.23	113.40
3	G	126	SER	N-CA-C	6.39	128.25	111.00
3	I	126	SER	N-CA-C	6.37	128.19	111.00
3	H	126	SER	N-CA-C	6.35	128.14	111.00
3	H	128	GLU	O-C-N	-6.07	112.98	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	128	GLU	O-C-N	-6.07	112.99	122.70
3	G	128	GLU	O-C-N	-6.03	113.06	122.70
1	A	393	SER	C-N-CA	-5.86	107.05	121.70
1	D	393	SER	C-N-CA	-5.84	107.10	121.70
1	C	393	SER	C-N-CA	-5.83	107.12	121.70
2	F	653	GLN	N-CA-C	5.73	126.46	111.00
2	B	653	GLN	N-CA-C	5.71	126.42	111.00
2	E	653	GLN	N-CA-C	5.69	126.36	111.00
1	C	351	LYS	C-N-CA	5.51	135.49	121.70
1	D	351	LYS	C-N-CA	5.48	135.39	121.70
1	A	351	LYS	C-N-CA	5.46	135.36	121.70
3	H	224	PRO	N-CA-C	5.41	126.18	112.10
3	G	224	PRO	N-CA-C	5.38	126.10	112.10
3	I	224	PRO	N-CA-C	5.38	126.10	112.10
3	G	129	ILE	CB-CA-C	-5.07	101.46	111.60
3	I	129	ILE	CB-CA-C	-5.07	101.46	111.60
3	H	129	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	LEU	Mainchain
1	C	86	LEU	Mainchain
1	D	86	LEU	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/476 (90%)	387 (90%)	32 (8%)	9 (2%)	7	38
1	C	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	7	38
1	D	428/476 (90%)	386 (90%)	33 (8%)	9 (2%)	7	38
2	B	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	30
2	E	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	30
2	F	128/153 (84%)	102 (80%)	22 (17%)	4 (3%)	4	30
3	G	234/236 (99%)	218 (93%)	13 (6%)	3 (1%)	12	48
3	H	234/236 (99%)	218 (93%)	13 (6%)	3 (1%)	12	48
3	I	234/236 (99%)	218 (93%)	13 (6%)	3 (1%)	12	48
All	All	2370/2595 (91%)	2119 (89%)	203 (9%)	48 (2%)	11	39

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	A	396	ILE
1	C	167	ASP
1	C	396	ILE
1	D	167	ASP
1	D	396	ILE
3	G	130	VAL
3	H	130	VAL
3	I	130	VAL
1	A	464	THR
2	B	597	GLY
2	B	649	SER
1	C	464	THR
1	D	464	THR
2	E	597	GLY
2	E	649	SER
2	F	597	GLY
2	F	649	SER
3	G	126	SER
3	H	126	SER
3	I	126	SER
1	A	166	ARG
2	B	548	ILE
1	C	166	ARG
1	D	166	ARG
2	E	548	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	548	ILE
1	A	70	ALA
1	A	321	GLY
2	B	656	ASN
1	C	70	ALA
1	C	321	GLY
1	D	70	ALA
1	D	321	GLY
2	E	656	ASN
2	F	656	ASN
1	A	84	ILE
1	A	351	LYS
1	C	84	ILE
1	C	351	LYS
1	D	84	ILE
1	D	351	LYS
1	C	326	ILE
1	D	326	ILE
1	A	326	ILE
3	G	125	VAL
3	H	125	VAL
3	I	125	VAL

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	393/423 (93%)	392 (100%)	1 (0%)	92	95
1	C	393/423 (93%)	392 (100%)	1 (0%)	92	95
1	D	393/423 (93%)	392 (100%)	1 (0%)	92	95
2	B	114/129 (88%)	114 (100%)	0	100	100
2	E	114/129 (88%)	114 (100%)	0	100	100
2	F	114/129 (88%)	114 (100%)	0	100	100
3	G	193/193 (100%)	189 (98%)	4 (2%)	53	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	193/193 (100%)	189 (98%)	4 (2%)	53	72
3	I	193/193 (100%)	189 (98%)	4 (2%)	53	72
All	All	2100/2235 (94%)	2085 (99%)	15 (1%)	84	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	C	197	ASN
1	D	197	ASN
3	G	65	GLN
3	G	129	ILE
3	G	166	LYS
3	G	175	ILE
3	H	65	GLN
3	H	129	ILE
3	H	166	LYS
3	H	175	ILE
3	I	65	GLN
3	I	129	ILE
3	I	166	LYS
3	I	175	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	C	279	ASN
1	D	279	ASN
3	G	32	ASN
3	G	54	HIS
3	G	159	ASN
3	G	217	GLN
3	G	219	ASN
3	H	32	ASN
3	H	54	HIS
3	H	159	ASN
3	H	217	GLN
3	H	219	ASN
3	I	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	54	HIS
3	I	159	ASN
3	I	217	GLN
3	I	219	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](#)

183 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	9	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
9	MAN	0	10	9	11,11,12	0.33	0	15,15,17	0.92	2 (13%)
9	NAG	0	2	9	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
9	BMA	0	3	9	11,11,12	0.42	0	15,15,17	0.63	0
9	MAN	0	4	9	11,11,12	0.45	0	15,15,17	1.08	1 (6%)
9	MAN	0	5	9	11,11,12	0.49	0	15,15,17	1.05	2 (13%)
9	MAN	0	6	9	11,11,12	0.49	0	15,15,17	1.20	1 (6%)
9	MAN	0	7	9	11,11,12	0.29	0	15,15,17	1.13	1 (6%)
9	MAN	0	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	0	9	9	11,11,12	0.35	0	15,15,17	0.77	0
5	NAG	1	1	5,1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
5	NAG	1	2	5	14,14,15	0.52	0	17,19,21	1.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	2	1	4,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
4	NAG	2	2	4	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	BMA	2	3	4	11,11,12	0.66	0	15,15,17	1.48	3 (20%)
4	NAG	3	1	4,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
4	NAG	3	2	4	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
4	BMA	3	3	4	11,11,12	0.65	0	15,15,17	1.48	3 (20%)
5	NAG	4	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	4	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	NAG	5	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	5	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	NAG	6	1	2,5	14,14,15	0.53	0	17,19,21	2.22	3 (17%)
5	NAG	6	2	5	14,14,15	0.53	0	17,19,21	1.37	3 (17%)
5	NAG	7	1	2,5	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	7	2	5	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
4	NAG	J	1	4,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
4	NAG	J	2	4	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
4	BMA	J	3	4	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
5	NAG	K	1	5,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
5	NAG	K	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	NAG	L	1	4,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
4	NAG	L	2	4	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
4	BMA	L	3	4	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
4	NAG	M	1	4,1	14,14,15	0.51	0	17,19,21	2.22	3 (17%)
4	NAG	M	2	4	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
4	BMA	M	3	4	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
5	NAG	N	1	5,1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
5	NAG	N	2	5	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
5	NAG	O	1	5	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	O	2	5	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
6	NAG	P	1	6	14,14,15	0.60	0	17,19,21	0.67	0
6	NAG	P	2	6	14,14,15	0.57	0	17,19,21	0.89	0
6	BMA	P	3	6	11,11,12	0.65	0	15,15,17	0.86	0
6	MAN	P	4	6	11,11,12	0.60	0	15,15,17	0.68	0
6	MAN	P	5	6	11,11,12	0.55	0	15,15,17	0.74	0
6	MAN	P	6	6	11,11,12	0.65	0	15,15,17	1.10	2 (13%)
6	MAN	P	7	6	11,11,12	0.62	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Q	1	4,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
4	NAG	Q	2	4	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
4	BMA	Q	3	4	11,11,12	0.63	0	15,15,17	1.46	3 (20%)
7	NAG	R	1	7,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
7	NAG	R	2	7	14,14,15	0.52	0	17,19,21	1.38	3 (17%)
7	BMA	R	3	7	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
7	MAN	R	4	7	11,11,12	0.56	0	15,15,17	1.72	4 (26%)
7	MAN	R	5	7	11,11,12	0.62	0	15,15,17	2.54	4 (26%)
8	NAG	S	1	8,1	14,14,15	0.29	0	17,19,21	0.63	0
8	NAG	S	2	8	14,14,15	0.33	0	17,19,21	2.40	4 (23%)
8	BMA	S	3	8	11,11,12	0.45	0	15,15,17	1.21	2 (13%)
8	MAN	S	4	8	11,11,12	0.41	0	15,15,17	0.90	1 (6%)
8	MAN	S	5	8	11,11,12	0.44	0	15,15,17	0.85	1 (6%)
8	MAN	S	6	8	11,11,12	0.48	0	15,15,17	0.83	1 (6%)
8	MAN	S	7	8	11,11,12	0.33	0	15,15,17	1.31	2 (13%)
9	NAG	T	1	9	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
9	MAN	T	10	9	11,11,12	0.33	0	15,15,17	0.92	2 (13%)
9	NAG	T	2	9	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
9	BMA	T	3	9	11,11,12	0.42	0	15,15,17	0.63	0
9	MAN	T	4	9	11,11,12	0.44	0	15,15,17	1.08	1 (6%)
9	MAN	T	5	9	11,11,12	0.48	0	15,15,17	1.05	2 (13%)
9	MAN	T	6	9	11,11,12	0.49	0	15,15,17	1.20	1 (6%)
9	MAN	T	7	9	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
9	MAN	T	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	T	9	9	11,11,12	0.34	0	15,15,17	0.78	0
5	NAG	U	1	5,1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
5	NAG	U	2	5	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	NAG	V	1	4,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
4	NAG	V	2	4	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	BMA	V	3	4	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
4	NAG	W	1	4,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
4	NAG	W	2	4	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
4	BMA	W	3	4	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
5	NAG	X	1	5,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	X	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Y	1	5,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	Y	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	NAG	Z	1	2,5	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
5	NAG	Z	2	5	14,14,15	0.53	0	17,19,21	1.37	3 (17%)
4	NAG	a	1	4,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
4	NAG	a	2	4	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
4	BMA	a	3	4	11,11,12	0.65	0	15,15,17	1.48	3 (20%)
5	NAG	b	1	5,1	14,14,15	0.50	0	17,19,21	2.22	3 (17%)
5	NAG	b	2	5	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
4	NAG	c	1	4,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
4	NAG	c	2	4	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
4	BMA	c	3	4	11,11,12	0.63	0	15,15,17	1.46	3 (20%)
4	NAG	d	1	4,1	14,14,15	0.49	0	17,19,21	2.22	3 (17%)
4	NAG	d	2	4	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
4	BMA	d	3	4	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
5	NAG	e	1	5,1	14,14,15	0.52	0	17,19,21	2.25	3 (17%)
5	NAG	e	2	5	14,14,15	0.54	0	17,19,21	1.37	3 (17%)
5	NAG	f	1	5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	f	2	5	14,14,15	0.49	0	17,19,21	1.38	3 (17%)
6	NAG	g	1	6	14,14,15	0.60	0	17,19,21	0.68	0
6	NAG	g	2	6	14,14,15	0.57	0	17,19,21	0.90	0
6	BMA	g	3	6	11,11,12	0.64	0	15,15,17	0.87	0
6	MAN	g	4	6	11,11,12	0.62	0	15,15,17	0.66	0
6	MAN	g	5	6	11,11,12	0.53	0	15,15,17	0.74	0
6	MAN	g	6	6	11,11,12	0.65	0	15,15,17	1.09	2 (13%)
6	MAN	g	7	6	11,11,12	0.61	0	15,15,17	0.62	0
4	NAG	h	1	4,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
4	NAG	h	2	4	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
4	BMA	h	3	4	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
7	NAG	i	1	7,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
7	NAG	i	2	7	14,14,15	0.53	0	17,19,21	1.37	3 (17%)
7	BMA	i	3	7	11,11,12	0.64	0	15,15,17	1.45	3 (20%)
7	MAN	i	4	7	11,11,12	0.57	0	15,15,17	1.72	4 (26%)
7	MAN	i	5	7	11,11,12	0.65	0	15,15,17	2.52	4 (26%)
8	NAG	j	1	8,1	14,14,15	0.29	0	17,19,21	0.63	0
8	NAG	j	2	8	14,14,15	0.33	0	17,19,21	2.40	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	j	3	8	11,11,12	0.45	0	15,15,17	1.22	2 (13%)
8	MAN	j	4	8	11,11,12	0.41	0	15,15,17	0.90	1 (6%)
8	MAN	j	5	8	11,11,12	0.44	0	15,15,17	0.86	1 (6%)
8	MAN	j	6	8	11,11,12	0.48	0	15,15,17	0.82	1 (6%)
8	MAN	j	7	8	11,11,12	0.33	0	15,15,17	1.30	2 (13%)
9	NAG	k	1	9	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
9	MAN	k	10	9	11,11,12	0.33	0	15,15,17	0.92	2 (13%)
9	NAG	k	2	9	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
9	BMA	k	3	9	11,11,12	0.42	0	15,15,17	0.63	0
9	MAN	k	4	9	11,11,12	0.45	0	15,15,17	1.08	1 (6%)
9	MAN	k	5	9	11,11,12	0.48	0	15,15,17	1.05	2 (13%)
9	MAN	k	6	9	11,11,12	0.48	0	15,15,17	1.20	1 (6%)
9	MAN	k	7	9	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
9	MAN	k	8	9	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
9	MAN	k	9	9	11,11,12	0.35	0	15,15,17	0.77	0
5	NAG	l	1	5,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	l	2	5	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
4	NAG	m	1	4,1	14,14,15	0.53	0	17,19,21	2.24	3 (17%)
4	NAG	m	2	4	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
4	BMA	m	3	4	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
4	NAG	n	1	4,1	14,14,15	0.48	0	17,19,21	2.24	3 (17%)
4	NAG	n	2	4	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
4	BMA	n	3	4	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
5	NAG	o	1	5,1	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
5	NAG	o	2	5	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
5	NAG	p	1	5,1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
5	NAG	p	2	5	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
4	NAG	q	1	4,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
4	NAG	q	2	4	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
4	BMA	q	3	4	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
5	NAG	r	1	5,1	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
5	NAG	r	2	5	14,14,15	0.52	0	17,19,21	1.37	3 (17%)
4	NAG	s	1	4,1	14,14,15	0.50	0	17,19,21	2.25	3 (17%)
4	NAG	s	2	4	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
4	BMA	s	3	4	11,11,12	0.65	0	15,15,17	1.46	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	t	1	4,1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
4	NAG	t	2	4	14,14,15	0.53	0	17,19,21	1.36	3 (17%)
4	BMA	t	3	4	11,11,12	0.67	0	15,15,17	1.47	3 (20%)
5	NAG	u	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	u	2	5	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
5	NAG	v	1	5	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	v	2	5	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
6	NAG	w	1	6	14,14,15	0.60	0	17,19,21	0.69	0
6	NAG	w	2	6	14,14,15	0.57	0	17,19,21	0.88	0
6	BMA	w	3	6	11,11,12	0.67	0	15,15,17	0.86	0
6	MAN	w	4	6	11,11,12	0.60	0	15,15,17	0.68	0
6	MAN	w	5	6	11,11,12	0.53	0	15,15,17	0.74	0
6	MAN	w	6	6	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
6	MAN	w	7	6	11,11,12	0.61	0	15,15,17	0.62	0
4	NAG	x	1	4,1	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
4	NAG	x	2	4	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	BMA	x	3	4	11,11,12	0.63	0	15,15,17	1.47	3 (20%)
7	NAG	y	1	7,1	14,14,15	0.48	0	17,19,21	2.23	3 (17%)
7	NAG	y	2	7	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
7	BMA	y	3	7	11,11,12	0.63	0	15,15,17	1.46	3 (20%)
7	MAN	y	4	7	11,11,12	0.56	0	15,15,17	1.73	4 (26%)
7	MAN	y	5	7	11,11,12	0.61	0	15,15,17	2.53	4 (26%)
8	NAG	z	1	8	14,14,15	0.29	0	17,19,21	0.62	0
8	NAG	z	2	8	14,14,15	0.34	0	17,19,21	2.39	4 (23%)
8	BMA	z	3	8	11,11,12	0.45	0	15,15,17	1.21	2 (13%)
8	MAN	z	4	8	11,11,12	0.42	0	15,15,17	0.90	1 (6%)
8	MAN	z	5	8	11,11,12	0.45	0	15,15,17	0.86	1 (6%)
8	MAN	z	6	8	11,11,12	0.49	0	15,15,17	0.82	1 (6%)
8	MAN	z	7	8	11,11,12	0.32	0	15,15,17	1.31	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	9	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	0	10	9	-	1/2/19/22	0/1/1/1
9	NAG	0	2	9	-	1/6/23/26	0/1/1/1
9	BMA	0	3	9	-	0/2/19/22	0/1/1/1
9	MAN	0	4	9	-	1/2/19/22	0/1/1/1
9	MAN	0	5	9	-	0/2/19/22	0/1/1/1
9	MAN	0	6	9	-	0/2/19/22	0/1/1/1
9	MAN	0	7	9	-	0/2/19/22	0/1/1/1
9	MAN	0	8	9	-	0/2/19/22	0/1/1/1
9	MAN	0	9	9	-	1/2/19/22	0/1/1/1
5	NAG	1	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	1	2	5	-	0/6/23/26	0/1/1/1
4	NAG	2	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	2	2	4	-	0/6/23/26	0/1/1/1
4	BMA	2	3	4	-	2/2/19/22	0/1/1/1
4	NAG	3	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	3	2	4	-	0/6/23/26	0/1/1/1
4	BMA	3	3	4	-	2/2/19/22	0/1/1/1
5	NAG	4	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	NAG	5	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
5	NAG	6	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	NAG	7	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	7	2	5	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	2/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
6	NAG	P	1	6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	2	NAG	C1-C2-N2	8.44	124.90	110.49
8	S	2	NAG	C1-C2-N2	8.40	124.84	110.49
8	z	2	NAG	C1-C2-N2	8.39	124.81	110.49
4	n	1	NAG	O5-C1-C2	-7.41	99.58	111.29
4	s	1	NAG	O5-C1-C2	-7.41	99.59	111.29
4	3	1	NAG	O5-C1-C2	-7.40	99.60	111.29
5	p	1	NAG	O5-C1-C2	-7.40	99.61	111.29
5	e	1	NAG	O5-C1-C2	-7.40	99.61	111.29
4	c	1	NAG	O5-C1-C2	-7.40	99.61	111.29
5	r	1	NAG	O5-C1-C2	-7.39	99.61	111.29
5	K	1	NAG	O5-C1-C2	-7.39	99.62	111.29
5	u	1	NAG	O5-C1-C2	-7.39	99.62	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	1	NAG	O5-C1-C2	-7.39	99.62	111.29
5	v	1	NAG	O5-C1-C2	-7.39	99.62	111.29
4	L	1	NAG	O5-C1-C2	-7.39	99.62	111.29
4	2	1	NAG	O5-C1-C2	-7.38	99.63	111.29
4	x	1	NAG	O5-C1-C2	-7.38	99.63	111.29
5	O	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	Y	1	NAG	O5-C1-C2	-7.38	99.64	111.29
4	q	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	X	1	NAG	O5-C1-C2	-7.38	99.64	111.29
4	Q	1	NAG	O5-C1-C2	-7.37	99.65	111.29
5	Z	1	NAG	O5-C1-C2	-7.37	99.65	111.29
4	h	1	NAG	O5-C1-C2	-7.37	99.65	111.29
5	7	1	NAG	O5-C1-C2	-7.36	99.66	111.29
5	1	1	NAG	O5-C1-C2	-7.36	99.66	111.29
4	J	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	5	1	NAG	O5-C1-C2	-7.36	99.67	111.29
5	f	1	NAG	O5-C1-C2	-7.36	99.67	111.29
7	i	1	NAG	O5-C1-C2	-7.35	99.67	111.29
5	o	1	NAG	O5-C1-C2	-7.35	99.68	111.29
4	m	1	NAG	O5-C1-C2	-7.35	99.68	111.29
5	4	1	NAG	O5-C1-C2	-7.35	99.69	111.29
4	V	1	NAG	O5-C1-C2	-7.35	99.69	111.29
5	U	1	NAG	O5-C1-C2	-7.35	99.69	111.29
4	a	1	NAG	O5-C1-C2	-7.34	99.69	111.29
5	l	1	NAG	O5-C1-C2	-7.34	99.69	111.29
5	N	1	NAG	O5-C1-C2	-7.34	99.70	111.29
7	R	1	NAG	O5-C1-C2	-7.34	99.70	111.29
7	y	1	NAG	O5-C1-C2	-7.34	99.70	111.29
5	b	1	NAG	O5-C1-C2	-7.34	99.70	111.29
4	t	1	NAG	O5-C1-C2	-7.34	99.70	111.29
4	d	1	NAG	O5-C1-C2	-7.32	99.73	111.29
5	6	1	NAG	O5-C1-C2	-7.31	99.74	111.29
4	M	1	NAG	O5-C1-C2	-7.31	99.75	111.29
7	R	5	MAN	C1-C2-C3	6.98	118.24	109.67
7	y	5	MAN	C1-C2-C3	6.95	118.22	109.67
7	i	5	MAN	C1-C2-C3	6.89	118.14	109.67
9	0	8	MAN	C1-O5-C5	4.49	118.28	112.19
9	k	8	MAN	C1-O5-C5	4.48	118.26	112.19
9	T	8	MAN	C1-O5-C5	4.47	118.25	112.19
7	R	5	MAN	C2-C3-C4	-4.08	103.84	110.89
7	i	5	MAN	C2-C3-C4	-4.06	103.86	110.89
7	y	5	MAN	C2-C3-C4	-4.05	103.89	110.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	4	MAN	C1-O5-C5	3.87	117.44	112.19
9	0	4	MAN	C1-O5-C5	3.87	117.44	112.19
9	T	4	MAN	C1-O5-C5	3.87	117.43	112.19
9	k	6	MAN	C1-C2-C3	3.67	114.17	109.67
9	0	6	MAN	C1-C2-C3	3.65	114.15	109.67
9	T	6	MAN	C1-C2-C3	3.64	114.14	109.67
4	J	2	NAG	O5-C5-C6	-3.56	101.62	107.20
4	2	2	NAG	O5-C5-C6	-3.55	101.63	107.20
9	0	7	MAN	C1-O5-C5	3.55	117.00	112.19
4	L	2	NAG	O5-C5-C6	-3.55	101.64	107.20
4	q	2	NAG	O5-C5-C6	-3.55	101.65	107.20
7	y	2	NAG	O5-C5-C6	-3.54	101.65	107.20
4	V	2	NAG	O5-C5-C6	-3.54	101.65	107.20
5	1	2	NAG	O5-C5-C6	-3.54	101.65	107.20
5	Y	2	NAG	O5-C5-C6	-3.54	101.65	107.20
4	a	2	NAG	O5-C5-C6	-3.54	101.65	107.20
5	o	2	NAG	O5-C5-C6	-3.54	101.66	107.20
5	U	2	NAG	O5-C5-C6	-3.53	101.66	107.20
4	M	2	NAG	O5-C5-C6	-3.53	101.67	107.20
5	f	2	NAG	O5-C5-C6	-3.53	101.67	107.20
4	c	2	NAG	O5-C5-C6	-3.53	101.68	107.20
4	s	2	NAG	O5-C5-C6	-3.52	101.68	107.20
5	N	2	NAG	O5-C5-C6	-3.52	101.68	107.20
9	T	7	MAN	C1-O5-C5	3.52	116.97	112.19
4	x	2	NAG	O5-C5-C6	-3.52	101.68	107.20
4	Q	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	X	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	K	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	u	2	NAG	O5-C5-C6	-3.52	101.69	107.20
5	e	2	NAG	O5-C5-C6	-3.51	101.69	107.20
4	m	2	NAG	O5-C5-C6	-3.51	101.69	107.20
5	v	2	NAG	O5-C5-C6	-3.51	101.69	107.20
4	d	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	4	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	p	2	NAG	O5-C5-C6	-3.51	101.70	107.20
5	O	2	NAG	O5-C5-C6	-3.51	101.70	107.20
9	k	7	MAN	C1-O5-C5	3.51	116.94	112.19
5	l	2	NAG	O5-C5-C6	-3.50	101.71	107.20
4	h	2	NAG	O5-C5-C6	-3.50	101.71	107.20
5	b	2	NAG	O5-C5-C6	-3.50	101.71	107.20
4	t	2	NAG	O5-C5-C6	-3.50	101.72	107.20
4	W	2	NAG	O5-C5-C6	-3.50	101.72	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	2	NAG	O5-C5-C6	-3.50	101.72	107.20
4	3	2	NAG	O5-C5-C6	-3.50	101.72	107.20
4	n	2	NAG	O5-C5-C6	-3.49	101.73	107.20
7	R	2	NAG	O5-C5-C6	-3.49	101.73	107.20
5	7	2	NAG	O5-C5-C6	-3.49	101.73	107.20
5	6	2	NAG	O5-C5-C6	-3.49	101.74	107.20
7	i	2	NAG	O5-C5-C6	-3.48	101.75	107.20
5	r	2	NAG	O5-C5-C6	-3.48	101.75	107.20
7	R	5	MAN	O5-C1-C2	-3.46	105.42	110.77
5	Z	2	NAG	O5-C5-C6	-3.44	101.80	107.20
7	i	5	MAN	O5-C1-C2	-3.42	105.50	110.77
8	z	7	MAN	C1-O5-C5	3.41	116.81	112.19
7	y	5	MAN	O5-C1-C2	-3.41	105.51	110.77
7	y	4	MAN	O5-C5-C6	3.38	112.51	107.20
8	S	7	MAN	C1-O5-C5	3.38	116.77	112.19
8	j	7	MAN	C1-O5-C5	3.37	116.76	112.19
7	R	4	MAN	O5-C5-C6	3.37	112.48	107.20
7	i	4	MAN	O5-C5-C6	3.35	112.46	107.20
4	n	3	BMA	O2-C2-C3	3.00	116.15	110.14
4	3	3	BMA	O2-C2-C3	2.99	116.13	110.14
4	a	3	BMA	O2-C2-C3	2.99	116.13	110.14
4	2	3	BMA	O2-C2-C3	2.99	116.12	110.14
8	S	4	MAN	C1-O5-C5	2.98	116.24	112.19
8	z	4	MAN	C1-O5-C5	2.98	116.23	112.19
8	j	4	MAN	C1-O5-C5	2.97	116.22	112.19
4	t	3	BMA	O2-C2-C3	2.97	116.08	110.14
4	V	3	BMA	O2-C2-C3	2.97	116.08	110.14
4	q	3	BMA	O2-C2-C3	2.97	116.08	110.14
4	J	3	BMA	O2-C2-C3	2.96	116.06	110.14
4	L	3	BMA	O2-C2-C3	2.95	116.06	110.14
4	W	3	BMA	O2-C2-C3	2.95	116.05	110.14
4	m	3	BMA	O2-C2-C3	2.94	116.03	110.14
4	M	3	BMA	O2-C2-C3	2.94	116.03	110.14
4	x	3	BMA	O2-C2-C3	2.94	116.03	110.14
4	h	3	BMA	O2-C2-C3	2.94	116.02	110.14
4	Q	3	BMA	O2-C2-C3	2.93	116.02	110.14
7	y	3	BMA	O2-C2-C3	2.93	116.02	110.14
4	s	3	BMA	O2-C2-C3	2.93	116.00	110.14
4	d	3	BMA	O2-C2-C3	2.92	115.99	110.14
4	c	3	BMA	O2-C2-C3	2.92	115.98	110.14
7	R	3	BMA	O2-C2-C3	2.92	115.98	110.14
7	i	3	BMA	O2-C2-C3	2.92	115.98	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	w	6	MAN	O5-C5-C6	2.84	111.65	107.20
6	P	6	MAN	O5-C5-C6	2.83	111.64	107.20
4	V	1	NAG	O7-C7-C8	-2.83	116.80	122.06
6	g	6	MAN	O5-C5-C6	2.81	111.61	107.20
5	6	1	NAG	O7-C7-C8	-2.81	116.84	122.06
4	t	1	NAG	O7-C7-C8	-2.81	116.84	122.06
5	Z	1	NAG	O7-C7-C8	-2.81	116.84	122.06
5	5	1	NAG	O7-C7-C8	-2.80	116.85	122.06
5	X	1	NAG	O7-C7-C8	-2.80	116.86	122.06
5	N	1	NAG	O7-C7-C8	-2.79	116.87	122.06
4	d	1	NAG	O7-C7-C8	-2.79	116.87	122.06
4	2	1	NAG	O7-C7-C8	-2.79	116.87	122.06
4	c	1	NAG	O7-C7-C8	-2.79	116.88	122.06
4	M	1	NAG	O7-C7-C8	-2.78	116.89	122.06
4	a	1	NAG	O7-C7-C8	-2.78	116.90	122.06
4	Q	1	NAG	O7-C7-C8	-2.78	116.90	122.06
7	R	1	NAG	O7-C7-C8	-2.78	116.90	122.06
4	x	1	NAG	O7-C7-C8	-2.77	116.90	122.06
4	s	1	NAG	O7-C7-C8	-2.77	116.90	122.06
7	i	1	NAG	O7-C7-C8	-2.77	116.91	122.06
4	L	1	NAG	O7-C7-C8	-2.77	116.91	122.06
5	Y	1	NAG	O7-C7-C8	-2.77	116.91	122.06
8	j	3	BMA	O3-C3-C2	2.77	115.30	109.99
4	q	1	NAG	O7-C7-C8	-2.77	116.92	122.06
5	e	1	NAG	O7-C7-C8	-2.77	116.92	122.06
5	K	1	NAG	O7-C7-C8	-2.77	116.92	122.06
5	f	1	NAG	O7-C7-C8	-2.77	116.92	122.06
5	u	1	NAG	O7-C7-C8	-2.77	116.92	122.06
8	S	3	BMA	O3-C3-C2	2.76	115.29	109.99
4	h	1	NAG	O7-C7-C8	-2.76	116.92	122.06
5	4	1	NAG	O7-C7-C8	-2.76	116.93	122.06
9	0	2	NAG	O5-C1-C2	-2.76	106.93	111.29
5	7	1	NAG	O7-C7-C8	-2.76	116.94	122.06
5	U	1	NAG	O7-C7-C8	-2.76	116.94	122.06
4	m	1	NAG	O7-C7-C8	-2.75	116.94	122.06
8	z	3	BMA	O3-C3-C2	2.75	115.26	109.99
5	o	1	NAG	O7-C7-C8	-2.75	116.95	122.06
4	W	1	NAG	O7-C7-C8	-2.75	116.95	122.06
9	k	2	NAG	O5-C1-C2	-2.75	106.95	111.29
4	n	1	NAG	O7-C7-C8	-2.75	116.95	122.06
5	f	1	NAG	C4-C3-C2	-2.75	106.99	111.02
5	v	1	NAG	O7-C7-C8	-2.75	116.95	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	y	1	NAG	O7-C7-C8	-2.75	116.95	122.06
4	J	1	NAG	O7-C7-C8	-2.74	116.96	122.06
9	T	2	NAG	O5-C1-C2	-2.74	106.95	111.29
5	v	1	NAG	C4-C3-C2	-2.74	107.00	111.02
5	O	1	NAG	O7-C7-C8	-2.74	116.97	122.06
5	l	1	NAG	O7-C7-C8	-2.74	116.97	122.06
4	3	1	NAG	O7-C7-C8	-2.73	116.99	122.06
5	r	1	NAG	O7-C7-C8	-2.72	117.01	122.06
5	l	1	NAG	C4-C3-C2	-2.72	107.03	111.02
5	l	1	NAG	O7-C7-C8	-2.71	117.02	122.06
5	e	1	NAG	C4-C3-C2	-2.71	107.04	111.02
5	p	1	NAG	O7-C7-C8	-2.71	117.02	122.06
5	p	1	NAG	C4-C3-C2	-2.71	107.05	111.02
5	N	1	NAG	C4-C3-C2	-2.71	107.05	111.02
5	Z	1	NAG	C4-C3-C2	-2.70	107.06	111.02
5	b	1	NAG	O7-C7-C8	-2.70	117.05	122.06
5	5	1	NAG	C4-C3-C2	-2.70	107.06	111.02
4	s	1	NAG	C4-C3-C2	-2.70	107.07	111.02
4	c	1	NAG	C4-C3-C2	-2.69	107.07	111.02
4	Q	1	NAG	C4-C3-C2	-2.69	107.08	111.02
5	O	1	NAG	C4-C3-C2	-2.69	107.08	111.02
5	U	1	NAG	C4-C3-C2	-2.69	107.08	111.02
4	h	1	NAG	C4-C3-C2	-2.68	107.09	111.02
4	L	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	l	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	r	1	NAG	C4-C3-C2	-2.67	107.10	111.02
4	2	1	NAG	C4-C3-C2	-2.67	107.11	111.02
5	Y	1	NAG	C4-C3-C2	-2.67	107.11	111.02
5	b	1	NAG	C4-C3-C2	-2.67	107.11	111.02
4	t	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	u	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	K	1	NAG	C4-C3-C2	-2.66	107.11	111.02
4	V	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	6	1	NAG	C4-C3-C2	-2.66	107.12	111.02
4	x	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	7	1	NAG	C4-C3-C2	-2.66	107.12	111.02
7	i	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	o	1	NAG	C4-C3-C2	-2.65	107.13	111.02
4	m	1	NAG	C4-C3-C2	-2.65	107.13	111.02
4	h	3	BMA	O4-C4-C5	-2.65	102.72	109.30
4	2	3	BMA	O4-C4-C5	-2.65	102.72	109.30
4	d	3	BMA	O4-C4-C5	-2.64	102.74	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	x	3	BMA	O4-C4-C5	-2.64	102.74	109.30
4	c	3	BMA	O4-C4-C5	-2.64	102.74	109.30
4	Q	3	BMA	O4-C4-C5	-2.64	102.74	109.30
4	n	1	NAG	C4-C3-C2	-2.64	107.15	111.02
4	q	1	NAG	C4-C3-C2	-2.64	107.15	111.02
4	J	1	NAG	C4-C3-C2	-2.64	107.15	111.02
4	V	3	BMA	O4-C4-C5	-2.64	102.75	109.30
4	W	3	BMA	O4-C4-C5	-2.64	102.75	109.30
5	X	1	NAG	C4-C3-C2	-2.64	107.16	111.02
7	y	1	NAG	C4-C3-C2	-2.64	107.16	111.02
9	0	1	NAG	C1-O5-C5	2.63	115.76	112.19
4	d	1	NAG	C4-C3-C2	-2.63	107.16	111.02
4	a	3	BMA	O4-C4-C5	-2.63	102.76	109.30
4	W	1	NAG	C4-C3-C2	-2.63	107.16	111.02
9	k	1	NAG	C1-O5-C5	2.63	115.76	112.19
4	q	3	BMA	O4-C4-C5	-2.63	102.77	109.30
5	4	1	NAG	C4-C3-C2	-2.62	107.17	111.02
4	M	1	NAG	C4-C3-C2	-2.62	107.18	111.02
7	y	3	BMA	O4-C4-C5	-2.62	102.79	109.30
7	R	1	NAG	C4-C3-C2	-2.62	107.18	111.02
4	3	3	BMA	O4-C4-C5	-2.62	102.80	109.30
7	R	3	BMA	O4-C4-C5	-2.62	102.80	109.30
4	J	3	BMA	O4-C4-C5	-2.61	102.80	109.30
4	a	1	NAG	C4-C3-C2	-2.61	107.19	111.02
4	M	3	BMA	O4-C4-C5	-2.61	102.81	109.30
7	i	3	BMA	O4-C4-C5	-2.61	102.81	109.30
4	L	3	BMA	O4-C4-C5	-2.61	102.81	109.30
4	n	3	BMA	O4-C4-C5	-2.61	102.83	109.30
7	y	4	MAN	O5-C1-C2	2.60	114.79	110.77
4	m	3	BMA	O4-C4-C5	-2.60	102.83	109.30
4	t	3	BMA	O4-C4-C5	-2.60	102.83	109.30
4	3	1	NAG	C4-C3-C2	-2.59	107.23	111.02
4	s	3	BMA	O4-C4-C5	-2.57	102.91	109.30
9	T	1	NAG	C1-O5-C5	2.57	115.67	112.19
8	j	2	NAG	C1-O5-C5	2.56	115.65	112.19
8	S	2	NAG	C1-O5-C5	2.55	115.65	112.19
8	z	2	NAG	C1-O5-C5	2.55	115.65	112.19
7	i	4	MAN	O5-C1-C2	2.54	114.69	110.77
7	R	4	MAN	O5-C1-C2	2.51	114.65	110.77
8	z	2	NAG	O5-C1-C2	-2.49	107.36	111.29
8	j	5	MAN	C1-C2-C3	2.49	112.72	109.67
9	T	5	MAN	O2-C2-C3	-2.49	105.16	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	5	MAN	O2-C2-C3	-2.48	105.17	110.14
9	0	5	MAN	O2-C2-C3	-2.48	105.18	110.14
8	S	5	MAN	C1-C2-C3	2.46	112.69	109.67
8	z	5	MAN	C1-C2-C3	2.46	112.69	109.67
8	S	2	NAG	O5-C1-C2	-2.46	107.40	111.29
4	q	3	BMA	C6-C5-C4	-2.45	107.26	113.00
4	W	3	BMA	C6-C5-C4	-2.45	107.27	113.00
8	j	2	NAG	O5-C1-C2	-2.45	107.42	111.29
4	M	3	BMA	C6-C5-C4	-2.45	107.28	113.00
4	n	3	BMA	C6-C5-C4	-2.45	107.28	113.00
4	3	3	BMA	C6-C5-C4	-2.44	107.28	113.00
4	s	3	BMA	C6-C5-C4	-2.44	107.29	113.00
4	2	3	BMA	C6-C5-C4	-2.44	107.29	113.00
4	a	3	BMA	C6-C5-C4	-2.42	107.33	113.00
8	z	3	BMA	O3-C3-C4	2.42	115.95	110.35
4	Q	3	BMA	C6-C5-C4	-2.42	107.33	113.00
7	y	3	BMA	C6-C5-C4	-2.42	107.33	113.00
4	x	3	BMA	C6-C5-C4	-2.42	107.34	113.00
8	j	3	BMA	O3-C3-C4	2.42	115.94	110.35
4	L	3	BMA	C6-C5-C4	-2.42	107.34	113.00
8	S	3	BMA	O3-C3-C4	2.42	115.94	110.35
8	S	7	MAN	O5-C1-C2	-2.42	107.04	110.77
4	h	3	BMA	C6-C5-C4	-2.41	107.35	113.00
4	d	3	BMA	C6-C5-C4	-2.41	107.36	113.00
4	J	3	BMA	C6-C5-C4	-2.41	107.36	113.00
8	z	7	MAN	O5-C1-C2	-2.41	107.05	110.77
4	V	3	BMA	C6-C5-C4	-2.41	107.36	113.00
7	R	3	BMA	C6-C5-C4	-2.41	107.36	113.00
4	c	3	BMA	C6-C5-C4	-2.41	107.36	113.00
4	t	3	BMA	C6-C5-C4	-2.41	107.37	113.00
4	m	3	BMA	C6-C5-C4	-2.40	107.38	113.00
8	j	7	MAN	O5-C1-C2	-2.40	107.07	110.77
7	i	3	BMA	C6-C5-C4	-2.39	107.41	113.00
5	O	2	NAG	O5-C1-C2	-2.33	107.61	111.29
5	v	2	NAG	O5-C1-C2	-2.33	107.61	111.29
4	L	2	NAG	O5-C1-C2	-2.31	107.64	111.29
9	k	10	MAN	C1-O5-C5	2.30	115.30	112.19
5	l	2	NAG	O5-C1-C2	-2.30	107.66	111.29
4	a	2	NAG	O5-C1-C2	-2.29	107.67	111.29
5	f	2	NAG	O5-C1-C2	-2.29	107.67	111.29
5	X	2	NAG	O5-C1-C2	-2.29	107.68	111.29
4	W	2	NAG	O5-C1-C2	-2.28	107.68	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	2	NAG	O5-C1-C2	-2.28	107.68	111.29
9	T	10	MAN	C1-O5-C5	2.28	115.28	112.19
9	0	10	MAN	C1-O5-C5	2.28	115.28	112.19
5	b	2	NAG	C4-C3-C2	-2.28	107.68	111.02
4	2	2	NAG	O5-C1-C2	-2.28	107.69	111.29
7	R	2	NAG	O5-C1-C2	-2.28	107.69	111.29
4	s	2	NAG	O5-C1-C2	-2.28	107.69	111.29
7	i	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	4	2	NAG	O5-C1-C2	-2.27	107.70	111.29
4	c	2	NAG	O5-C1-C2	-2.27	107.70	111.29
4	n	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	Y	2	NAG	O5-C1-C2	-2.27	107.70	111.29
5	5	2	NAG	O5-C1-C2	-2.27	107.71	111.29
5	4	2	NAG	C4-C3-C2	-2.27	107.70	111.02
5	o	2	NAG	O5-C1-C2	-2.27	107.71	111.29
4	d	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	1	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	u	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	o	2	NAG	C4-C3-C2	-2.26	107.70	111.02
5	N	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	U	2	NAG	O5-C1-C2	-2.26	107.72	111.29
4	M	2	NAG	O5-C1-C2	-2.26	107.72	111.29
4	q	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	e	2	NAG	O5-C1-C2	-2.26	107.72	111.29
5	p	2	NAG	O5-C1-C2	-2.26	107.73	111.29
5	7	2	NAG	O5-C1-C2	-2.25	107.73	111.29
4	V	2	NAG	O5-C1-C2	-2.25	107.73	111.29
4	W	2	NAG	C4-C3-C2	-2.25	107.73	111.02
8	z	2	NAG	C4-C3-C2	-2.25	107.73	111.02
4	m	2	NAG	O5-C1-C2	-2.25	107.74	111.29
7	y	2	NAG	O5-C1-C2	-2.24	107.74	111.29
5	K	2	NAG	O5-C1-C2	-2.24	107.75	111.29
4	3	2	NAG	O5-C1-C2	-2.24	107.75	111.29
4	h	2	NAG	O5-C1-C2	-2.24	107.75	111.29
4	J	2	NAG	O5-C1-C2	-2.24	107.75	111.29
8	S	2	NAG	C4-C3-C2	-2.23	107.75	111.02
4	c	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	5	2	NAG	C4-C3-C2	-2.23	107.75	111.02
4	x	2	NAG	O5-C1-C2	-2.23	107.77	111.29
4	Q	2	NAG	O5-C1-C2	-2.23	107.77	111.29
4	s	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	X	2	NAG	C4-C3-C2	-2.23	107.75	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	2	NAG	O5-C1-C2	-2.22	107.78	111.29
5	6	2	NAG	O5-C1-C2	-2.22	107.78	111.29
4	t	2	NAG	O5-C1-C2	-2.22	107.78	111.29
5	Z	2	NAG	C4-C3-C2	-2.22	107.77	111.02
8	j	2	NAG	C4-C3-C2	-2.22	107.77	111.02
7	R	4	MAN	O3-C3-C4	2.22	115.47	110.35
4	J	2	NAG	C4-C3-C2	-2.21	107.78	111.02
7	R	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	m	2	NAG	C4-C3-C2	-2.21	107.78	111.02
7	y	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	3	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	q	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	r	2	NAG	O5-C1-C2	-2.21	107.80	111.29
4	Q	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	p	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	r	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	a	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	l	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	1	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	O	2	NAG	C4-C3-C2	-2.20	107.79	111.02
4	x	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	6	2	NAG	C4-C3-C2	-2.20	107.79	111.02
7	i	4	MAN	O3-C3-C4	2.19	115.42	110.35
5	U	2	NAG	C4-C3-C2	-2.19	107.80	111.02
9	0	5	MAN	C1-O5-C5	2.19	115.17	112.19
5	Y	2	NAG	C4-C3-C2	-2.19	107.80	111.02
4	n	2	NAG	C4-C3-C2	-2.19	107.81	111.02
9	k	5	MAN	C1-O5-C5	2.19	115.15	112.19
4	2	2	NAG	C4-C3-C2	-2.18	107.82	111.02
7	i	2	NAG	C4-C3-C2	-2.18	107.82	111.02
4	V	2	NAG	C4-C3-C2	-2.18	107.82	111.02
9	T	5	MAN	C1-O5-C5	2.18	115.15	112.19
5	7	2	NAG	C4-C3-C2	-2.18	107.82	111.02
5	K	2	NAG	C4-C3-C2	-2.18	107.82	111.02
5	u	2	NAG	C4-C3-C2	-2.18	107.83	111.02
4	L	2	NAG	C4-C3-C2	-2.18	107.83	111.02
7	y	4	MAN	O3-C3-C4	2.17	115.37	110.35
5	N	2	NAG	C4-C3-C2	-2.17	107.84	111.02
5	v	2	NAG	C4-C3-C2	-2.17	107.84	111.02
4	h	2	NAG	C4-C3-C2	-2.17	107.84	111.02
5	e	2	NAG	C4-C3-C2	-2.16	107.86	111.02
9	0	10	MAN	C1-C2-C3	2.14	112.30	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	2	NAG	C4-C3-C2	-2.14	107.88	111.02
9	k	10	MAN	C1-C2-C3	2.14	112.30	109.67
9	T	10	MAN	C1-C2-C3	2.14	112.30	109.67
8	S	6	MAN	C1-O5-C5	2.14	115.09	112.19
5	f	2	NAG	C4-C3-C2	-2.14	107.89	111.02
8	j	6	MAN	C1-O5-C5	2.14	115.08	112.19
4	M	2	NAG	C4-C3-C2	-2.11	107.92	111.02
8	z	6	MAN	C1-O5-C5	2.11	115.05	112.19
4	t	2	NAG	C4-C3-C2	-2.10	107.94	111.02
7	i	4	MAN	O4-C4-C3	-2.06	105.58	110.35
7	y	5	MAN	O5-C5-C6	-2.06	103.98	107.20
7	R	4	MAN	O4-C4-C3	-2.05	105.61	110.35
7	R	5	MAN	O5-C5-C6	-2.04	104.01	107.20
7	i	5	MAN	O5-C5-C6	-2.03	104.02	107.20
7	y	4	MAN	O4-C4-C3	-2.03	105.65	110.35
6	P	6	MAN	C1-O5-C5	-2.03	109.44	112.19
6	g	6	MAN	C1-O5-C5	-2.03	109.44	112.19

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	1	NAG	O7-C7-N2-C2
8	j	1	NAG	O7-C7-N2-C2
8	z	1	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	j	1	NAG	C8-C7-N2-C2
8	z	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
8	z	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	x	1	NAG	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
8	z	1	NAG	C4-C5-C6-O6
6	g	5	MAN	O5-C5-C6-O6
6	w	5	MAN	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
4	x	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	P	5	MAN	O5-C5-C6-O6
8	S	6	MAN	O5-C5-C6-O6
8	j	6	MAN	O5-C5-C6-O6
8	z	6	MAN	O5-C5-C6-O6
6	P	2	NAG	C8-C7-N2-C2
6	g	2	NAG	C8-C7-N2-C2
6	w	2	NAG	C8-C7-N2-C2
8	S	2	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
8	z	2	NAG	C1-C2-N2-C7
6	P	3	BMA	C4-C5-C6-O6
6	w	3	BMA	C4-C5-C6-O6
6	w	6	MAN	C4-C5-C6-O6
6	P	6	MAN	C4-C5-C6-O6
6	g	3	BMA	C4-C5-C6-O6
6	g	6	MAN	C4-C5-C6-O6
9	k	4	MAN	O5-C5-C6-O6
9	0	4	MAN	O5-C5-C6-O6
9	T	4	MAN	O5-C5-C6-O6
6	P	6	MAN	O5-C5-C6-O6
6	g	6	MAN	O5-C5-C6-O6
6	w	6	MAN	O5-C5-C6-O6
9	0	10	MAN	O5-C5-C6-O6
6	P	2	NAG	O7-C7-N2-C2
6	g	2	NAG	O7-C7-N2-C2
6	w	2	NAG	O7-C7-N2-C2
9	k	10	MAN	O5-C5-C6-O6
9	T	10	MAN	O5-C5-C6-O6
8	S	7	MAN	O5-C5-C6-O6
8	j	7	MAN	O5-C5-C6-O6
8	z	7	MAN	O5-C5-C6-O6
9	k	2	NAG	O5-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
9	0	2	NAG	O5-C5-C6-O6
6	w	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
4	s	3	BMA	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	L	3	BMA	C4-C5-C6-O6
4	M	3	BMA	C4-C5-C6-O6
4	Q	3	BMA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	V	3	BMA	C4-C5-C6-O6
4	m	3	BMA	C4-C5-C6-O6
4	q	3	BMA	C4-C5-C6-O6
4	t	3	BMA	C4-C5-C6-O6
4	x	3	BMA	C4-C5-C6-O6
4	2	3	BMA	C4-C5-C6-O6
7	R	3	BMA	C4-C5-C6-O6
7	i	3	BMA	C4-C5-C6-O6
7	y	3	BMA	C4-C5-C6-O6
4	W	3	BMA	C4-C5-C6-O6
4	a	3	BMA	C4-C5-C6-O6
4	n	3	BMA	C4-C5-C6-O6
4	c	3	BMA	C4-C5-C6-O6
4	d	3	BMA	C4-C5-C6-O6
4	3	3	BMA	C4-C5-C6-O6
4	h	3	BMA	C4-C5-C6-O6
8	z	4	MAN	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	5	1	NAG	C4-C5-C6-O6
8	S	4	MAN	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
8	j	4	MAN	C4-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
4	W	3	BMA	O5-C5-C6-O6
4	2	3	BMA	O5-C5-C6-O6
4	M	3	BMA	O5-C5-C6-O6
4	s	3	BMA	O5-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
4	m	3	BMA	O5-C5-C6-O6
4	q	3	BMA	O5-C5-C6-O6
4	x	3	BMA	O5-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
4	a	3	BMA	O5-C5-C6-O6
4	3	3	BMA	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
7	y	3	BMA	O5-C5-C6-O6
4	d	3	BMA	O5-C5-C6-O6
4	h	3	BMA	O5-C5-C6-O6
4	n	3	BMA	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	c	3	BMA	O5-C5-C6-O6
4	t	3	BMA	O5-C5-C6-O6

Continued on next page...

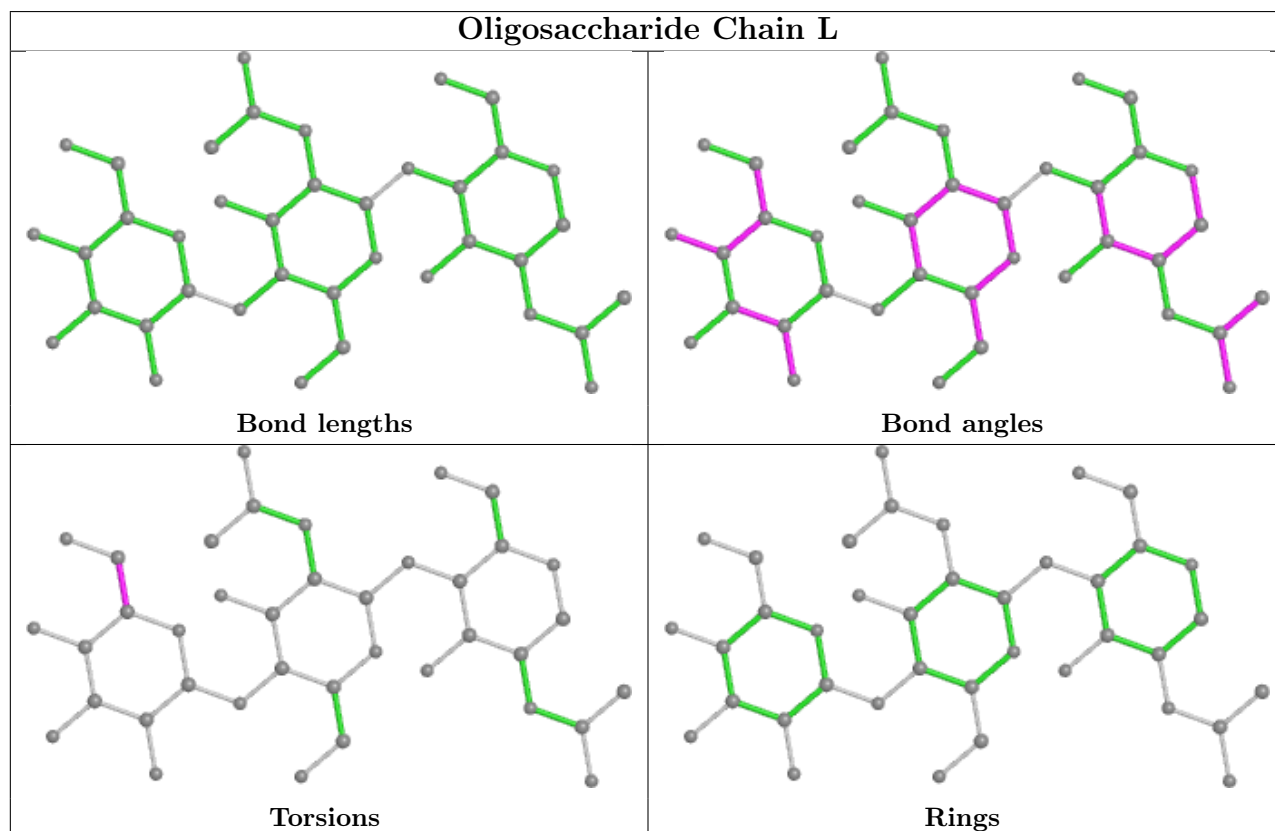
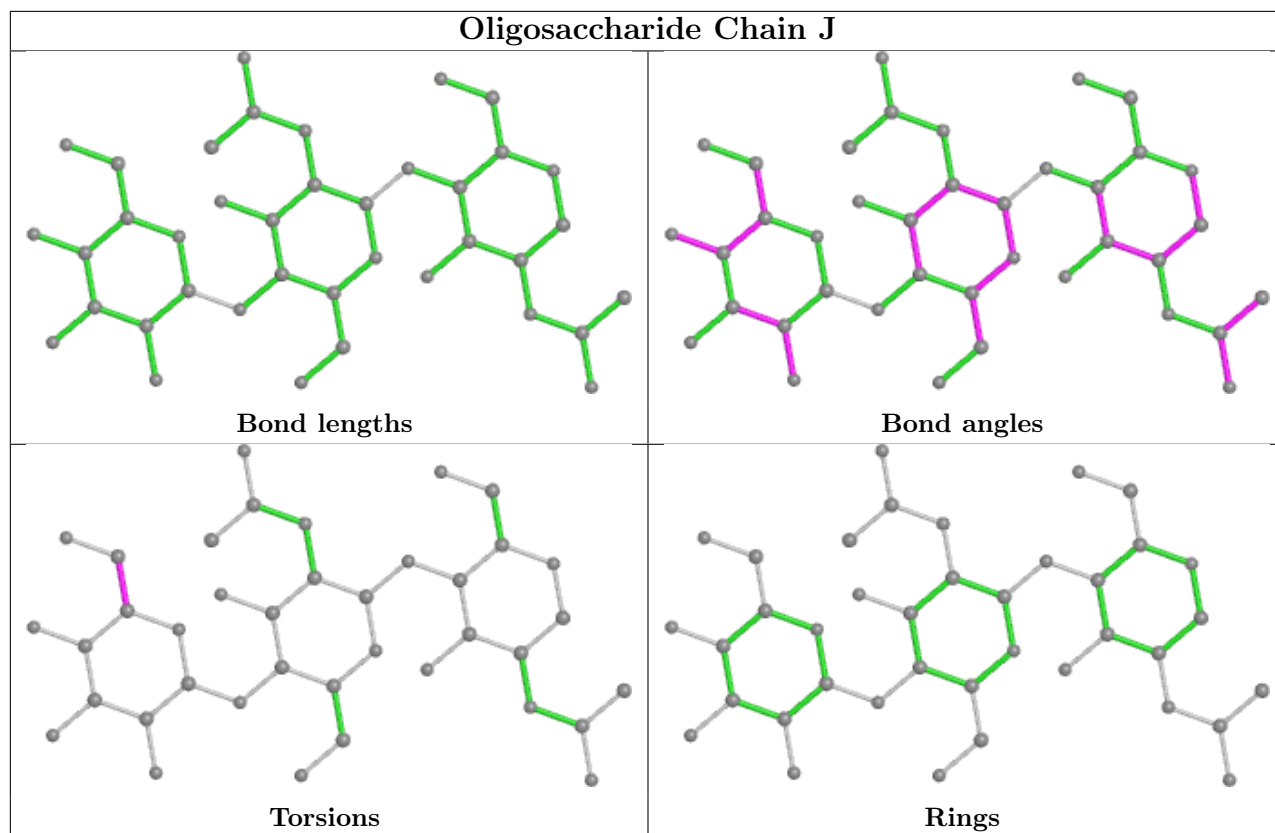
Continued from previous page...

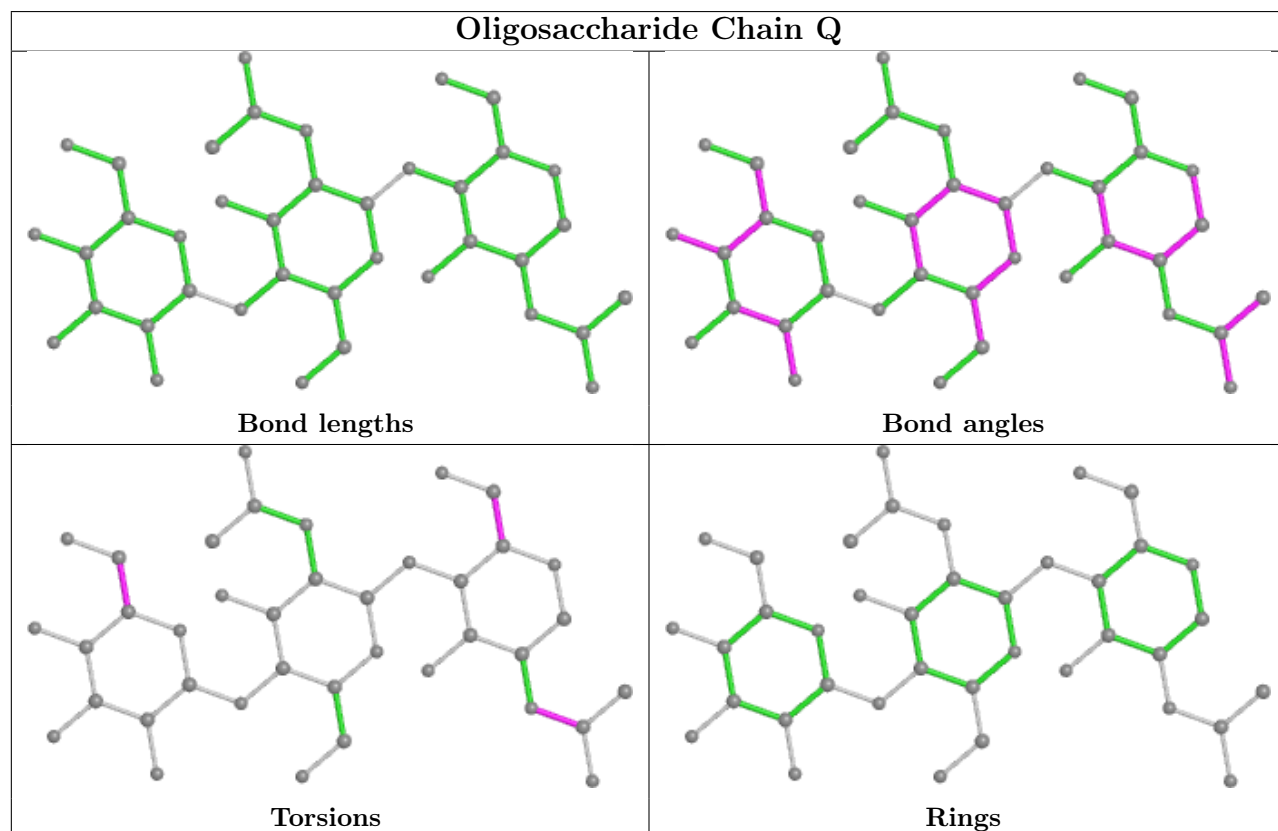
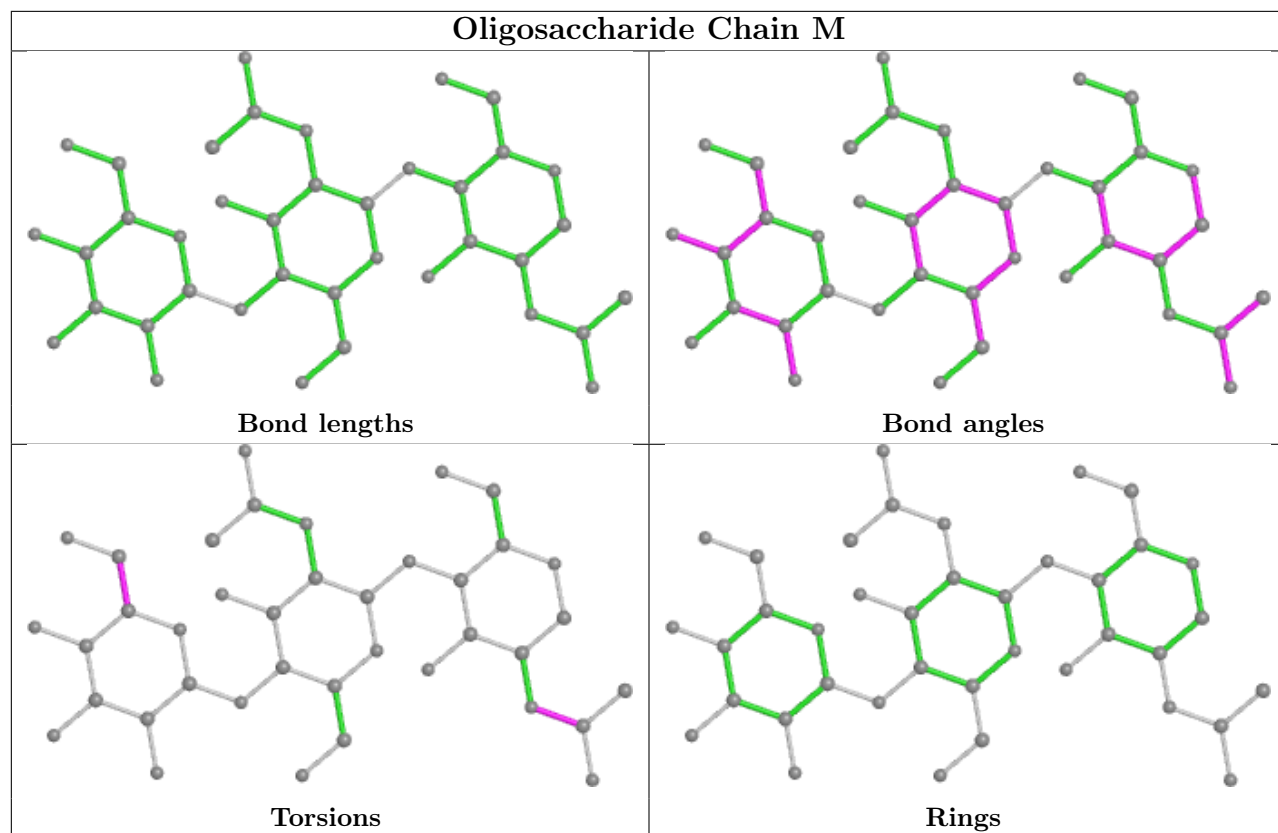
Mol	Chain	Res	Type	Atoms
7	i	3	BMA	O5-C5-C6-O6
8	S	1	NAG	C1-C2-N2-C7
8	j	1	NAG	C1-C2-N2-C7
8	z	1	NAG	C1-C2-N2-C7
6	P	5	MAN	C4-C5-C6-O6
6	w	5	MAN	C4-C5-C6-O6
6	g	5	MAN	C4-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
8	j	4	MAN	O5-C5-C6-O6
5	5	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
8	S	4	MAN	O5-C5-C6-O6
8	z	4	MAN	O5-C5-C6-O6
8	z	6	MAN	C4-C5-C6-O6
8	S	6	MAN	C4-C5-C6-O6
8	j	6	MAN	C4-C5-C6-O6
8	S	1	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
8	z	1	NAG	C3-C2-N2-C7
9	T	9	MAN	C4-C5-C6-O6
9	k	9	MAN	C4-C5-C6-O6
9	0	9	MAN	C4-C5-C6-O6
4	M	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	c	1	NAG	O7-C7-N2-C2
4	h	1	NAG	O7-C7-N2-C2
4	s	1	NAG	O7-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	l	1	NAG	O7-C7-N2-C2
5	5	1	NAG	O7-C7-N2-C2
5	6	1	NAG	O7-C7-N2-C2

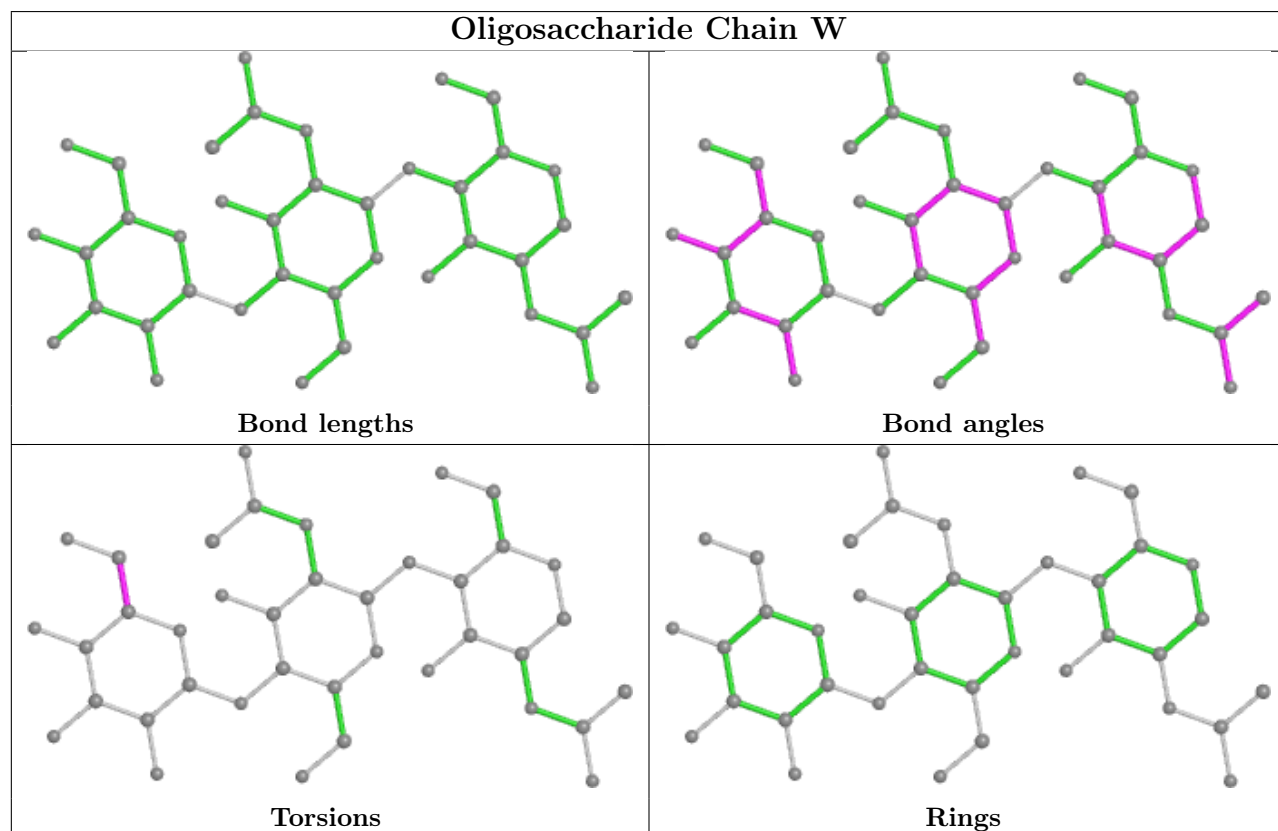
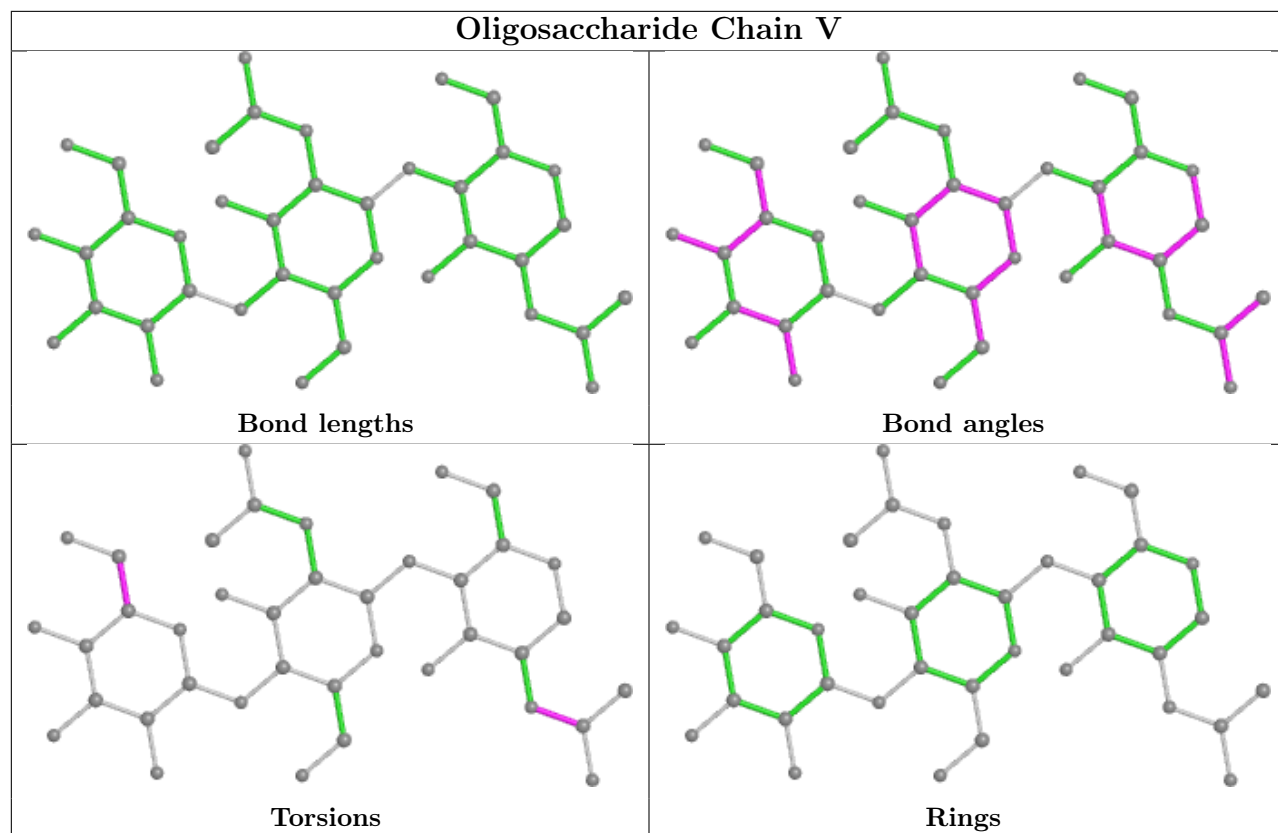
There are no ring outliers.

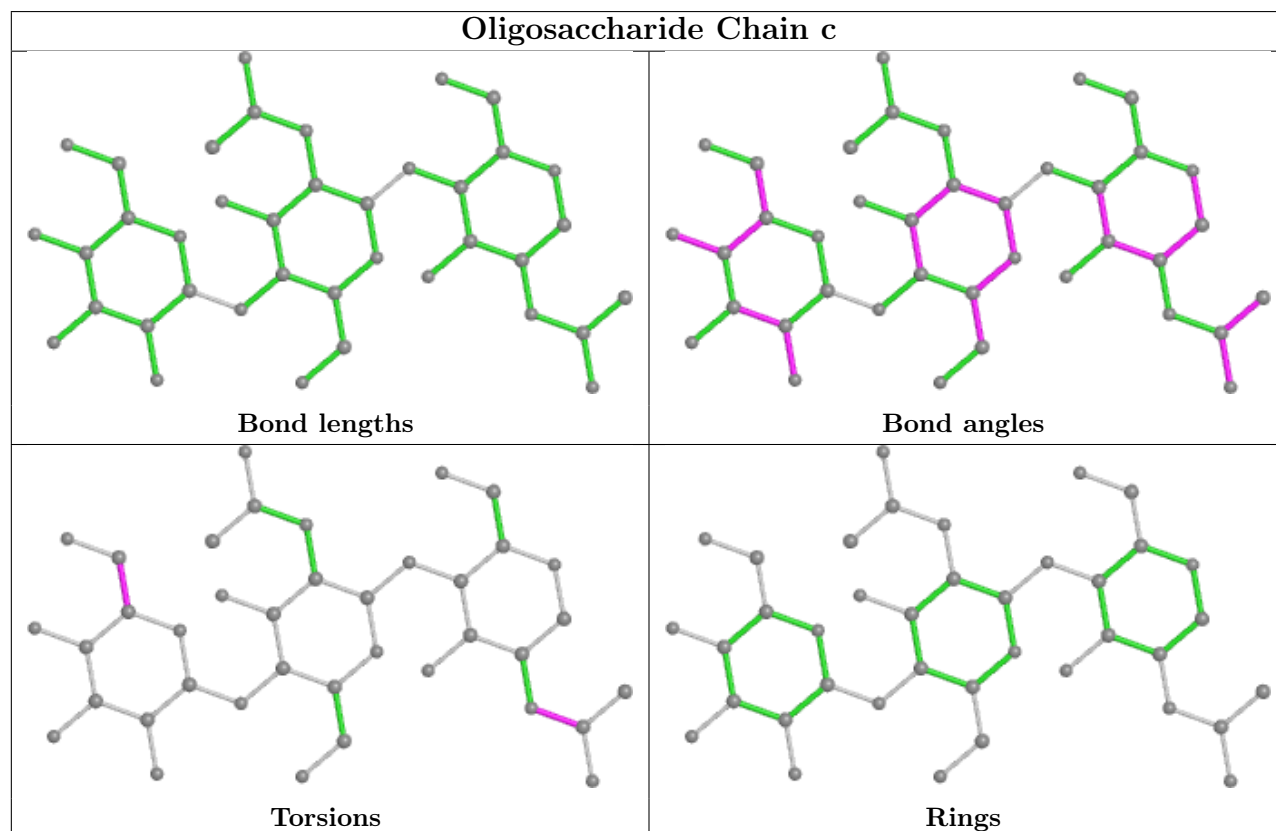
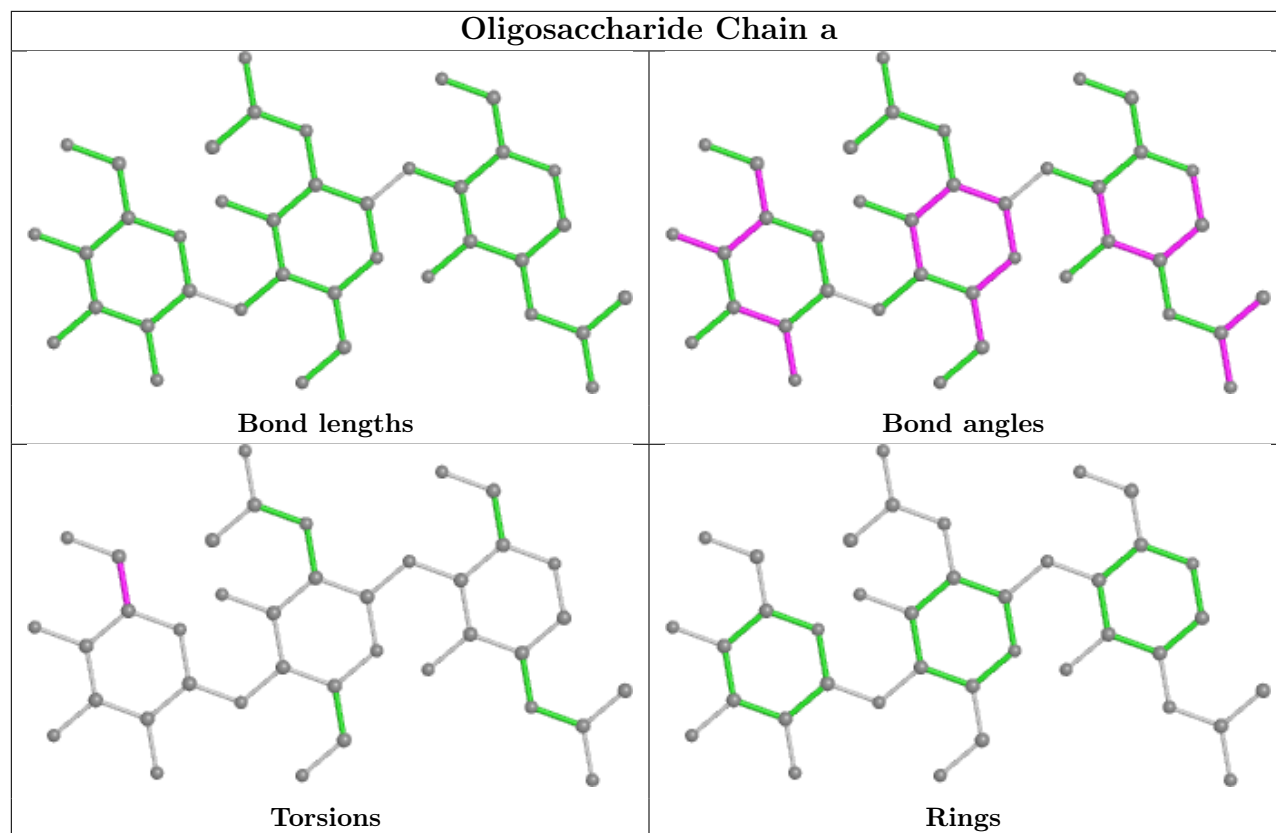
No monomer is involved in short contacts.

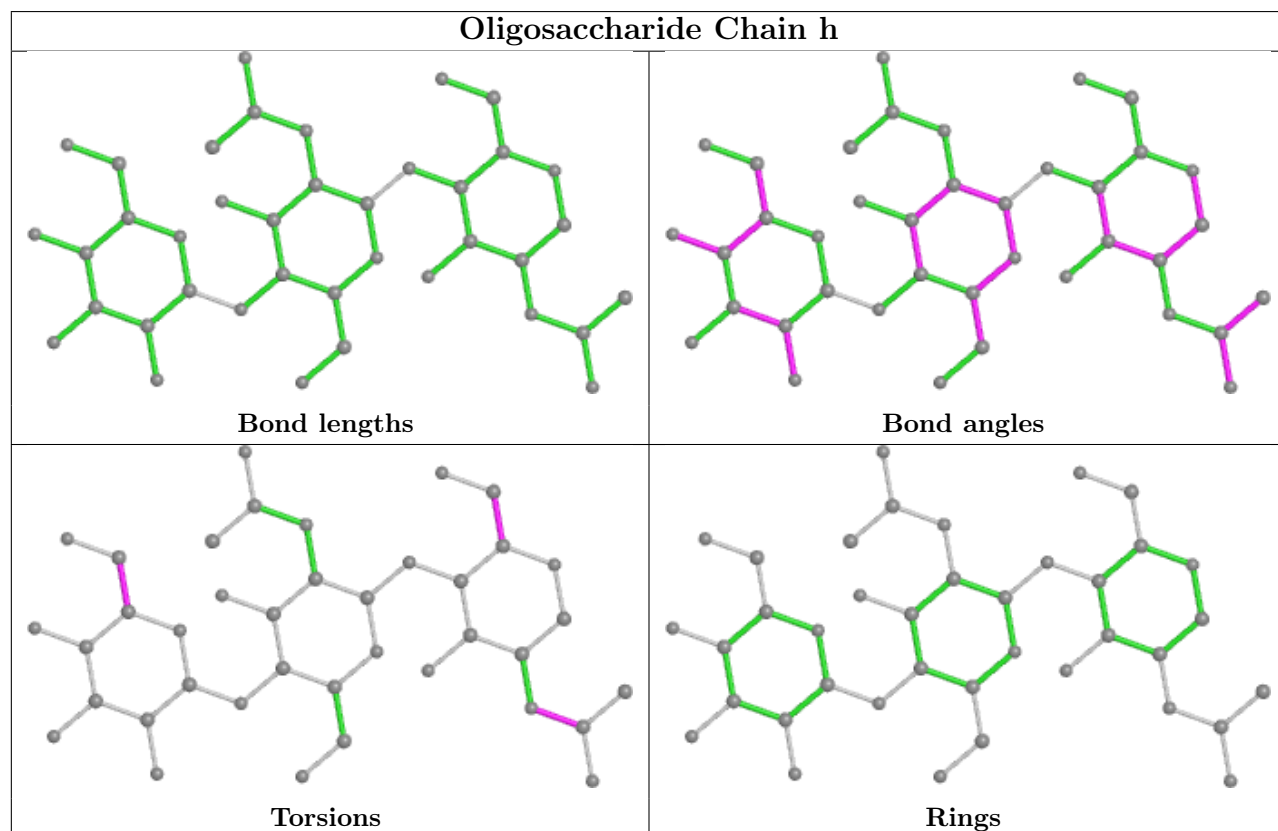
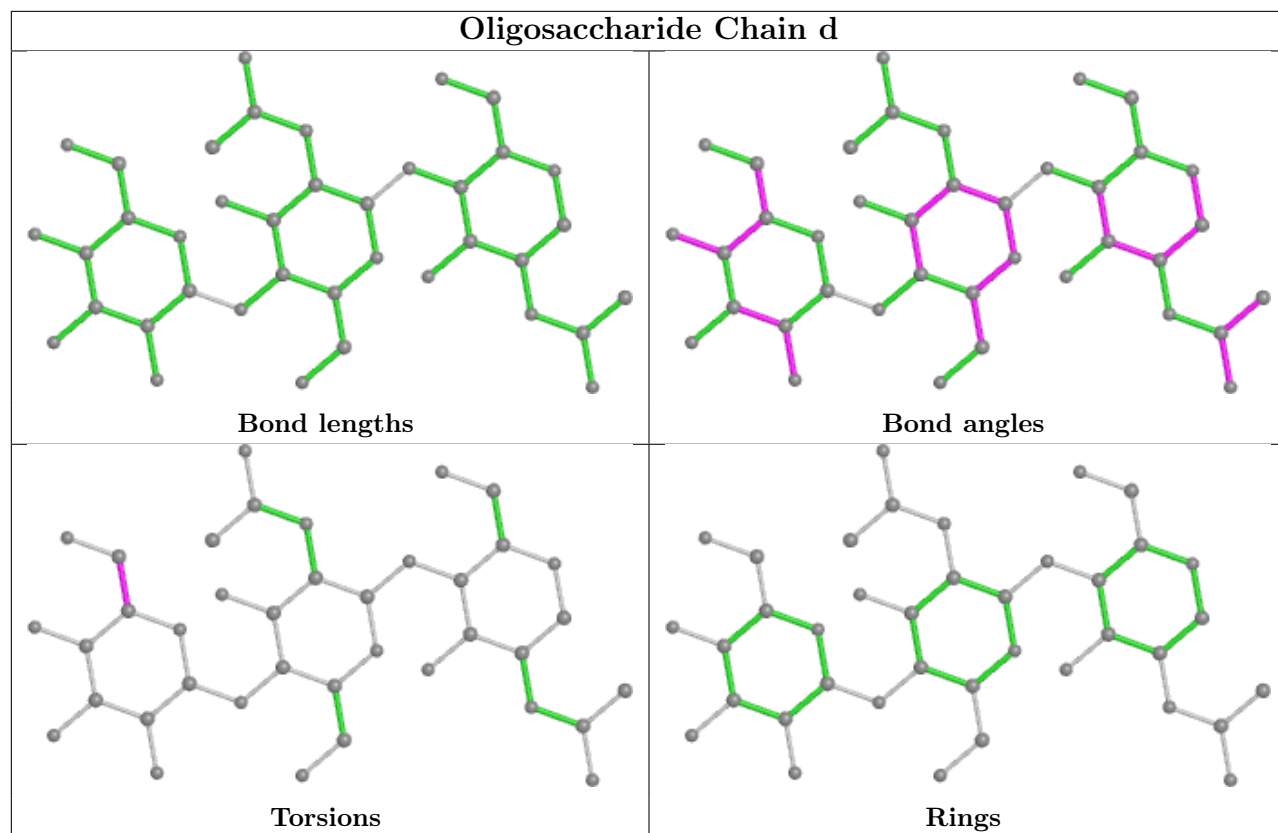
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

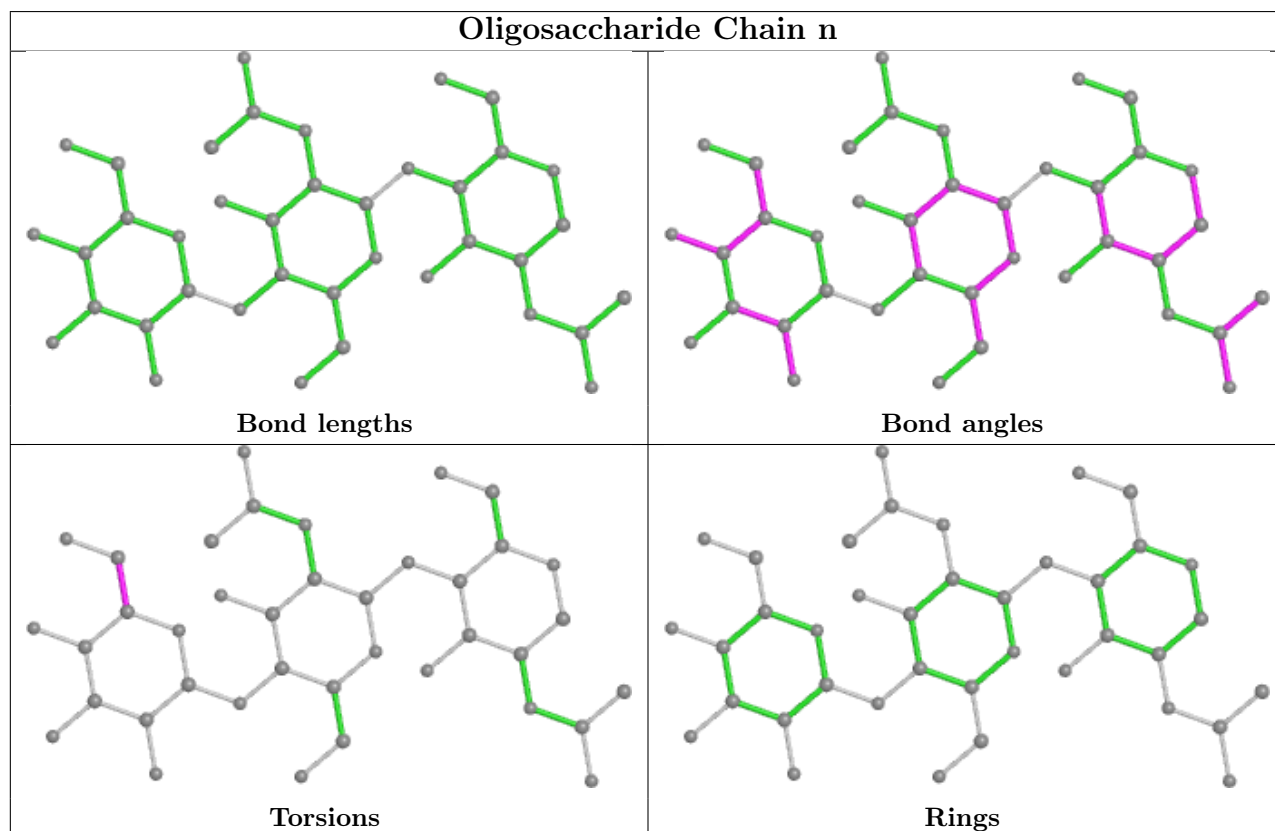
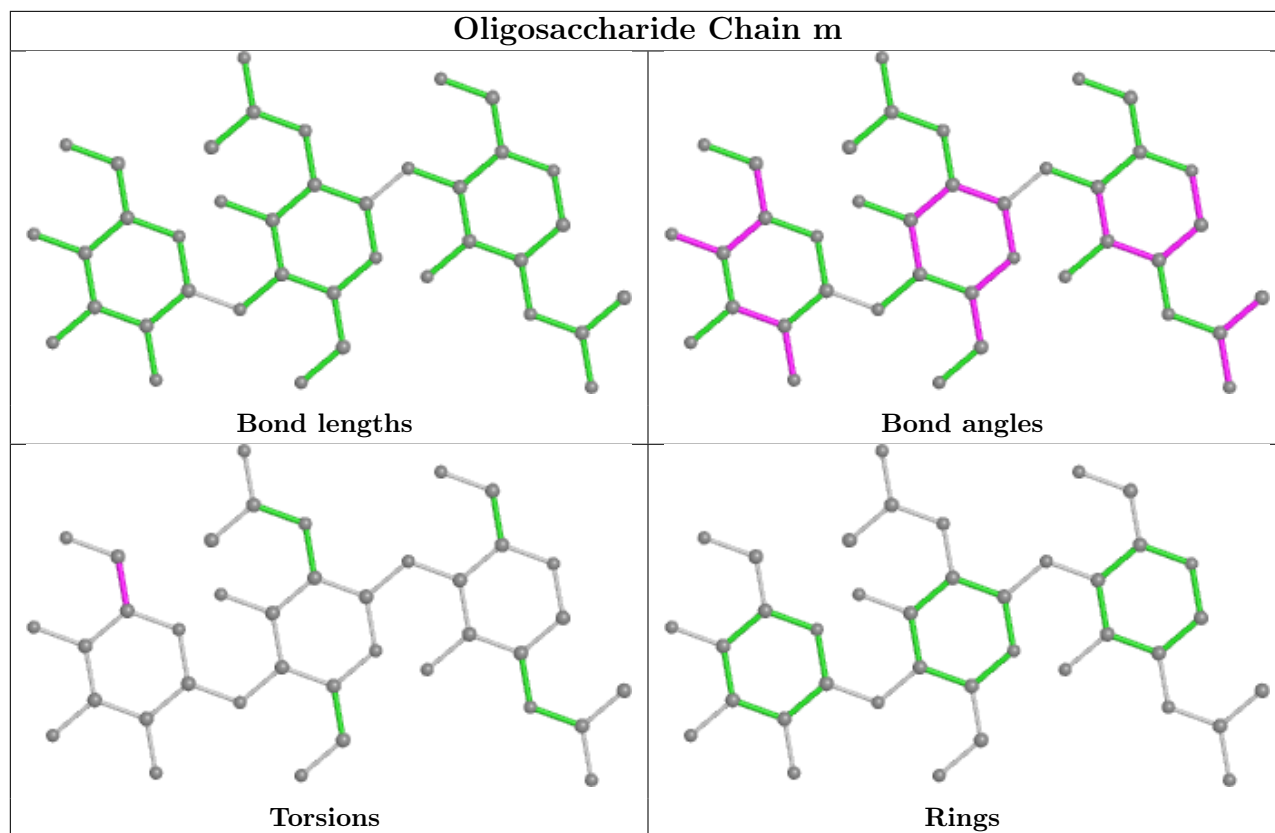


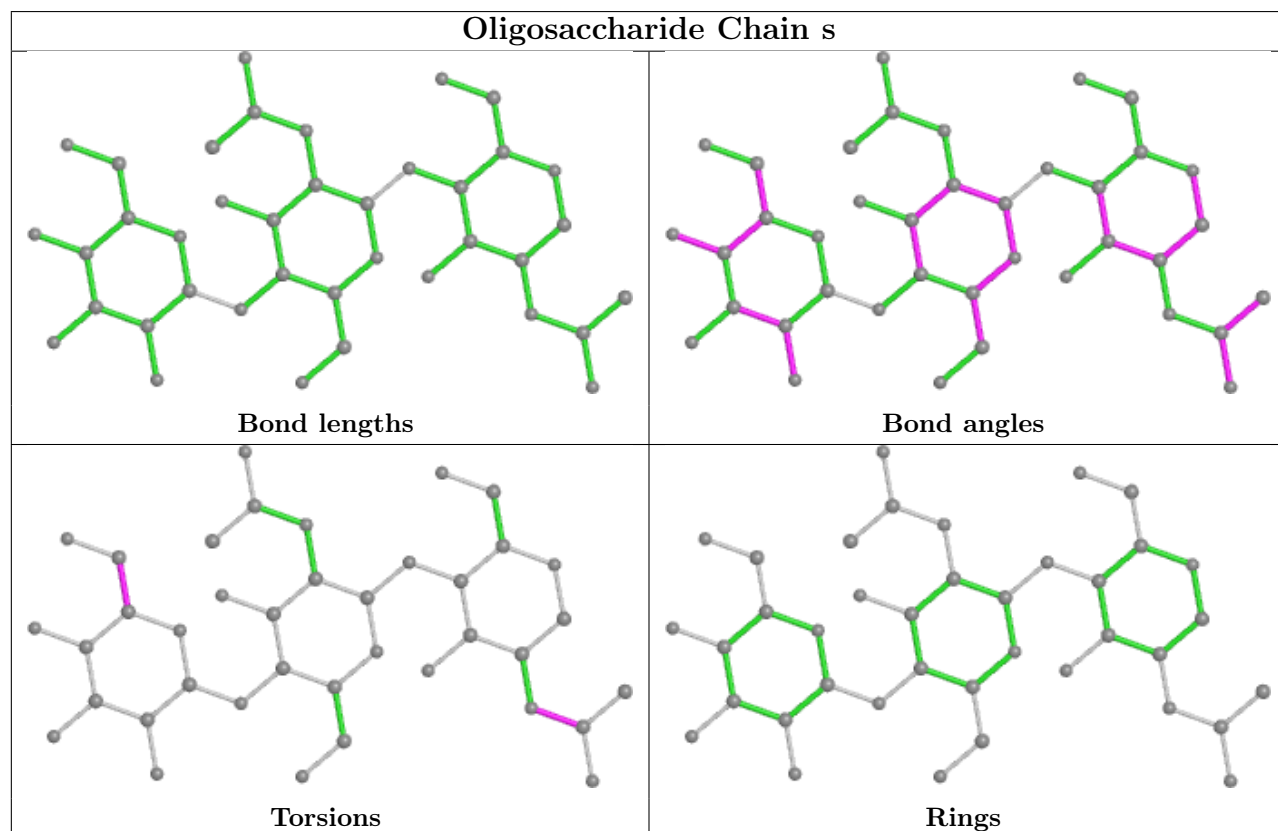
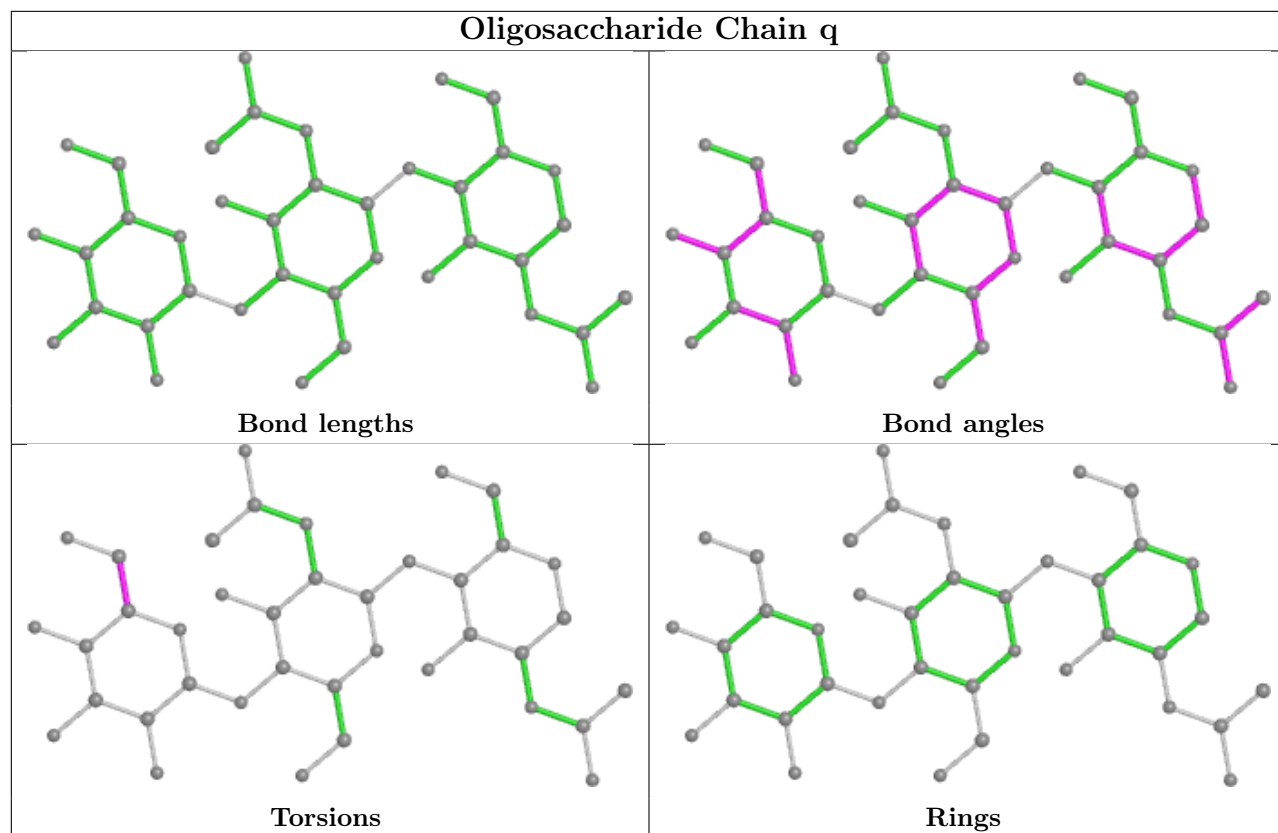


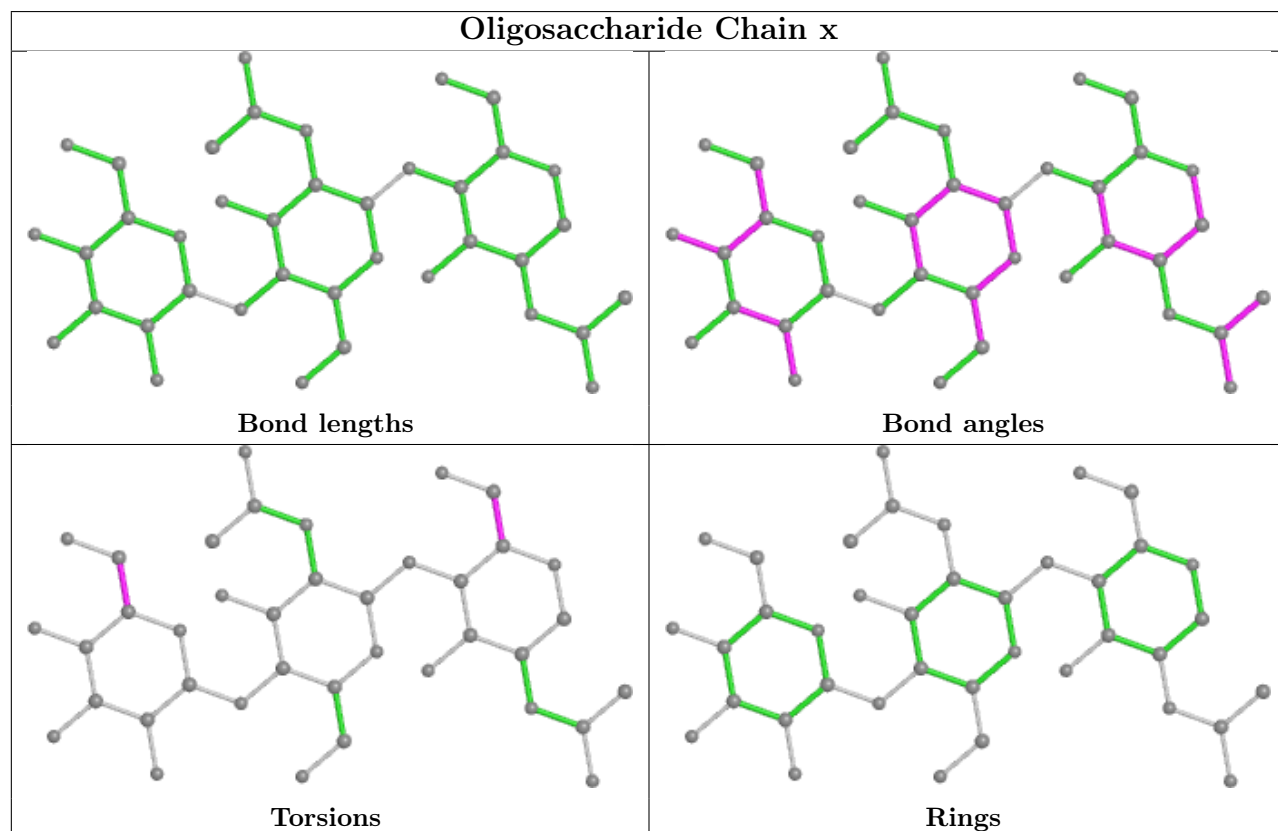
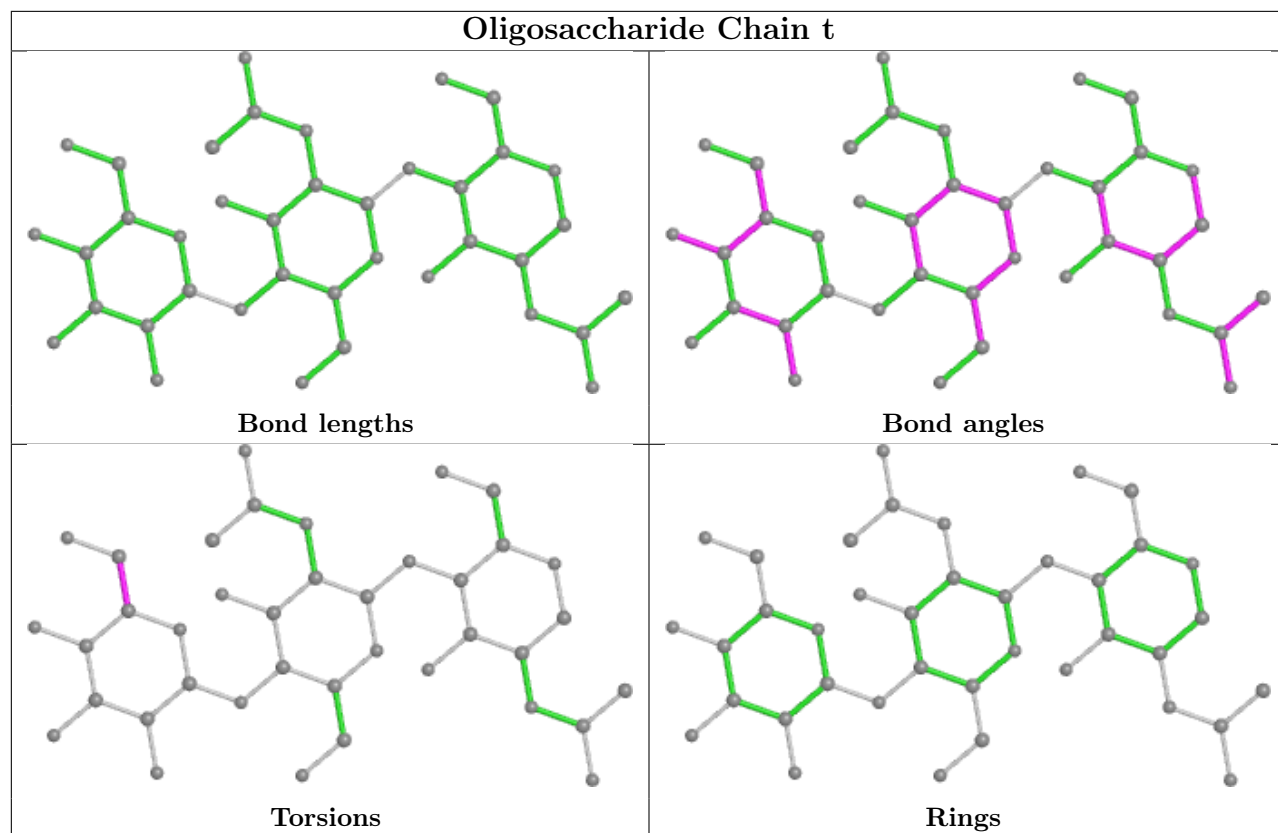


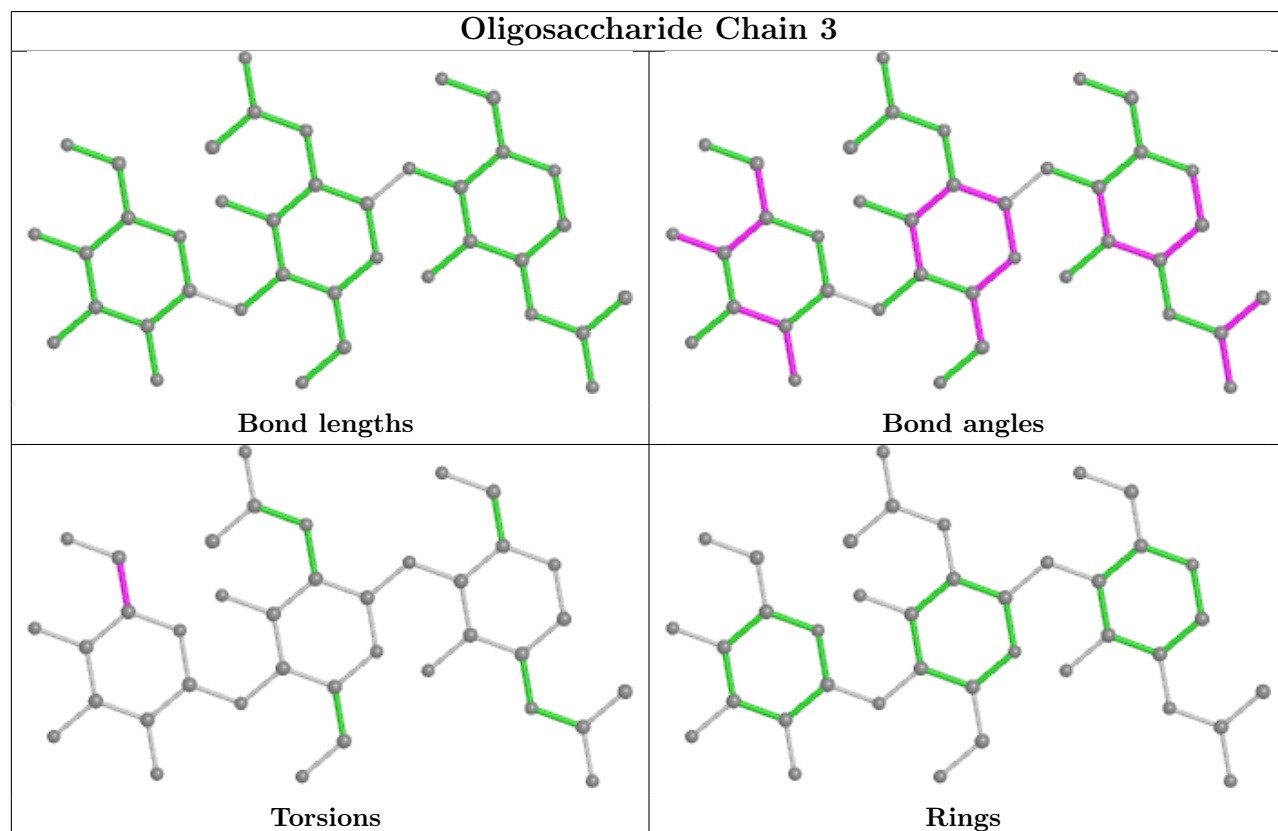
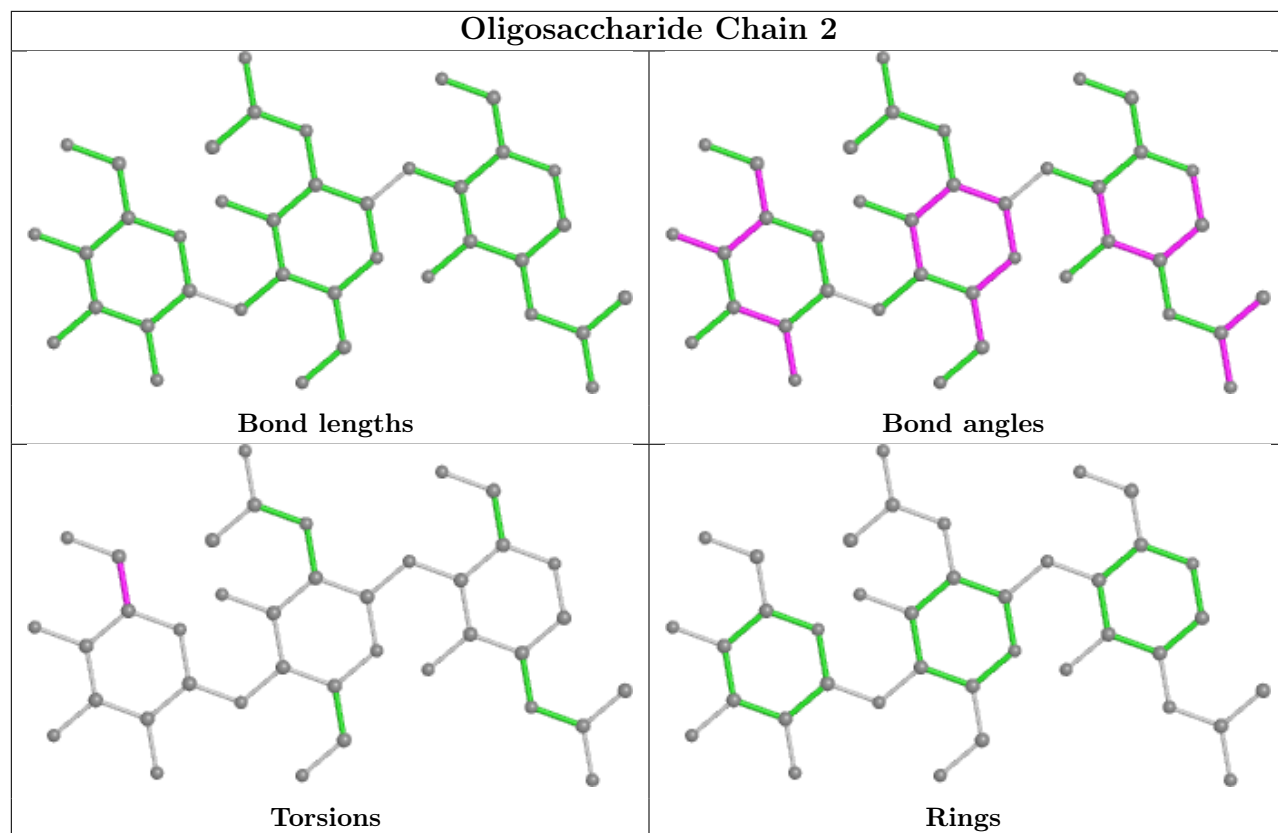


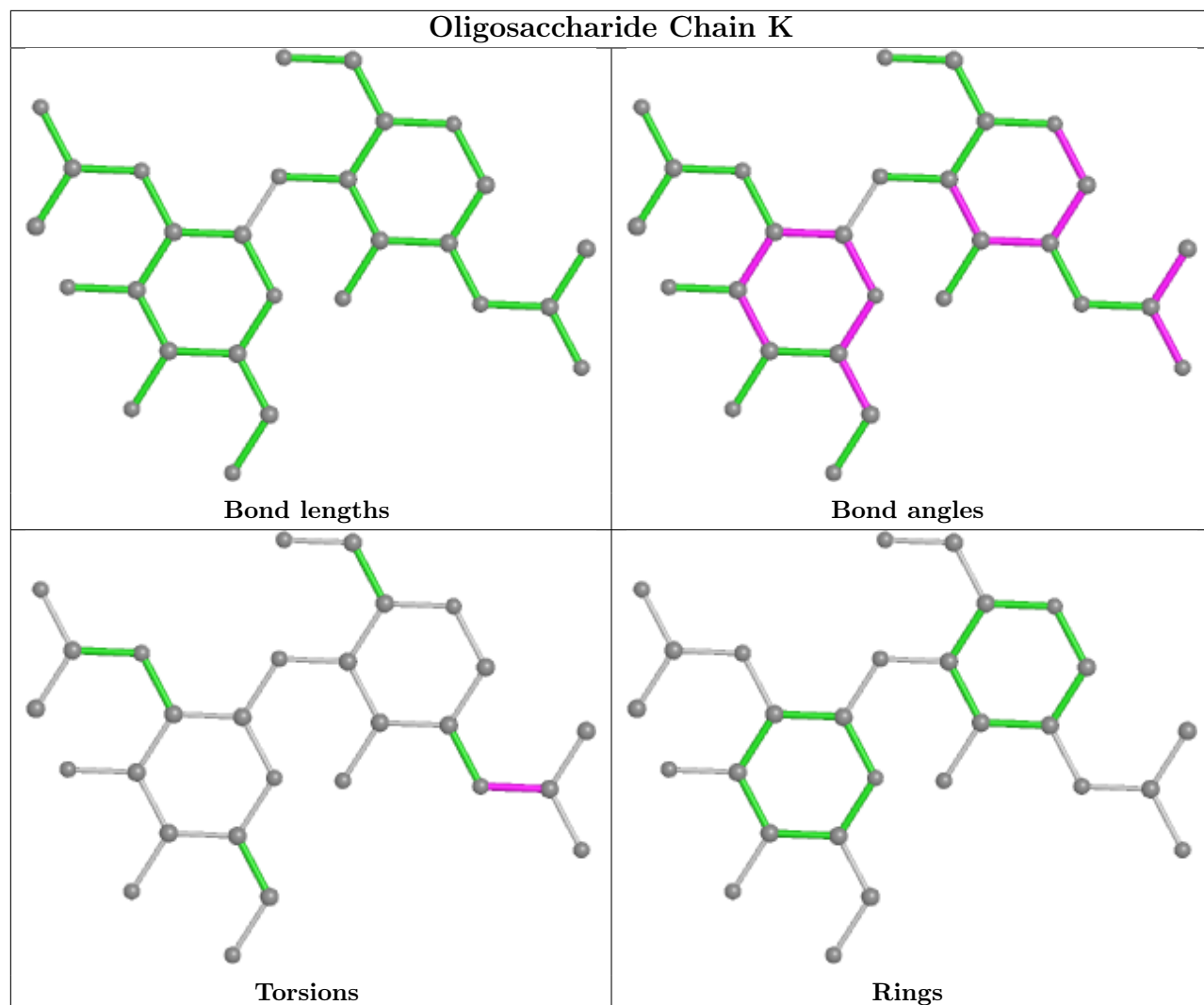


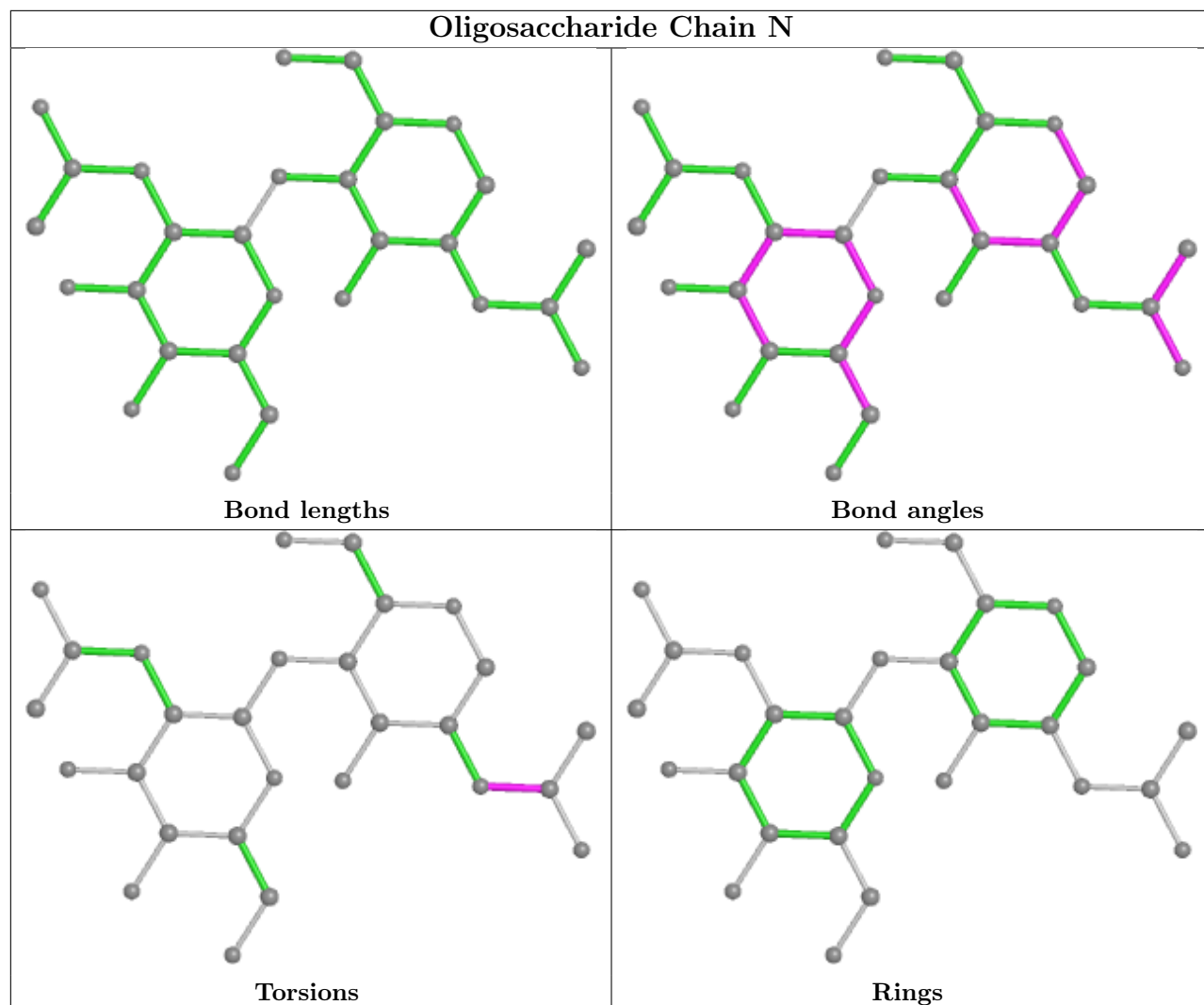


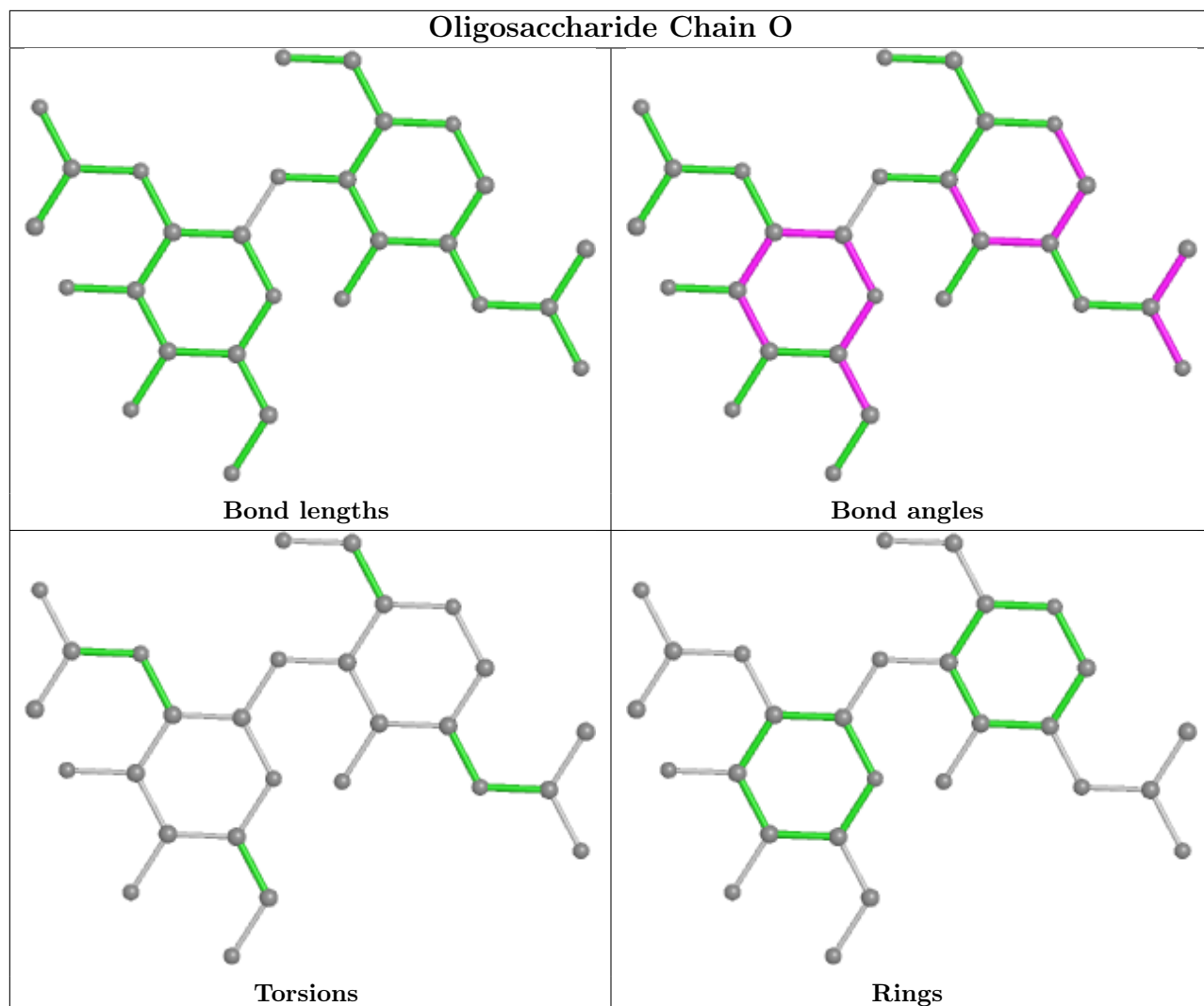


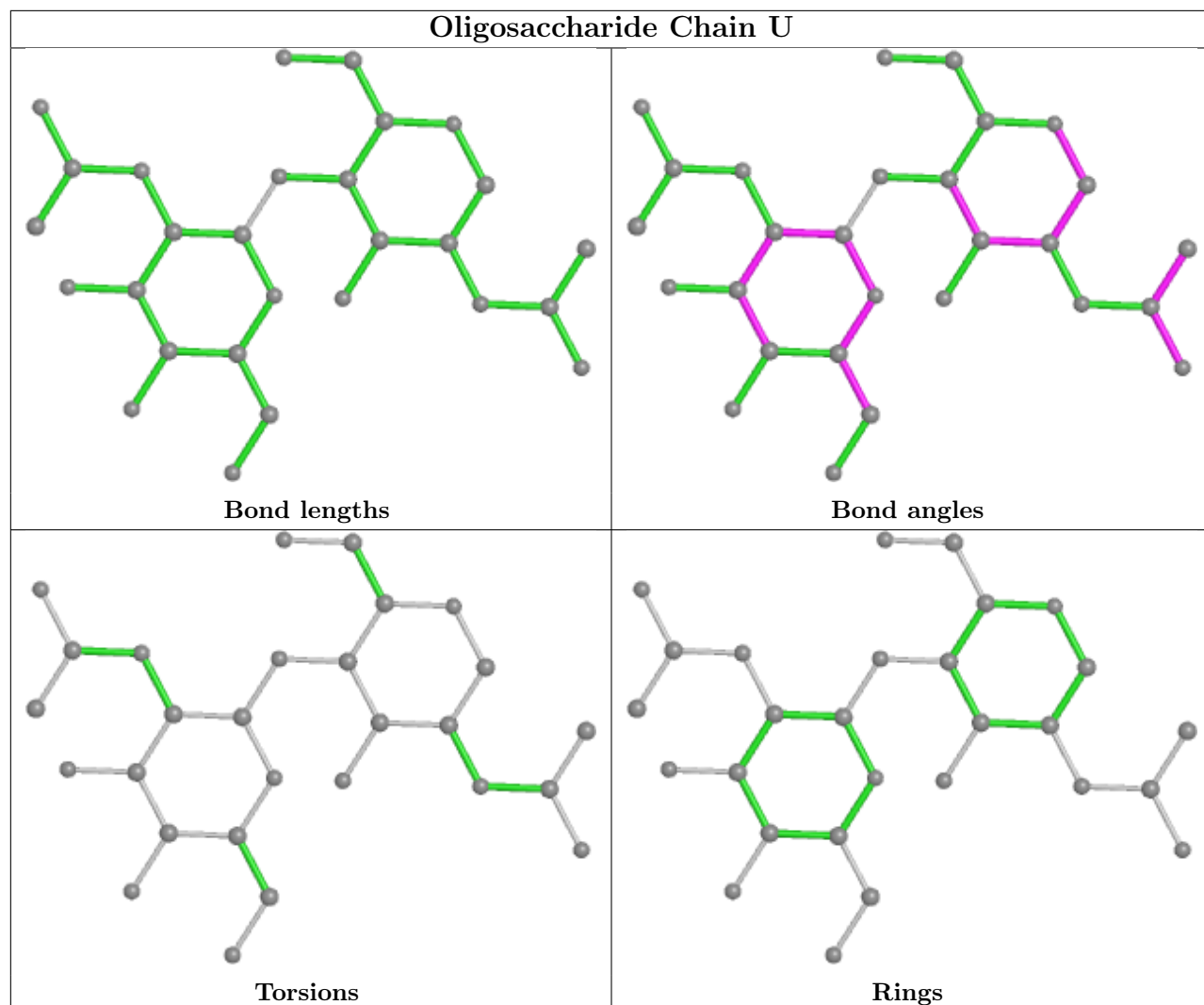


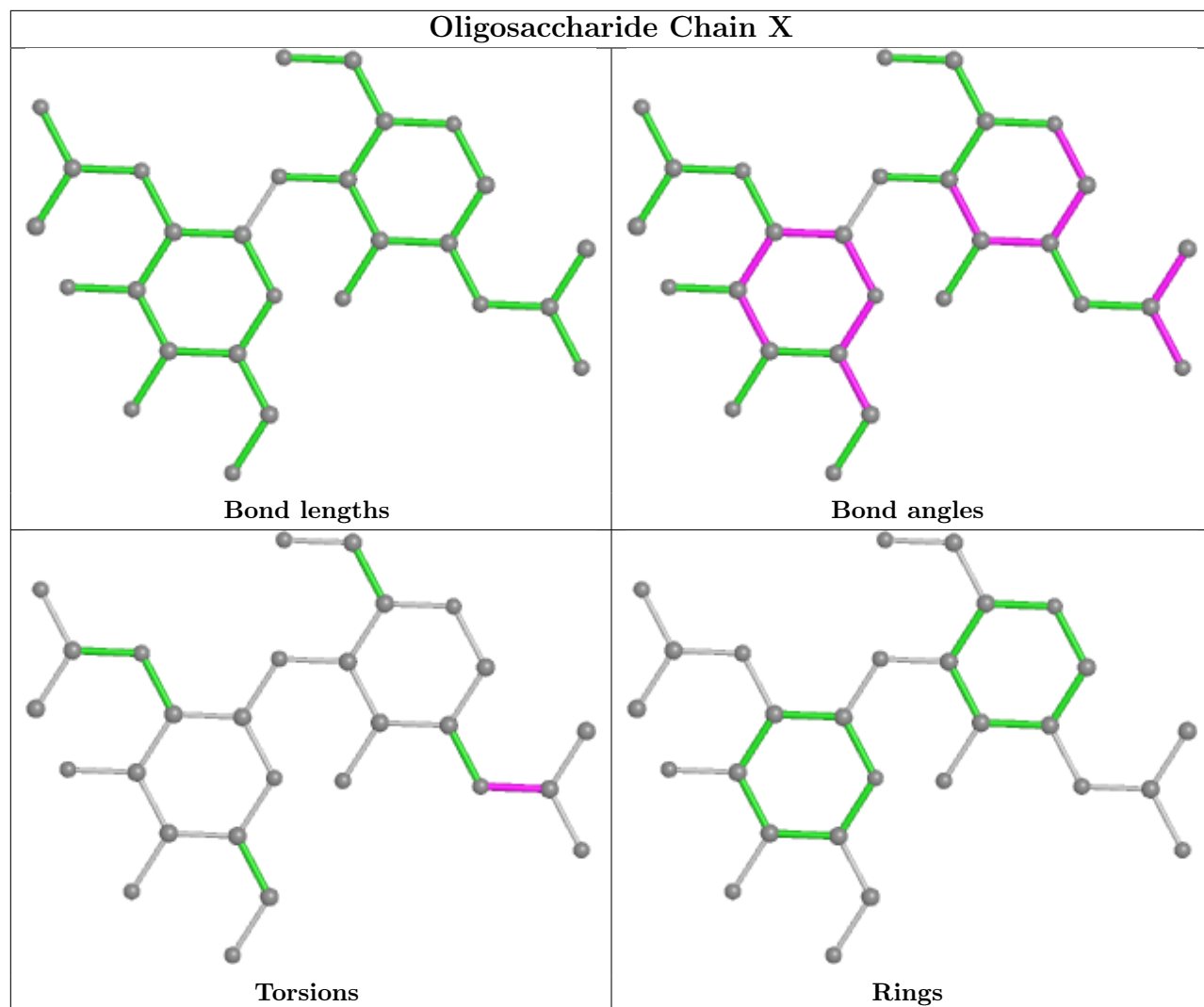


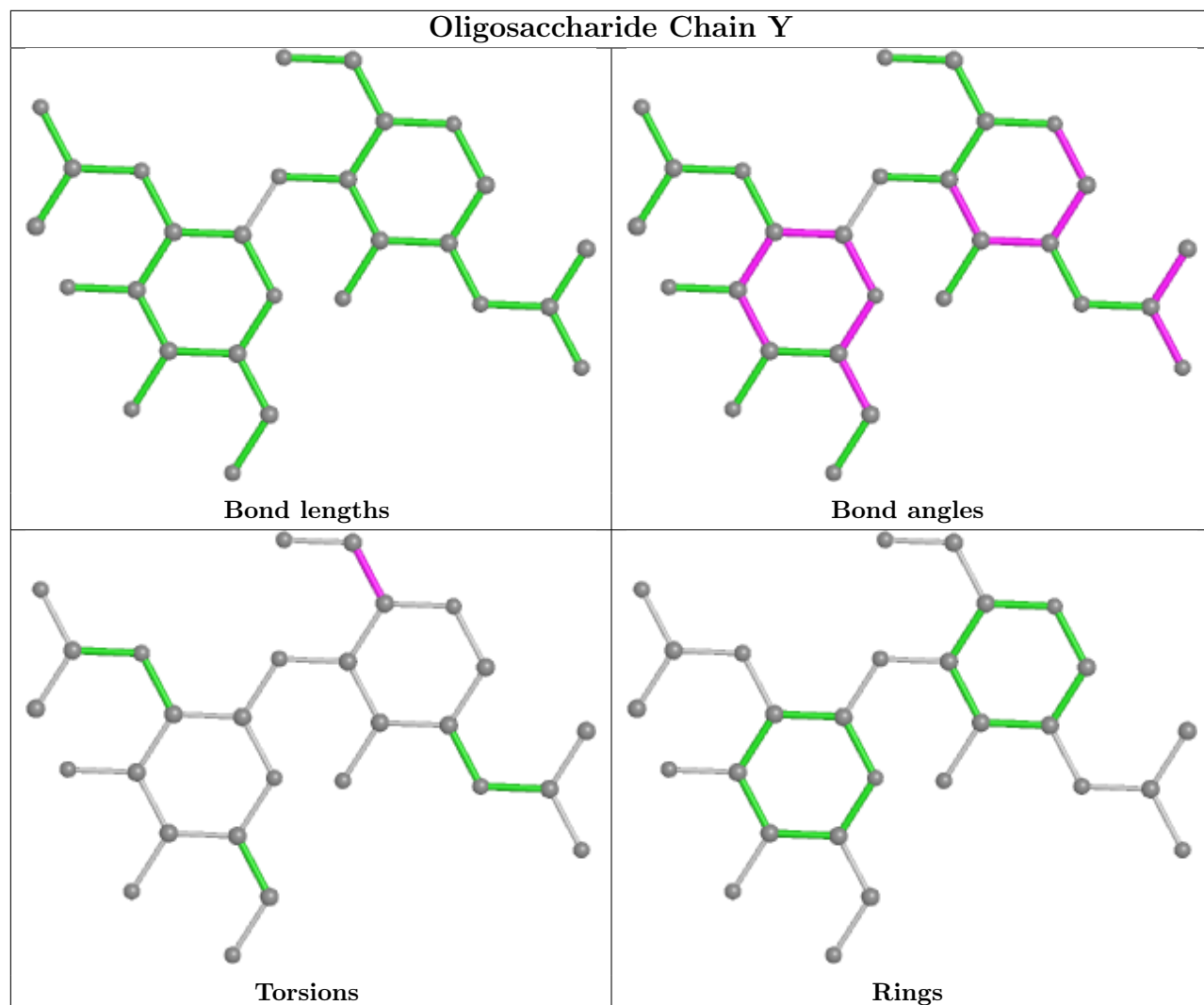


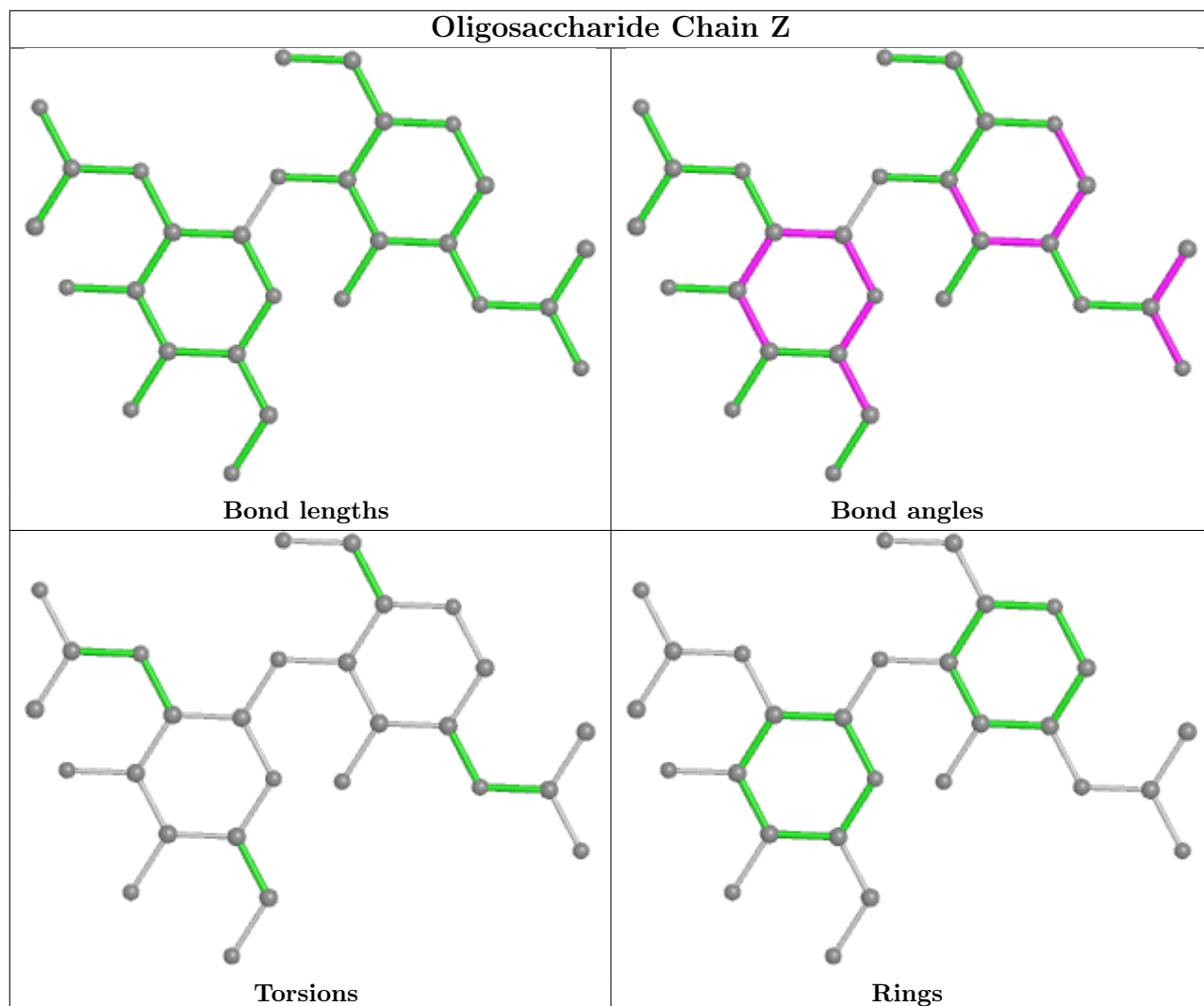


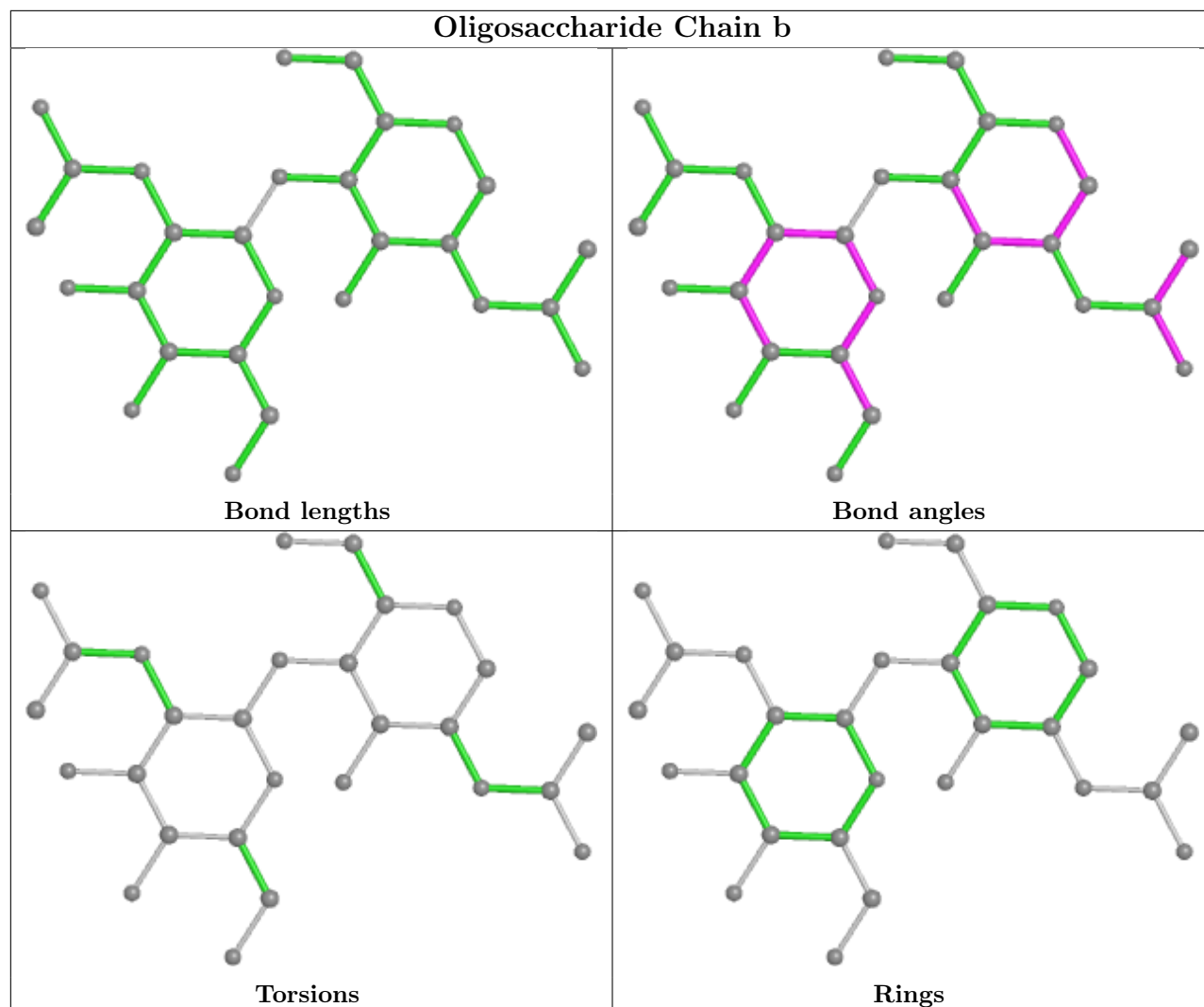


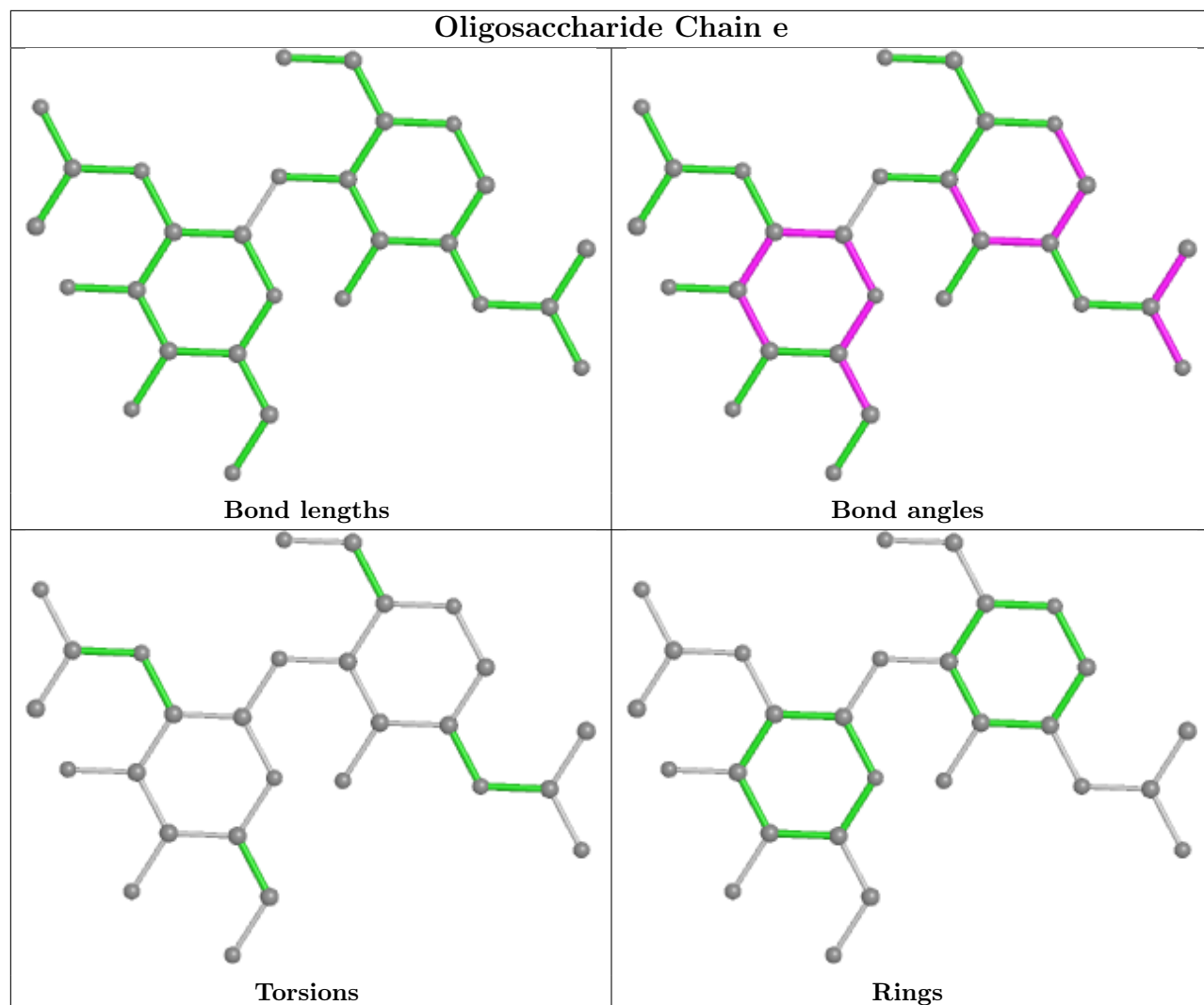


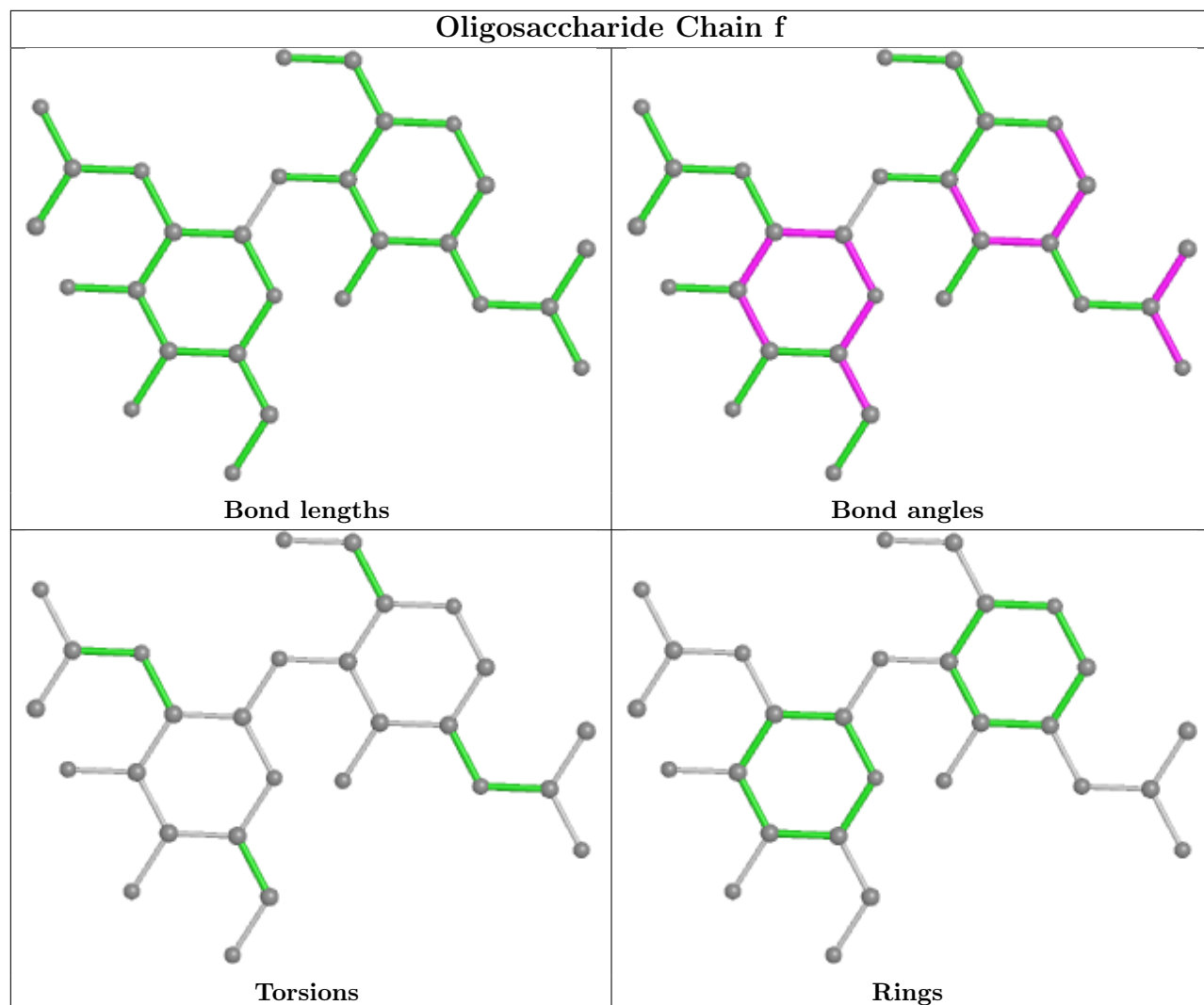


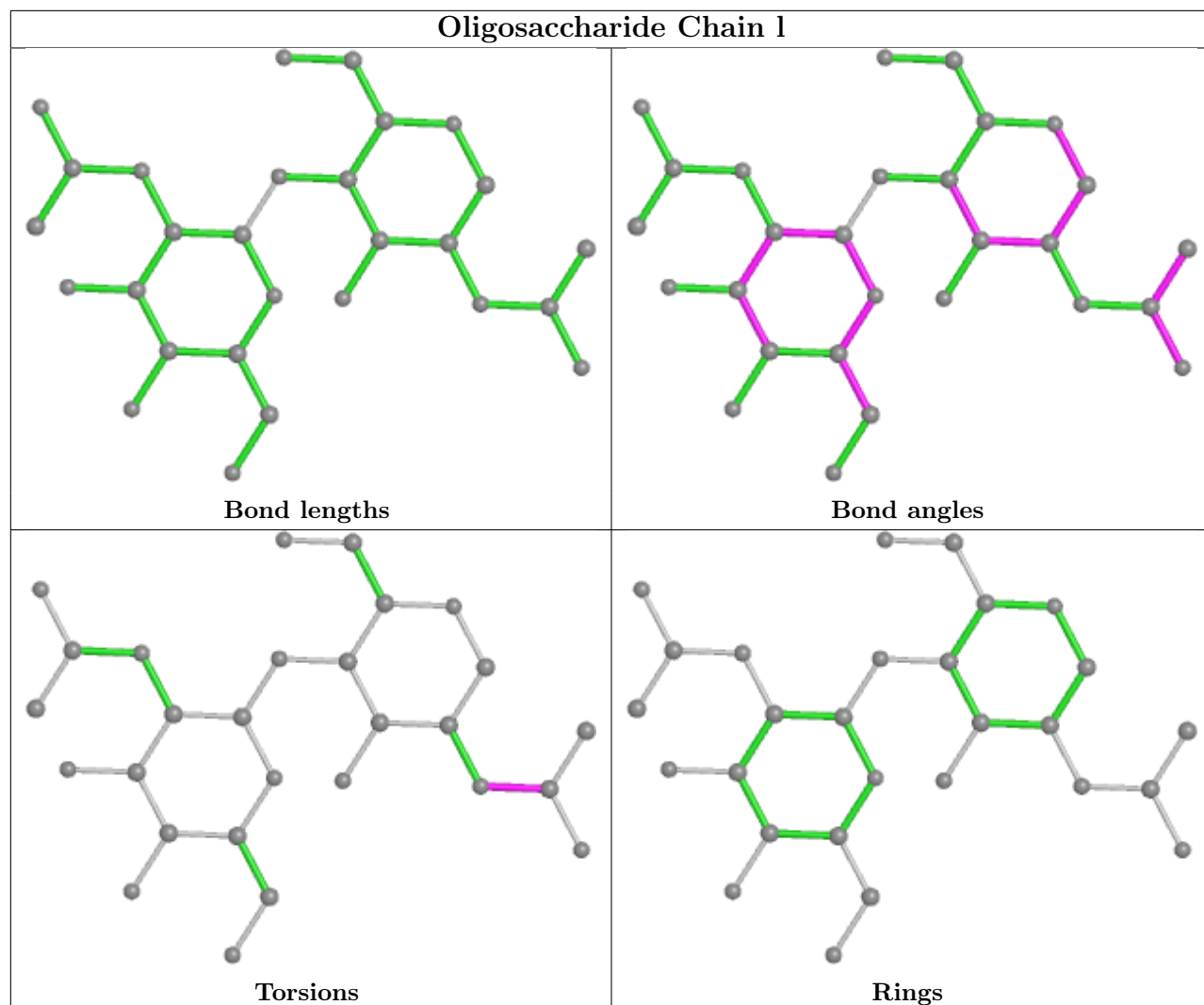


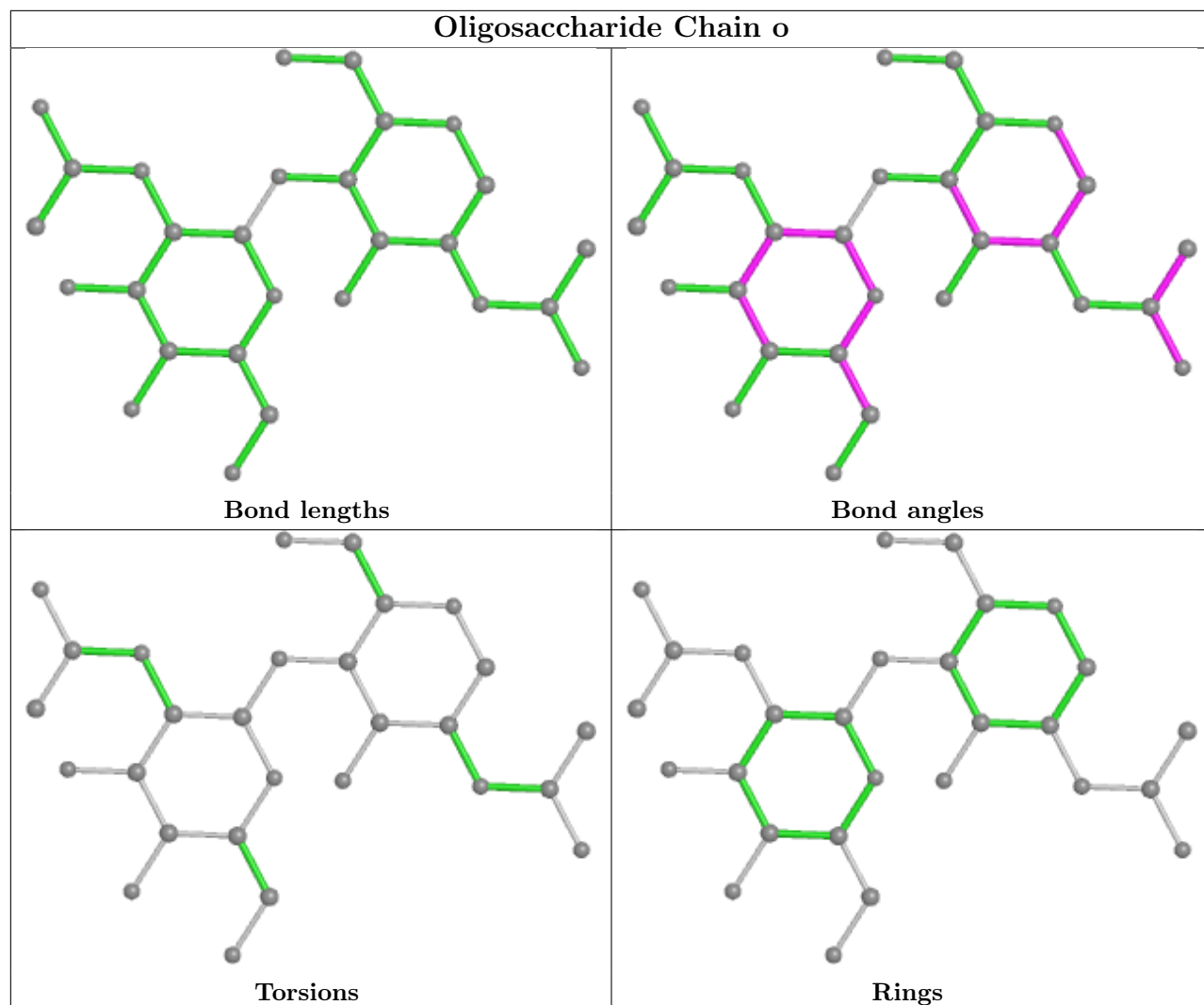


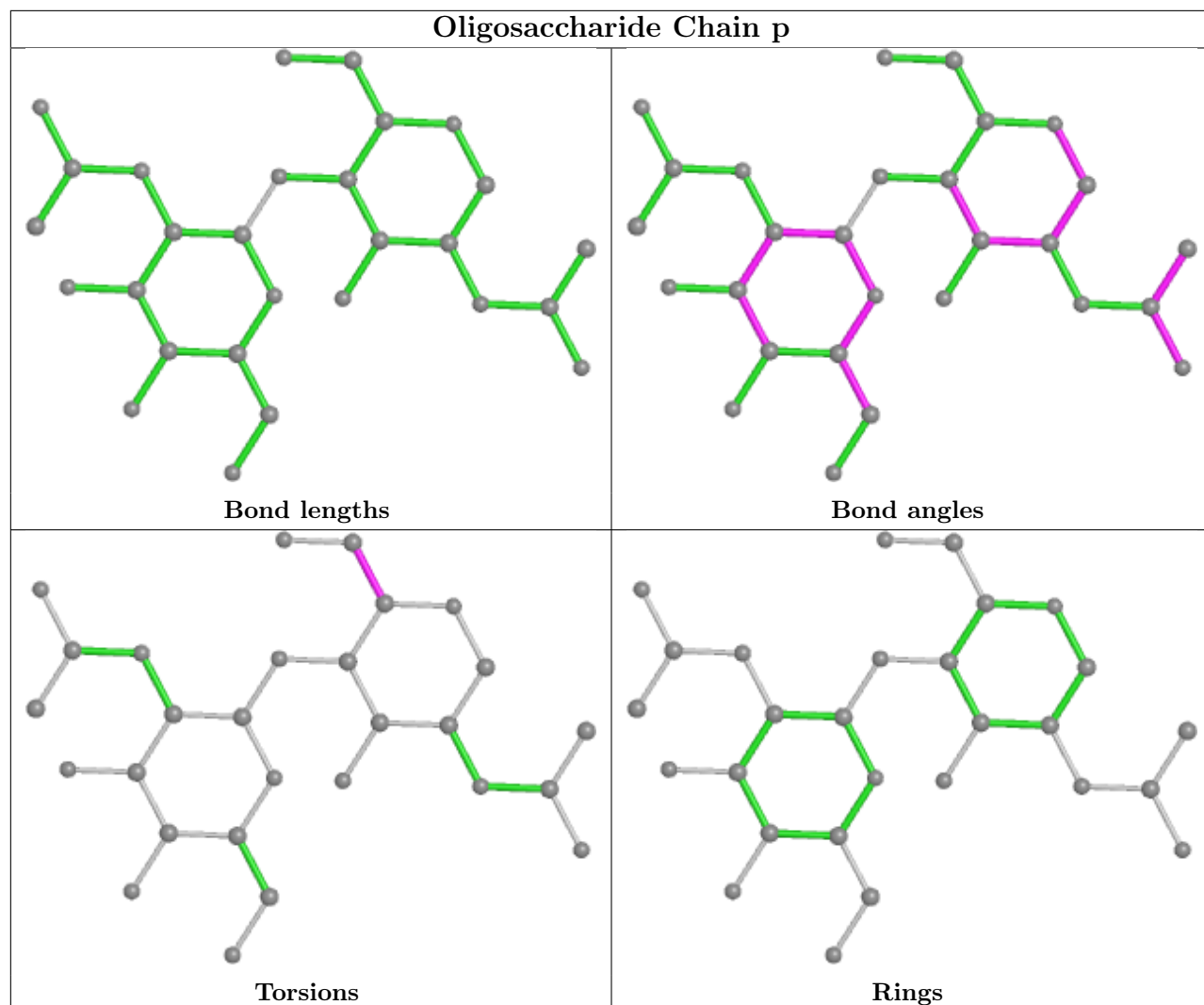


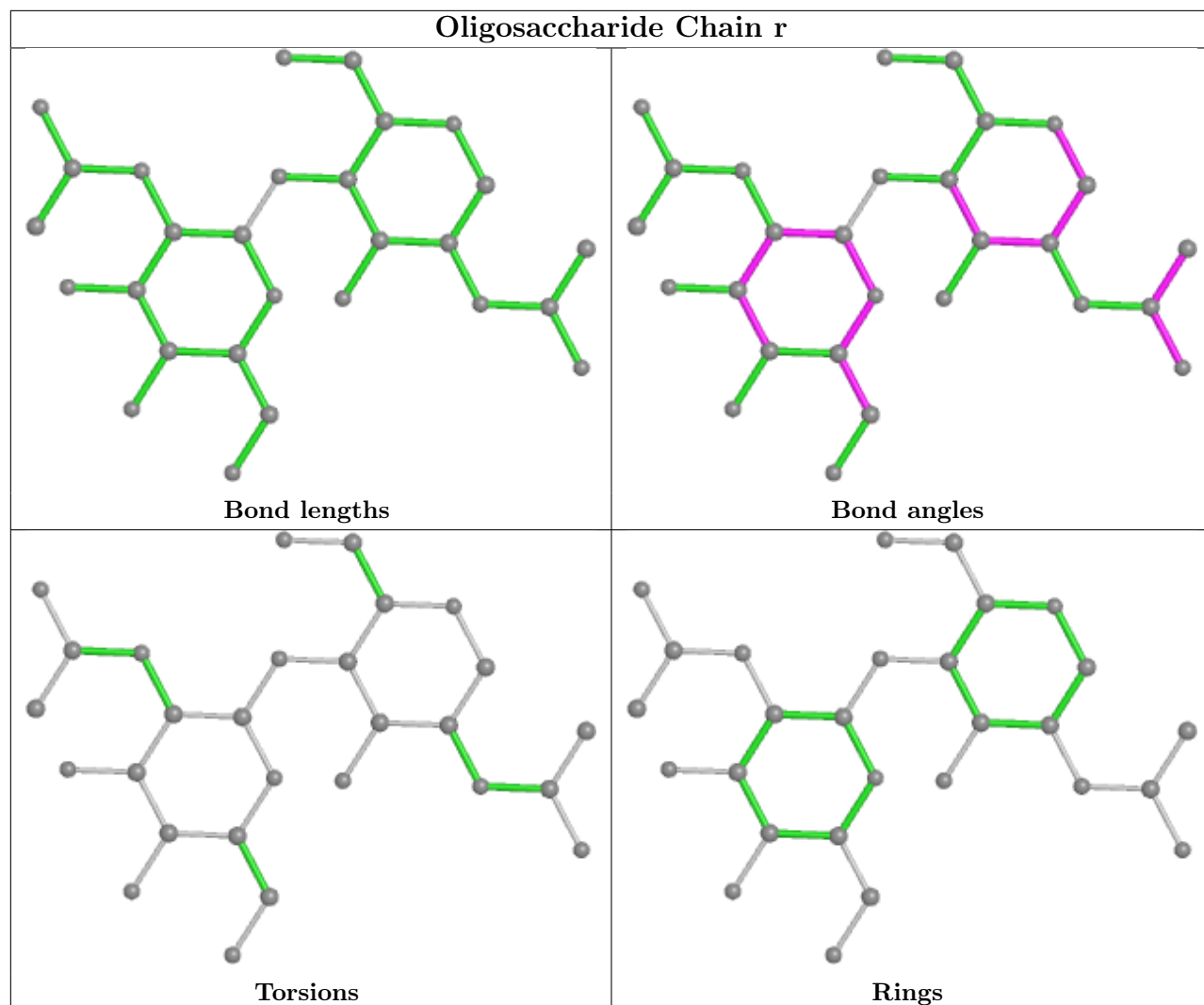


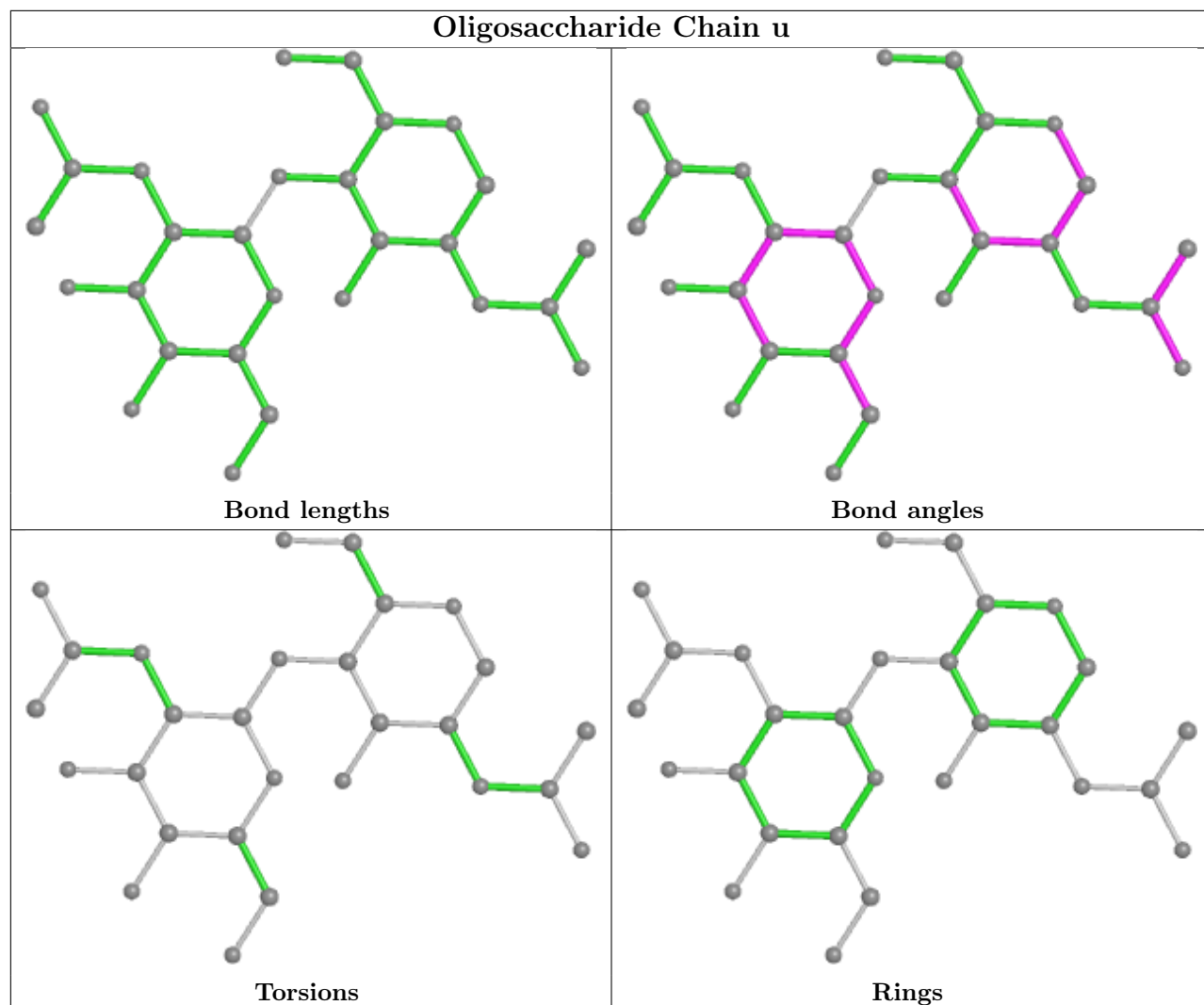


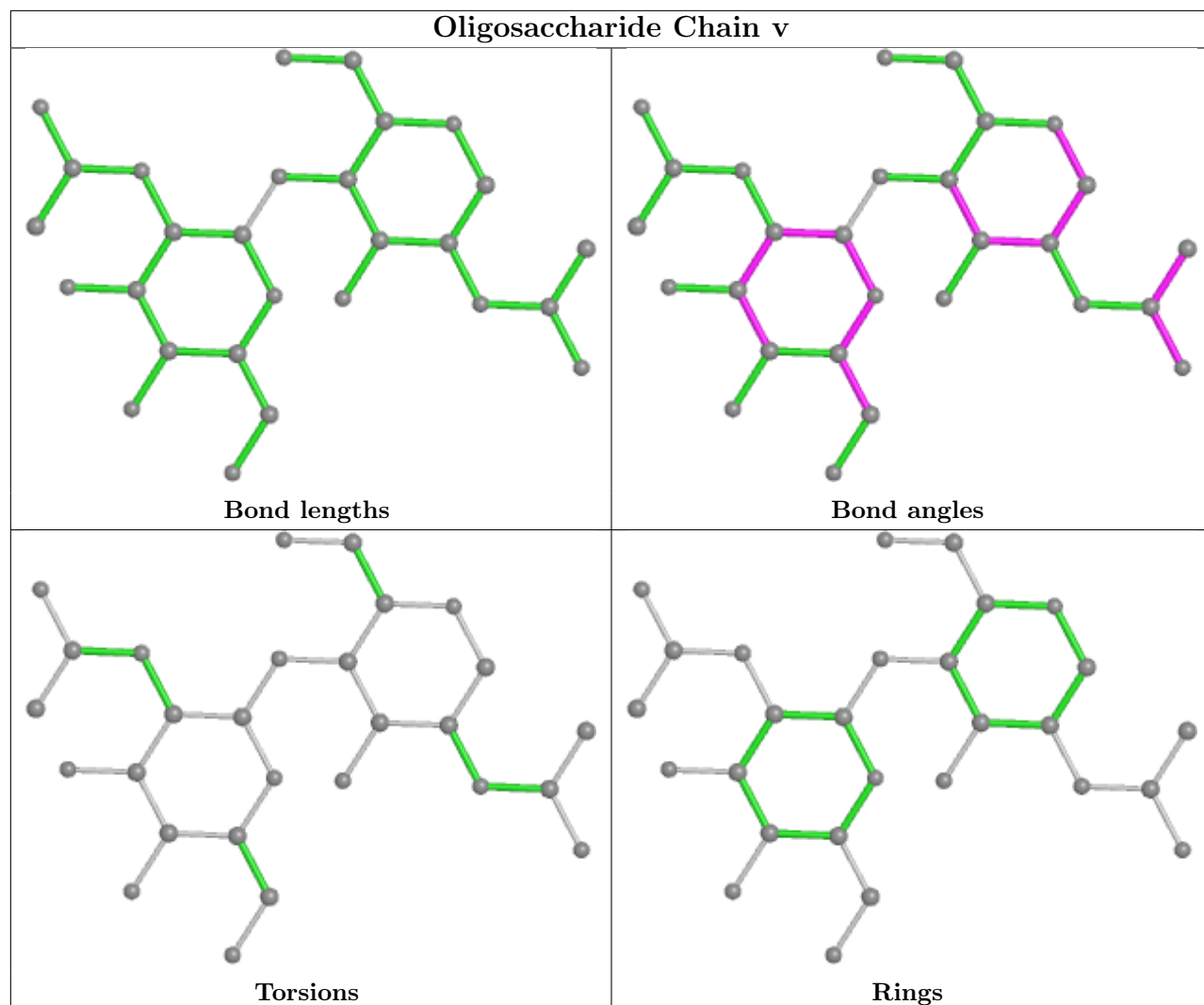


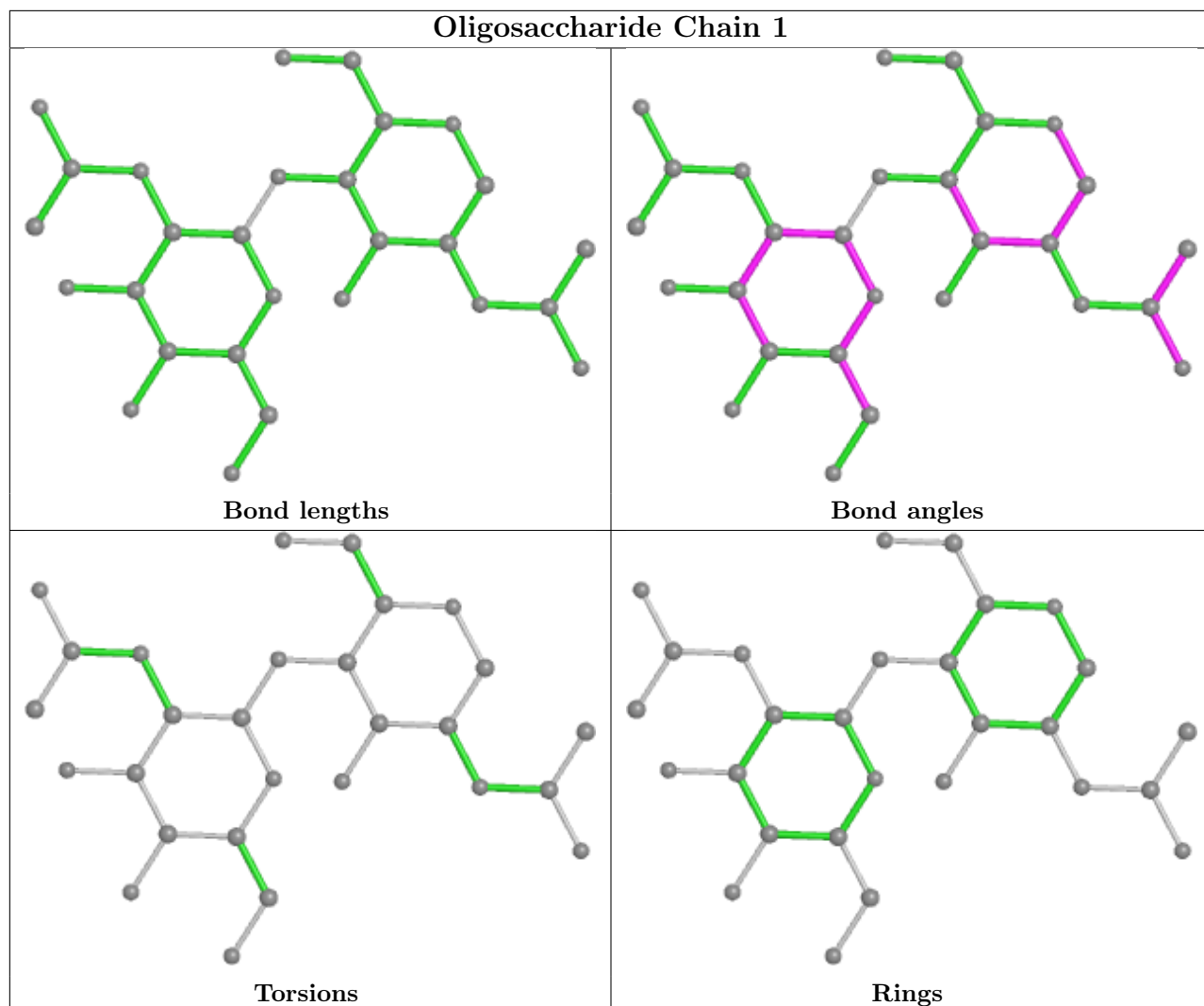


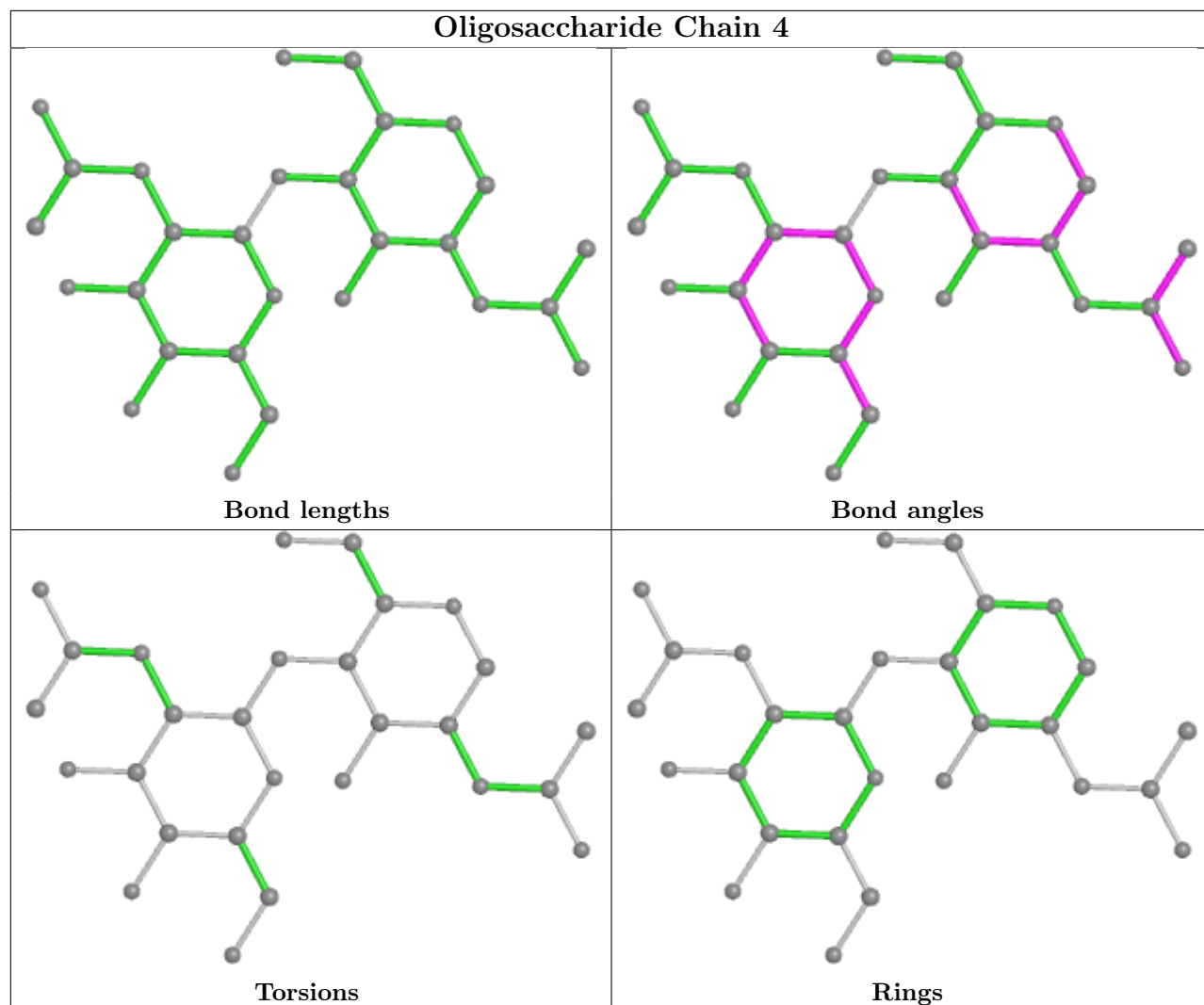


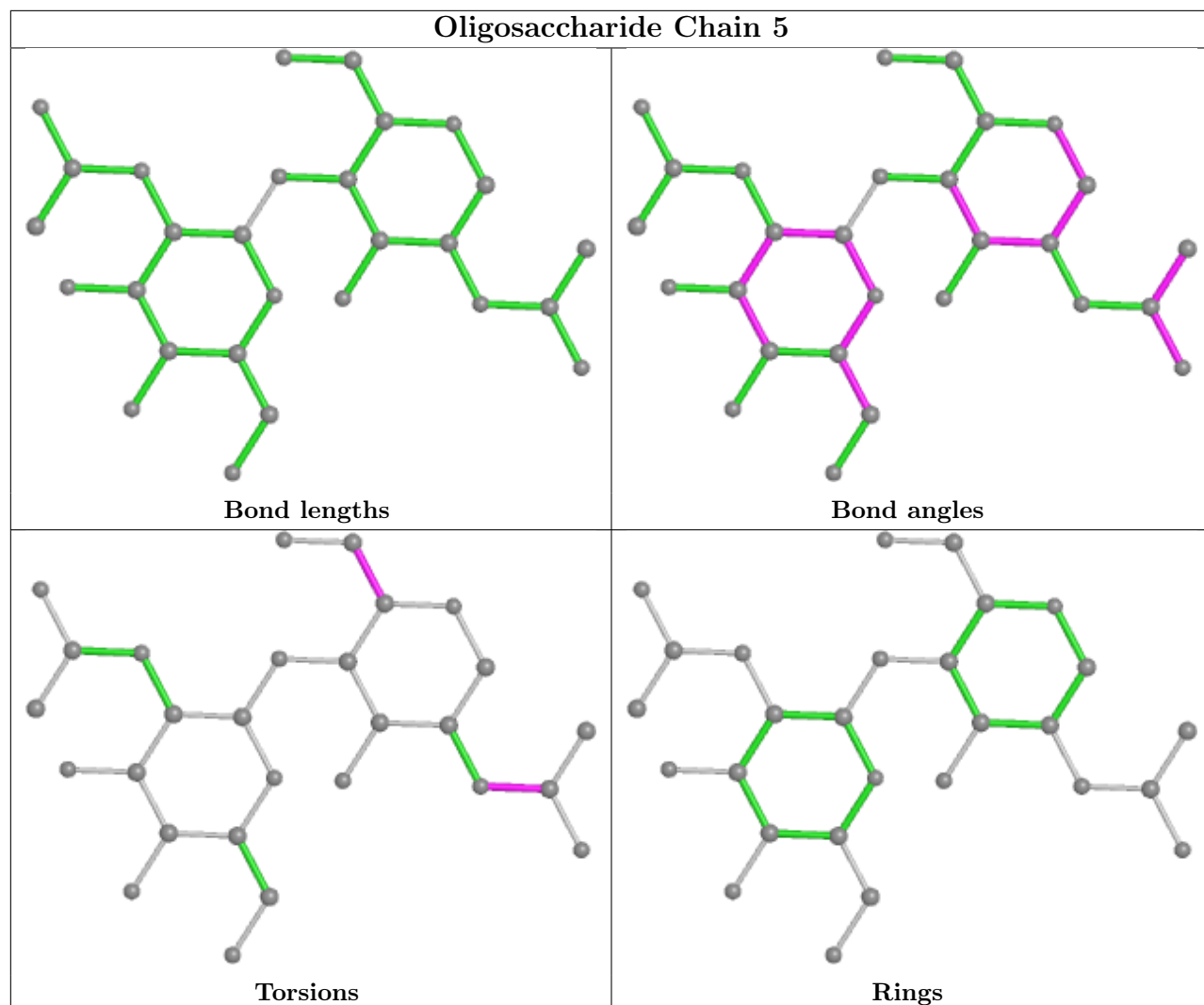


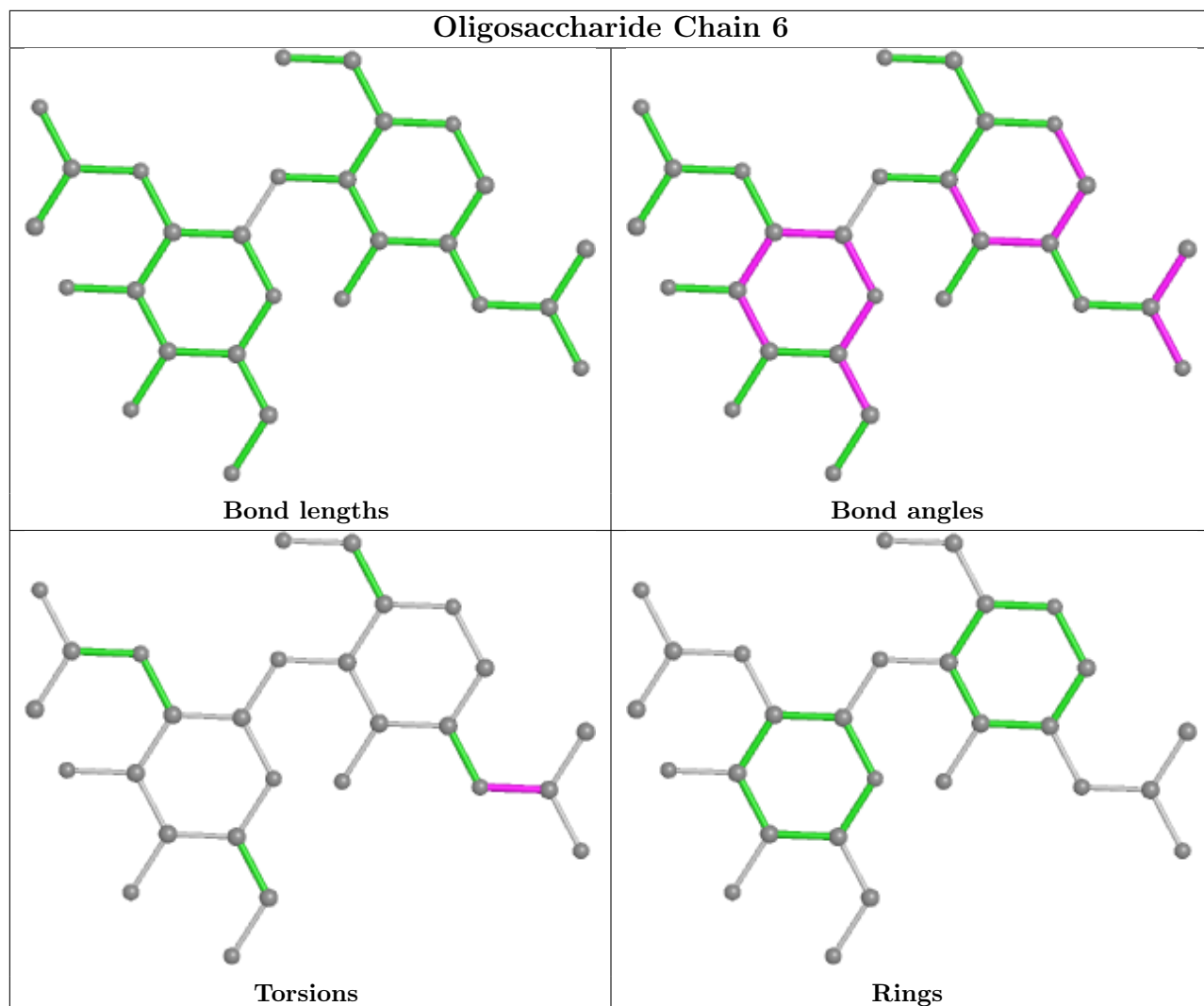


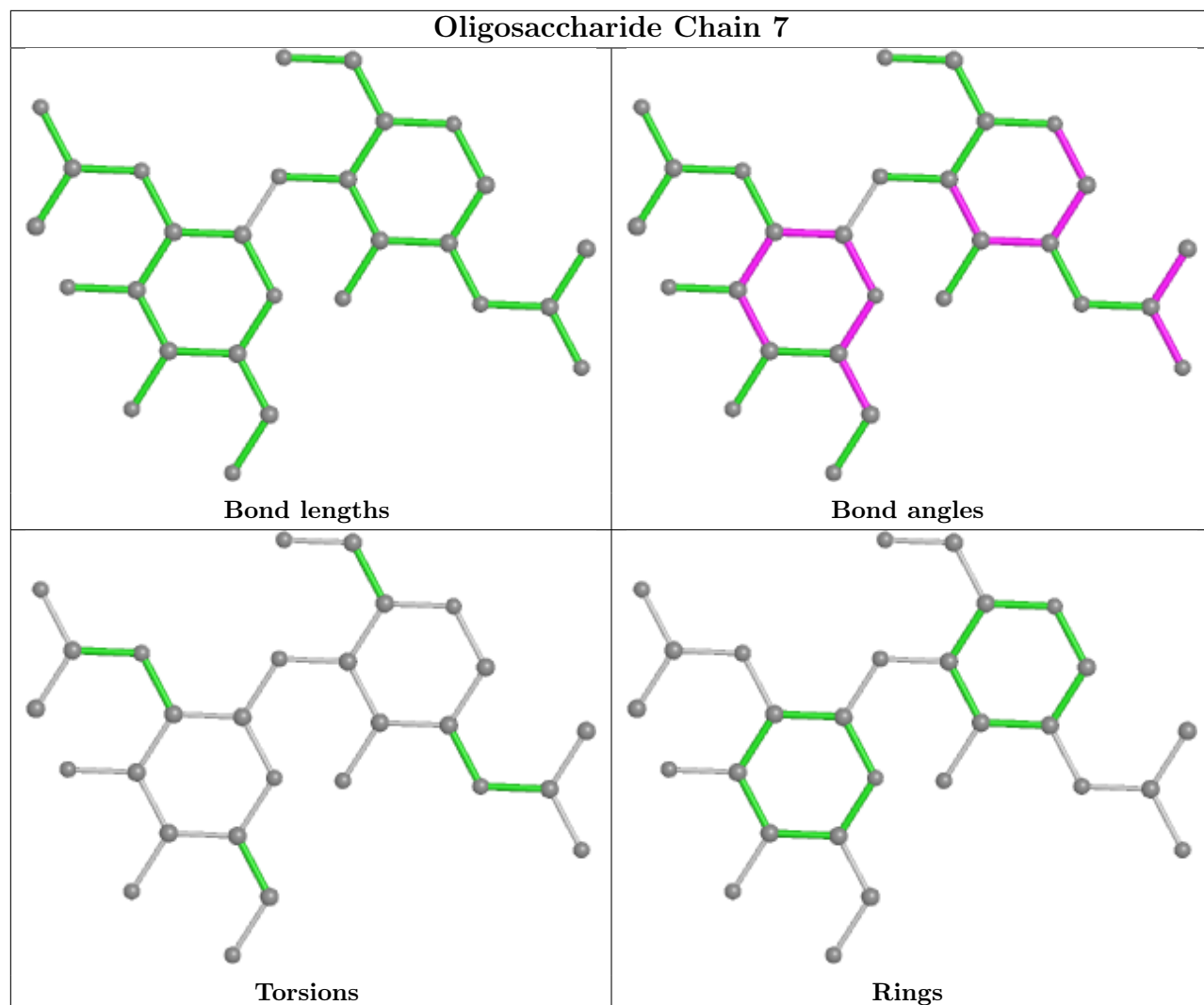


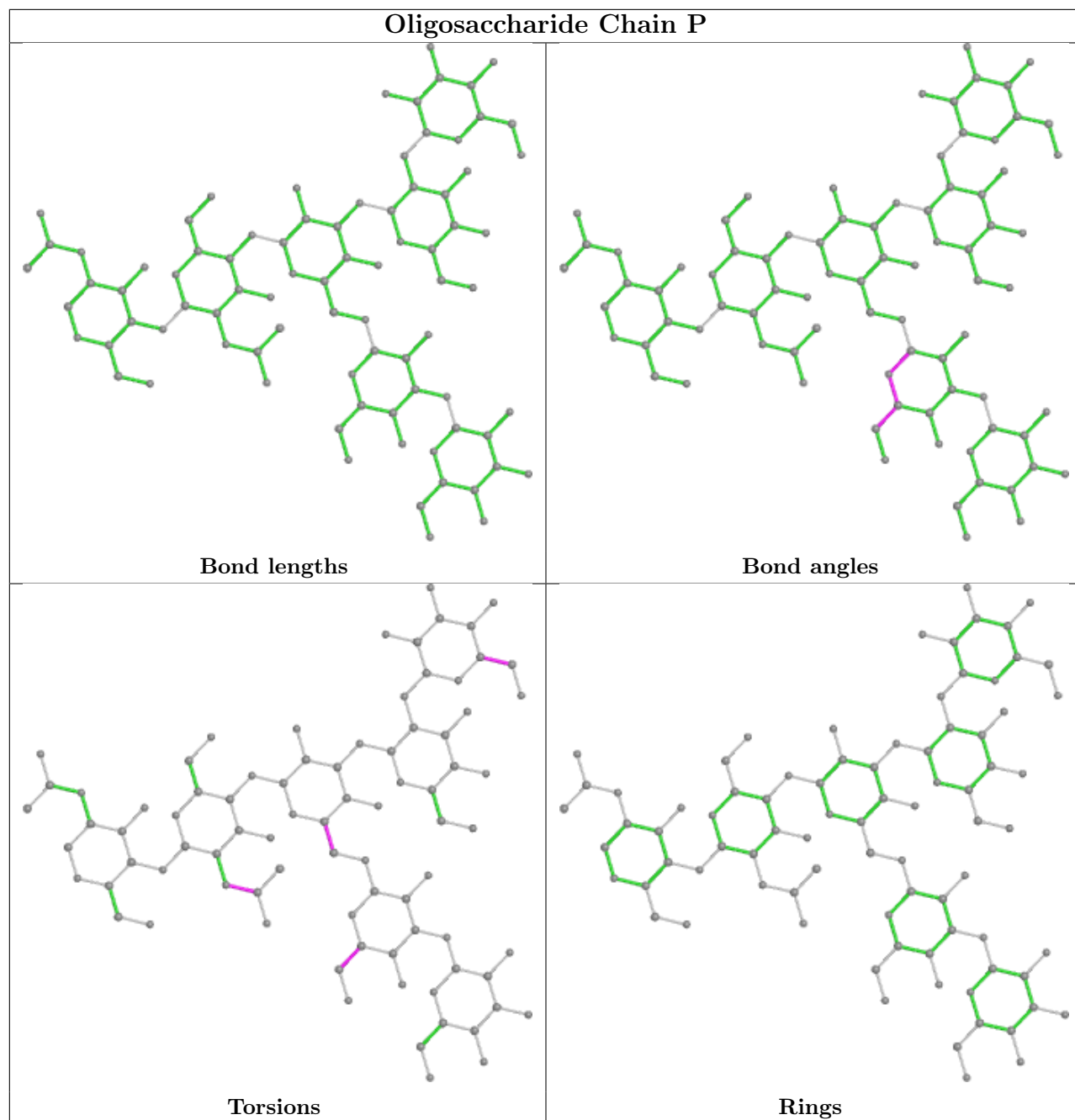


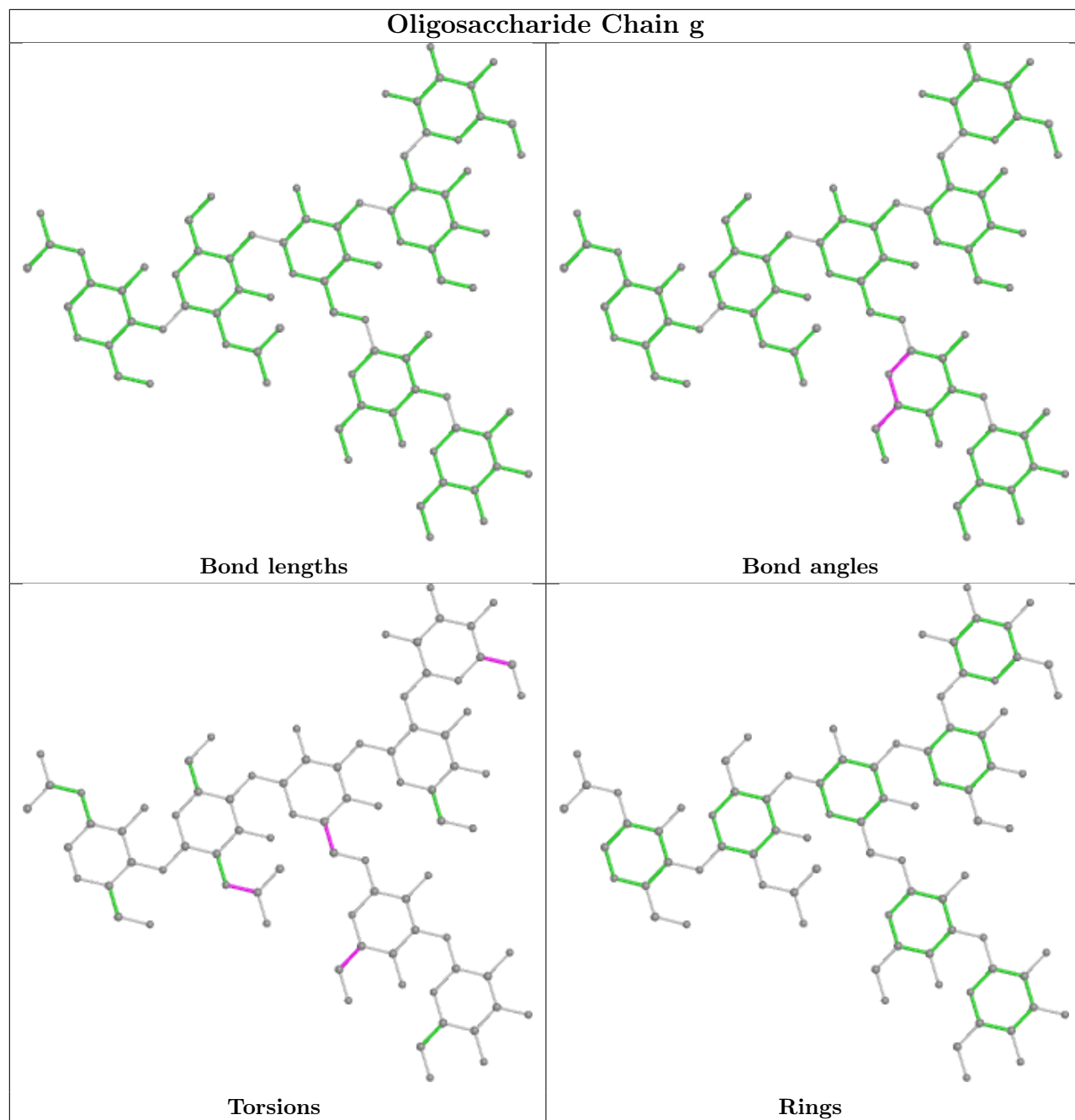


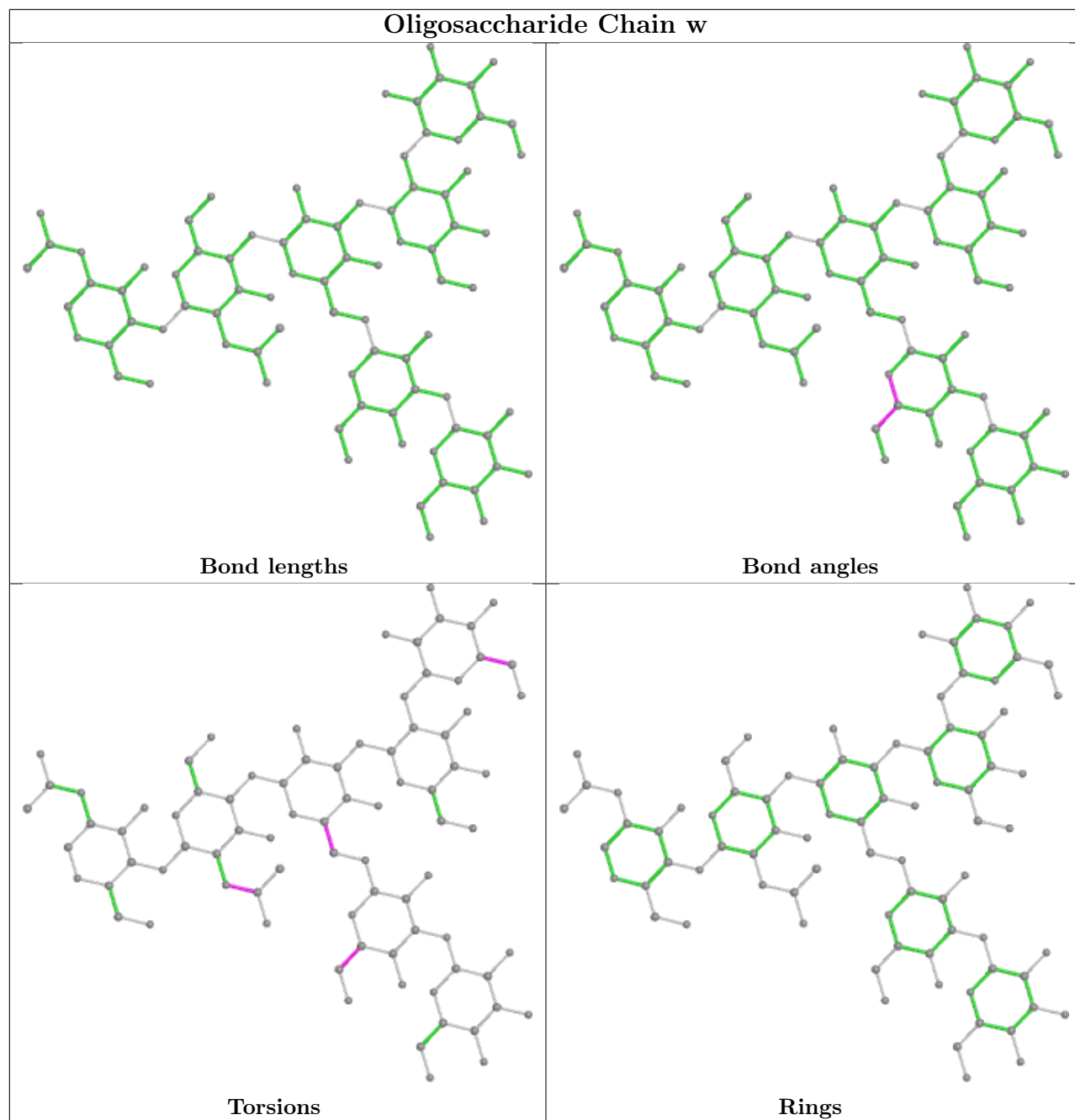


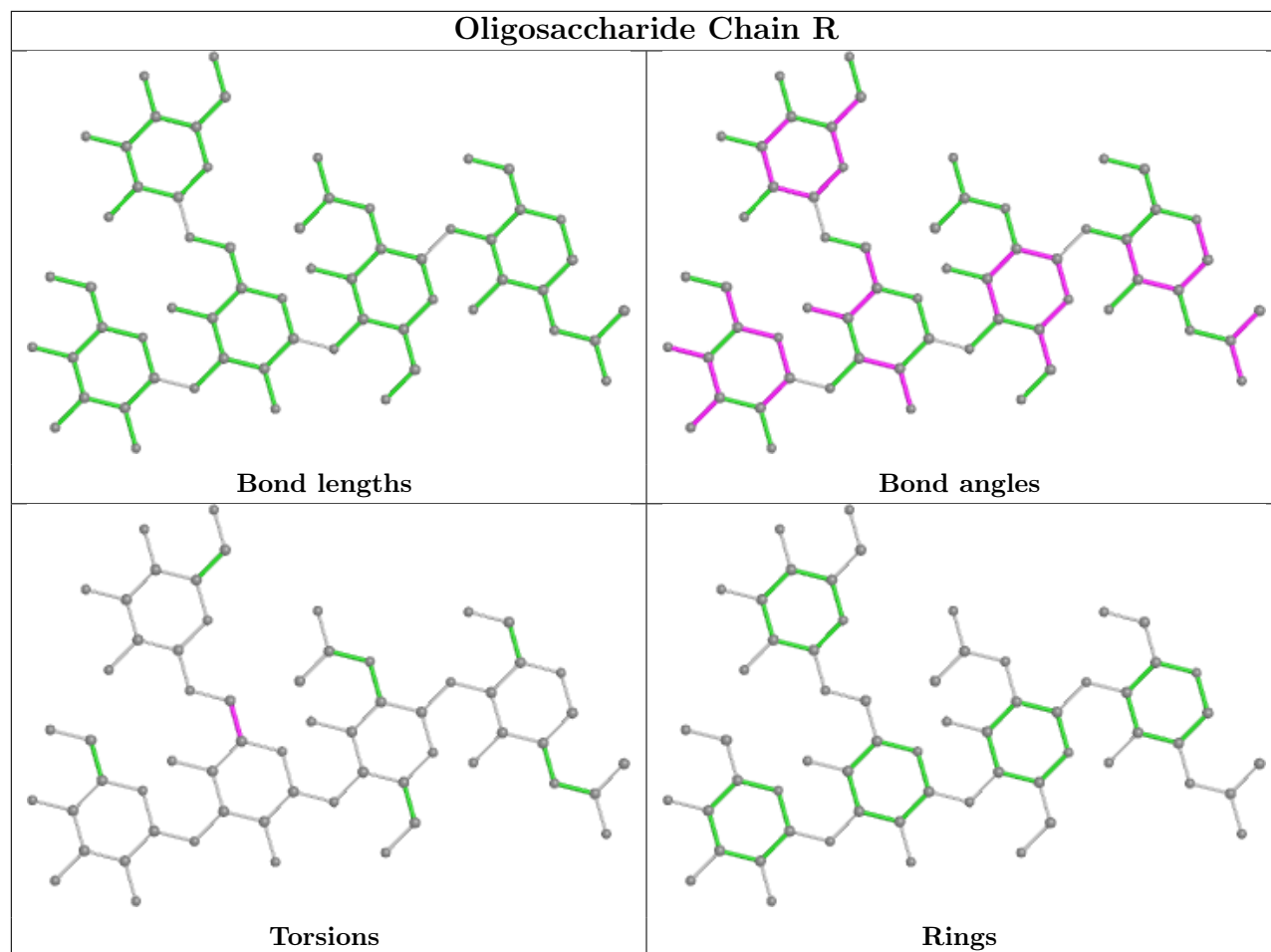


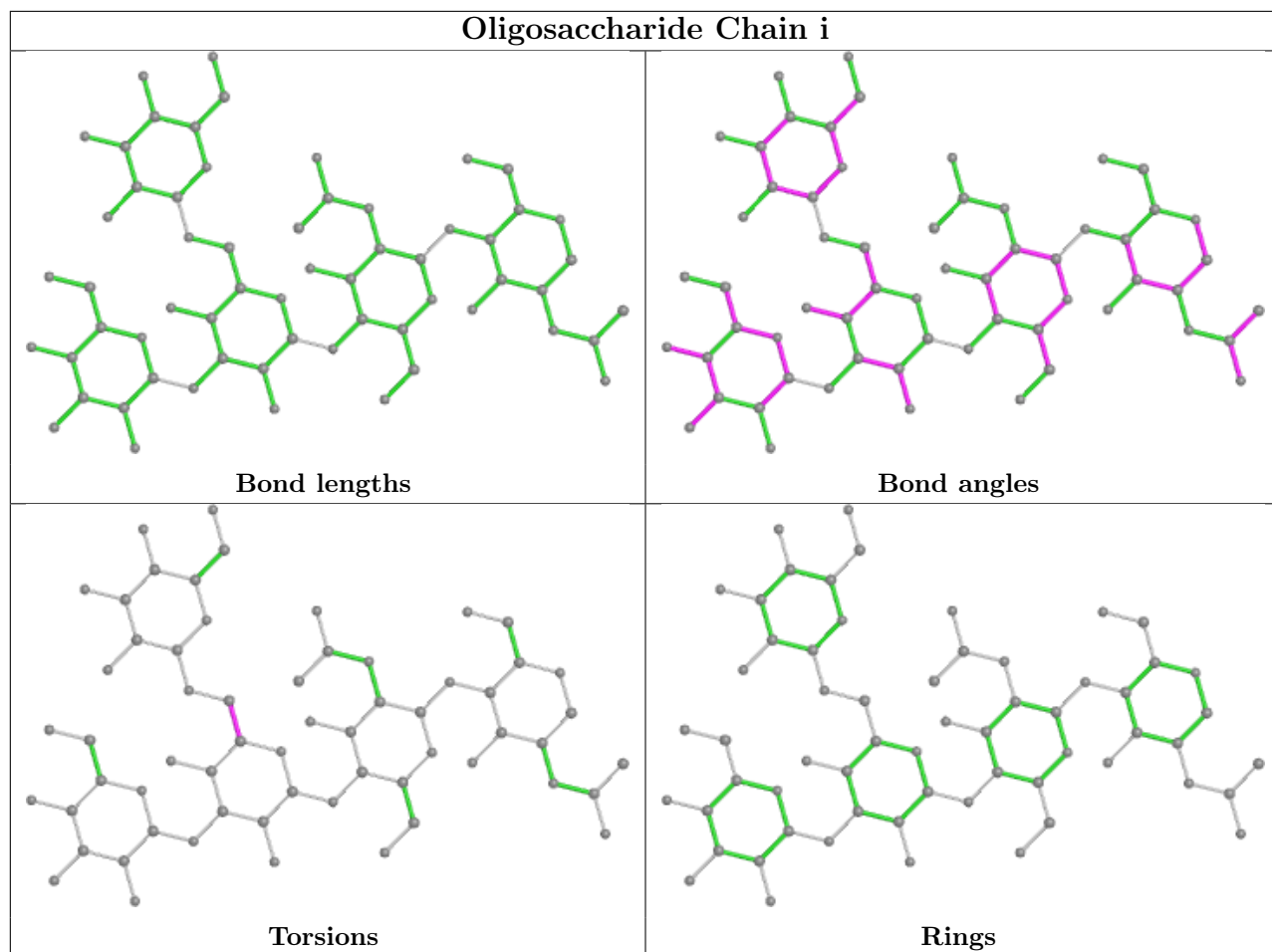


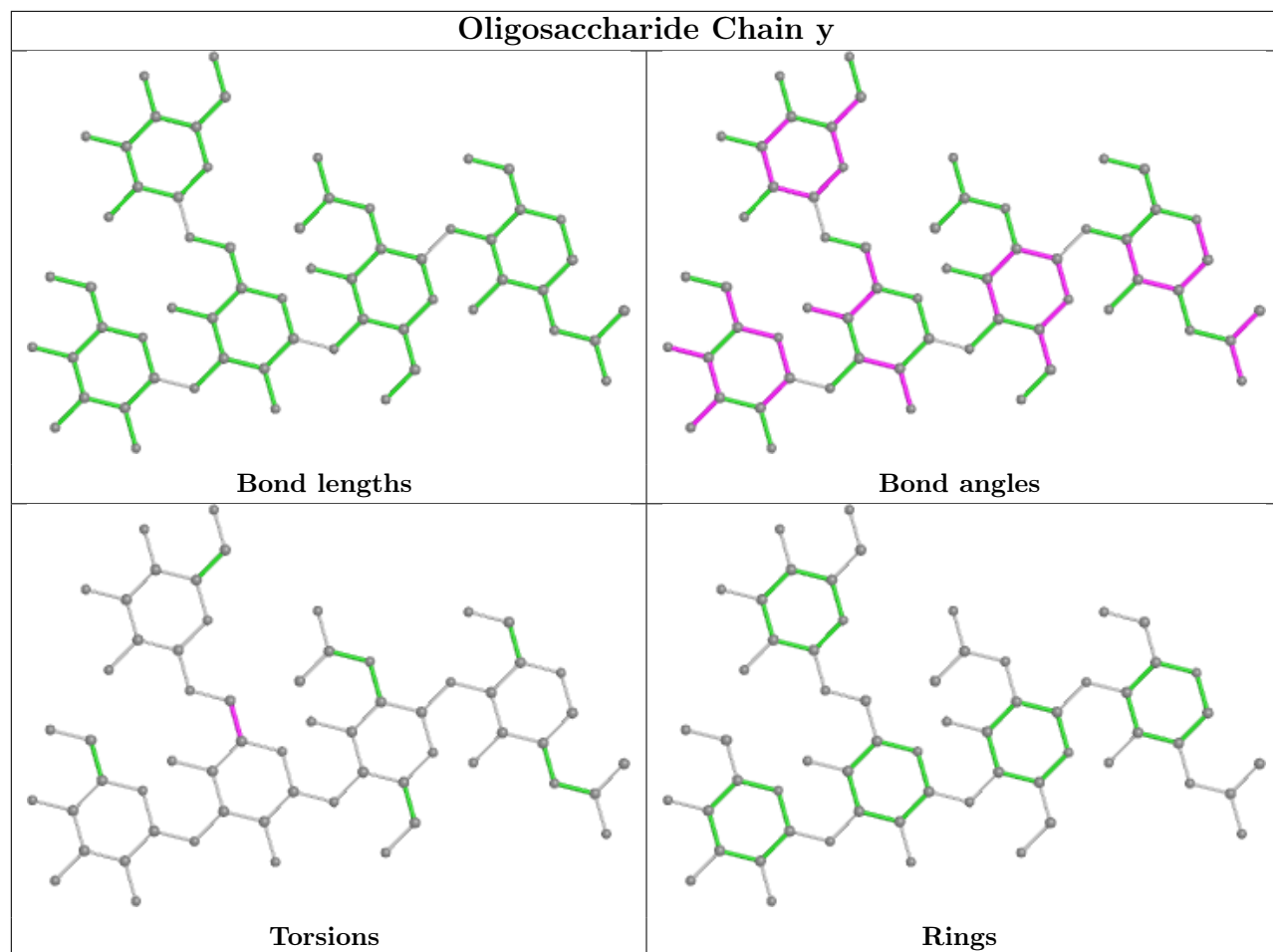


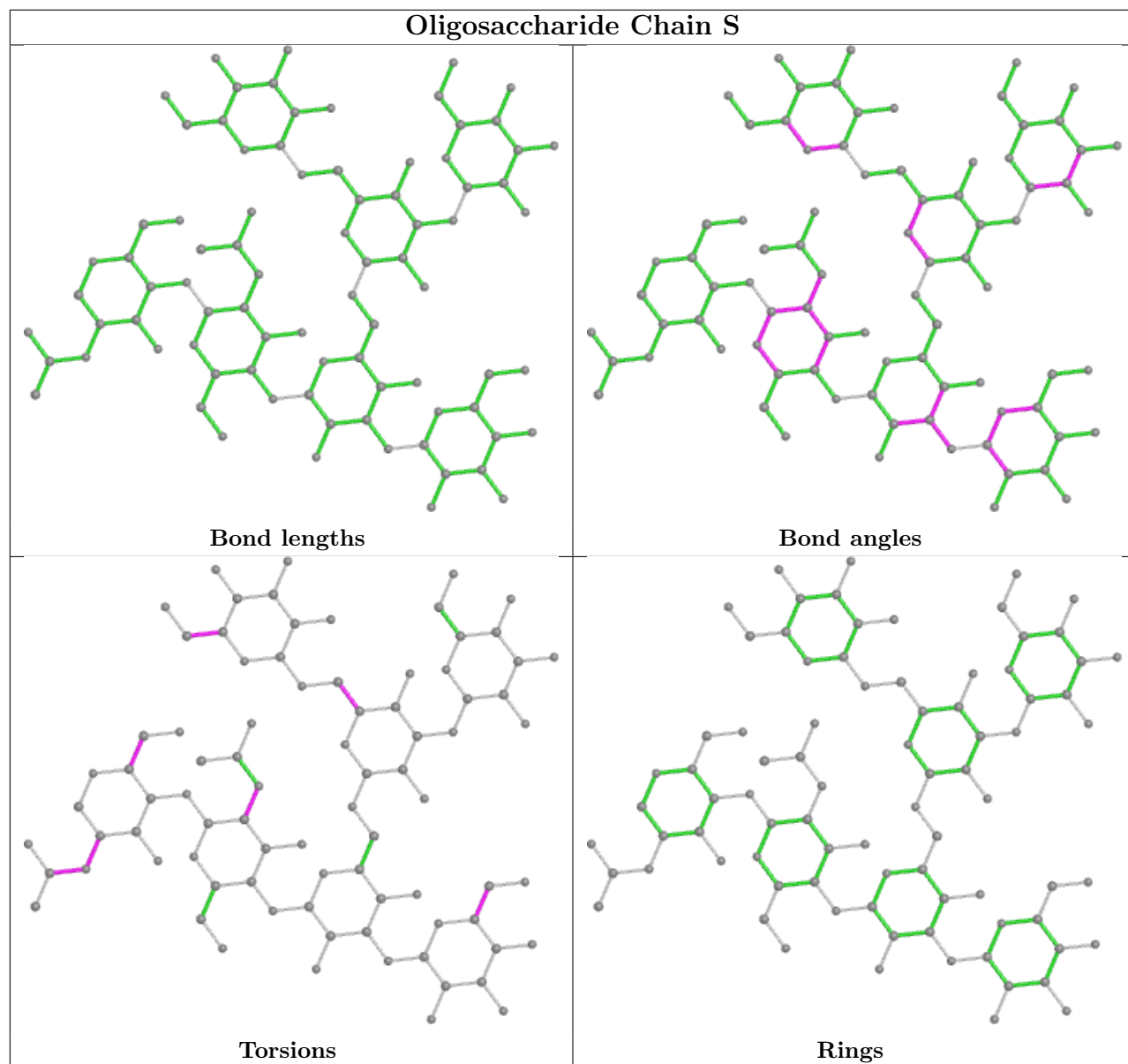


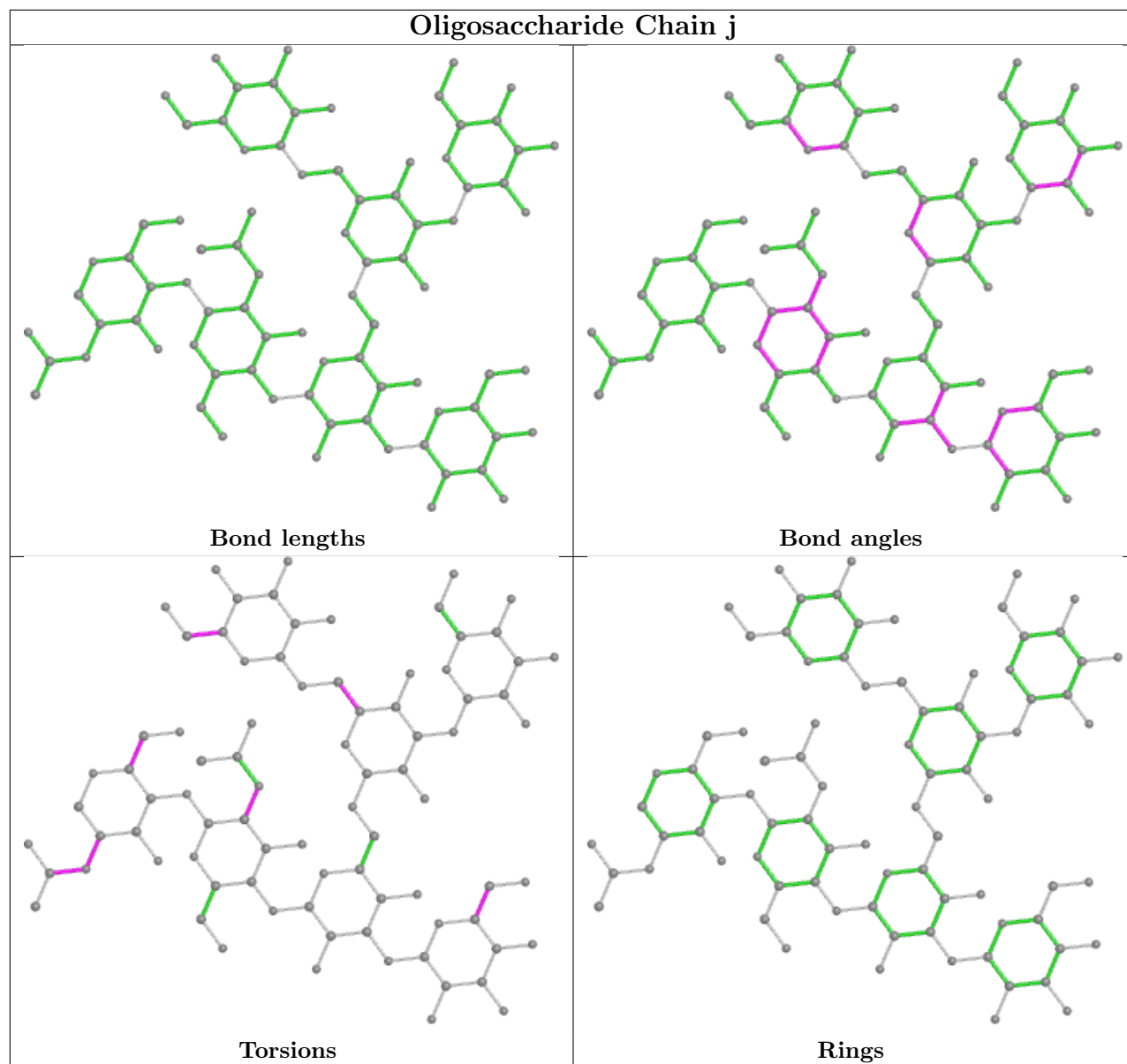


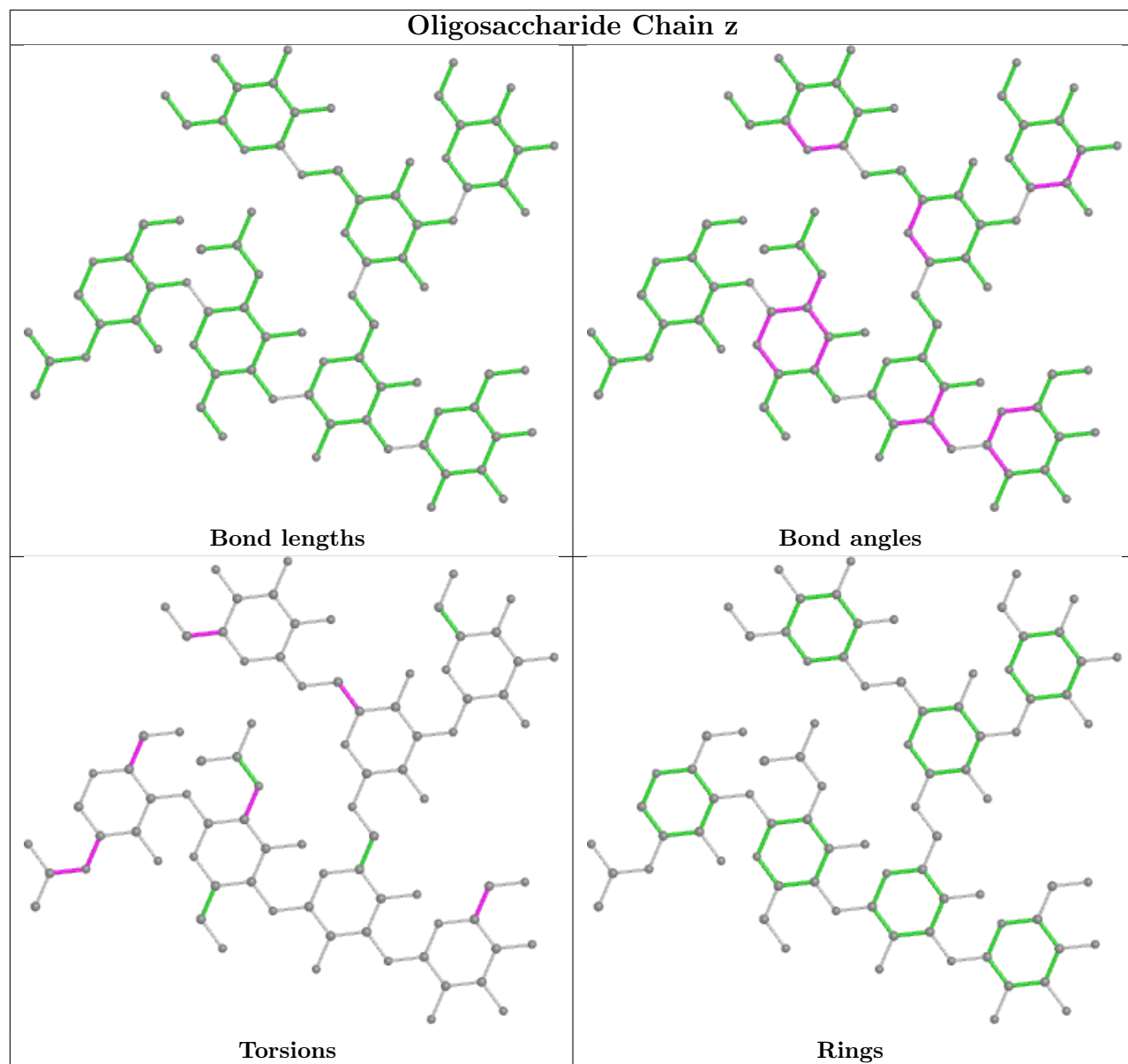


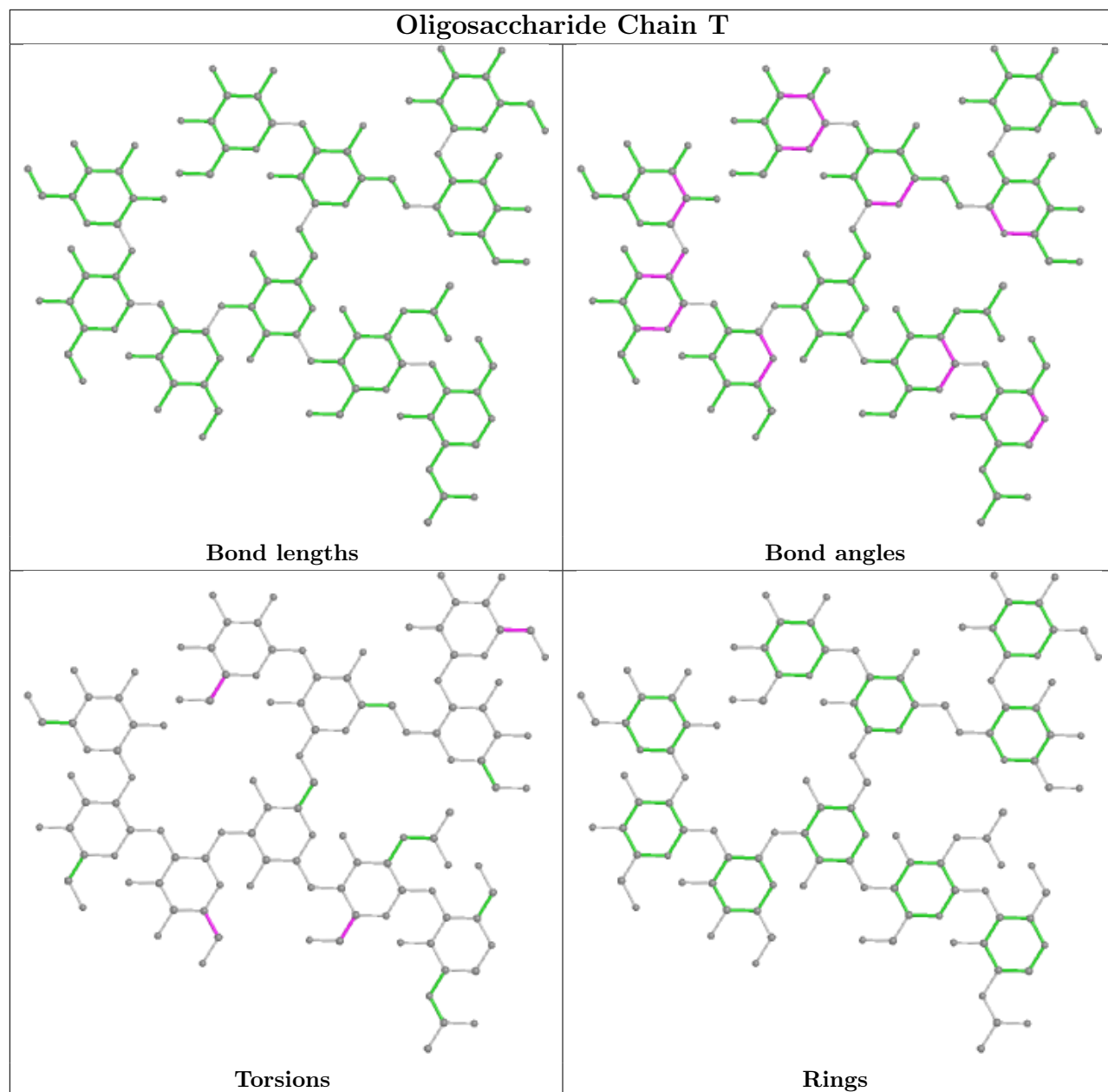


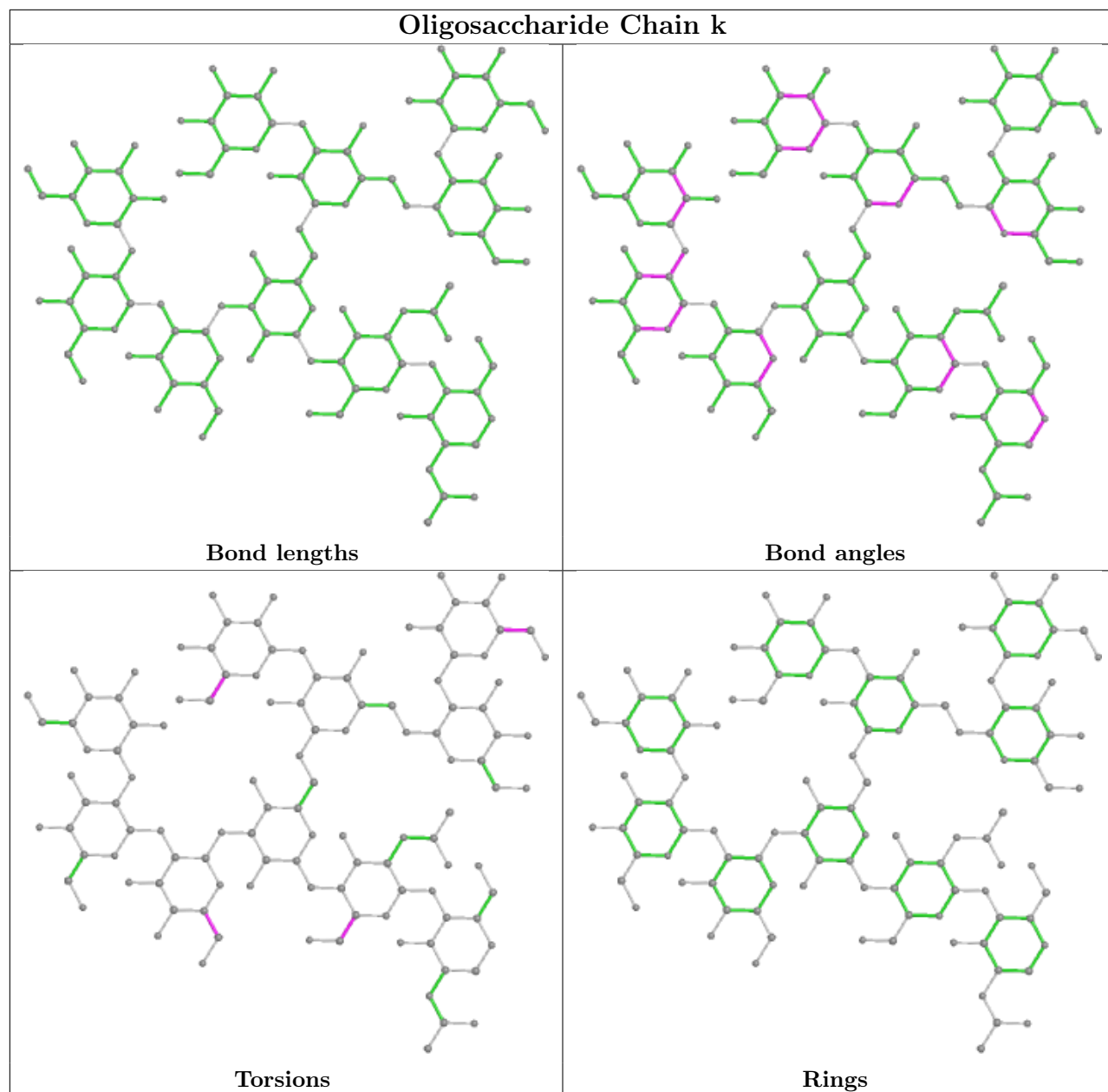


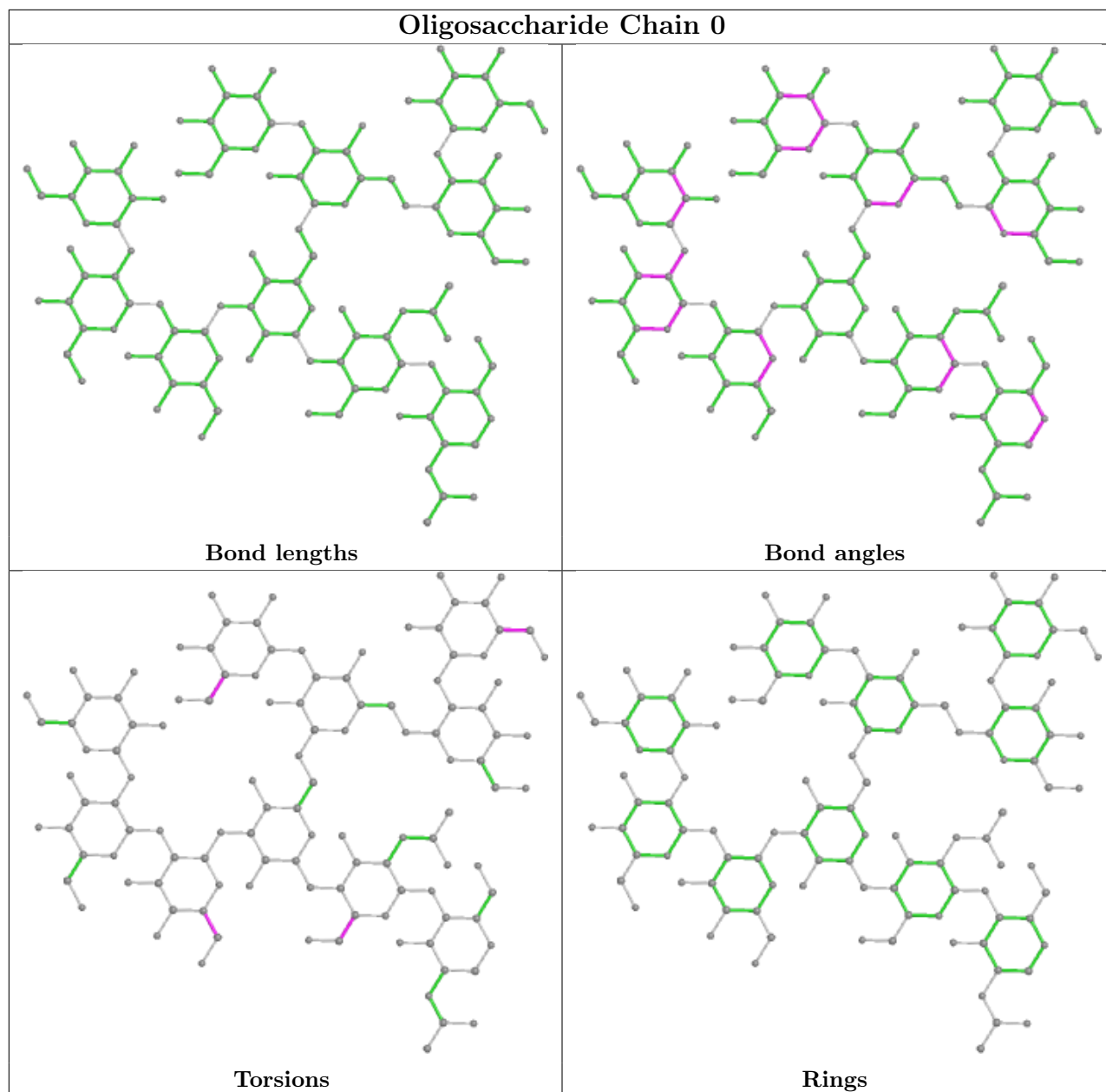












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	C	648	1	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
10	NAG	A	648	1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
10	NAG	F	704	2	14,14,15	0.49	0	17,19,21	2.24	3 (17%)
10	NAG	E	704	2	14,14,15	0.48	0	17,19,21	2.24	3 (17%)
10	NAG	B	704	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	D	648	1	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
10	NAG	F	703	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
10	NAG	B	703	2	14,14,15	0.52	0	17,19,21	2.24	3 (17%)
10	NAG	E	703	2	14,14,15	0.51	0	17,19,21	2.24	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	648	1	-	0/6/23/26	0/1/1/1
10	NAG	A	648	1	-	0/6/23/26	0/1/1/1
10	NAG	F	704	2	-	0/6/23/26	0/1/1/1
10	NAG	E	704	2	-	0/6/23/26	0/1/1/1
10	NAG	B	704	2	-	0/6/23/26	0/1/1/1
10	NAG	D	648	1	-	0/6/23/26	0/1/1/1
10	NAG	F	703	2	-	3/6/23/26	0/1/1/1
10	NAG	B	703	2	-	2/6/23/26	0/1/1/1
10	NAG	E	703	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	704	NAG	O5-C1-C2	-7.43	99.56	111.29
10	E	704	NAG	O5-C1-C2	-7.42	99.57	111.29
10	F	703	NAG	O5-C1-C2	-7.39	99.62	111.29
10	C	648	NAG	O5-C1-C2	-7.38	99.63	111.29
10	B	703	NAG	O5-C1-C2	-7.38	99.64	111.29
10	E	703	NAG	O5-C1-C2	-7.38	99.64	111.29
10	B	704	NAG	O5-C1-C2	-7.37	99.65	111.29
10	A	648	NAG	O5-C1-C2	-7.37	99.65	111.29
10	D	648	NAG	O5-C1-C2	-7.37	99.66	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	648	NAG	O7-C7-C8	-2.79	116.87	122.06
10	B	704	NAG	O7-C7-C8	-2.79	116.88	122.06
10	B	703	NAG	O7-C7-C8	-2.77	116.91	122.06
10	A	648	NAG	O7-C7-C8	-2.77	116.91	122.06
10	F	704	NAG	O7-C7-C8	-2.77	116.92	122.06
10	F	703	NAG	O7-C7-C8	-2.76	116.93	122.06
10	E	703	NAG	O7-C7-C8	-2.76	116.93	122.06
10	E	704	NAG	O7-C7-C8	-2.75	116.94	122.06
10	D	648	NAG	O7-C7-C8	-2.74	116.96	122.06
10	D	648	NAG	C4-C3-C2	-2.70	107.06	111.02
10	C	648	NAG	C4-C3-C2	-2.69	107.07	111.02
10	A	648	NAG	C4-C3-C2	-2.69	107.08	111.02
10	F	703	NAG	C4-C3-C2	-2.66	107.11	111.02
10	E	703	NAG	C4-C3-C2	-2.66	107.12	111.02
10	B	703	NAG	C4-C3-C2	-2.66	107.12	111.02
10	F	704	NAG	C4-C3-C2	-2.64	107.15	111.02
10	B	704	NAG	C4-C3-C2	-2.63	107.16	111.02
10	E	704	NAG	C4-C3-C2	-2.62	107.18	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	703	NAG	C1-C2-N2-C7
10	E	703	NAG	C1-C2-N2-C7
10	F	703	NAG	C1-C2-N2-C7
10	B	703	NAG	C3-C2-N2-C7
10	E	703	NAG	C3-C2-N2-C7
10	F	703	NAG	C3-C2-N2-C7
10	E	703	NAG	O7-C7-N2-C2
10	F	703	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1
3	H	1
3	I	1
2	B	1
2	E	1
2	F	1
1	A	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	127:SER	C	128:GLU	N	1.62
1	H	127:SER	C	128:GLU	N	1.62
1	I	127:SER	C	128:GLU	N	1.62
1	B	658:GLN	C	659:ASP	N	1.61
1	E	658:GLN	C	659:ASP	N	1.61
1	F	658:GLN	C	659:ASP	N	1.61
1	A	92:GLU	C	93:PHE	N	1.19
1	C	92:GLU	C	93:PHE	N	1.19
1	D	92:GLU	C	93:PHE	N	1.19

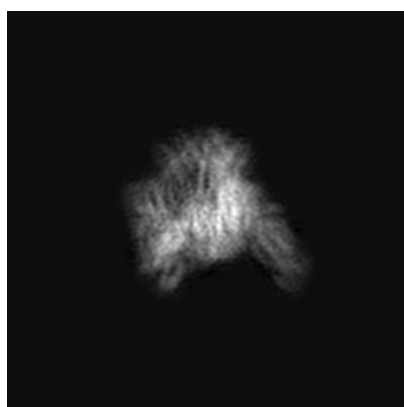
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9166. These allow visual inspection of the internal detail of the map and identification of artifacts.

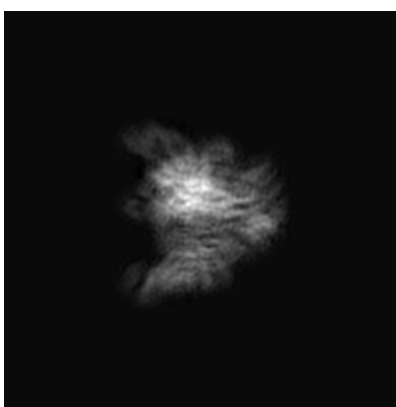
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

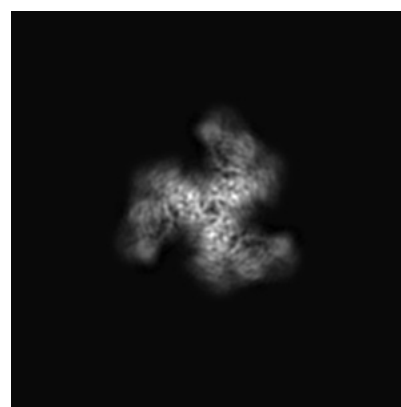
6.1.1 Primary map



X



Y

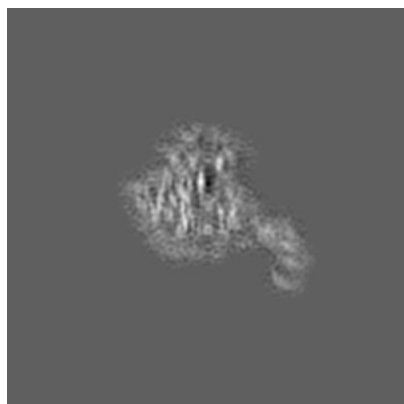


Z

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

6.2 Central slices [i](#)

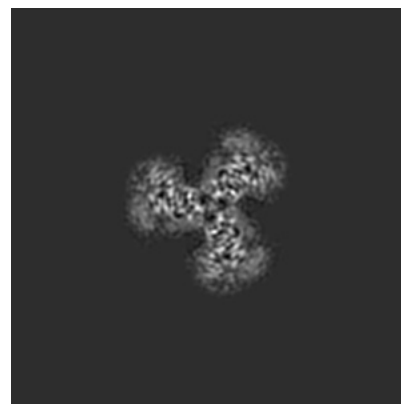
6.2.1 Primary map



X Index: 80



Y Index: 80

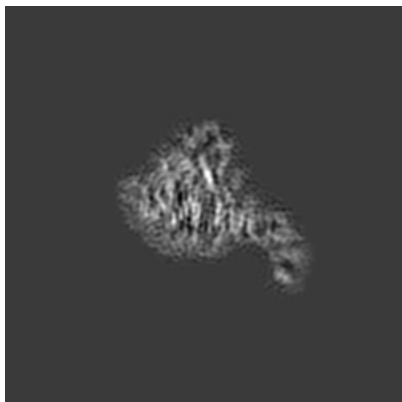


Z Index: 80

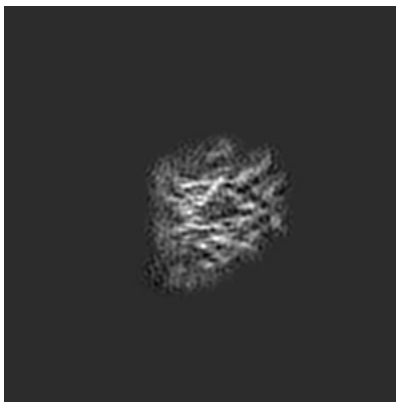
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

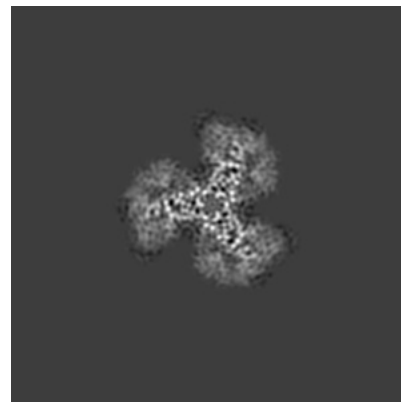
6.3.1 Primary map



X Index: 83



Y Index: 85

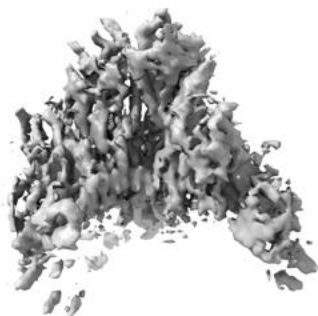


Z Index: 74

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

6.4 Orthogonal surface views [i](#)

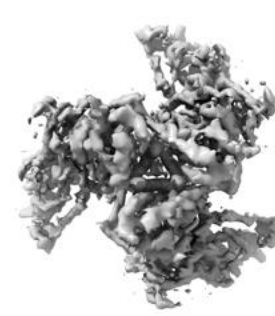
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.102. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

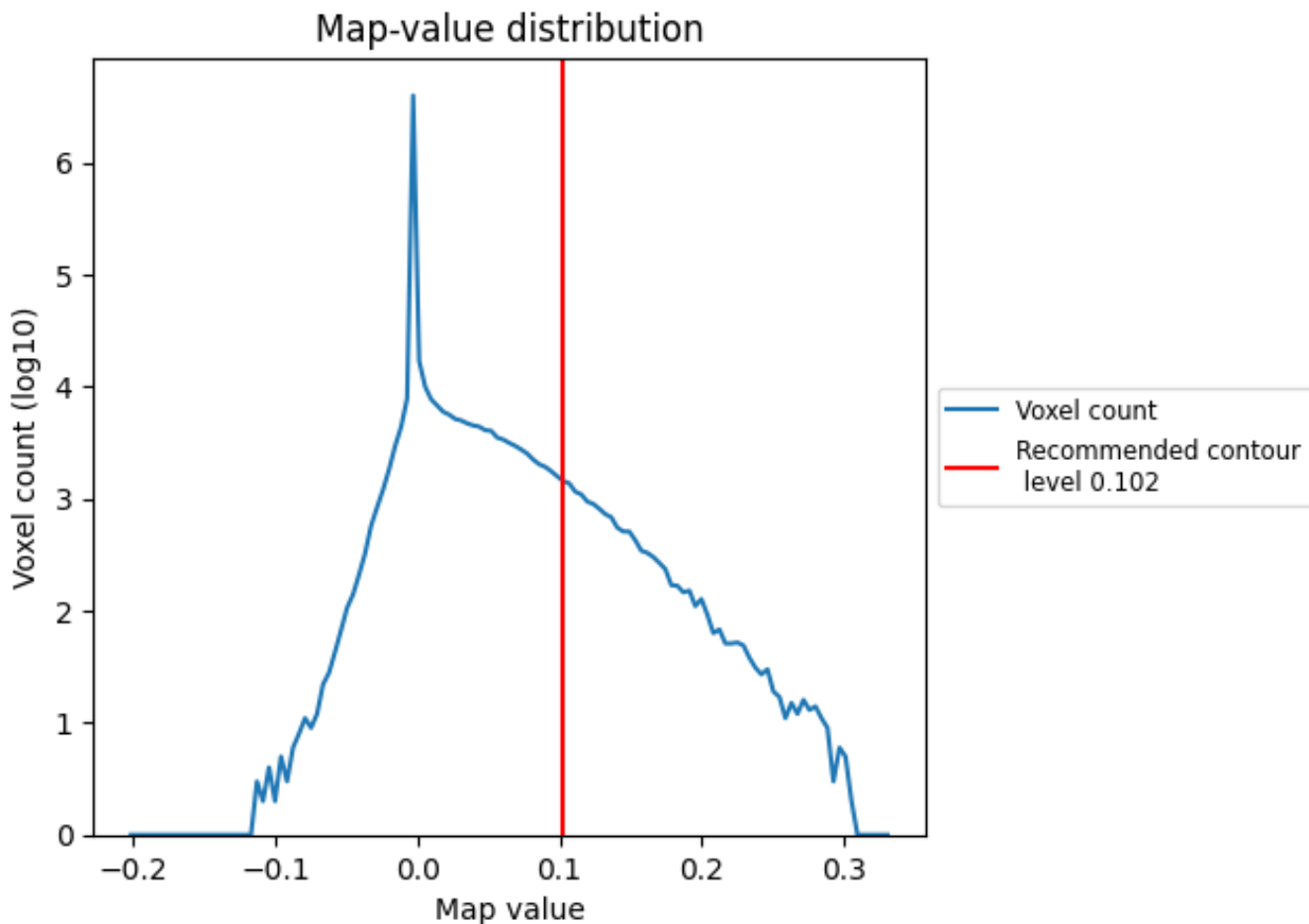
6.5 Mask visualisation

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

7 Map analysis [i](#)

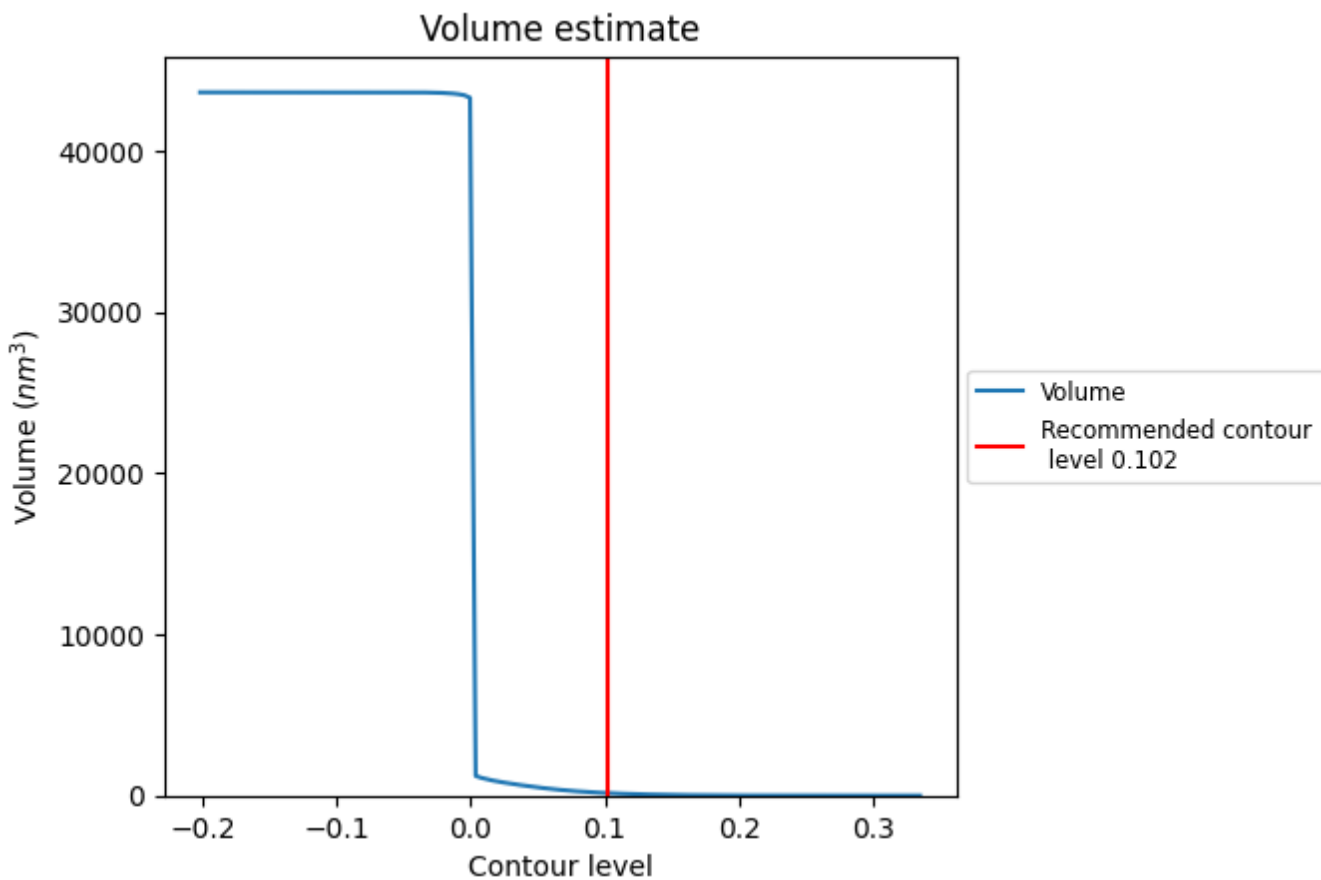
This section contains the results of statistical analysis of the map.

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.

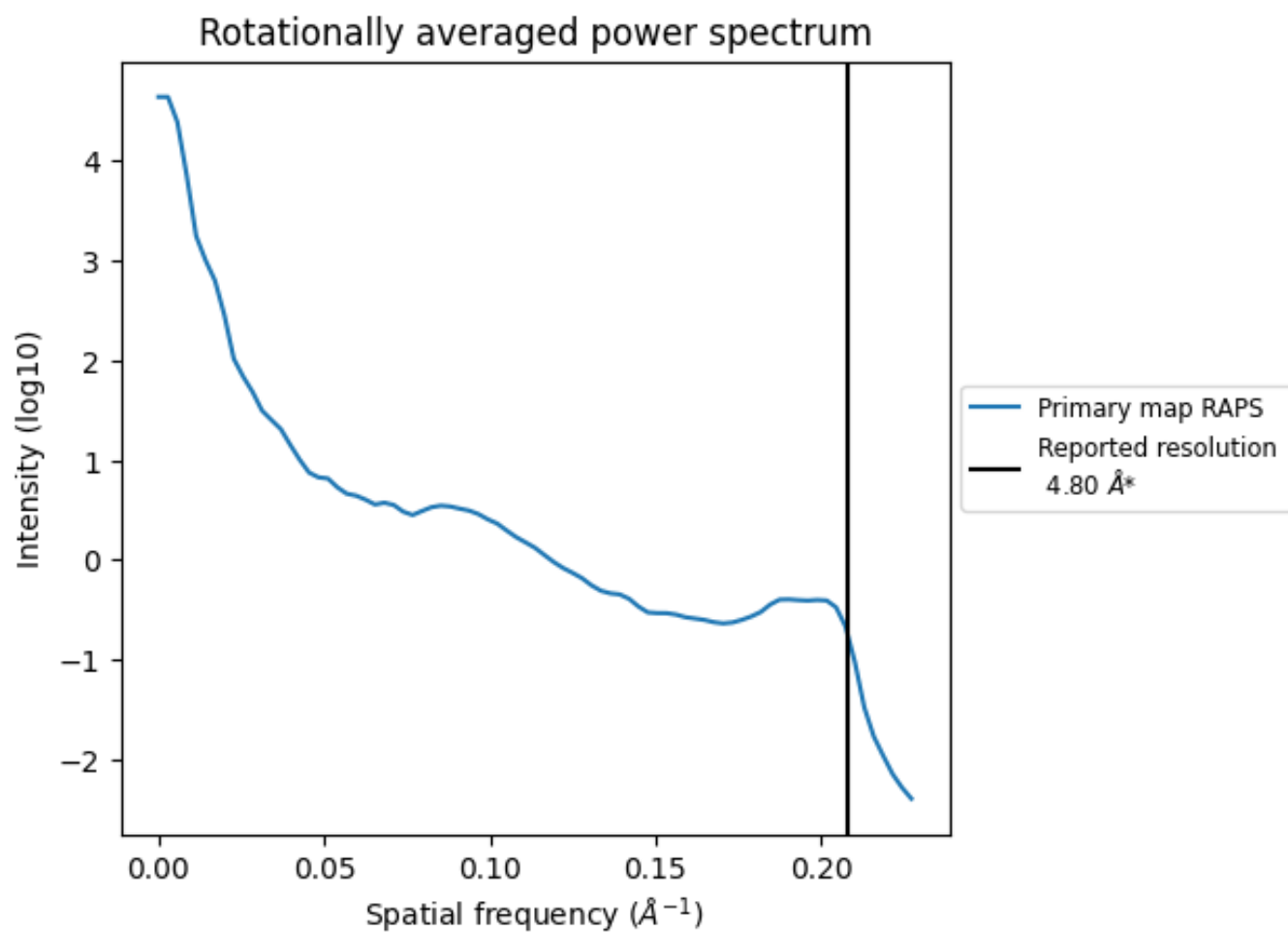
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm^3 ; this corresponds to an approximate mass of 138 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](#)

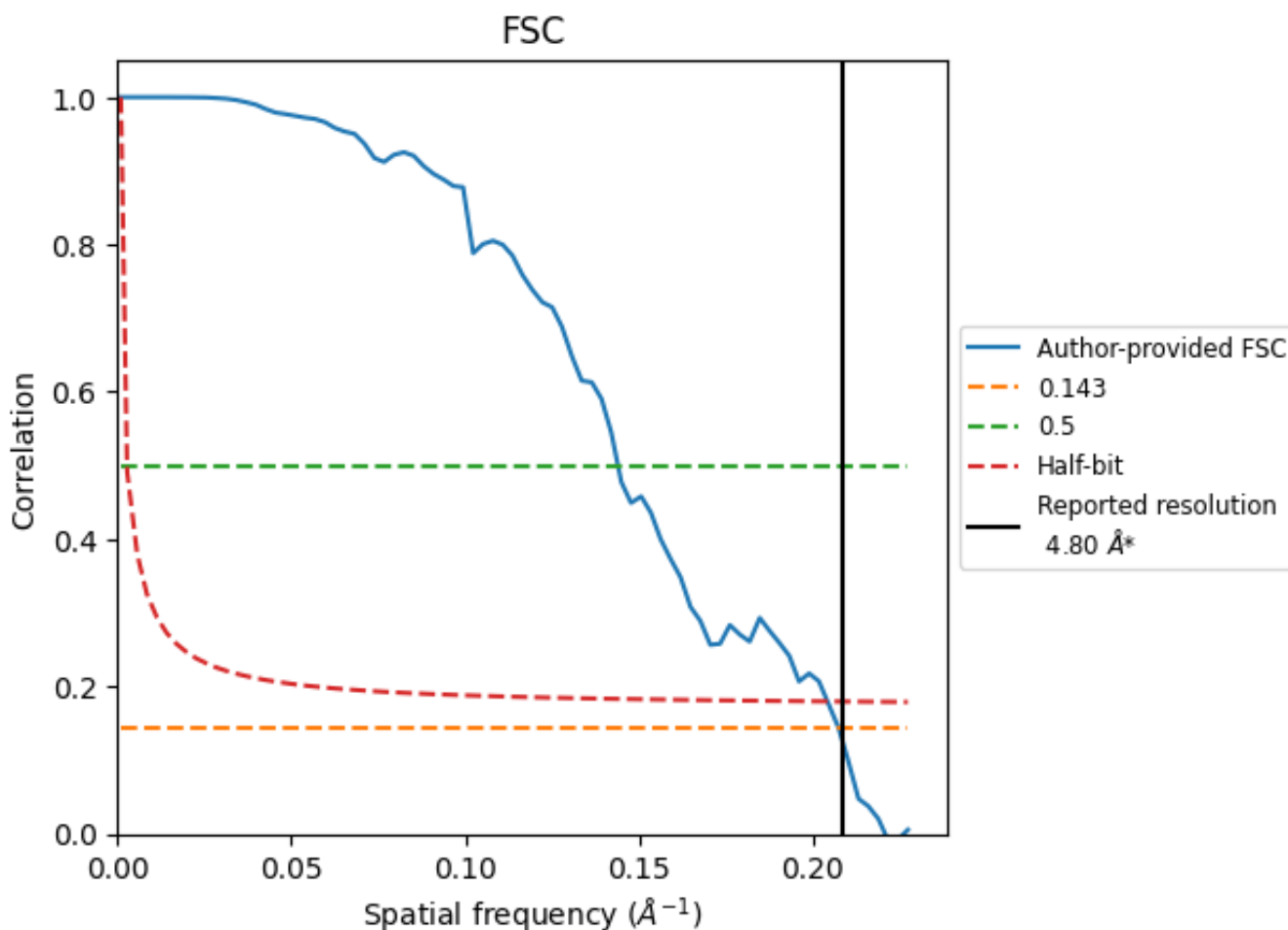


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

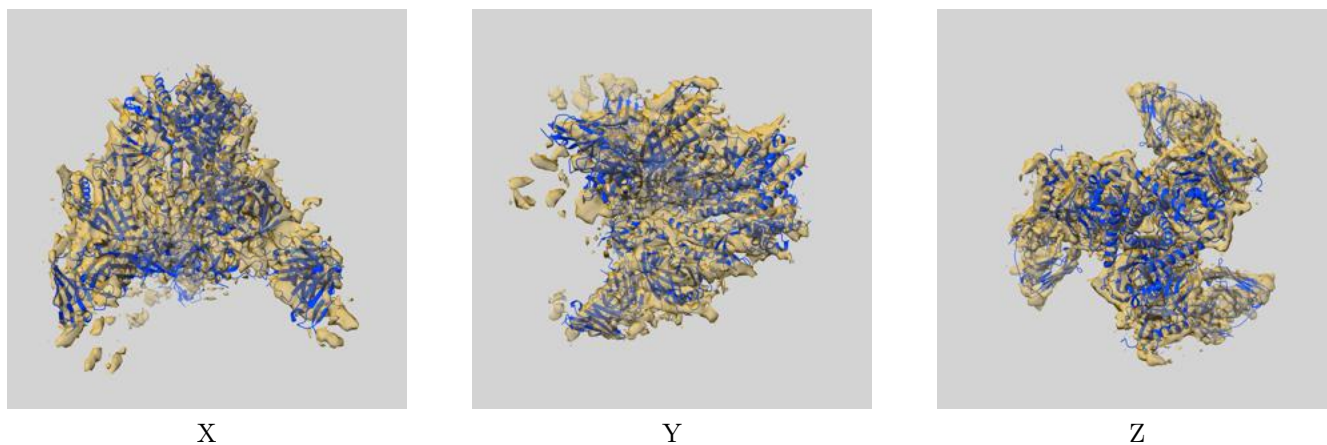
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.82	6.95	4.90
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

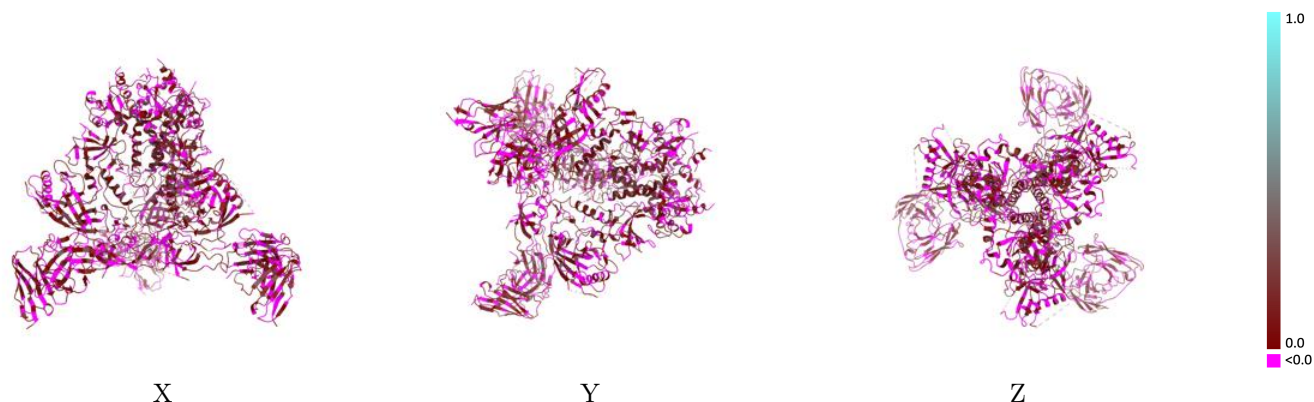
This section contains information regarding the fit between EMDB map EMD-9166 and PDB model 6MN7. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



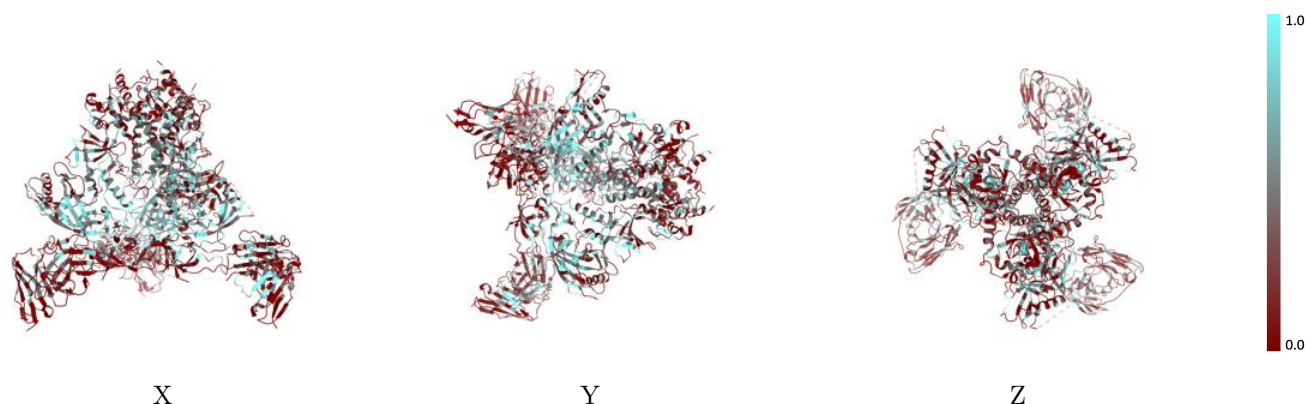
The images above show the 3D surface view of the map at the recommended contour level 0.102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



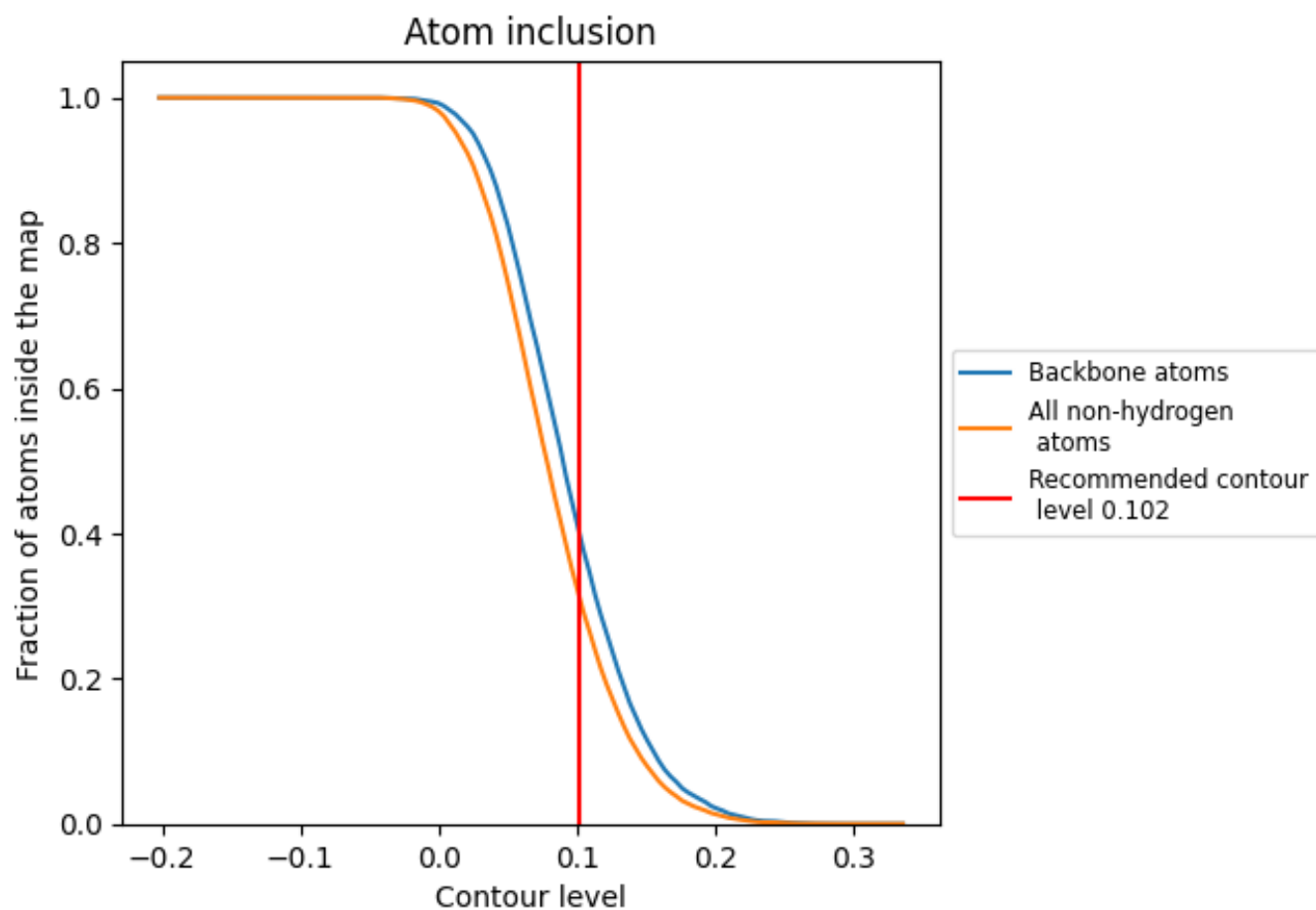
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.102).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 31% 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 (0.102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3087	 0.0490
0	 0.3103	 0.0330
1	 0.2143	 0.0520
2	 0.1795	 -0.0490
3	 0.0000	 -0.0320
4	 0.1786	 0.1260
5	 0.0714	 0.1900
6	 0.0357	 0.1920
7	 0.0357	 0.2130
A	 0.4082	 0.0650
B	 0.2890	 0.0540
C	 0.3965	 0.0560
D	 0.4082	 0.0640
E	 0.2927	 0.0560
F	 0.2871	 0.0610
G	 0.2172	 0.0300
H	 0.2195	 0.0250
I	 0.2184	 0.0310
J	 0.0000	 -0.0140
K	 0.0000	 -0.0160
L	 0.0000	 -0.0170
M	 0.0000	 -0.0370
N	 0.0000	 0.0840
O	 0.1071	 -0.0330
P	 0.1084	 0.0370
Q	 0.0000	 -0.0010
R	 0.1967	 -0.0440
S	 0.1687	 0.1300
T	 0.3621	 0.0550
U	 0.1786	 0.0160
V	 0.1795	 -0.0960
W	 0.0000	 -0.0200
X	 0.1071	 0.0870
Y	 0.1071	 0.1700
Z	 0.0000	 0.1910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.0000	-0.0160
b	0.0000	-0.0220
c	0.0000	-0.0770
d	0.0000	-0.0100
e	0.0000	0.0600
f	0.0357	-0.0770
g	0.1205	0.0140
h	0.0000	0.0450
i	0.1967	-0.0510
j	0.1687	0.1170
k	0.3276	0.0780
l	0.2143	0.0340
m	0.1282	-0.1200
n	0.0000	0.0080
o	0.1071	0.0450
p	0.1429	0.1870
q	0.0000	-0.0140
r	0.0000	-0.0760
s	0.0000	-0.0600
t	0.0000	0.0220
u	0.0000	0.0520
v	0.0357	-0.0940
w	0.1084	0.0260
x	0.0000	0.0430
y	0.2131	-0.0330
z	0.1566	0.1090