



# wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 08:59 PM UTC

PDB ID : 7PC2 / pdb\_00007pc2  
EMDB ID : EMD-13316  
Title : HIV-1 Env (BG505 SOSIP.664) in complex with the IgA bNAbs 7-269 and the antibody 3BNC117.  
Authors : Fernandez, I.; Bontems, F.; Pehau-Arnaudet, G.; Rey, F.  
Deposited on : 2021-08-03  
Resolution : 2.80 Å (reported)  
Based on initial model : 5V8M

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

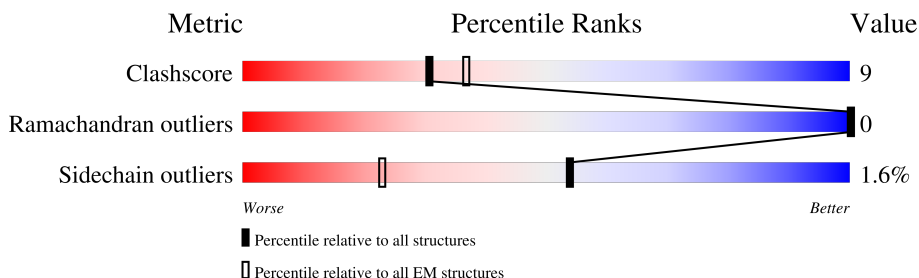
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	240	<div> <div>48%</div> <div> <div></div> <div>36%</div> <div>18%</div> <div>46%</div> </div> </div>
1	O	240	<div> <div>36%</div> <div> <div></div> <div>38%</div> <div>17%</div> <div>46%</div> </div> </div>
1	Q	240	<div> <div>41%</div> <div> <div></div> <div>34%</div> <div>20%</div> <div>46%</div> </div> </div>
2	N	215	<div> <div>37%</div> <div> <div></div> <div>38%</div> <div>12%</div> <div>50%</div> </div> </div>
2	P	215	<div> <div>33%</div> <div> <div></div> <div>35%</div> <div>15%</div> <div>50%</div> </div> </div>
2	R	215	<div> <div>40%</div> <div> <div></div> <div>37%</div> <div>13%</div> <div>50%</div> </div> </div>
3	A	481	<div> <div>65%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
3	B	481	<div> <div>62%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	C	481	
4	D	153	
4	E	153	
4	F	153	
5	G	226	
5	I	226	
5	K	226	
6	H	206	
6	J	206	
6	L	206	
7	4	2	
7	7	2	
7	8	2	
7	9	2	
7	S	2	
7	T	2	
7	U	2	
7	V	2	
7	Z	2	
7	d	2	
7	g	2	
7	h	2	
7	i	2	
7	j	2	
7	k	2	

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Mol	Chain	Length	Quality of chain
7	p	2	100% 
7	v	2	100% 
7	w	2	50% 
7	x	2	100% 
8	W	9	78% 
8	s	9	89% 
8	y	9	89% 
9	X	8	100% 
9	l	8	100% 
9	z	8	75% 
10	0	3	100% 
10	2	3	67% 
10	3	3	100% 
10	Y	3	67% 
10	c	3	100% 
10	f	3	100% 
10	m	3	100% 
10	o	3	67% 
10	t	3	67% 
10	u	3	100% 
11	6	11	82% 
11	a	11	82% 
11	r	11	64% 
12	b	7	71% 
13	1	5	100% 

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Mol	Chain	Length	Quality of chain
13	e	5	<div><div></div><div>40%</div><div>60%</div><div>40%</div></div>
13	n	5	<div><div></div><div>100%</div><div>60%</div><div>40%</div></div>
14	5	8	<div><div></div><div>62%</div><div>12%</div><div>75%</div><div>12%</div></div>
14	q	8	<div><div></div><div>62%</div><div>12%</div><div>88%</div></div>

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 27063 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 7-269 IgA Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		
1	M	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		
1	Q	130	Total	C	N	O	S	0	0
			1031	646	181	195	9		

- Molecule 2 is a protein called 7-269 IgA Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	108	Total	C	N	O	S	0	0
			821	515	140	163	3		
2	N	108	Total	C	N	O	S	0	0
			821	515	140	163	3		
2	R	108	Total	C	N	O	S	0	0
			821	515	140	163	3		

- Molecule 3 is a protein called gp120, BG505 SOSIP.664 T332N.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		
3	B	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		
3	C	445	Total	C	N	O	S	0	0
			3499	2195	618	658	28		

- Molecule 4 is a protein called gp41 BG505 T332N SOSIP.664.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
4	F	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		

- Molecule 5 is a protein called 3BNC IgG Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
5	G	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
5	I	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 6 is a protein called 3BNC117 IgG Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
6	H	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
6	J	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



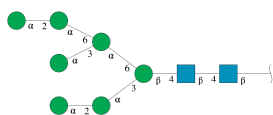
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	k	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		
7	x	2	Total	C	N	O	0	0
			28	16	2	10		
7	4	2	Total	C	N	O	0	0
			28	16	2	10		
7	7	2	Total	C	N	O	0	0
			28	16	2	10		
7	8	2	Total	C	N	O	0	0
			28	16	2	10		
7	9	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	W	9	Total	C	N	O	0	0
			105	58	2	45		

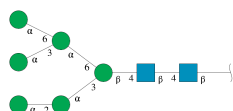
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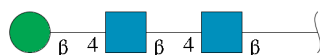
Mol	Chain	Residues	Atoms				AltConf	Trace
8	s	9	Total	C	N	O	0	0
			105	58	2	45		
8	y	9	Total	C	N	O	0	0
			105	58	2	45		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	8	Total	C	N	O	0	0
			94	52	2	40		
9	l	8	Total	C	N	O	0	0
			94	52	2	40		
9	z	8	Total	C	N	O	0	0
			94	52	2	40		

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



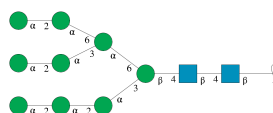
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	3	Total	C	N	O	0	0
			39	22	2	15		
10	c	3	Total	C	N	O	0	0
			39	22	2	15		
10	f	3	Total	C	N	O	0	0
			39	22	2	15		
10	m	3	Total	C	N	O	0	0
			39	22	2	15		
10	o	3	Total	C	N	O	0	0
			39	22	2	15		
10	t	3	Total	C	N	O	0	0
			39	22	2	15		

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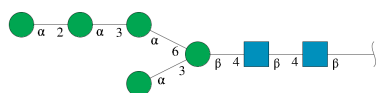
Mol	Chain	Residues	Atoms				AltConf	Trace
10	u	3	Total	C	N	O	0	0
			39	22	2	15		
10	0	3	Total	C	N	O	0	0
			39	22	2	15		
10	2	3	Total	C	N	O	0	0
			39	22	2	15		
10	3	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	11	Total	C	N	O	0	0
			127	70	2	55		
11	r	11	Total	C	N	O	0	0
			127	70	2	55		
11	6	11	Total	C	N	O	0	0
			127	70	2	55		

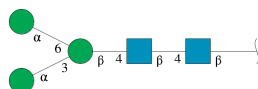
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	b	7	Total	C	N	O	0	0
			83	46	2	35		

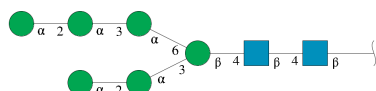
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	5	Total	C	N	O	0	0
			61	34	2	25		
13	n	5	Total	C	N	O	0	0
			61	34	2	25		
13	1	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	q	8	Total	C	N	O	0	0
			94	52	2	40		
14	5	8	Total	C	N	O	0	0
			94	52	2	40		

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



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

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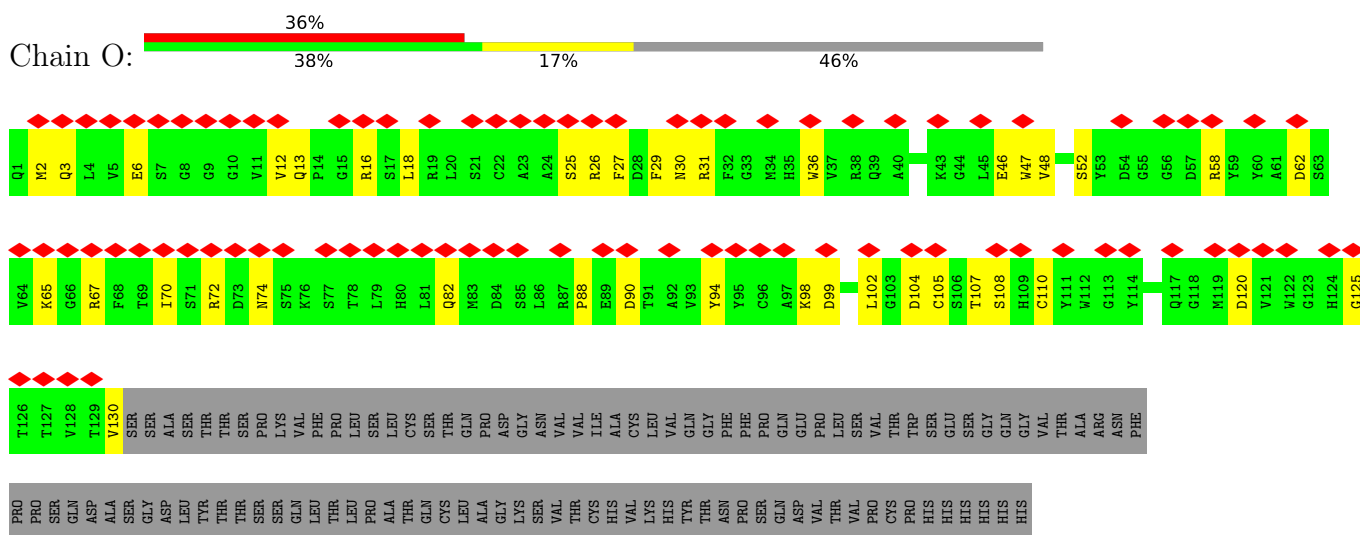
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Mol	Chain	Residues	Atoms				AltConf
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	

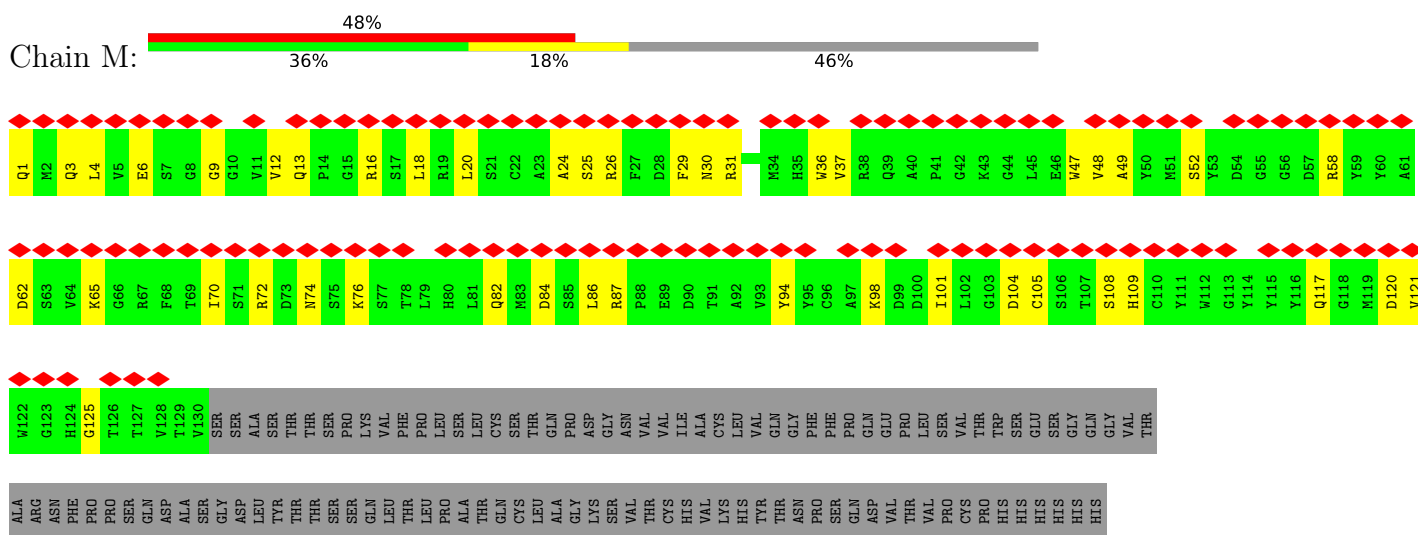
### 3 Residue-property plots

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.

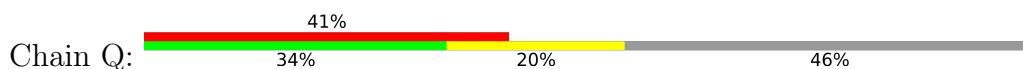
- Molecule 1: 7-269 IgA Fab heavy chain



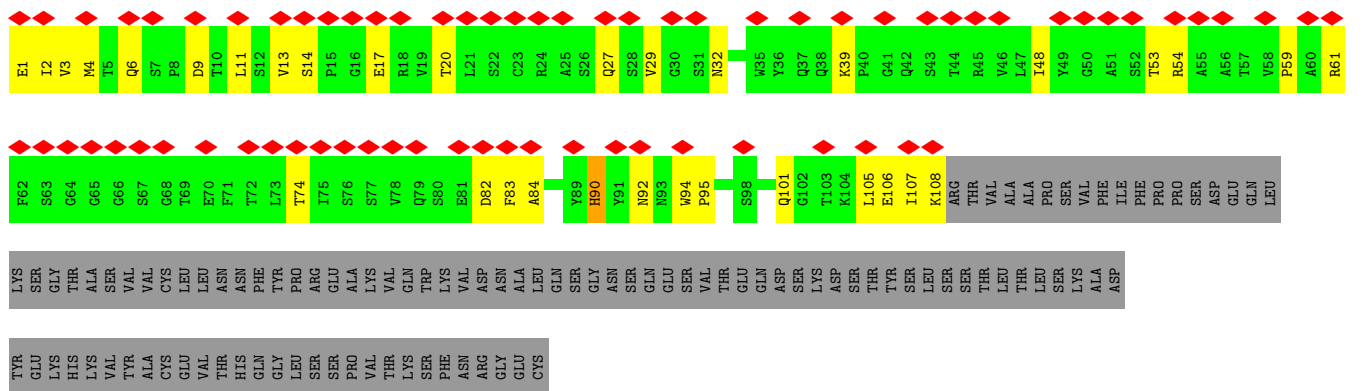
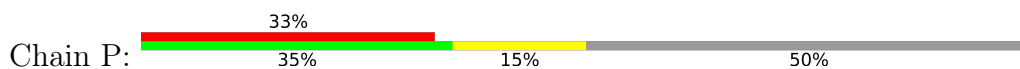
- Molecule 1: 7-269 IgA Fab heavy chain



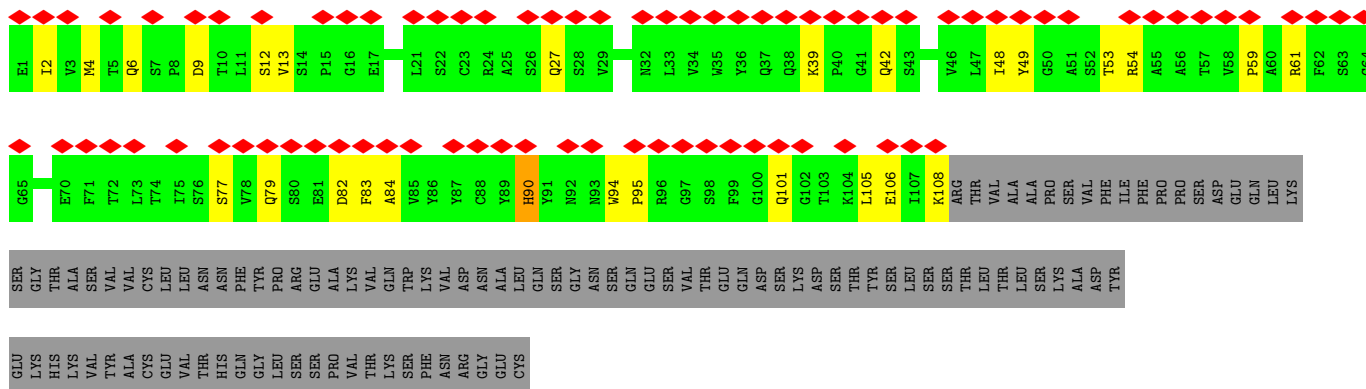
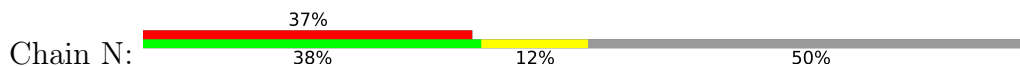
- Molecule 1: 7-269 IgA Fab heavy chain



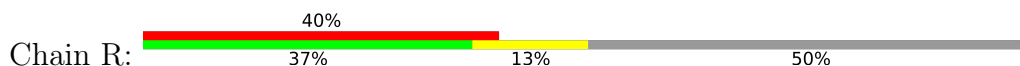
- Molecule 2: 7-269 IgA Fab light chain

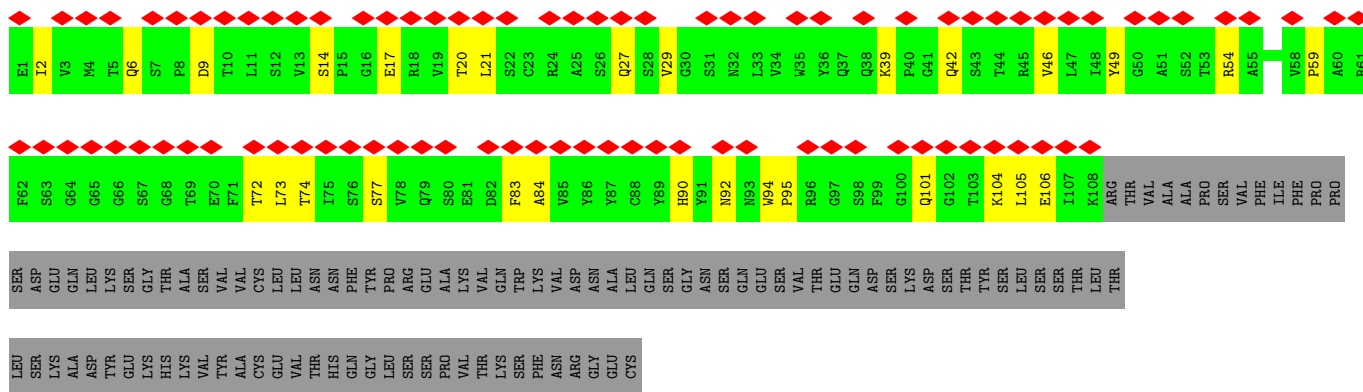


- Molecule 2: 7-269 IgA Fab light chain

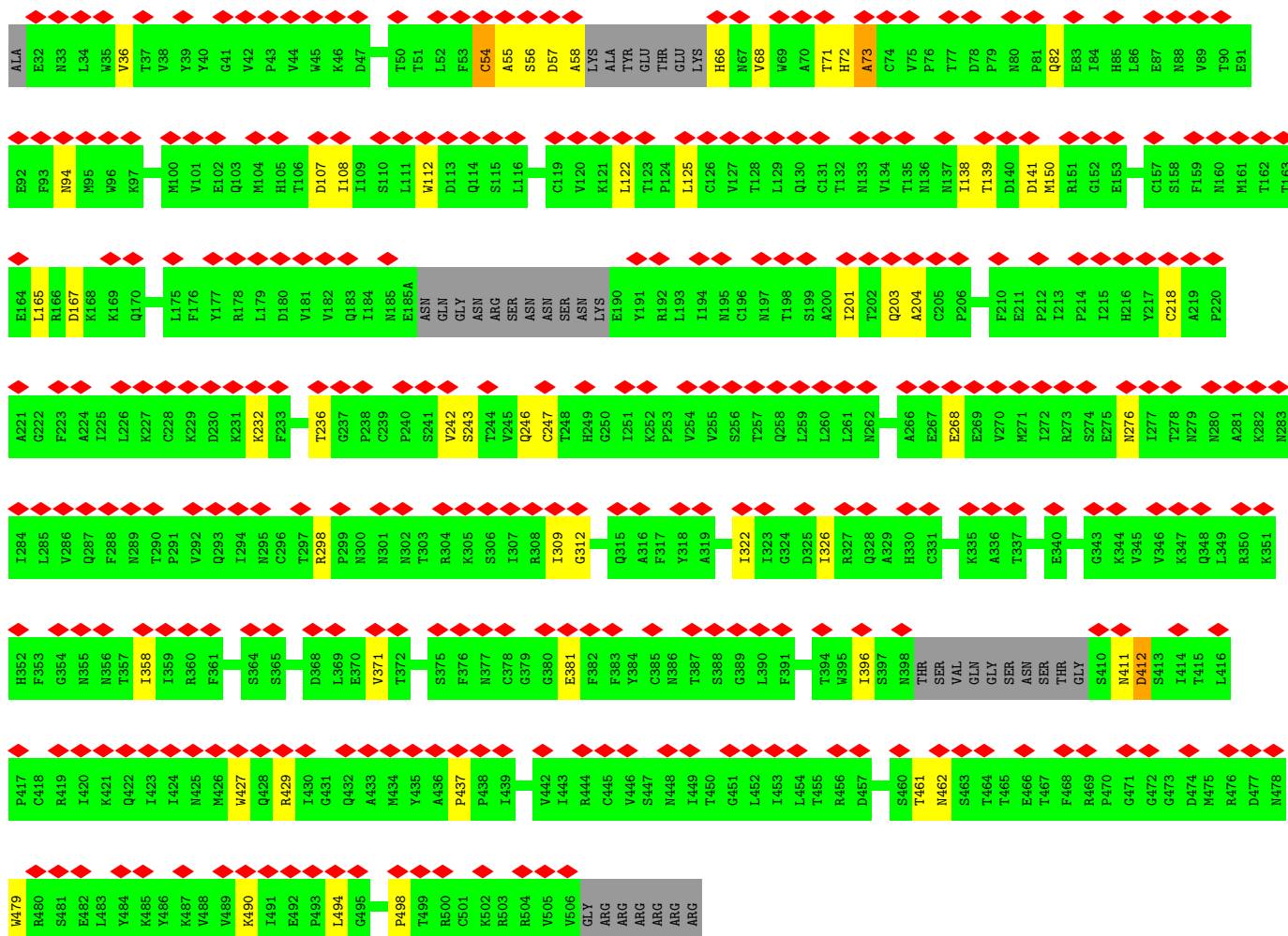
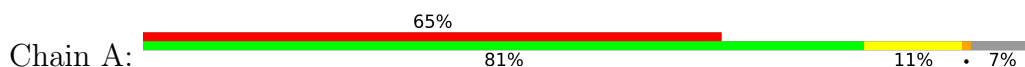


- Molecule 2: 7-269 IgA Fab light chain

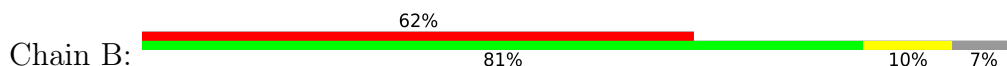




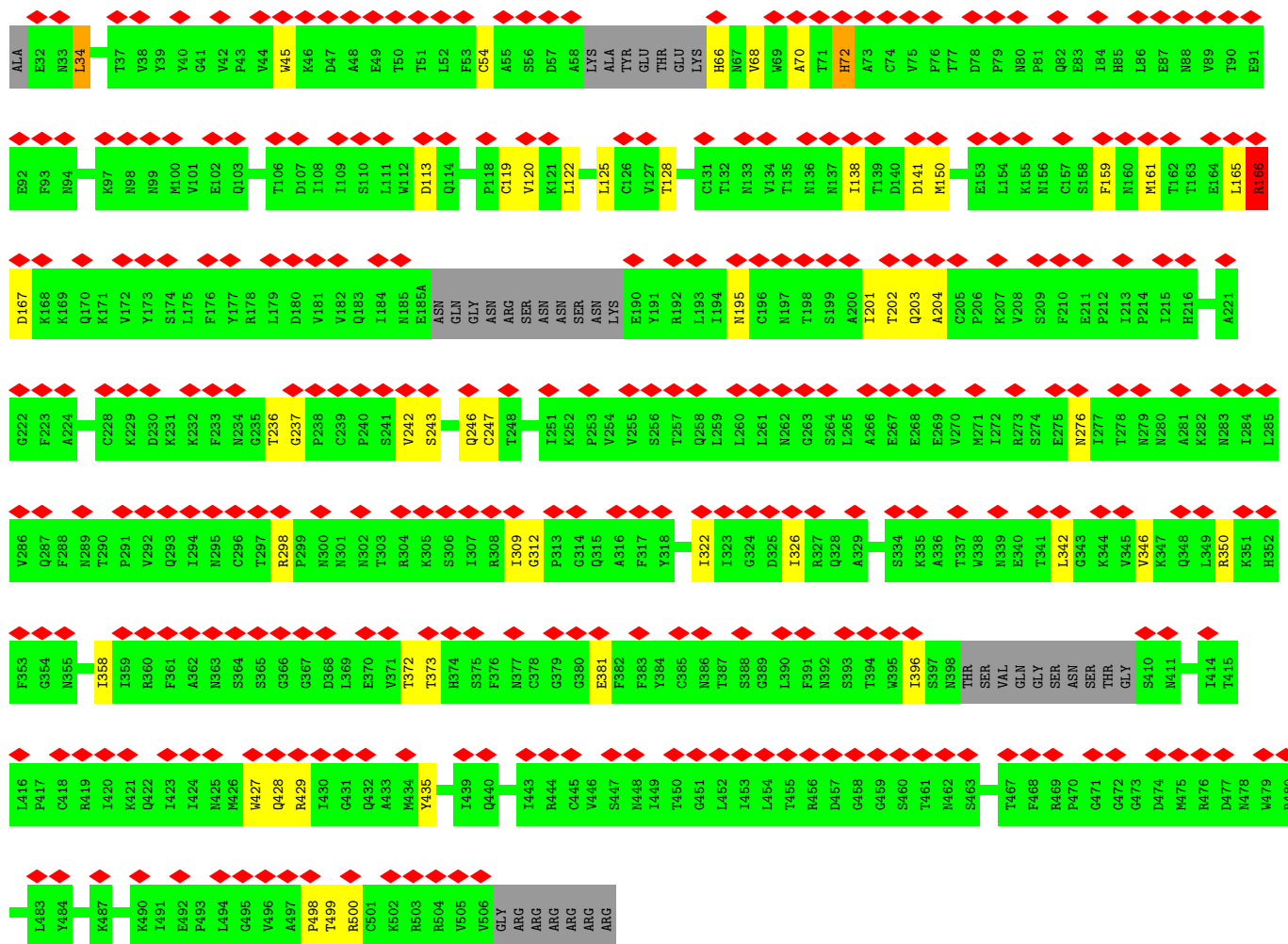
• Molecule 3: gp120, BG505 SOSIP.664 T332N



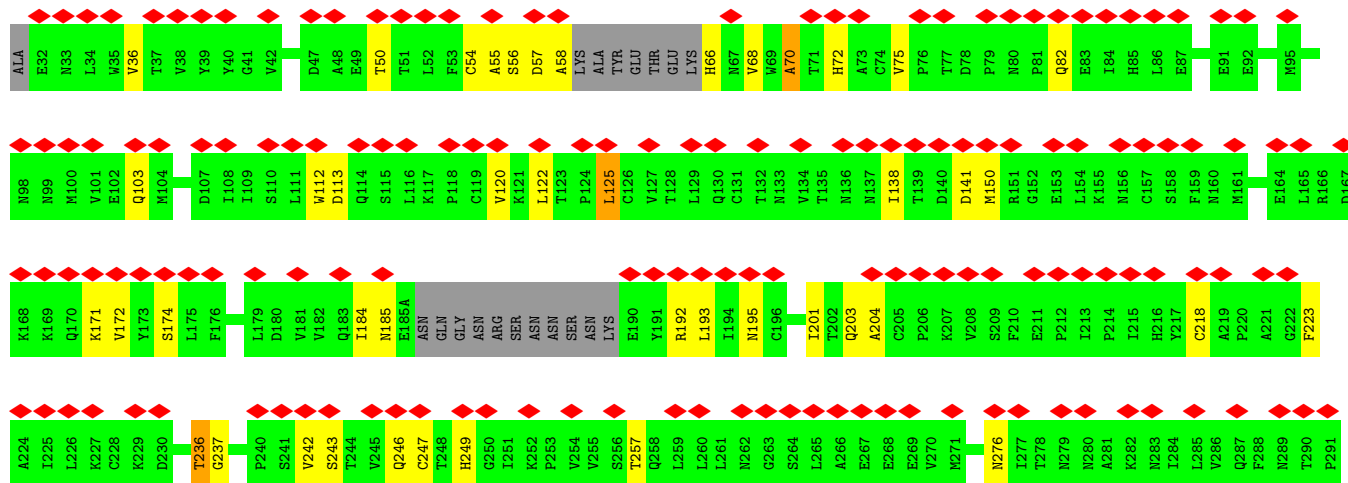
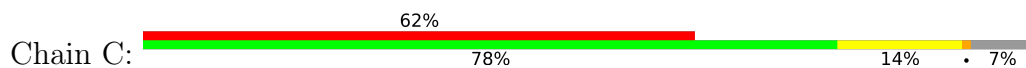
• Molecule 3: gp120, BG505 SOSIP.664 T332N

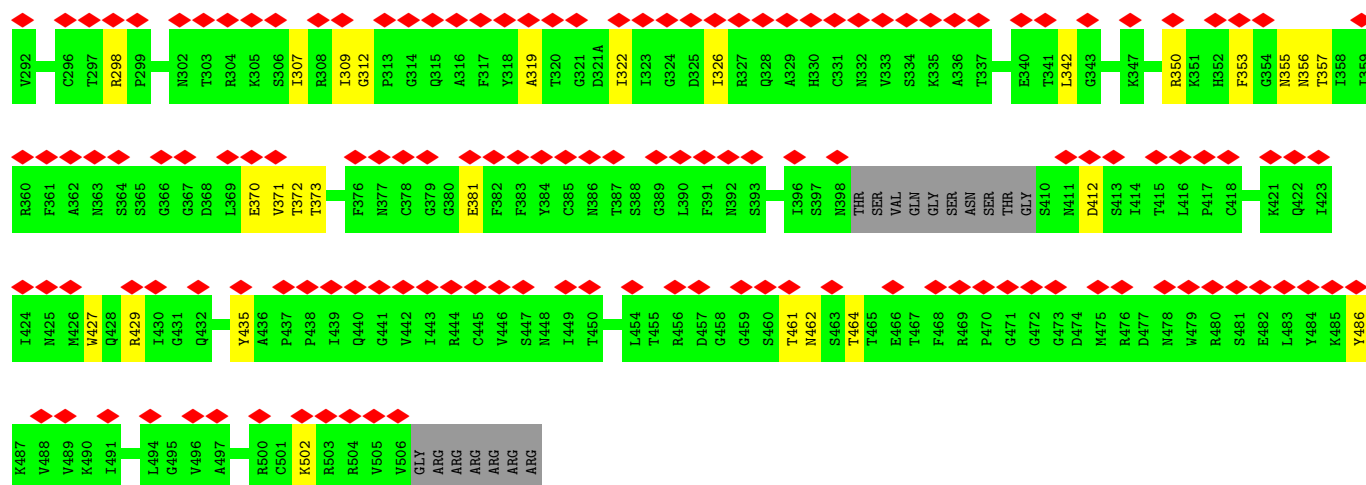




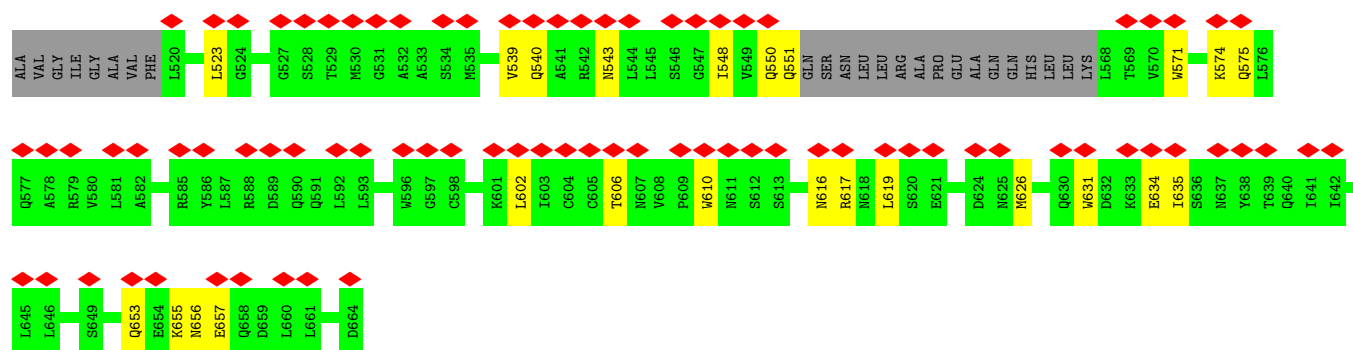


• Molecule 3: gp120, BG505 SOSIP.664 T332N

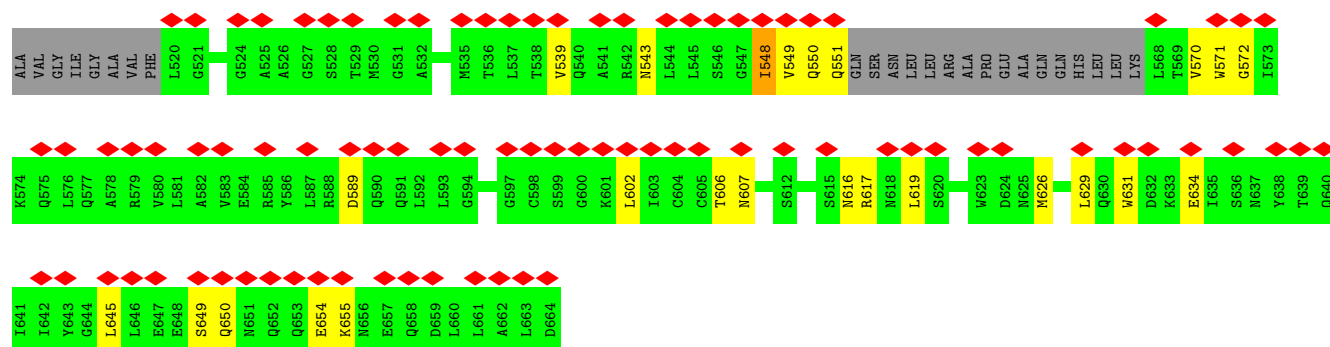




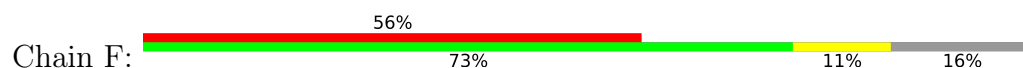
• Molecule 4: gp41 BG505 T332N SOSIP.664

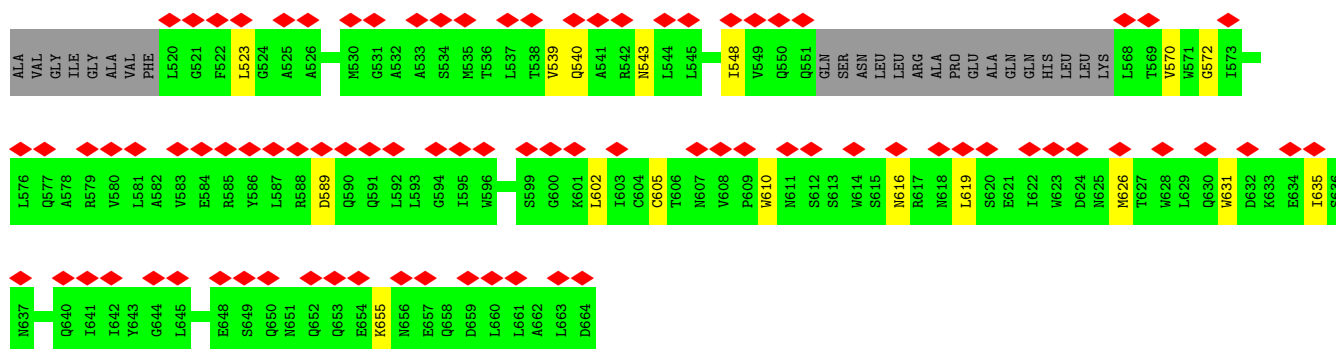


• Molecule 4: gp41 BG505 T332N SOSIP.664

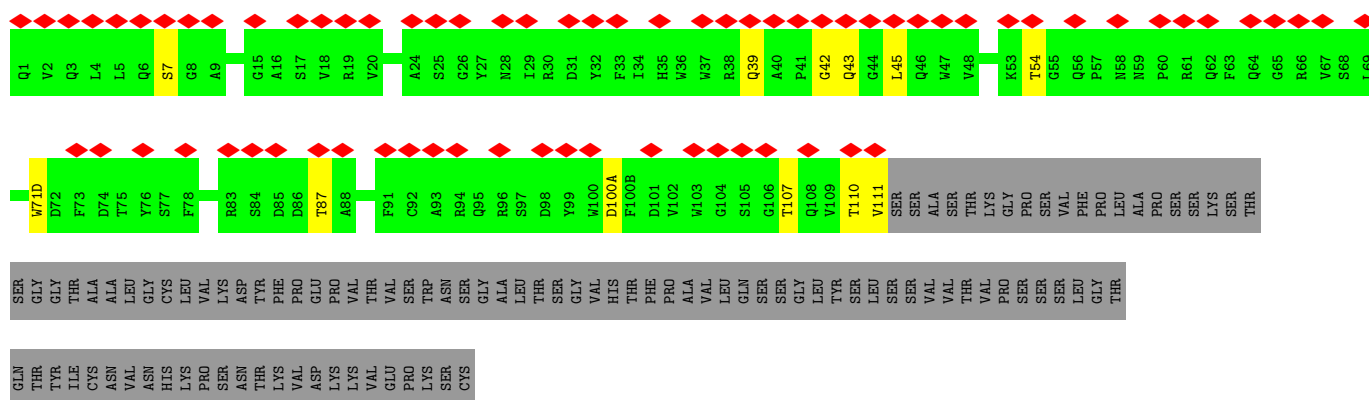


• Molecule 4: gp41 BG505 T332N SOSIP.664

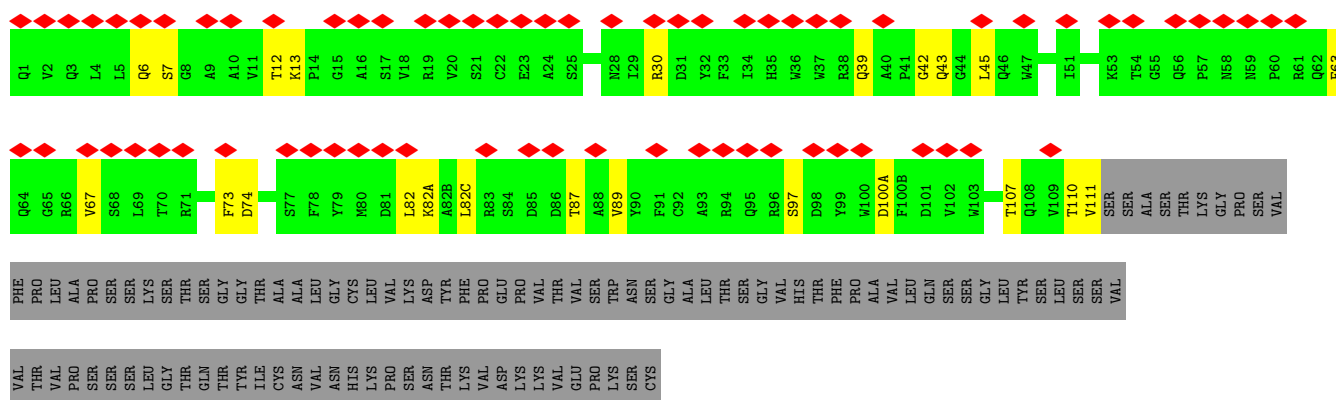
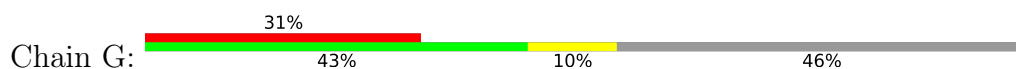




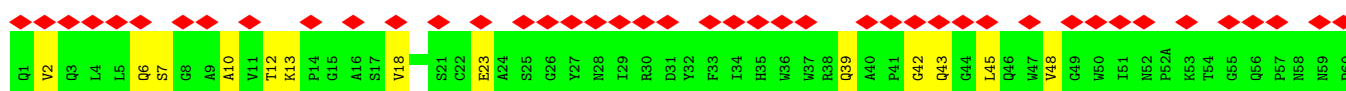
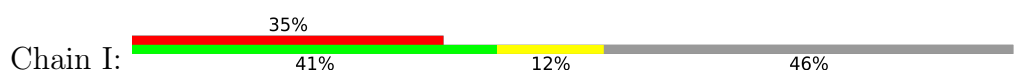
• Molecule 5: 3BNC IgG Fab heavy chain



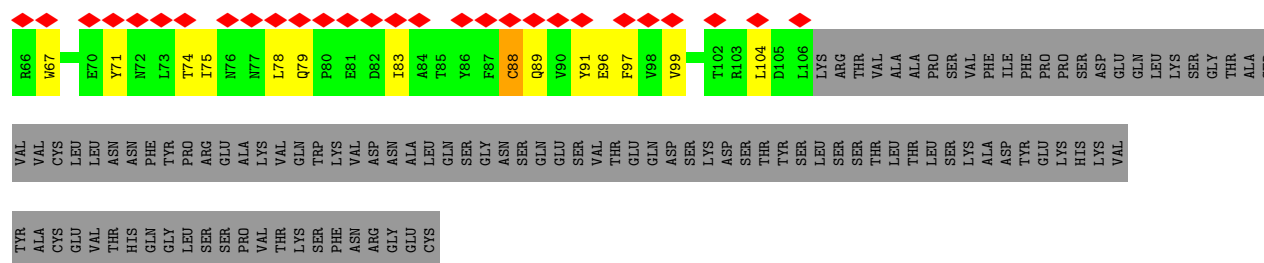
• Molecule 5: 3BNC IgG Fab heavy chain



• Molecule 5: 3BNC IgG Fab heavy chain







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



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



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



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



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





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



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



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



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



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



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



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



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



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



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



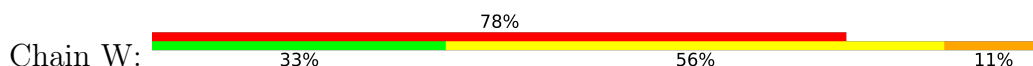
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



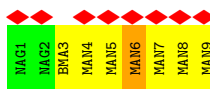
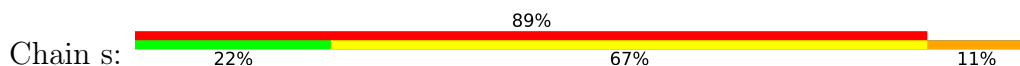
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



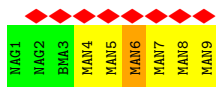
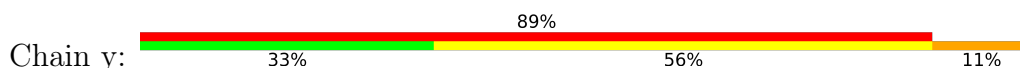
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



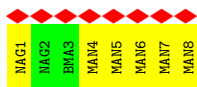
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



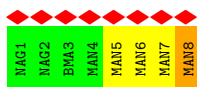
1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



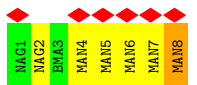
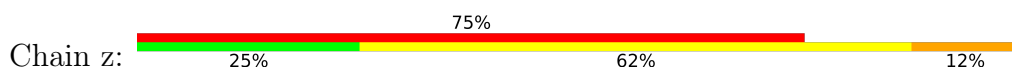
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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





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



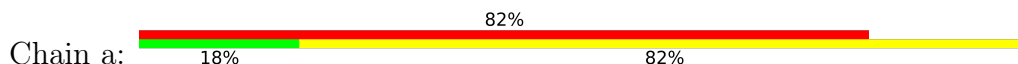
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

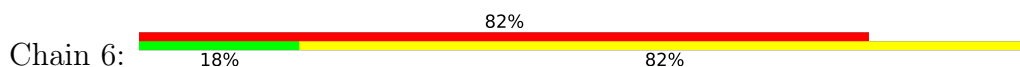


- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

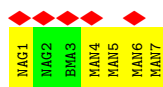




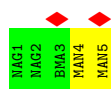
- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



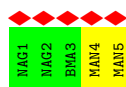
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 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

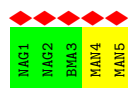


- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 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 14:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose



- Molecule 14:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	115394	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.634	Depositor
Minimum map value	-0.659	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	357.0, 357.0, 357.0	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	M	0.57	0/1059	0.76	2/1432 (0.1%)
1	O	0.19	0/1059	0.46	0/1432
1	Q	0.20	0/1059	0.47	0/1432
2	N	0.19	0/840	0.42	0/1142
2	P	0.19	0/840	0.41	0/1142
2	R	0.19	0/840	0.41	0/1142
3	A	0.47	1/3569 (0.0%)	0.47	4/4844 (0.1%)
3	B	0.61	4/3569 (0.1%)	0.52	3/4844 (0.1%)
3	C	0.53	4/3569 (0.1%)	0.49	1/4844 (0.0%)
4	D	0.24	0/1041	0.35	0/1412
4	E	0.24	0/1041	0.37	0/1412
4	F	0.25	0/1041	0.39	0/1412
5	G	0.26	0/1017	0.42	0/1386
5	I	0.26	0/1017	0.41	0/1386
5	K	0.26	0/1017	0.40	0/1386
6	H	0.28	0/798	0.85	5/1080 (0.5%)
6	J	0.19	0/798	0.35	0/1080
6	L	0.19	0/798	0.35	0/1080
All	All	0.41	9/24972 (0.0%)	0.48	15/33888 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	165	LEU	C-O	-6.14	1.16	1.24
3	B	166	ARG	C-O	-5.98	1.16	1.24
3	A	68	VAL	C-O	-5.52	1.17	1.24
3	C	68	VAL	C-O	-5.33	1.17	1.24
3	C	55	ALA	C-O	-5.32	1.17	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	7	SER	N-CA-C	17.23	147.88	109.81
6	H	7	SER	CB-CA-C	-15.00	80.62	110.17
1	M	108	SER	N-CA-C	14.57	132.09	112.13
1	M	108	SER	CB-CA-C	-10.06	94.93	110.83
3	B	68	VAL	N-CA-C	7.69	119.39	110.62

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1031	0	960	39	0
1	O	1031	0	958	32	0
1	Q	1031	0	958	39	0
2	N	821	0	788	18	0
2	P	821	0	788	20	0
2	R	821	0	788	20	0
3	A	3499	0	3427	43	0
3	B	3499	0	3425	41	0
3	C	3499	0	3429	52	0
4	D	1024	0	1005	19	0
4	E	1024	0	1005	19	0
4	F	1024	0	1005	10	0
5	G	985	0	919	11	0
5	I	985	0	919	16	0
5	K	985	0	919	9	0
6	H	783	0	761	47	0
6	J	783	0	761	21	0
6	L	783	0	761	23	0
7	4	28	0	25	0	0
7	7	28	0	25	1	0
7	8	28	0	25	2	0
7	9	28	0	25	1	0
7	S	28	0	25	1	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	28	0	25	0	0
7	Z	28	0	25	0	0
7	d	28	0	25	1	0
7	g	28	0	25	1	0
7	h	28	0	25	0	0
7	i	28	0	25	0	0
7	j	28	0	25	0	0
7	k	28	0	25	1	0
7	p	28	0	25	0	0
7	v	28	0	25	0	0
7	w	28	0	25	0	0
7	x	28	0	25	0	0
8	W	105	0	88	1	0
8	s	105	0	88	1	0
8	y	105	0	88	1	0
9	X	94	0	79	2	0
9	l	94	0	79	1	0
9	z	94	0	79	2	0
10	0	39	0	34	0	0
10	2	39	0	34	0	0
10	3	39	0	34	0	0
10	Y	39	0	34	0	0
10	c	39	0	34	1	0
10	f	39	0	34	0	0
10	m	39	0	34	0	0
10	o	39	0	34	0	0
10	t	39	0	34	0	0
10	u	39	0	34	1	0
11	6	127	0	106	0	0
11	a	127	0	106	0	0
11	r	127	0	106	0	0
12	b	83	0	70	1	0
13	1	61	0	52	0	0
13	e	61	0	52	0	0
13	n	61	0	52	0	0
14	5	94	0	79	1	0
14	q	94	0	79	1	0
15	A	70	0	65	1	0
15	B	70	0	65	0	0
15	C	56	0	52	0	0
15	D	28	0	26	0	0
15	E	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	F	28	0	26	0	0
All	All	27063	0	25854	465	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 465 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:62:PHE:CE2	6:J:75:ILE:HD12	1.67	1.29
6:H:62:PHE:CE2	6:H:75:ILE:HD12	1.82	1.14
1:M:104:ASP:OD1	1:M:105:CYS:N	1.81	1.13
3:B:499:THR:HG22	3:B:500:ARG:H	1.15	1.06
6:H:7:SER:HB3	6:H:8:PRO:CD	1.87	1.04

There are no symmetry-related clashes.

## 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	M	128/240 (53%)	114 (89%)	14 (11%)	0	100	100
1	O	128/240 (53%)	115 (90%)	13 (10%)	0	100	100
1	Q	128/240 (53%)	117 (91%)	11 (9%)	0	100	100
2	N	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
2	P	106/215 (49%)	97 (92%)	9 (8%)	0	100	100
2	R	106/215 (49%)	98 (92%)	8 (8%)	0	100	100
3	A	433/481 (90%)	398 (92%)	35 (8%)	0	100	100
3	B	433/481 (90%)	405 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	433/481 (90%)	405 (94%)	28 (6%)	0	100	100
4	D	125/153 (82%)	113 (90%)	12 (10%)	0	100	100
4	E	125/153 (82%)	114 (91%)	11 (9%)	0	100	100
4	F	125/153 (82%)	111 (89%)	14 (11%)	0	100	100
5	G	119/226 (53%)	112 (94%)	7 (6%)	0	100	100
5	I	119/226 (53%)	111 (93%)	8 (7%)	0	100	100
5	K	119/226 (53%)	112 (94%)	7 (6%)	0	100	100
6	H	92/206 (45%)	83 (90%)	9 (10%)	0	100	100
6	J	92/206 (45%)	86 (94%)	6 (6%)	0	100	100
6	L	92/206 (45%)	86 (94%)	6 (6%)	0	100	100
All	All	3009/4563 (66%)	2773 (92%)	236 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	108/206 (52%)	108 (100%)	0	100	100
1	O	108/206 (52%)	107 (99%)	1 (1%)	70	89
1	Q	108/206 (52%)	107 (99%)	1 (1%)	70	89
2	N	90/187 (48%)	89 (99%)	1 (1%)	65	87
2	P	90/187 (48%)	89 (99%)	1 (1%)	65	87
2	R	90/187 (48%)	89 (99%)	1 (1%)	65	87
3	A	398/428 (93%)	392 (98%)	6 (2%)	57	84
3	B	398/428 (93%)	392 (98%)	6 (2%)	57	84
3	C	398/428 (93%)	394 (99%)	4 (1%)	68	88
4	D	111/129 (86%)	109 (98%)	2 (2%)	51	82
4	E	111/129 (86%)	105 (95%)	6 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	111/129 (86%)	108 (97%)	3 (3%)	39	74
5	G	102/193 (53%)	98 (96%)	4 (4%)	28	64
5	I	102/193 (53%)	98 (96%)	4 (4%)	28	64
5	K	102/193 (53%)	102 (100%)	0	100	100
6	H	86/183 (47%)	85 (99%)	1 (1%)	63	87
6	J	86/183 (47%)	84 (98%)	2 (2%)	44	78
6	L	86/183 (47%)	85 (99%)	1 (1%)	63	87
All	All	2685/3978 (68%)	2641 (98%)	44 (2%)	54	83

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	654	GLU
5	G	82(C)	LEU
4	F	548	ILE
5	G	6	GLN
5	I	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	280	ASN
6	L	79	GLN
3	C	203	GLN
6	L	6	GLN
5	G	43	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

190 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	NAG	0	1	10,3	14,14,15	0.21	0	17,19,21	0.49	0
10	NAG	0	2	10	14,14,15	0.20	0	17,19,21	0.48	0
10	BMA	0	3	10	11,11,12	0.48	0	15,15,17	0.73	0
13	NAG	1	1	3,13	14,14,15	0.38	0	17,19,21	0.43	0
13	NAG	1	2	13	14,14,15	0.31	0	17,19,21	0.47	0
13	BMA	1	3	13	11,11,12	0.56	0	15,15,17	0.68	0
13	MAN	1	4	13	11,11,12	0.61	0	15,15,17	1.08	2 (13%)
13	MAN	1	5	13	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
10	NAG	2	1	10,3	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
10	NAG	2	2	10	14,14,15	0.22	0	17,19,21	0.42	0
10	BMA	2	3	10	11,11,12	0.50	0	15,15,17	0.71	0
10	NAG	3	1	10,3	14,14,15	0.25	0	17,19,21	0.46	0
10	NAG	3	2	10	14,14,15	0.18	0	17,19,21	0.43	0
10	BMA	3	3	10	11,11,12	0.58	0	15,15,17	0.86	0
7	NAG	4	1	3,7	14,14,15	0.19	0	17,19,21	0.60	0
7	NAG	4	2	7	14,14,15	0.27	0	17,19,21	0.45	0
14	NAG	5	1	3,14	14,14,15	0.40	0	17,19,21	1.38	2 (11%)
14	NAG	5	2	14	14,14,15	0.33	0	17,19,21	0.55	0
14	BMA	5	3	14	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
14	MAN	5	4	14	11,11,12	0.59	0	15,15,17	0.94	1 (6%)
14	MAN	5	5	14	11,11,12	0.60	0	15,15,17	1.13	2 (13%)
14	MAN	5	6	14	11,11,12	0.68	0	15,15,17	1.06	1 (6%)
14	MAN	5	7	14	11,11,12	0.83	1 (9%)	15,15,17	1.16	1 (6%)
14	MAN	5	8	14	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
11	NAG	6	1	3,11	14,14,15	0.48	0	17,19,21	0.42	0
11	MAN	6	10	11	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
11	MAN	6	11	11	11,11,12	0.72	1 (9%)	15,15,17	0.91	1 (6%)
11	NAG	6	2	11	14,14,15	0.32	0	17,19,21	0.51	0
11	BMA	6	3	11	11,11,12	0.56	0	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	6	4	11	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
11	MAN	6	5	11	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
11	MAN	6	6	11	11,11,12	0.53	0	15,15,17	1.11	2 (13%)
11	MAN	6	7	11	11,11,12	0.67	0	15,15,17	1.19	2 (13%)
11	MAN	6	8	11	11,11,12	0.57	0	15,15,17	1.17	2 (13%)
11	MAN	6	9	11	11,11,12	0.56	0	15,15,17	0.97	2 (13%)
7	NAG	7	1	6,7	14,14,15	0.22	0	17,19,21	0.40	0
7	NAG	7	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	8	1	6,7	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	8	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	9	1	6,7	14,14,15	0.23	0	17,19,21	0.38	0
7	NAG	9	2	7	14,14,15	0.21	0	17,19,21	0.39	0
7	NAG	S	1	3,7	14,14,15	0.23	0	17,19,21	0.49	0
7	NAG	S	2	7	14,14,15	0.43	0	17,19,21	1.33	2 (11%)
7	NAG	T	1	3,7	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	T	2	7	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	U	1	3,7	14,14,15	0.35	0	17,19,21	0.43	0
7	NAG	U	2	7	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	V	1	3,7	14,14,15	0.43	0	17,19,21	0.48	0
7	NAG	V	2	7	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	W	1	3,8	14,14,15	0.30	0	17,19,21	0.54	0
8	NAG	W	2	8	14,14,15	0.30	0	17,19,21	0.53	0
8	BMA	W	3	8	11,11,12	0.81	0	15,15,17	0.91	0
8	MAN	W	4	8	11,11,12	0.54	0	15,15,17	1.17	2 (13%)
8	MAN	W	5	8	11,11,12	0.56	0	15,15,17	1.06	2 (13%)
8	MAN	W	6	8	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
8	MAN	W	7	8	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
8	MAN	W	8	8	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
8	MAN	W	9	8	11,11,12	0.51	0	15,15,17	1.13	2 (13%)
9	NAG	X	1	9,3	14,14,15	0.37	0	17,19,21	0.44	0
9	NAG	X	2	9	14,14,15	0.17	0	17,19,21	0.44	0
9	BMA	X	3	9	11,11,12	0.55	0	15,15,17	0.68	0
9	MAN	X	4	9	11,11,12	0.66	0	15,15,17	1.21	2 (13%)
9	MAN	X	5	9	11,11,12	0.68	0	15,15,17	0.84	1 (6%)
9	MAN	X	6	9	11,11,12	0.58	0	15,15,17	1.04	2 (13%)
9	MAN	X	7	9	11,11,12	0.57	0	15,15,17	1.05	2 (13%)
9	MAN	X	8	9	11,11,12	0.58	0	15,15,17	0.96	2 (13%)
10	NAG	Y	1	10,3	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	Y	2	10	14,14,15	0.19	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	BMA	Y	3	10	11,11,12	0.52	0	15,15,17	0.72	0
7	NAG	Z	1	3,7	14,14,15	0.20	0	17,19,21	0.59	0
7	NAG	Z	2	7	14,14,15	0.27	0	17,19,21	0.45	0
11	NAG	a	1	3,11	14,14,15	0.50	0	17,19,21	0.41	0
11	MAN	a	10	11	11,11,12	0.82	0	15,15,17	1.45	2 (13%)
11	MAN	a	11	11	11,11,12	0.60	0	15,15,17	1.59	2 (13%)
11	NAG	a	2	11	14,14,15	0.33	0	17,19,21	0.50	0
11	BMA	a	3	11	11,11,12	0.57	0	15,15,17	0.92	1 (6%)
11	MAN	a	4	11	11,11,12	0.74	0	15,15,17	1.21	2 (13%)
11	MAN	a	5	11	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
11	MAN	a	6	11	11,11,12	0.54	0	15,15,17	1.18	2 (13%)
11	MAN	a	7	11	11,11,12	0.68	0	15,15,17	1.19	2 (13%)
11	MAN	a	8	11	11,11,12	0.54	0	15,15,17	1.17	2 (13%)
11	MAN	a	9	11	11,11,12	0.51	0	15,15,17	0.99	2 (13%)
12	NAG	b	1	3,12	14,14,15	0.58	0	17,19,21	0.46	0
12	NAG	b	2	12	14,14,15	0.24	0	17,19,21	0.58	0
12	BMA	b	3	12	11,11,12	0.71	0	15,15,17	0.89	0
12	MAN	b	4	12	11,11,12	0.53	0	15,15,17	1.00	2 (13%)
12	MAN	b	5	12	11,11,12	0.58	0	15,15,17	1.06	2 (13%)
12	MAN	b	6	12	11,11,12	0.64	0	15,15,17	1.07	2 (13%)
12	MAN	b	7	12	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
10	NAG	c	1	10,3	14,14,15	0.40	0	17,19,21	1.38	2 (11%)
10	NAG	c	2	10	14,14,15	0.20	0	17,19,21	0.45	0
10	BMA	c	3	10	11,11,12	0.58	0	15,15,17	0.65	0
7	NAG	d	1	3,7	14,14,15	0.29	0	17,19,21	0.49	0
7	NAG	d	2	7	14,14,15	0.23	0	17,19,21	0.40	0
13	NAG	e	1	3,13	14,14,15	0.40	0	17,19,21	0.41	0
13	NAG	e	2	13	14,14,15	0.27	0	17,19,21	0.52	0
13	BMA	e	3	13	11,11,12	0.60	0	15,15,17	0.67	0
13	MAN	e	4	13	11,11,12	0.62	0	15,15,17	0.93	1 (6%)
13	MAN	e	5	13	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
10	NAG	f	1	10,3	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
10	NAG	f	2	10	14,14,15	0.21	0	17,19,21	0.46	0
10	BMA	f	3	10	11,11,12	0.52	0	15,15,17	0.71	0
7	NAG	g	1	3,7	14,14,15	0.25	0	17,19,21	0.49	0
7	NAG	g	2	7	14,14,15	0.44	0	17,19,21	1.32	2 (11%)
7	NAG	h	1	3,7	14,14,15	0.16	0	17,19,21	0.51	0
7	NAG	h	2	7	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	i	1	3,7	14,14,15	0.32	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	i	2	7	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	j	1	3,7	14,14,15	0.40	0	17,19,21	0.47	0
7	NAG	j	2	7	14,14,15	0.26	0	17,19,21	0.39	0
7	NAG	k	1	3,7	14,14,15	0.43	0	17,19,21	1.40	2 (11%)
7	NAG	k	2	7	14,14,15	0.24	0	17,19,21	0.39	0
9	NAG	l	1	9,3	14,14,15	0.47	0	17,19,21	0.41	0
9	NAG	l	2	9	14,14,15	0.18	0	17,19,21	0.46	0
9	BMA	l	3	9	11,11,12	0.53	0	15,15,17	0.68	0
9	MAN	l	4	9	11,11,12	0.67	0	15,15,17	0.99	0
9	MAN	l	5	9	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
9	MAN	l	6	9	11,11,12	0.68	0	15,15,17	1.04	1 (6%)
9	MAN	l	7	9	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
9	MAN	l	8	9	11,11,12	0.58	0	15,15,17	0.96	2 (13%)
10	NAG	m	1	10,3	14,14,15	0.22	0	17,19,21	0.48	0
10	NAG	m	2	10	14,14,15	0.21	0	17,19,21	0.45	0
10	BMA	m	3	10	11,11,12	0.49	0	15,15,17	0.71	0
13	NAG	n	1	3,13	14,14,15	0.39	0	17,19,21	0.42	0
13	NAG	n	2	13	14,14,15	0.30	0	17,19,21	0.47	0
13	BMA	n	3	13	11,11,12	0.60	0	15,15,17	0.79	0
13	MAN	n	4	13	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
13	MAN	n	5	13	11,11,12	0.74	0	15,15,17	1.23	2 (13%)
10	NAG	o	1	10,3	14,14,15	0.32	0	17,19,21	0.65	0
10	NAG	o	2	10	14,14,15	0.23	0	17,19,21	0.41	0
10	BMA	o	3	10	11,11,12	0.53	0	15,15,17	0.72	0
7	NAG	p	1	3,7	14,14,15	0.20	0	17,19,21	0.59	0
7	NAG	p	2	7	14,14,15	0.25	0	17,19,21	0.46	0
14	NAG	q	1	3,14	14,14,15	0.49	0	17,19,21	0.48	0
14	NAG	q	2	14	14,14,15	0.27	0	17,19,21	0.54	0
14	BMA	q	3	14	11,11,12	0.61	0	15,15,17	0.93	1 (6%)
14	MAN	q	4	14	11,11,12	0.57	0	15,15,17	0.93	1 (6%)
14	MAN	q	5	14	11,11,12	0.59	0	15,15,17	1.11	2 (13%)
14	MAN	q	6	14	11,11,12	0.68	0	15,15,17	1.07	1 (6%)
14	MAN	q	7	14	11,11,12	0.58	0	15,15,17	1.06	2 (13%)
14	MAN	q	8	14	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
11	NAG	r	1	3,11	14,14,15	0.50	0	17,19,21	0.42	0
11	MAN	r	10	11	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
11	MAN	r	11	11	11,11,12	0.70	1 (9%)	15,15,17	0.89	1 (6%)
11	NAG	r	2	11	14,14,15	0.34	0	17,19,21	0.55	0
11	BMA	r	3	11	11,11,12	0.61	0	15,15,17	0.91	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	r	4	11	11,11,12	0.71	0	15,15,17	1.21	2 (13%)
11	MAN	r	5	11	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
11	MAN	r	6	11	11,11,12	0.52	0	15,15,17	1.15	2 (13%)
11	MAN	r	7	11	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
11	MAN	r	8	11	11,11,12	0.55	0	15,15,17	1.14	2 (13%)
11	MAN	r	9	11	11,11,12	0.49	0	15,15,17	1.01	2 (13%)
8	NAG	s	1	3,8	14,14,15	0.29	0	17,19,21	0.53	0
8	NAG	s	2	8	14,14,15	0.32	0	17,19,21	0.54	0
8	BMA	s	3	8	11,11,12	0.86	0	15,15,17	0.94	1 (6%)
8	MAN	s	4	8	11,11,12	0.60	0	15,15,17	1.15	2 (13%)
8	MAN	s	5	8	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
8	MAN	s	6	8	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
8	MAN	s	7	8	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
8	MAN	s	8	8	11,11,12	0.83	1 (9%)	15,15,17	1.31	2 (13%)
8	MAN	s	9	8	11,11,12	0.72	0	15,15,17	0.88	1 (6%)
10	NAG	t	1	10,3	14,14,15	0.27	0	17,19,21	0.45	0
10	NAG	t	2	10	14,14,15	0.19	0	17,19,21	0.42	0
10	BMA	t	3	10	11,11,12	0.54	0	15,15,17	0.68	0
10	NAG	u	1	10,3	14,14,15	0.25	0	17,19,21	0.45	0
10	NAG	u	2	10	14,14,15	0.41	0	17,19,21	1.33	2 (11%)
10	BMA	u	3	10	11,11,12	0.52	0	15,15,17	0.75	0
7	NAG	v	1	3,7	14,14,15	0.34	0	17,19,21	0.43	0
7	NAG	v	2	7	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	w	1	3,7	14,14,15	0.37	0	17,19,21	0.47	0
7	NAG	w	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	x	1	3,7	14,14,15	0.43	0	17,19,21	0.74	1 (5%)
7	NAG	x	2	7	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
8	NAG	y	1	3,8	14,14,15	0.29	0	17,19,21	0.54	0
8	NAG	y	2	8	14,14,15	0.32	0	17,19,21	0.57	0
8	BMA	y	3	8	11,11,12	0.77	0	15,15,17	0.88	0
8	MAN	y	4	8	11,11,12	0.63	0	15,15,17	1.12	2 (13%)
8	MAN	y	5	8	11,11,12	0.54	0	15,15,17	1.07	2 (13%)
8	MAN	y	6	8	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
8	MAN	y	7	8	11,11,12	0.61	0	15,15,17	0.89	1 (6%)
8	MAN	y	8	8	11,11,12	0.65	0	15,15,17	1.22	2 (13%)
8	MAN	y	9	8	11,11,12	0.66	0	15,15,17	1.27	2 (13%)
9	NAG	z	1	9,3	14,14,15	0.49	0	17,19,21	0.39	0
9	NAG	z	2	9	14,14,15	0.18	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BMA	z	3	9	11,11,12	0.49	0	15,15,17	0.70	0
9	MAN	z	4	9	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
9	MAN	z	5	9	11,11,12	0.78	1 (9%)	15,15,17	1.06	2 (13%)
9	MAN	z	6	9	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
9	MAN	z	7	9	11,11,12	0.52	0	15,15,17	1.13	2 (13%)
9	MAN	z	8	9	11,11,12	0.58	0	15,15,17	0.97	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	0	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	0	2	10	-	2/6/23/26	0/1/1/1
10	BMA	0	3	10	-	0/2/19/22	0/1/1/1
13	NAG	1	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	1	2	13	-	0/6/23/26	0/1/1/1
13	BMA	1	3	13	-	1/2/19/22	0/1/1/1
13	MAN	1	4	13	-	2/2/19/22	1/1/1/1
13	MAN	1	5	13	-	2/2/19/22	0/1/1/1
10	NAG	2	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	2	2	10	-	0/6/23/26	0/1/1/1
10	BMA	2	3	10	-	0/2/19/22	0/1/1/1
10	NAG	3	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	3	2	10	-	0/6/23/26	0/1/1/1
10	BMA	3	3	10	-	2/2/19/22	0/1/1/1
7	NAG	4	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	4	2	7	-	1/6/23/26	0/1/1/1
14	NAG	5	1	3,14	-	6/6/23/26	0/1/1/1
14	NAG	5	2	14	-	2/6/23/26	0/1/1/1
14	BMA	5	3	14	-	0/2/19/22	0/1/1/1
14	MAN	5	4	14	-	2/2/19/22	0/1/1/1
14	MAN	5	5	14	-	2/2/19/22	0/1/1/1
14	MAN	5	6	14	-	0/2/19/22	0/1/1/1
14	MAN	5	7	14	-	2/2/19/22	0/1/1/1
14	MAN	5	8	14	-	2/2/19/22	0/1/1/1
11	NAG	6	1	3,11	-	2/6/23/26	0/1/1/1
11	MAN	6	10	11	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	X	7	9	-	2/2/19/22	1/1/1/1
9	MAN	X	8	9	-	2/2/19/22	0/1/1/1
10	NAG	Y	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
11	NAG	a	1	3,11	-	2/6/23/26	0/1/1/1
11	MAN	a	10	11	-	0/2/19/22	0/1/1/1
11	MAN	a	11	11	-	0/2/19/22	1/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
11	BMA	a	3	11	-	2/2/19/22	0/1/1/1
11	MAN	a	4	11	-	0/2/19/22	0/1/1/1
11	MAN	a	5	11	-	0/2/19/22	0/1/1/1
11	MAN	a	6	11	-	2/2/19/22	0/1/1/1
11	MAN	a	7	11	-	0/2/19/22	1/1/1/1
11	MAN	a	8	11	-	0/2/19/22	0/1/1/1
11	MAN	a	9	11	-	0/2/19/22	0/1/1/1
12	NAG	b	1	3,12	-	3/6/23/26	0/1/1/1
12	NAG	b	2	12	-	2/6/23/26	0/1/1/1
12	BMA	b	3	12	-	0/2/19/22	0/1/1/1
12	MAN	b	4	12	-	2/2/19/22	0/1/1/1
12	MAN	b	5	12	-	2/2/19/22	0/1/1/1
12	MAN	b	6	12	-	0/2/19/22	0/1/1/1
12	MAN	b	7	12	-	1/2/19/22	0/1/1/1
10	NAG	c	1	10,3	-	4/6/23/26	0/1/1/1
10	NAG	c	2	10	-	0/6/23/26	0/1/1/1
10	BMA	c	3	10	-	1/2/19/22	0/1/1/1
7	NAG	d	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
13	NAG	e	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	e	2	13	-	0/6/23/26	0/1/1/1
13	BMA	e	3	13	-	0/2/19/22	0/1/1/1
13	MAN	e	4	13	-	2/2/19/22	0/1/1/1
13	MAN	e	5	13	-	0/2/19/22	0/1/1/1
10	NAG	f	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	0/6/23/26	0/1/1/1
10	BMA	f	3	10	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	g	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	4/6/23/26	0/1/1/1
7	NAG	h	1	3,7	-	3/6/23/26	0/1/1/1
7	NAG	h	2	7	-	0/6/23/26	0/1/1/1
7	NAG	i	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	1/6/23/26	0/1/1/1
7	NAG	j	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	NAG	k	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	k	2	7	-	2/6/23/26	0/1/1/1
9	NAG	l	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	0/2/19/22	0/1/1/1
9	MAN	l	4	9	-	2/2/19/22	0/1/1/1
9	MAN	l	5	9	-	1/2/19/22	1/1/1/1
9	MAN	l	6	9	-	2/2/19/22	0/1/1/1
9	MAN	l	7	9	-	2/2/19/22	1/1/1/1
9	MAN	l	8	9	-	0/2/19/22	0/1/1/1
10	NAG	m	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	m	2	10	-	0/6/23/26	0/1/1/1
10	BMA	m	3	10	-	0/2/19/22	0/1/1/1
13	NAG	n	1	3,13	-	2/6/23/26	0/1/1/1
13	NAG	n	2	13	-	0/6/23/26	0/1/1/1
13	BMA	n	3	13	-	2/2/19/22	0/1/1/1
13	MAN	n	4	13	-	2/2/19/22	0/1/1/1
13	MAN	n	5	13	-	1/2/19/22	1/1/1/1
10	NAG	o	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	o	2	10	-	0/6/23/26	0/1/1/1
10	BMA	o	3	10	-	1/2/19/22	0/1/1/1
7	NAG	p	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	p	2	7	-	2/6/23/26	0/1/1/1
14	NAG	q	1	3,14	-	2/6/23/26	0/1/1/1
14	NAG	q	2	14	-	2/6/23/26	0/1/1/1
14	BMA	q	3	14	-	0/2/19/22	0/1/1/1
14	MAN	q	4	14	-	0/2/19/22	0/1/1/1
14	MAN	q	5	14	-	2/2/19/22	0/1/1/1
14	MAN	q	6	14	-	1/2/19/22	0/1/1/1
14	MAN	q	7	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	q	8	14	-	1/2/19/22	0/1/1/1
11	NAG	r	1	3,11	-	1/6/23/26	0/1/1/1
11	MAN	r	10	11	-	2/2/19/22	0/1/1/1
11	MAN	r	11	11	-	2/2/19/22	0/1/1/1
11	NAG	r	2	11	-	2/6/23/26	0/1/1/1
11	BMA	r	3	11	-	2/2/19/22	0/1/1/1
11	MAN	r	4	11	-	2/2/19/22	0/1/1/1
11	MAN	r	5	11	-	1/2/19/22	0/1/1/1
11	MAN	r	6	11	-	2/2/19/22	0/1/1/1
11	MAN	r	7	11	-	0/2/19/22	1/1/1/1
11	MAN	r	8	11	-	1/2/19/22	0/1/1/1
11	MAN	r	9	11	-	2/2/19/22	0/1/1/1
8	NAG	s	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	s	2	8	-	0/6/23/26	0/1/1/1
8	BMA	s	3	8	-	0/2/19/22	0/1/1/1
8	MAN	s	4	8	-	0/2/19/22	0/1/1/1
8	MAN	s	5	8	-	1/2/19/22	0/1/1/1
8	MAN	s	6	8	-	2/2/19/22	0/1/1/1
8	MAN	s	7	8	-	0/2/19/22	0/1/1/1
8	MAN	s	8	8	-	0/2/19/22	0/1/1/1
8	MAN	s	9	8	-	2/2/19/22	0/1/1/1
10	NAG	t	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	t	2	10	-	2/6/23/26	0/1/1/1
10	BMA	t	3	10	-	0/2/19/22	0/1/1/1
10	NAG	u	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	u	2	10	-	4/6/23/26	0/1/1/1
10	BMA	u	3	10	-	0/2/19/22	0/1/1/1
7	NAG	v	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	1/6/23/26	0/1/1/1
7	NAG	w	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	2/6/23/26	0/1/1/1
7	NAG	x	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	x	2	7	-	2/6/23/26	0/1/1/1
8	NAG	y	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	y	5	8	-	1/2/19/22	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	5	MAN	C1-C2	2.23	1.57	1.52
14	5	7	MAN	O5-C1	-2.07	1.40	1.43
11	6	11	MAN	O5-C1	-2.05	1.40	1.43
8	s	8	MAN	O5-C1	-2.05	1.40	1.43
11	r	11	MAN	O5-C1	-2.03	1.40	1.43

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	11	MAN	C1-O5-C5	5.25	119.22	112.19
10	c	1	NAG	C2-N2-C7	4.65	129.13	122.90
14	5	1	NAG	C2-N2-C7	4.63	129.11	122.90
7	S	2	NAG	C2-N2-C7	4.55	129.00	122.90
10	u	2	NAG	C2-N2-C7	4.54	128.98	122.90

There are no chirality outliers.

5 of 206 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	k	2	NAG	C4-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
12	b	1	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
9	l	7	MAN	O5-C5-C6-O6

5 of 10 ring outliers are listed below:

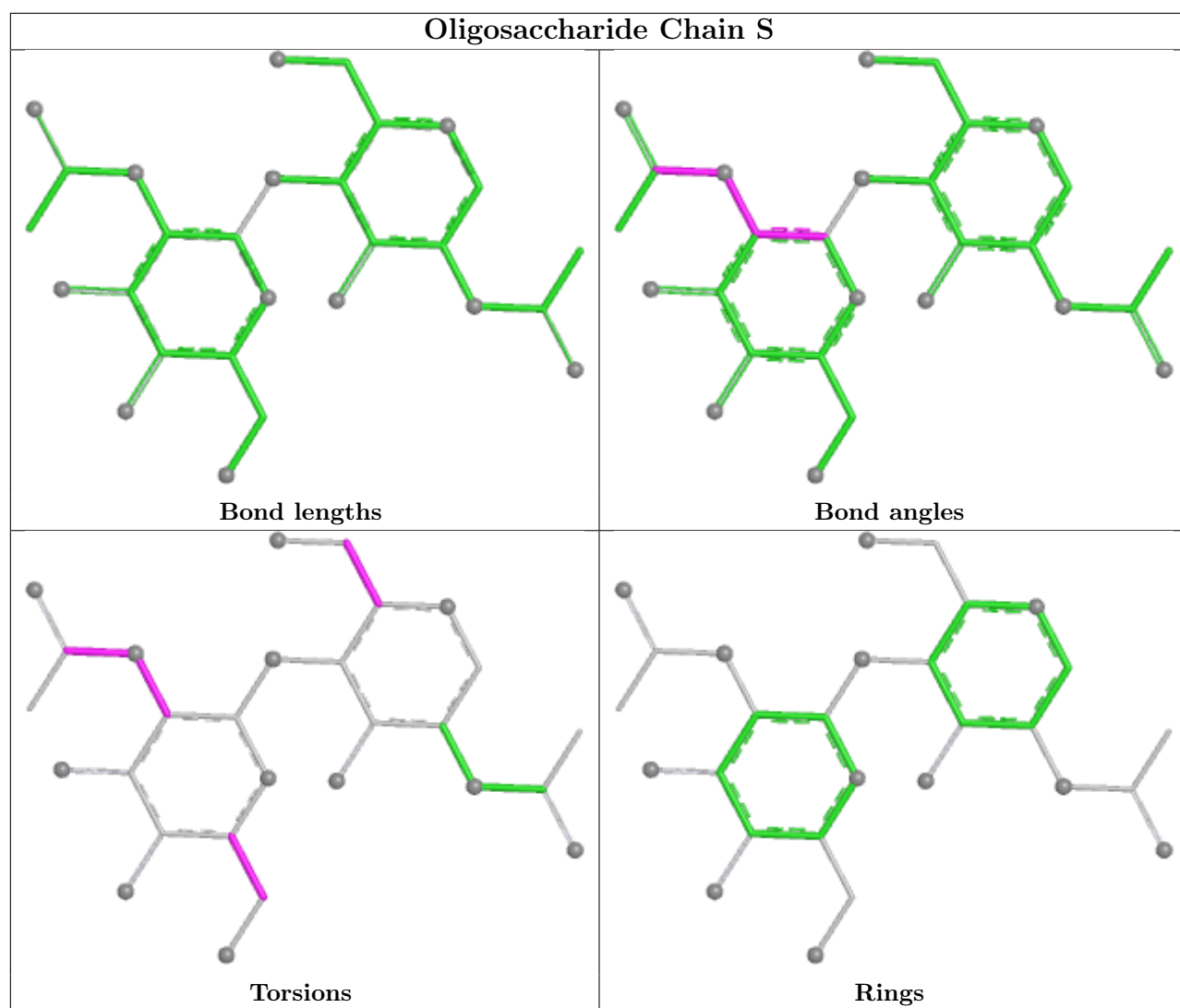
Mol	Chain	Res	Type	Atoms
9	l	7	MAN	C1-C2-C3-C4-C5-O5
8	y	9	MAN	C1-C2-C3-C4-C5-O5
9	X	7	MAN	C1-C2-C3-C4-C5-O5
11	a	11	MAN	C1-C2-C3-C4-C5-O5
9	l	5	MAN	C1-C2-C3-C4-C5-O5

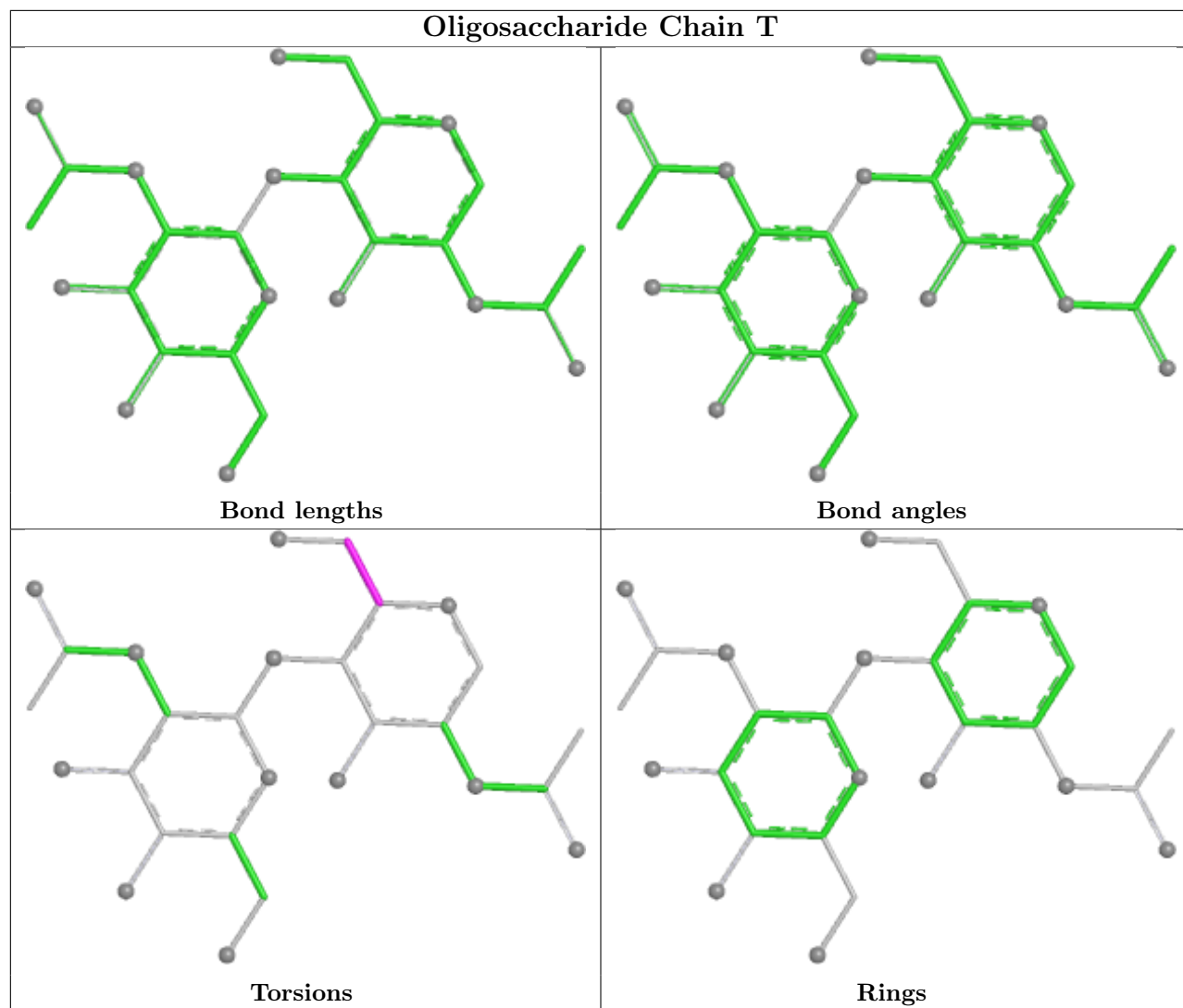
19 monomers are involved in 21 short contacts:

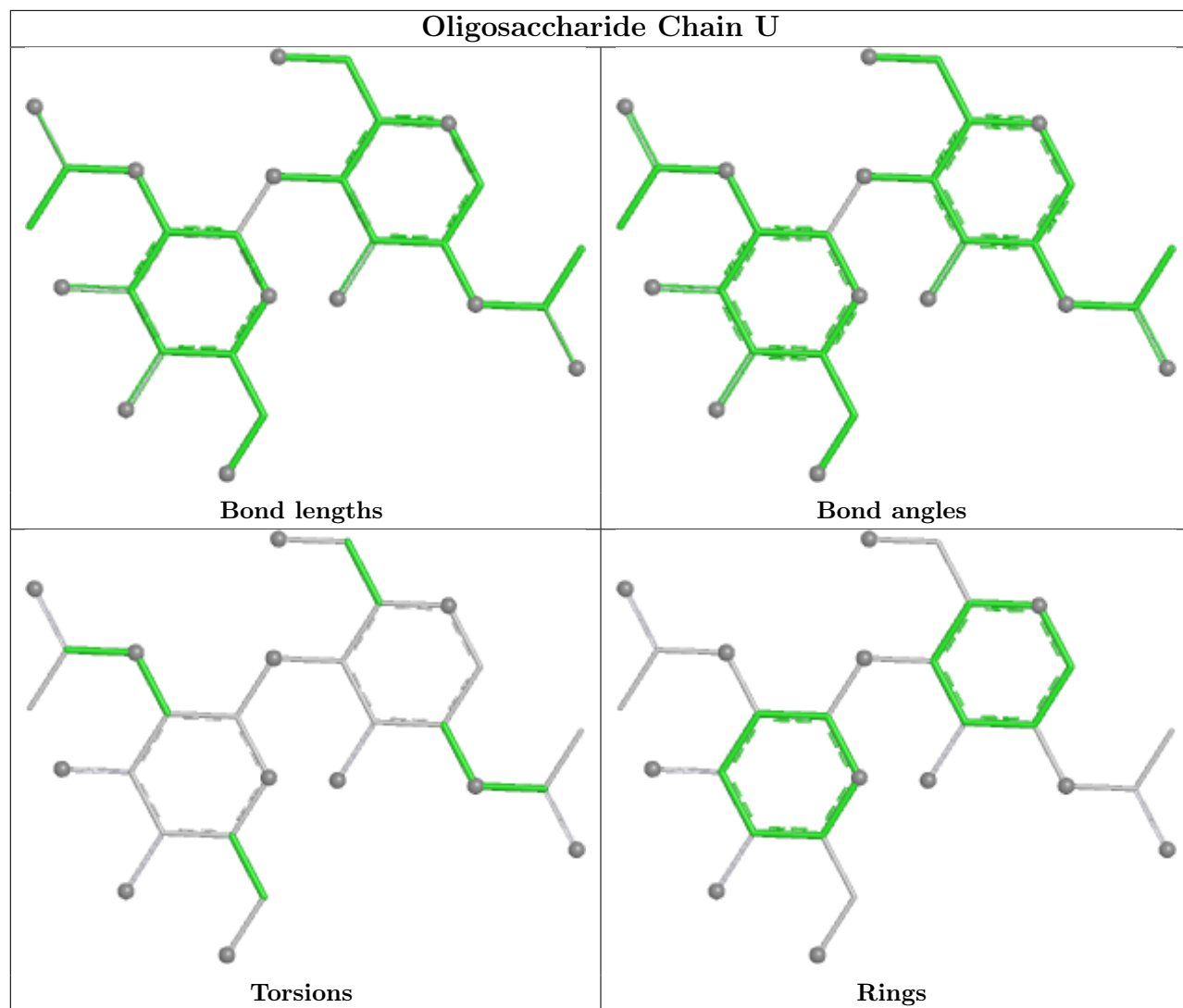
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	c	1	NAG	1	0
10	u	2	NAG	1	0
7	9	1	NAG	1	0
12	b	1	NAG	1	0
7	g	2	NAG	1	0
14	5	1	NAG	1	0
7	d	1	NAG	1	0
7	7	1	NAG	1	0
9	z	8	MAN	1	0
8	s	6	MAN	1	0
9	X	1	NAG	2	0
7	k	1	NAG	1	0
9	l	8	MAN	1	0
7	S	2	NAG	1	0
14	q	1	NAG	1	0
7	8	1	NAG	2	0
8	W	6	MAN	1	0
8	y	6	MAN	1	0
9	z	2	NAG	1	0

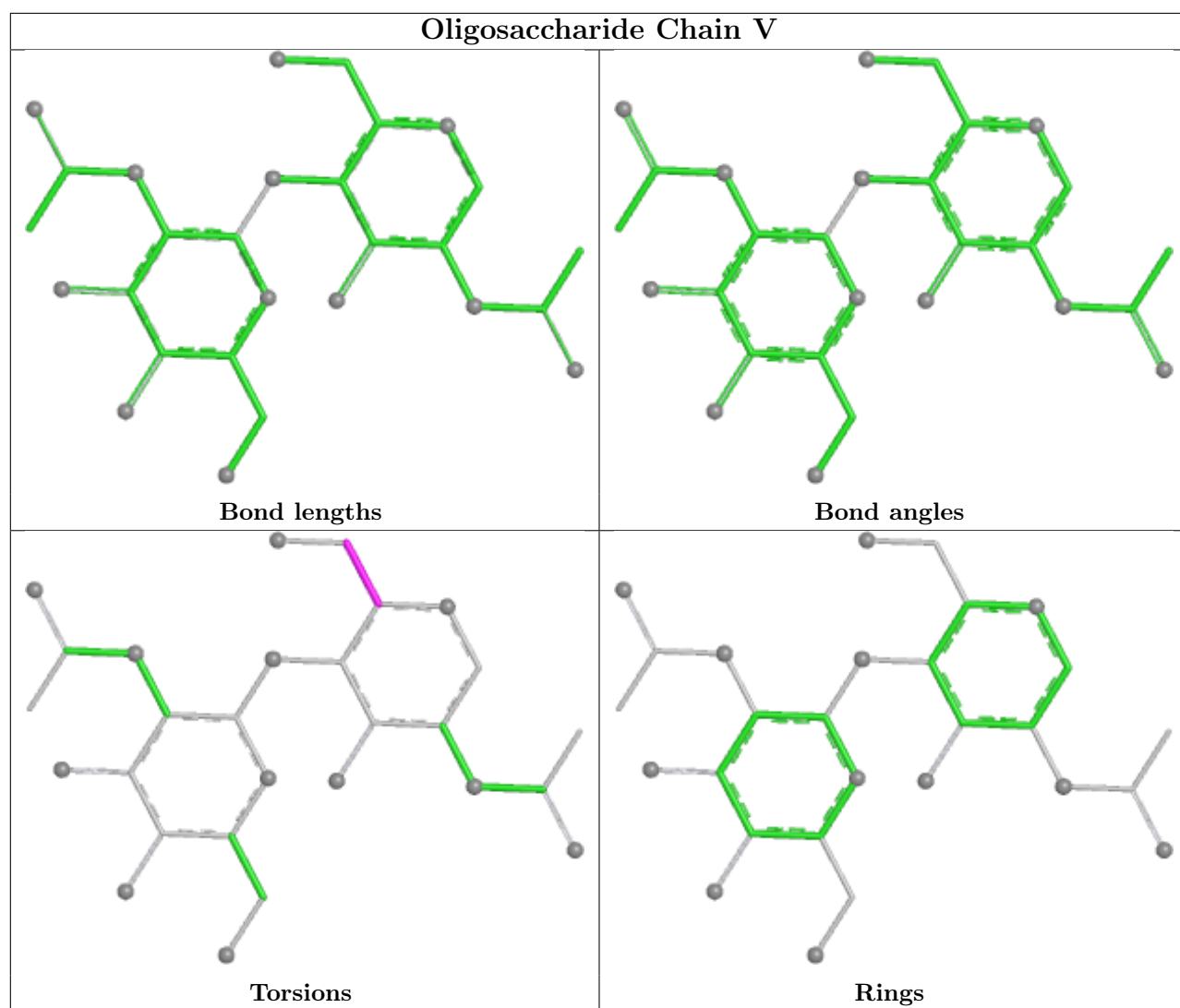
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

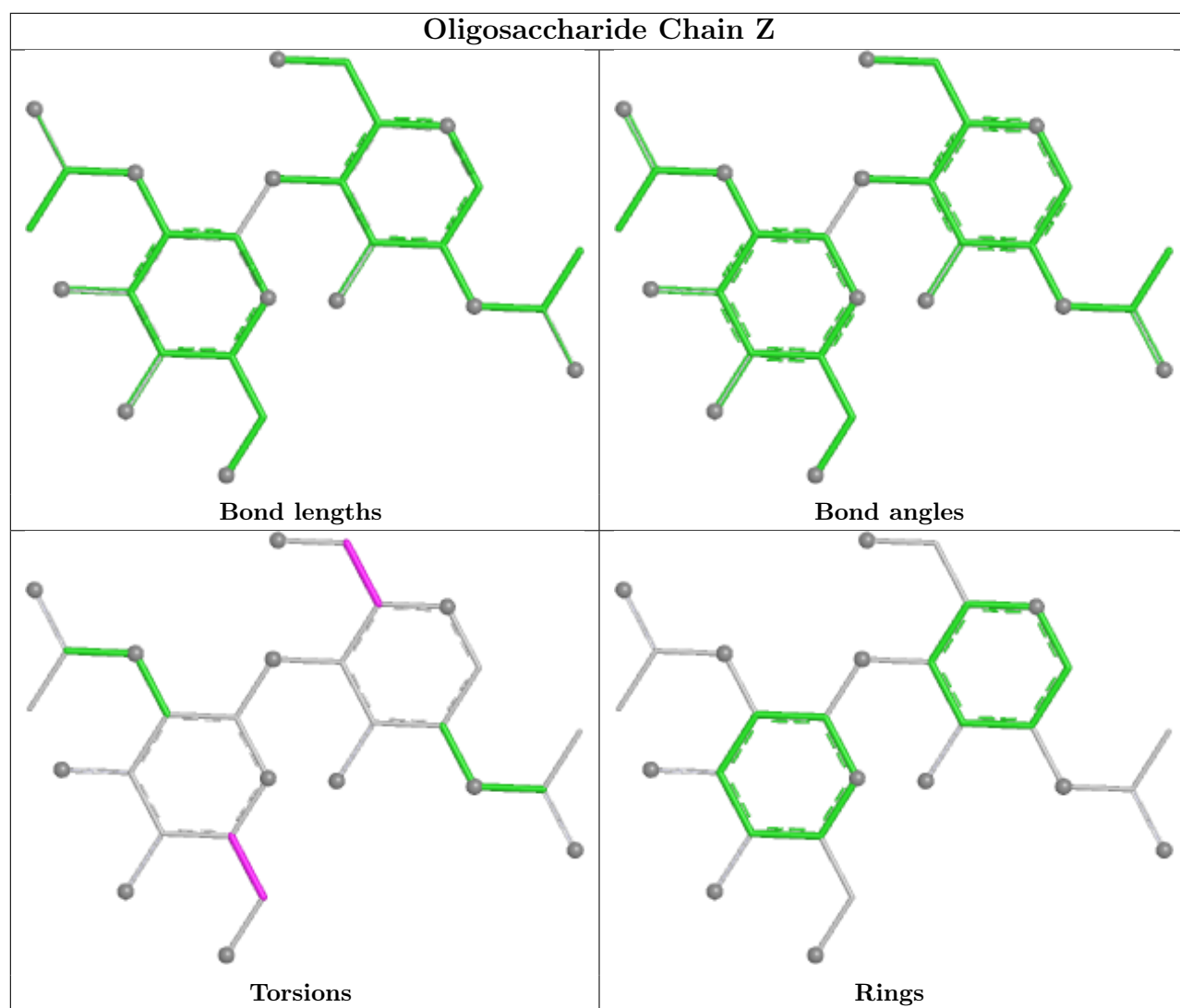


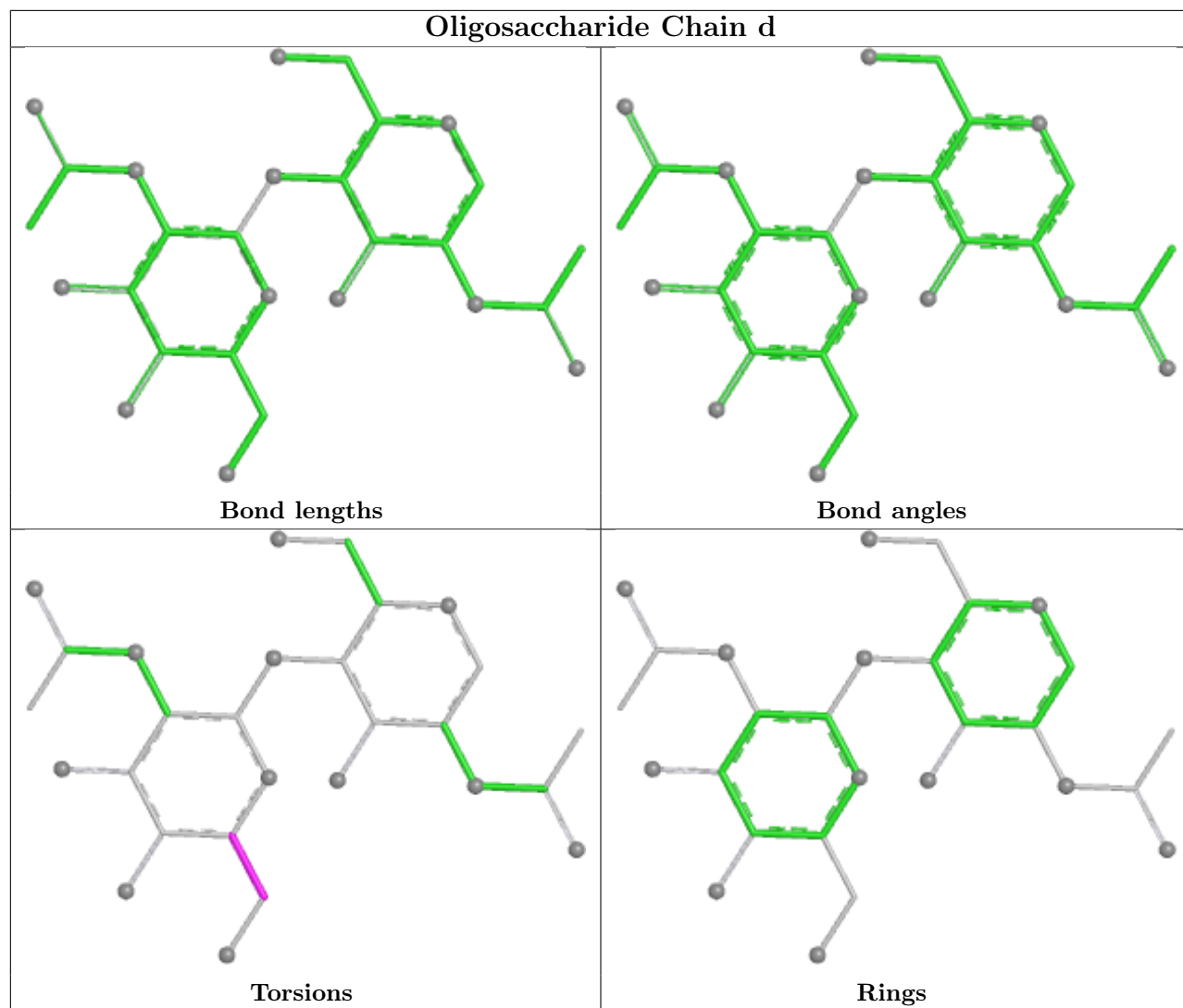


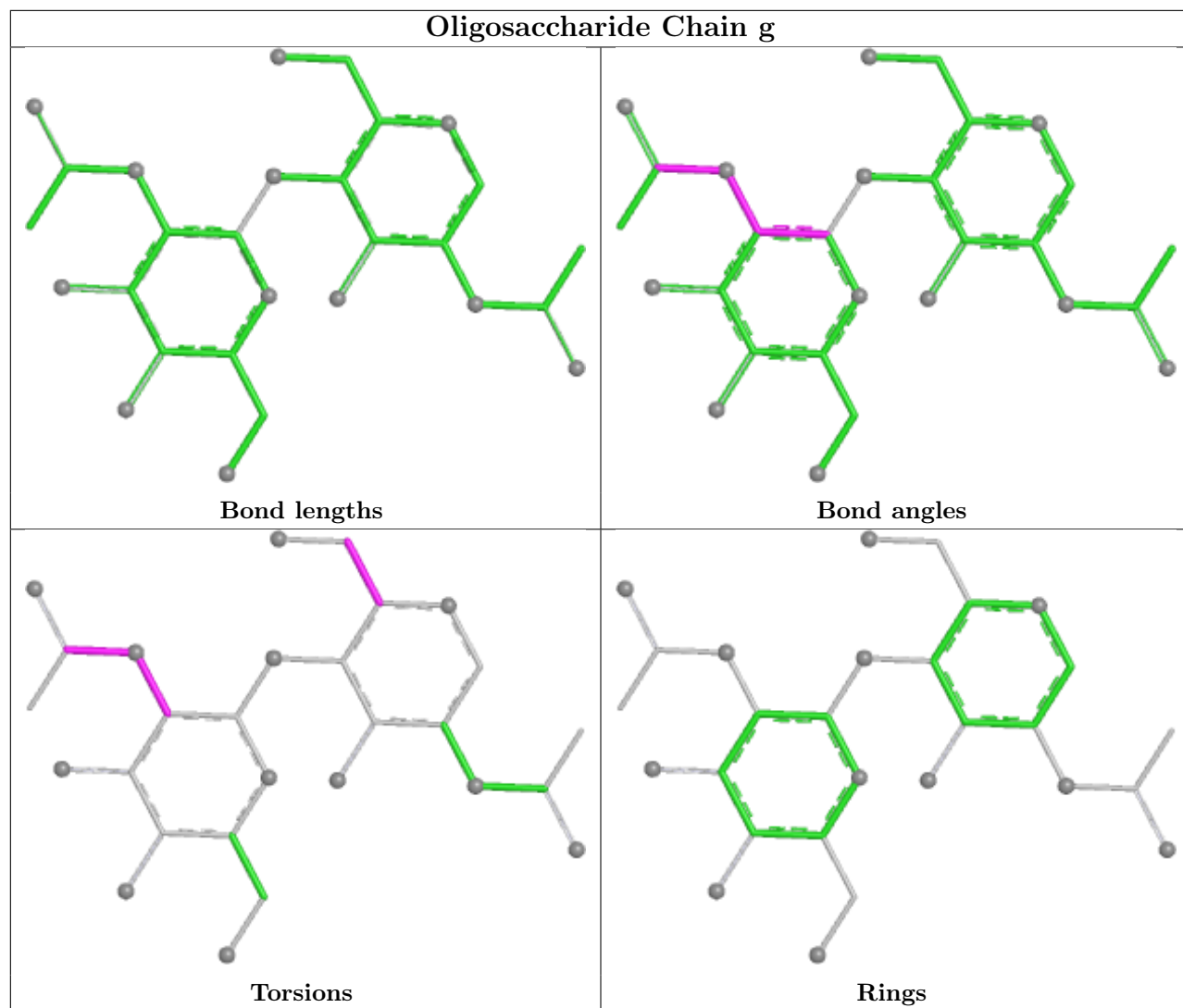


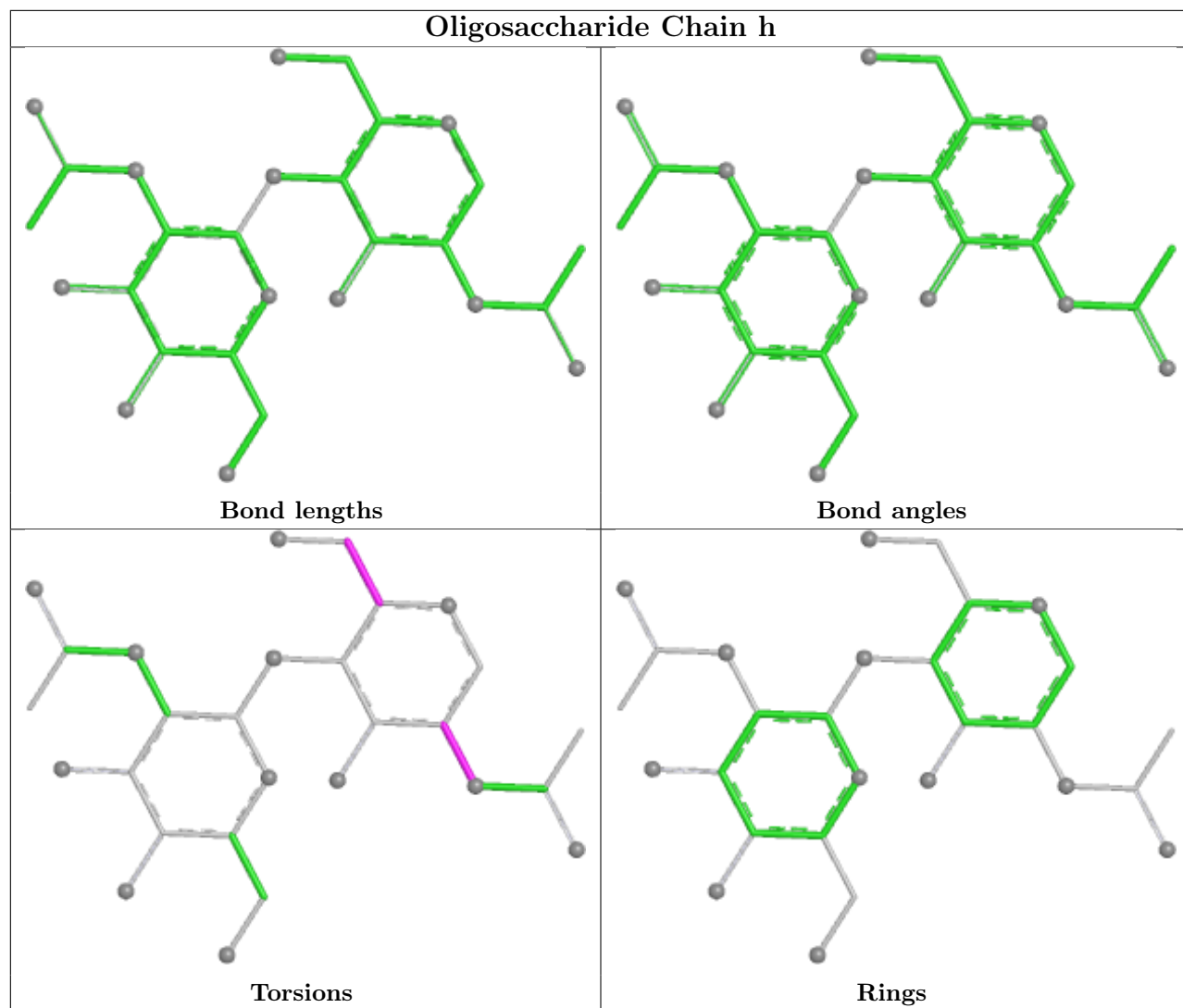




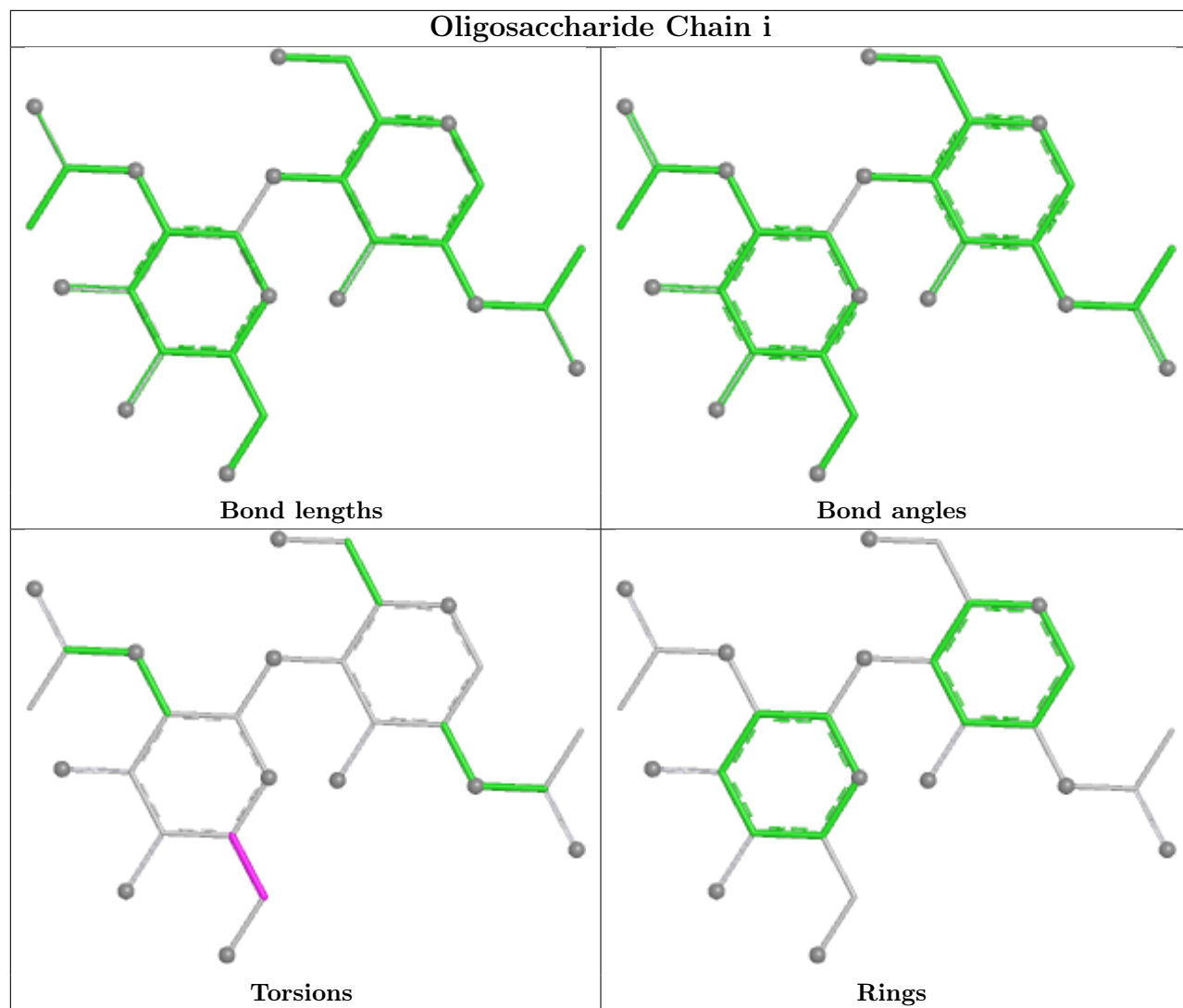


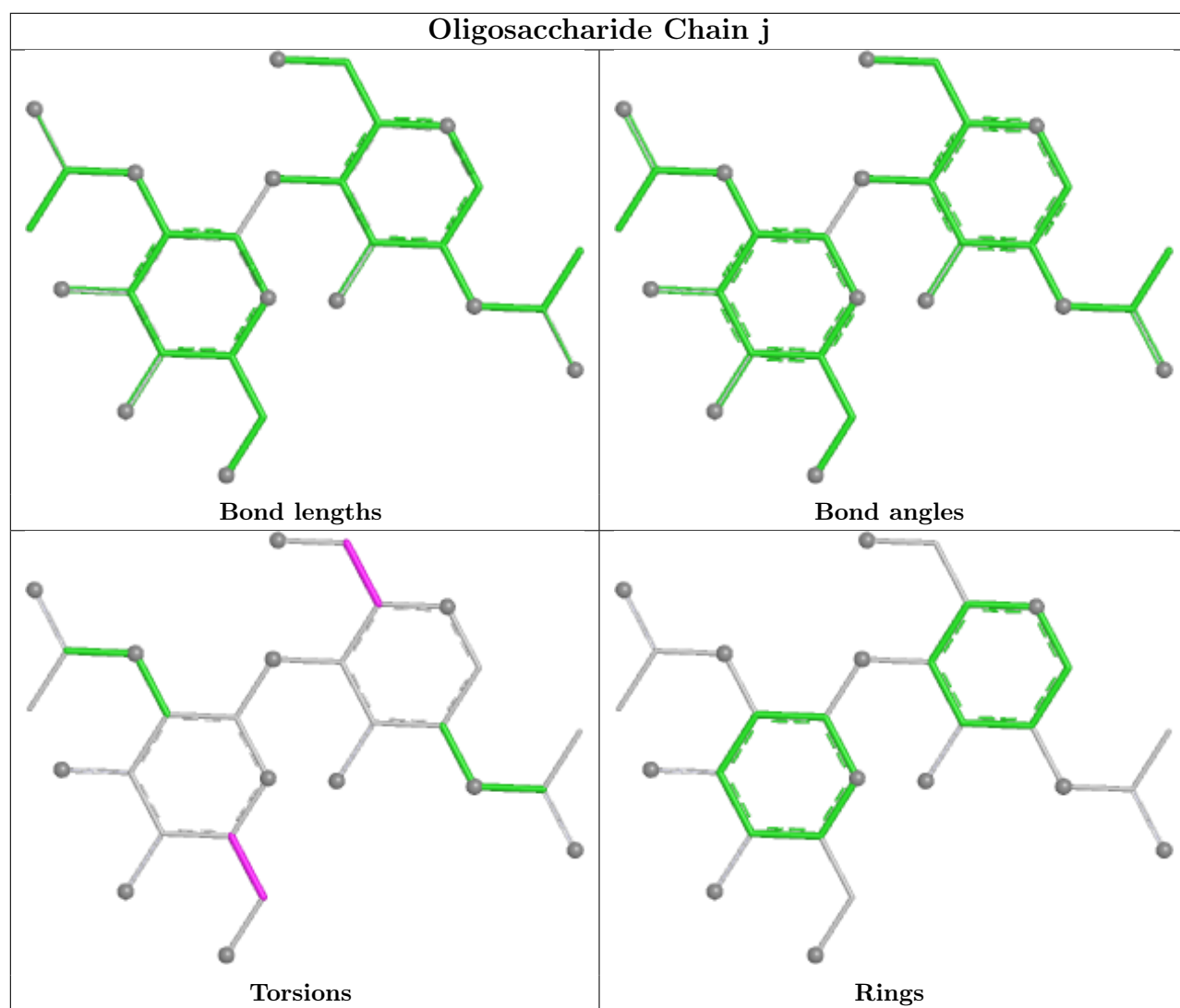


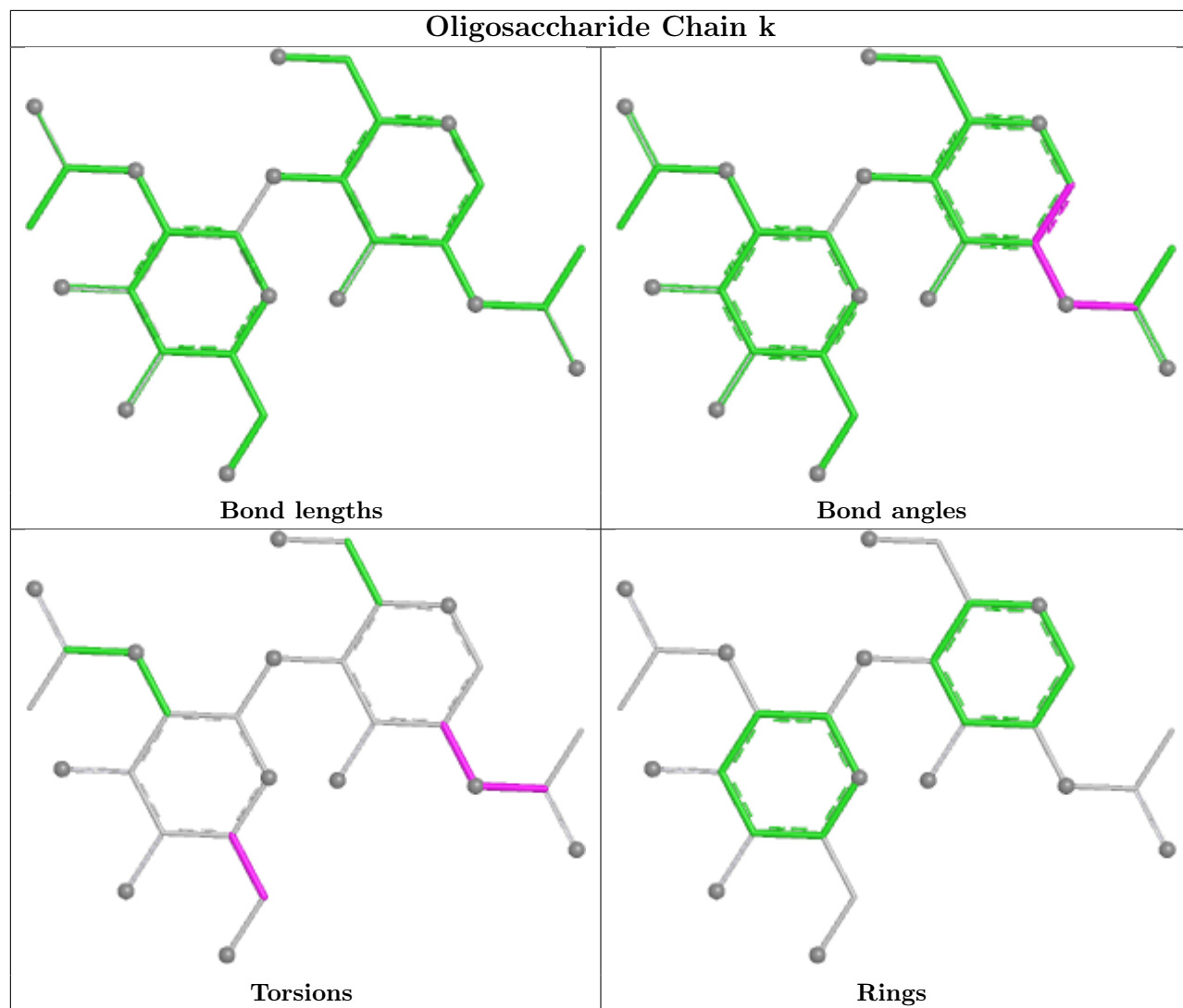


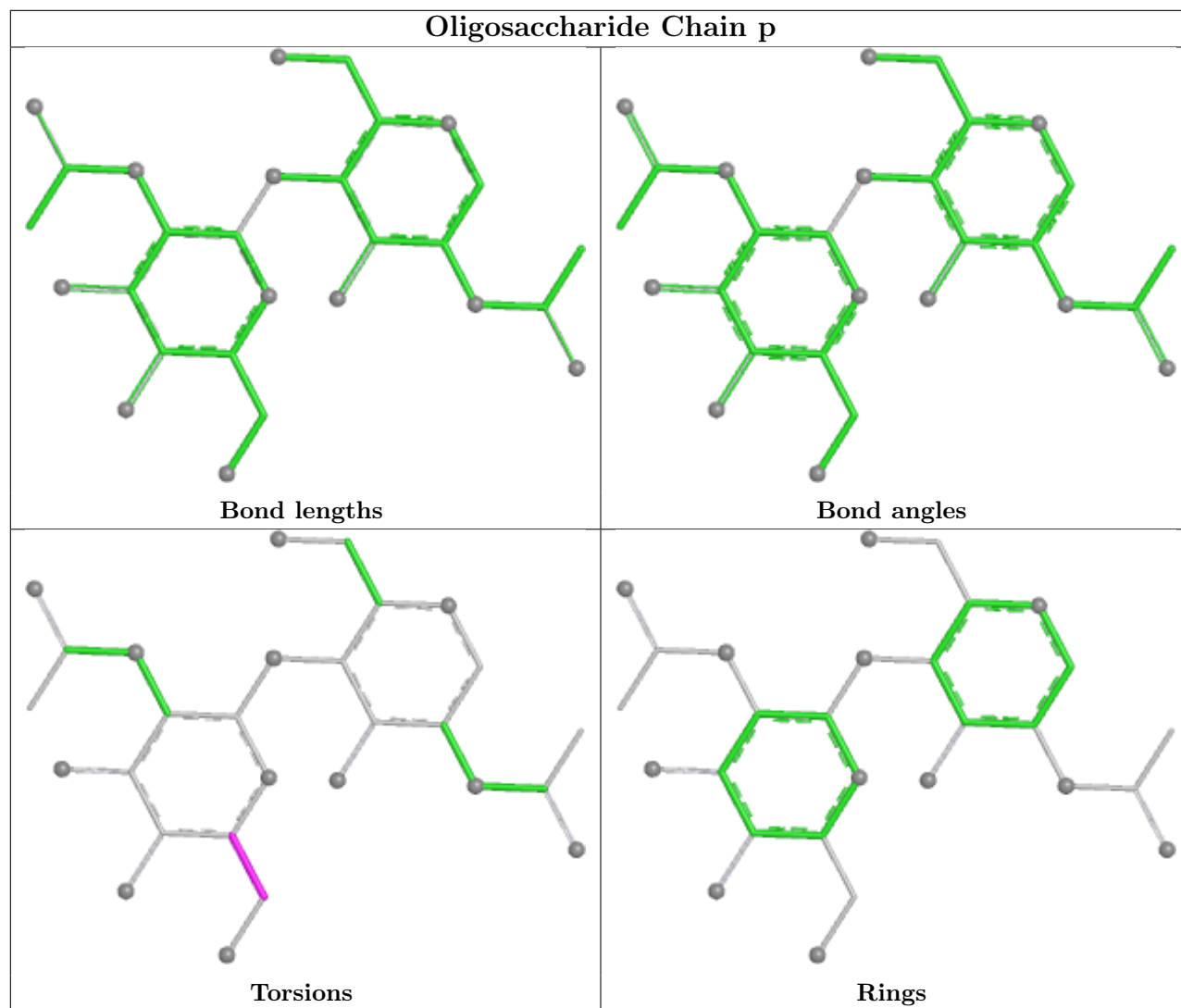


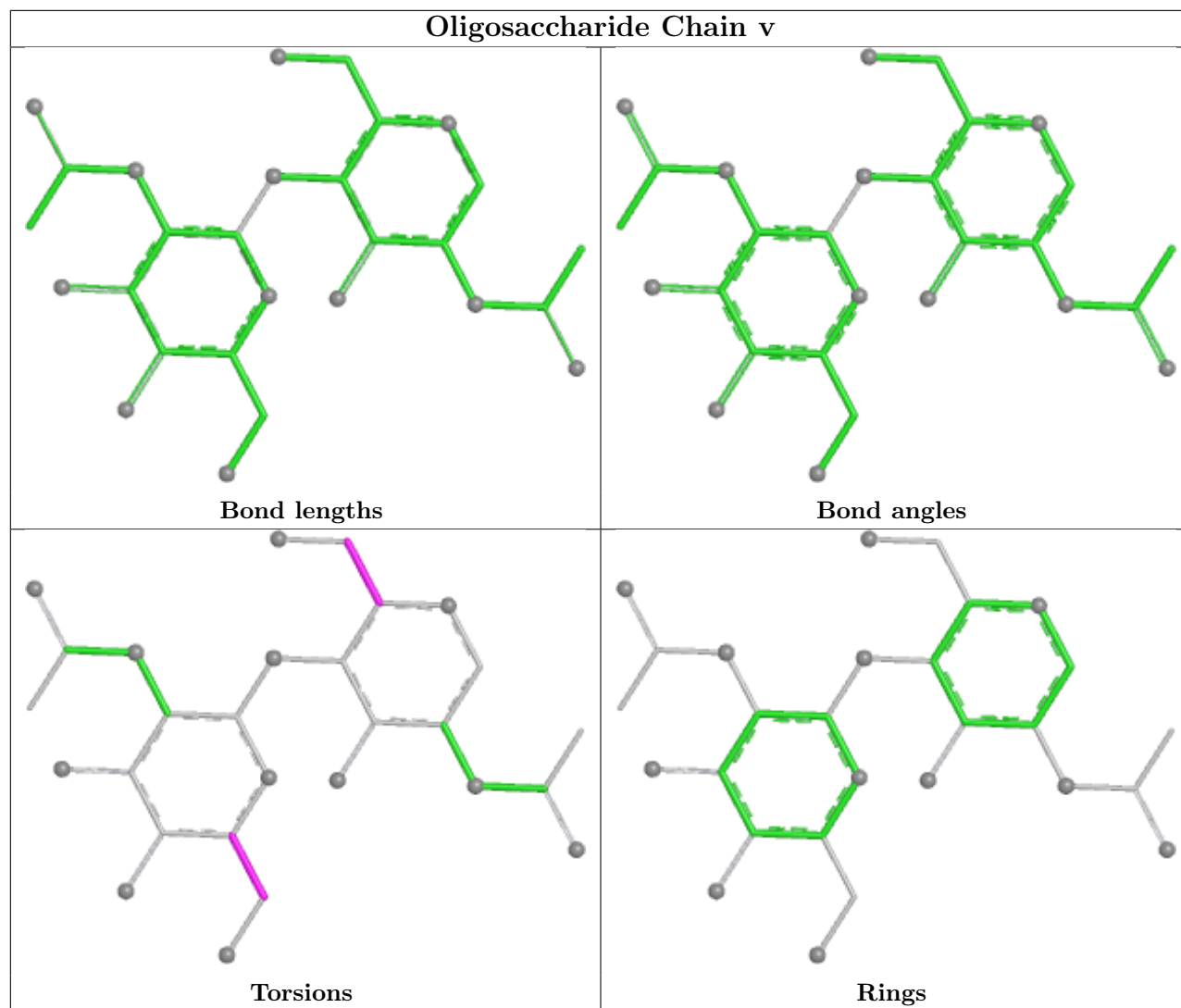


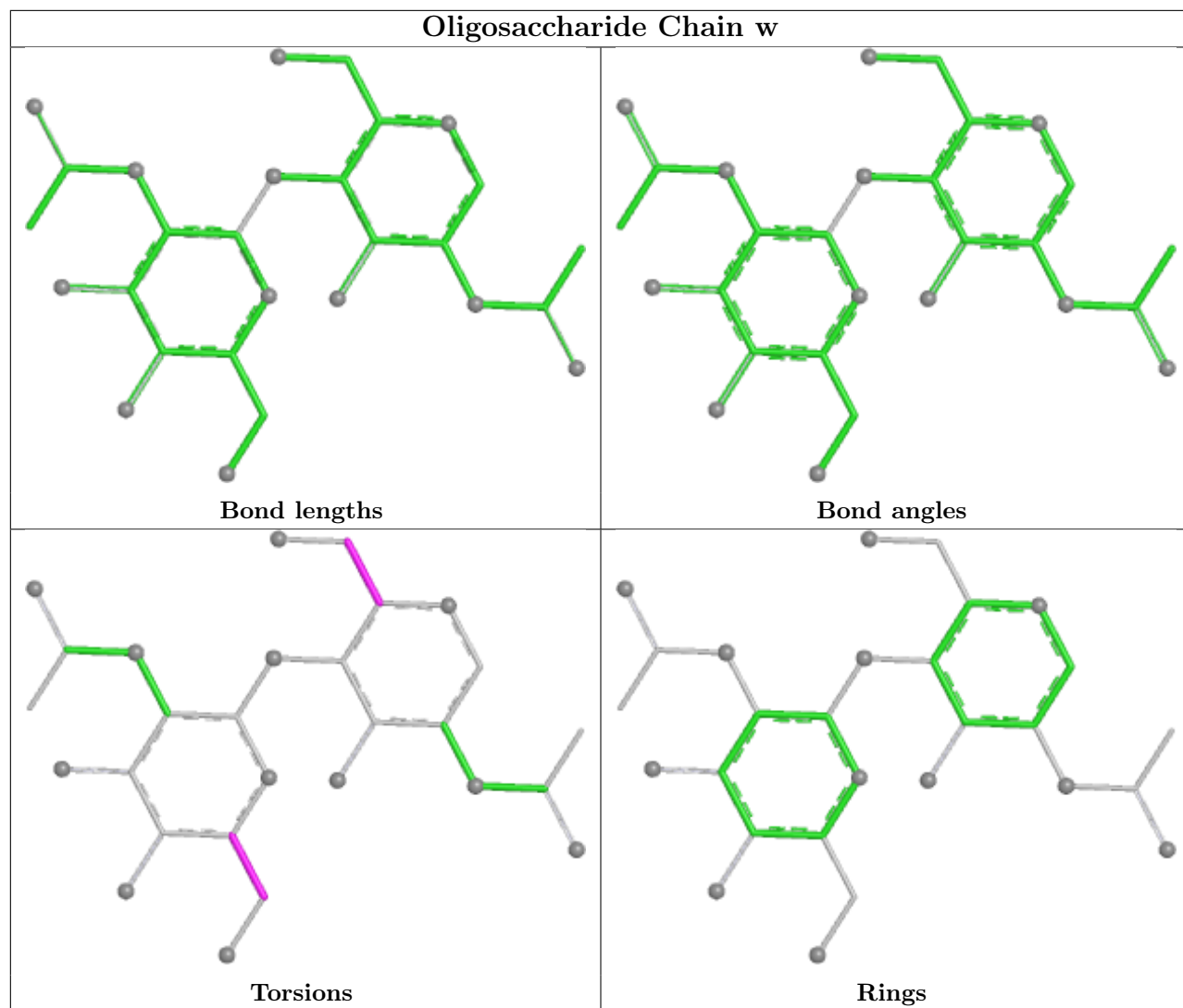


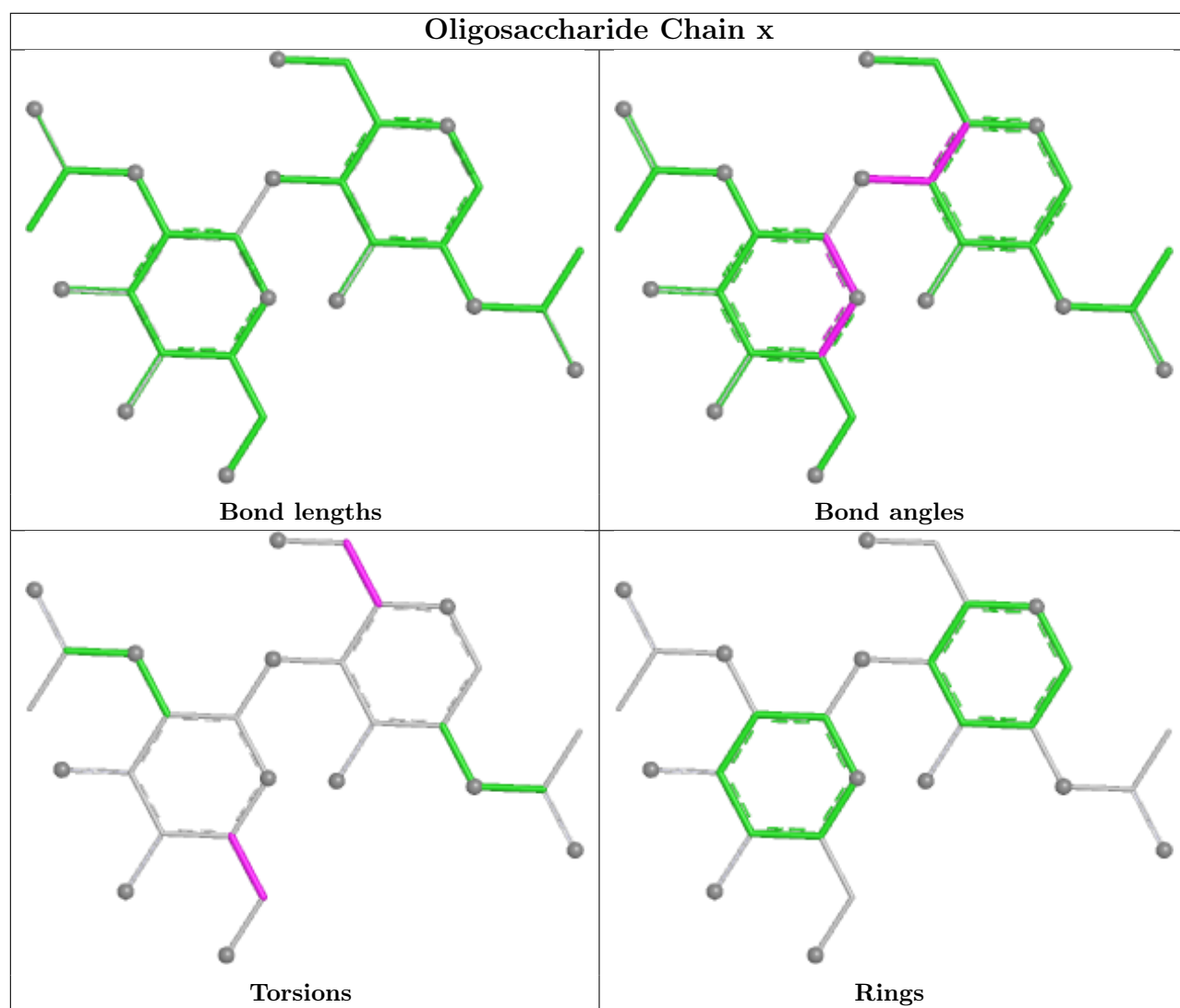


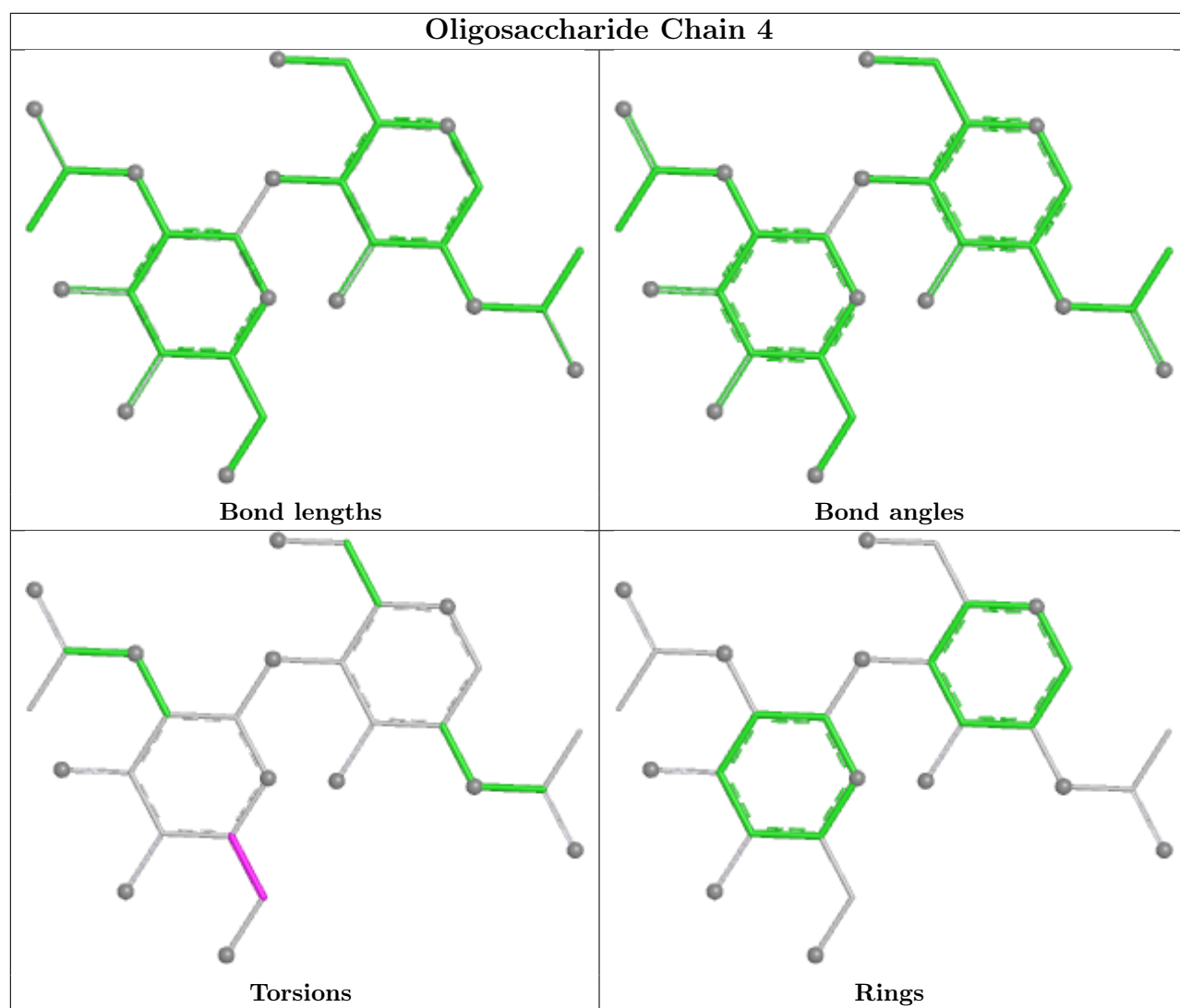




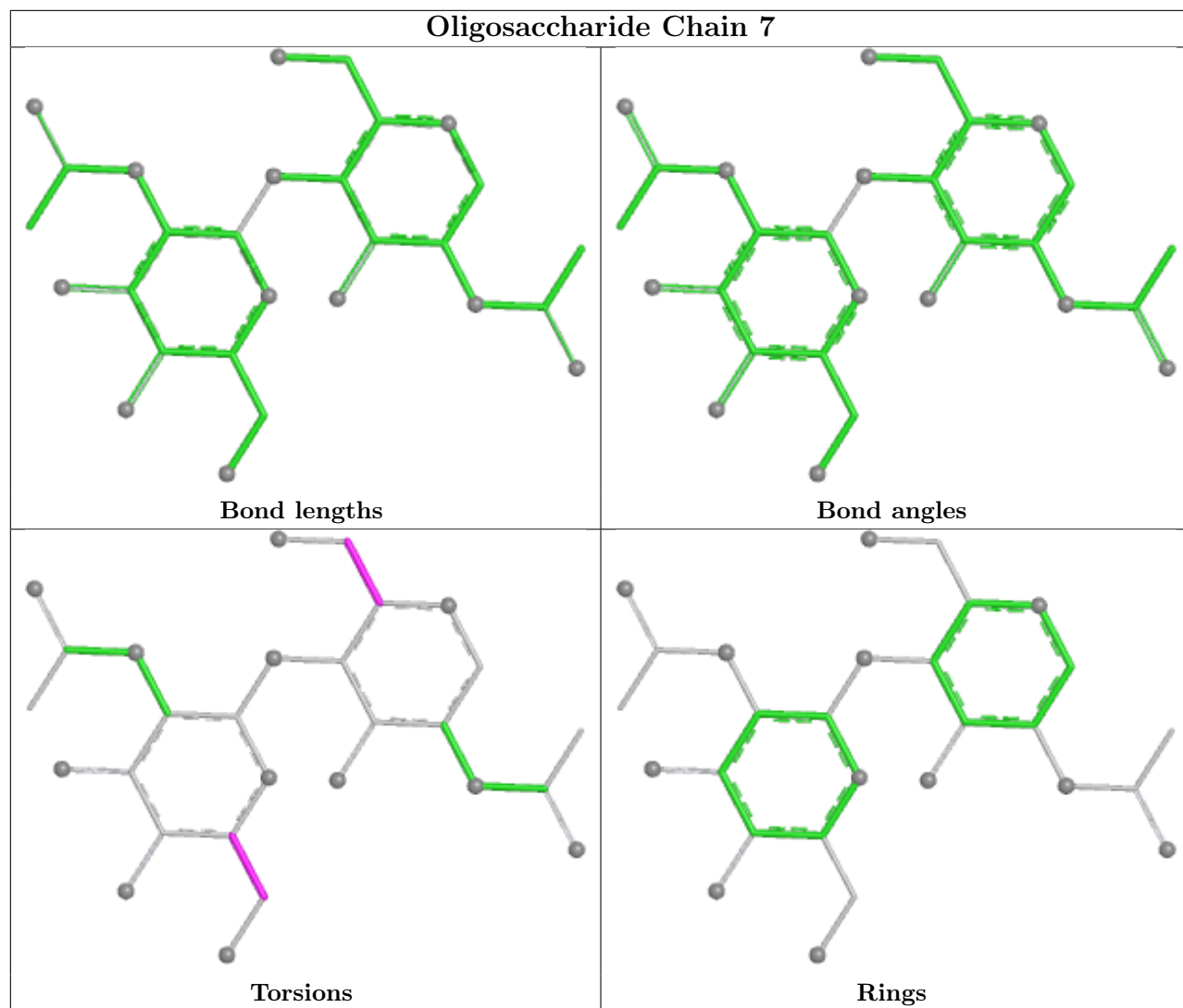


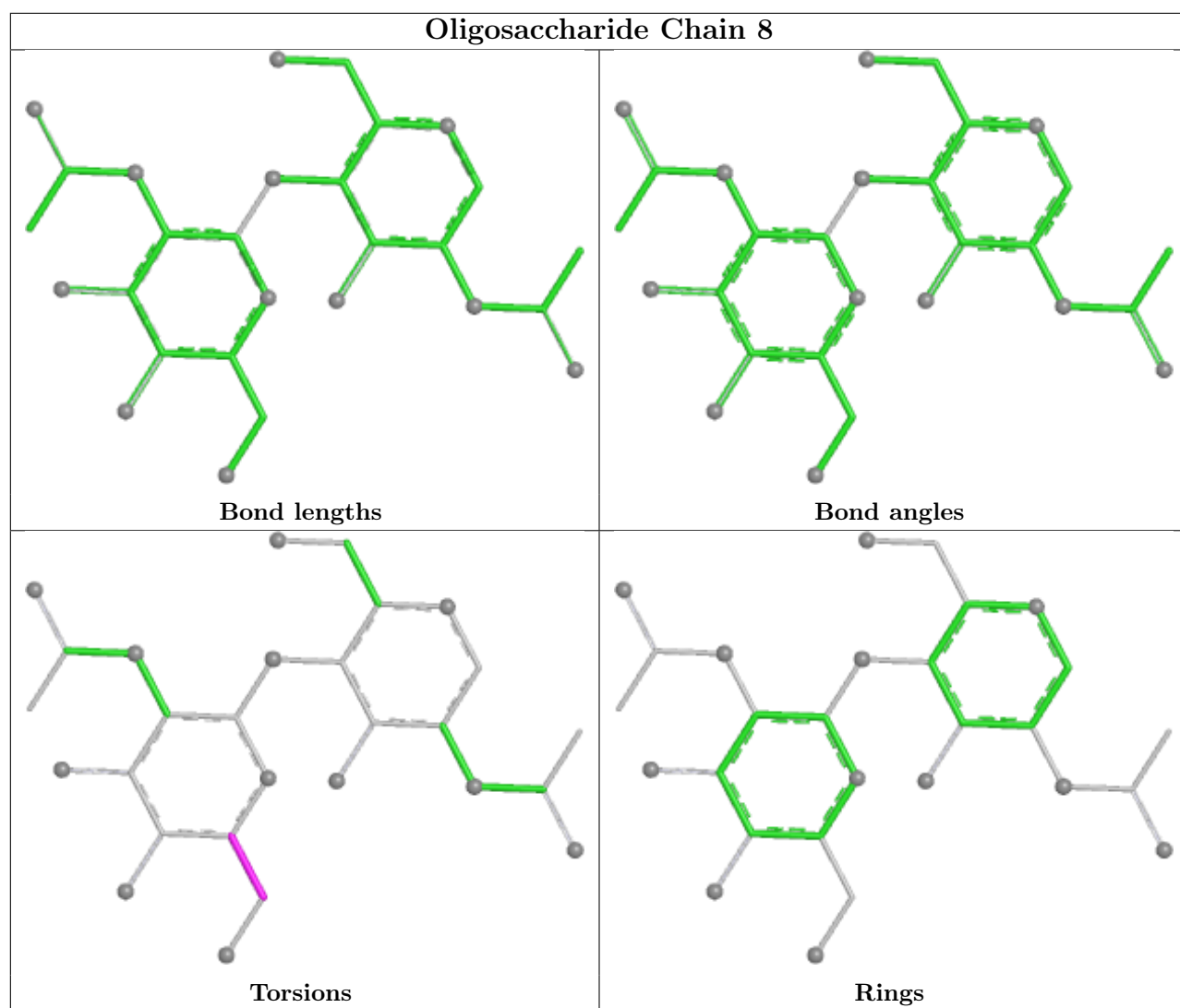


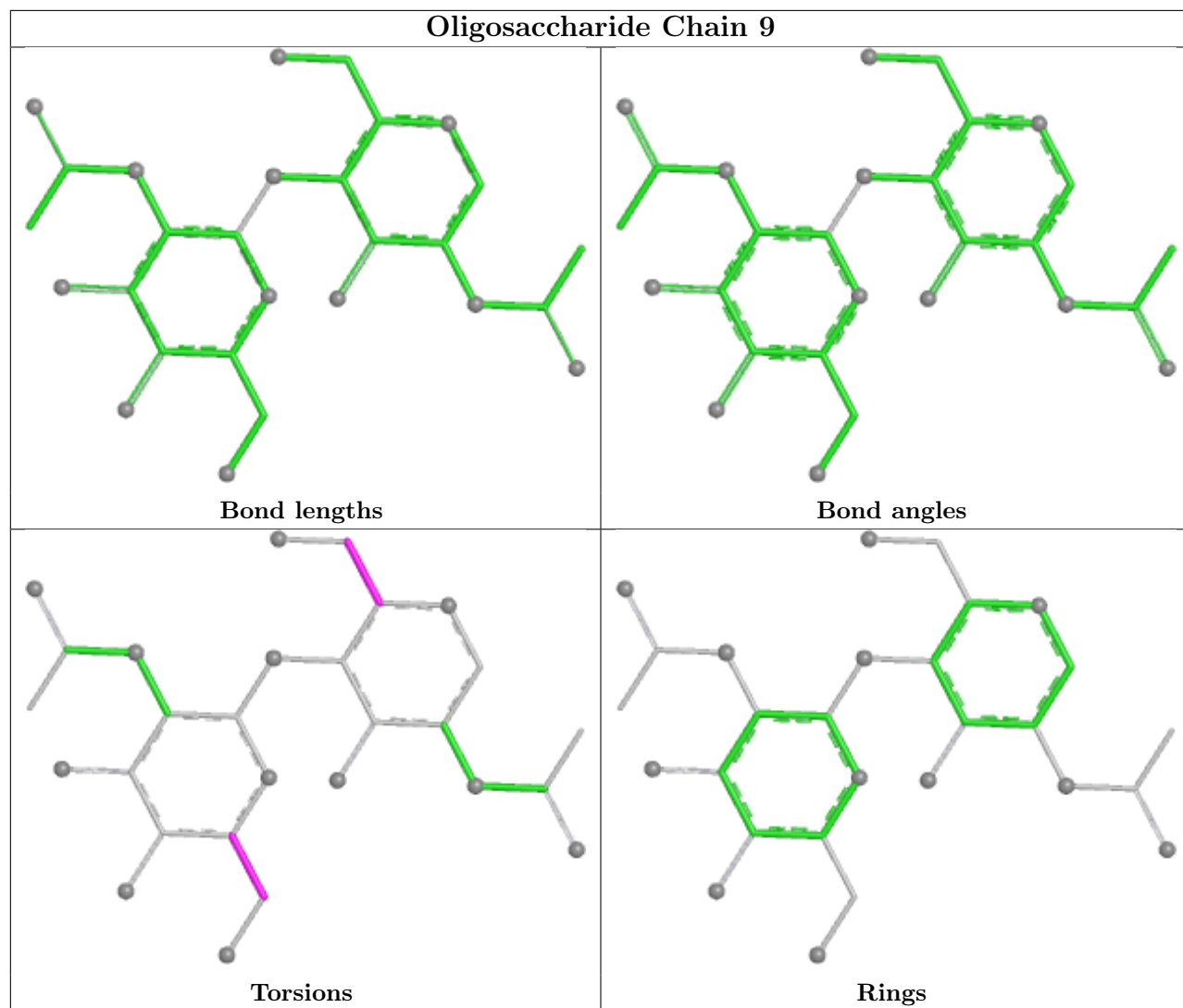


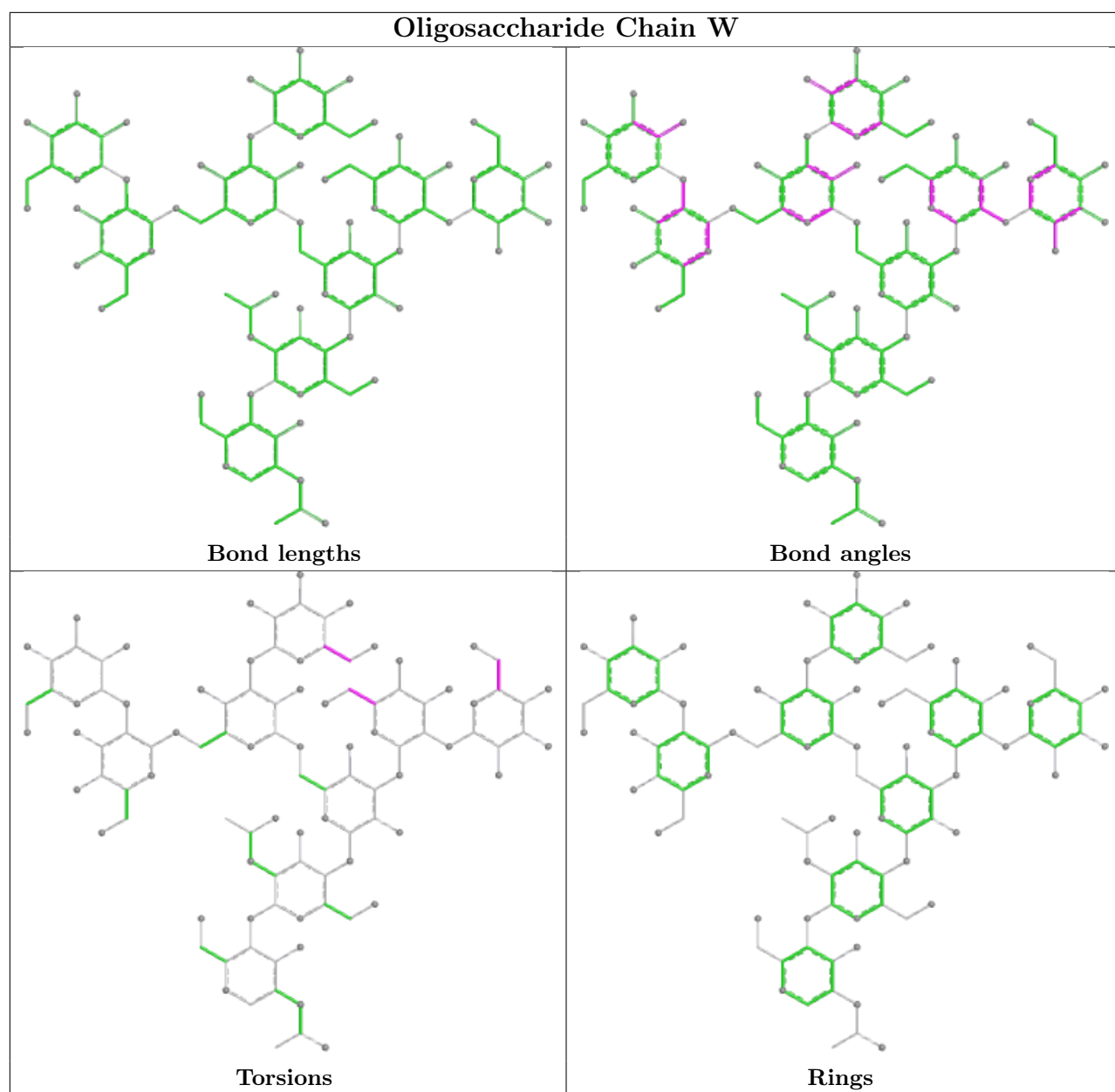


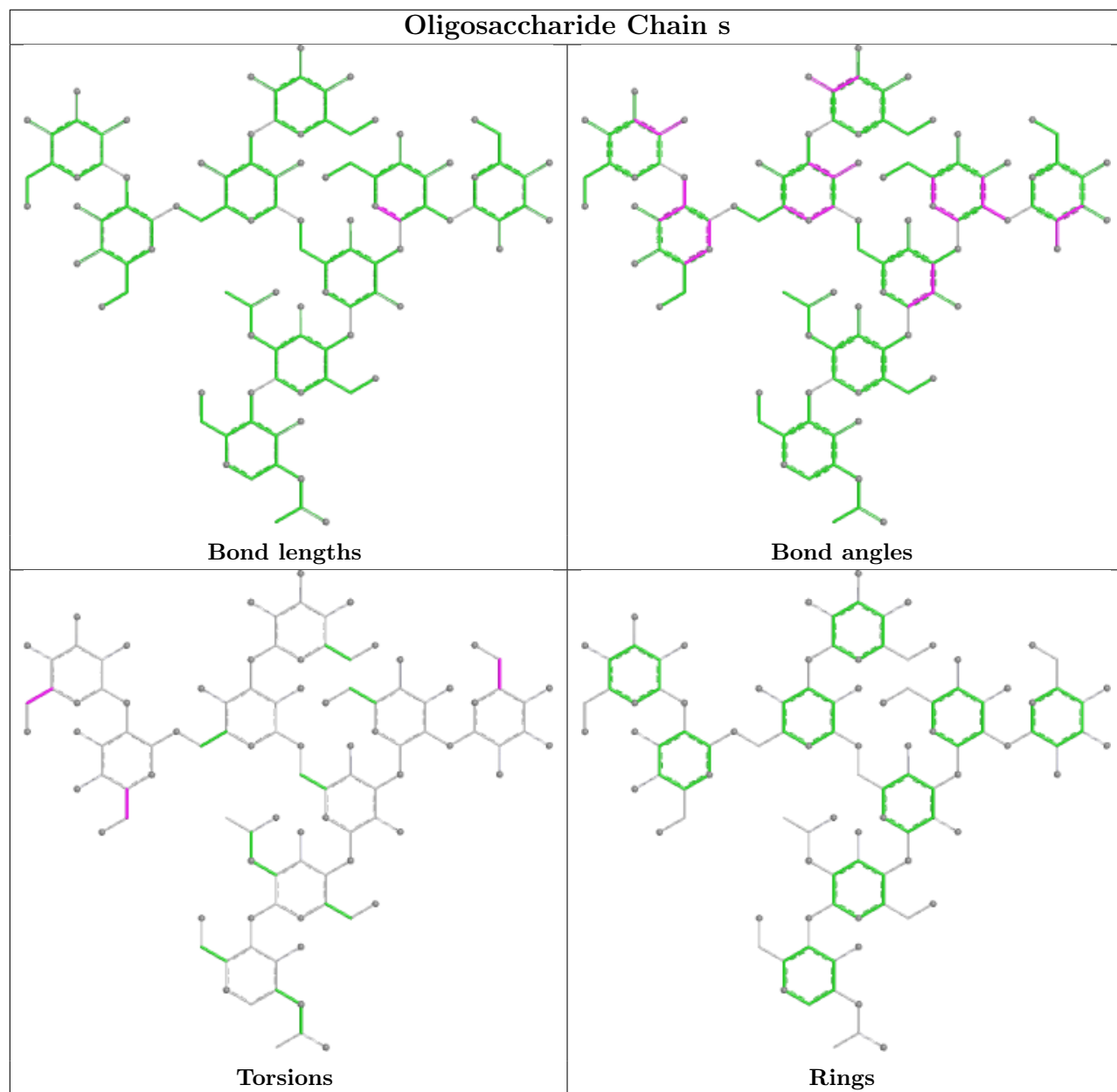


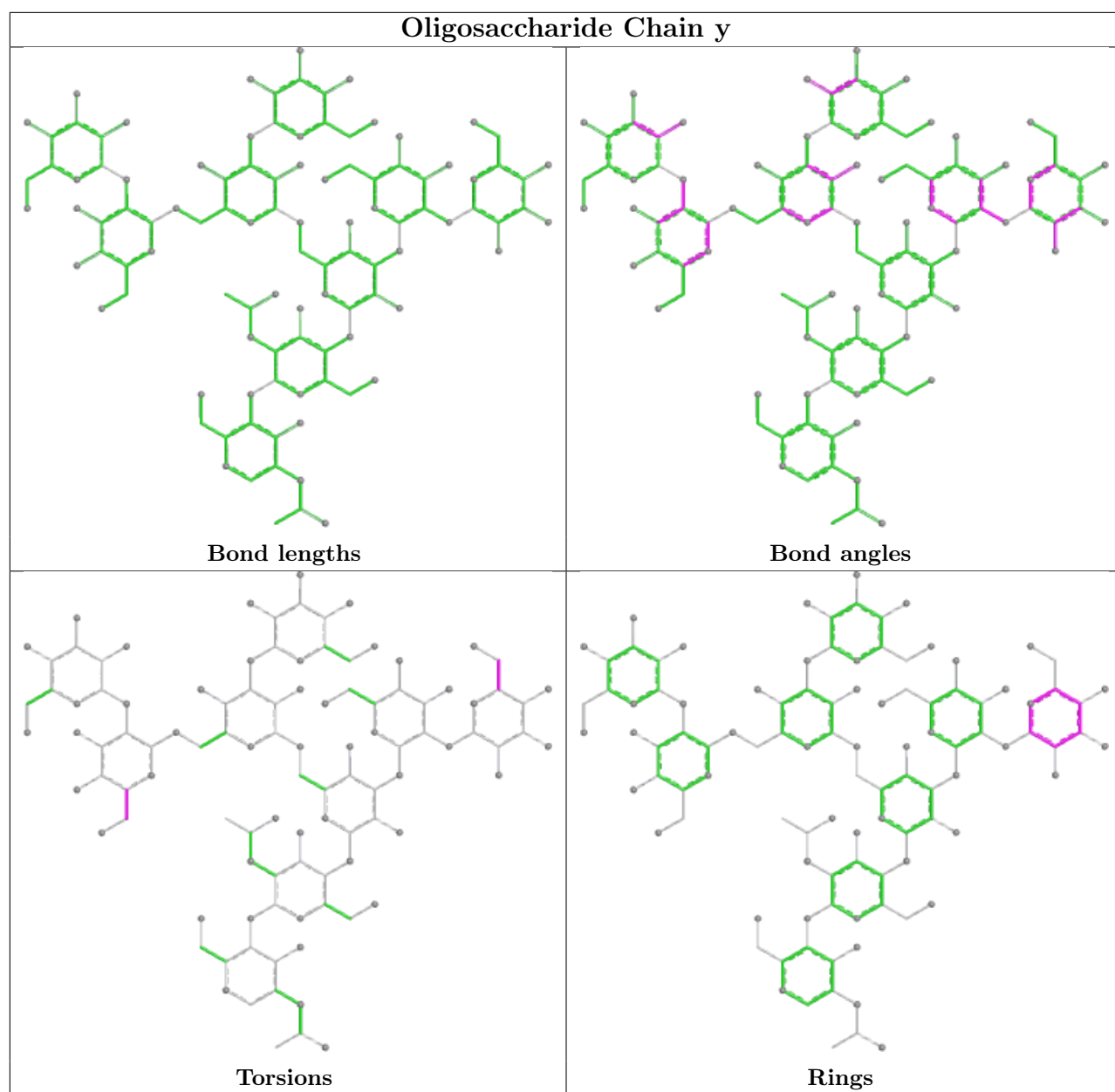


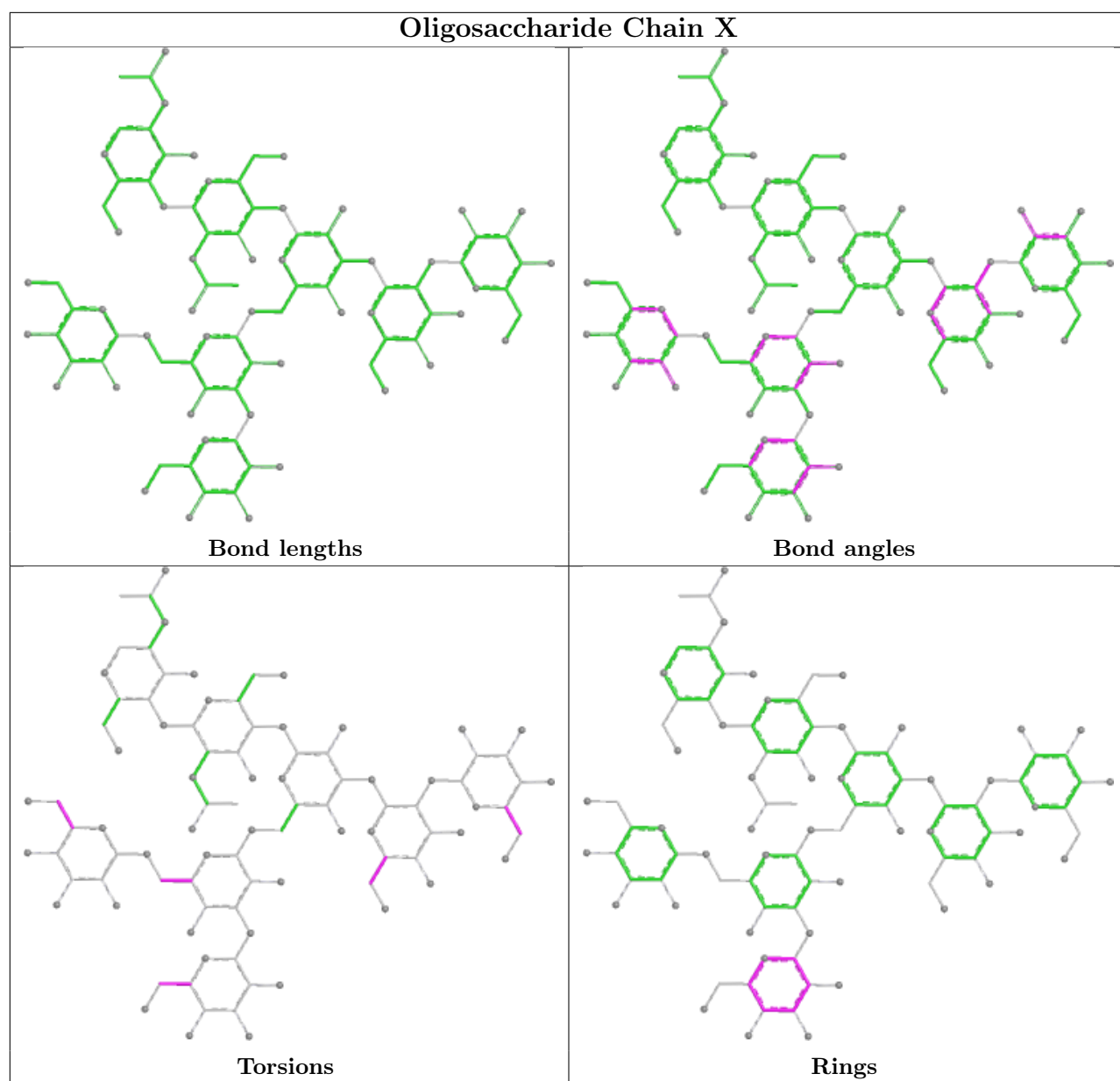


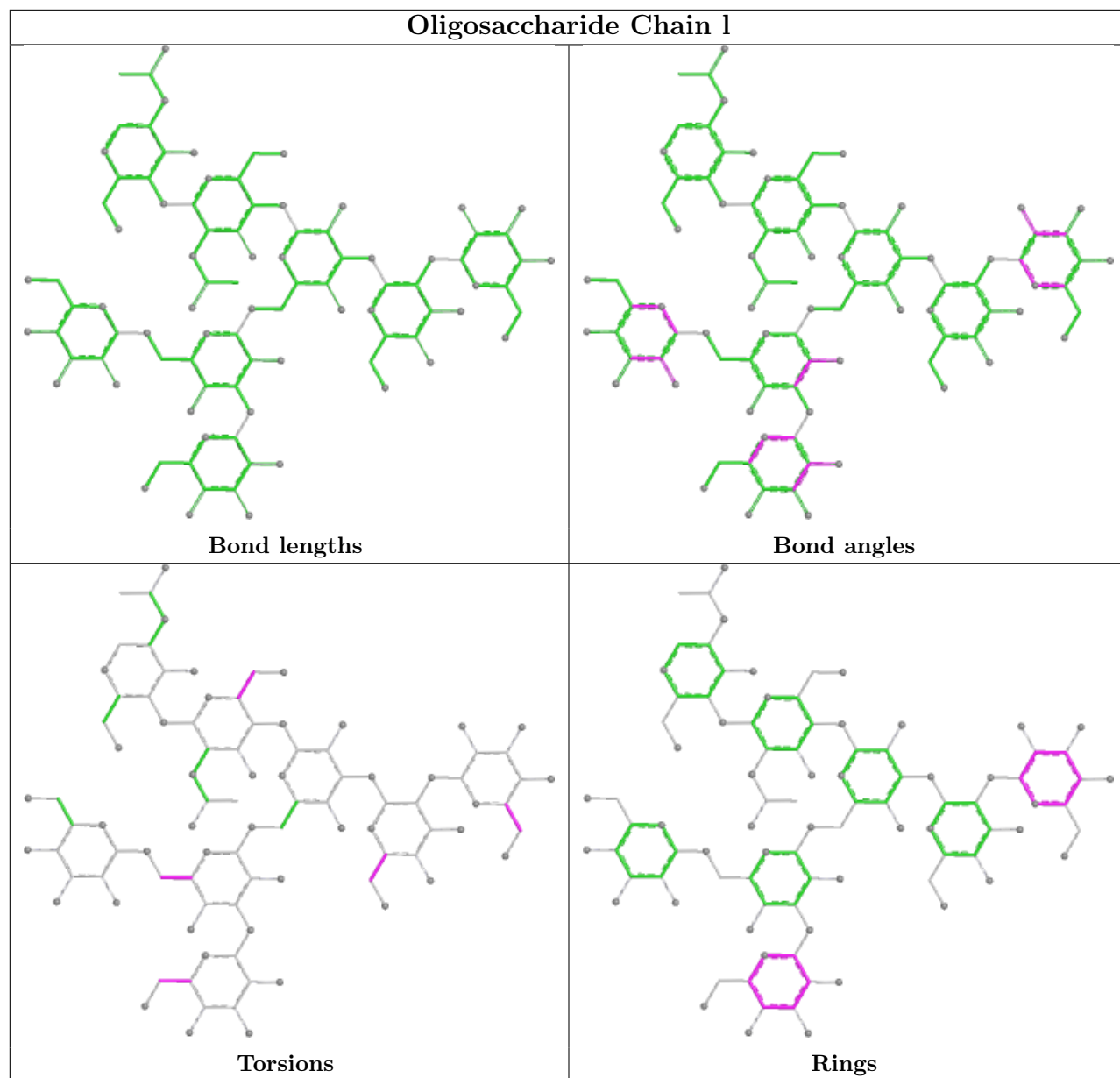




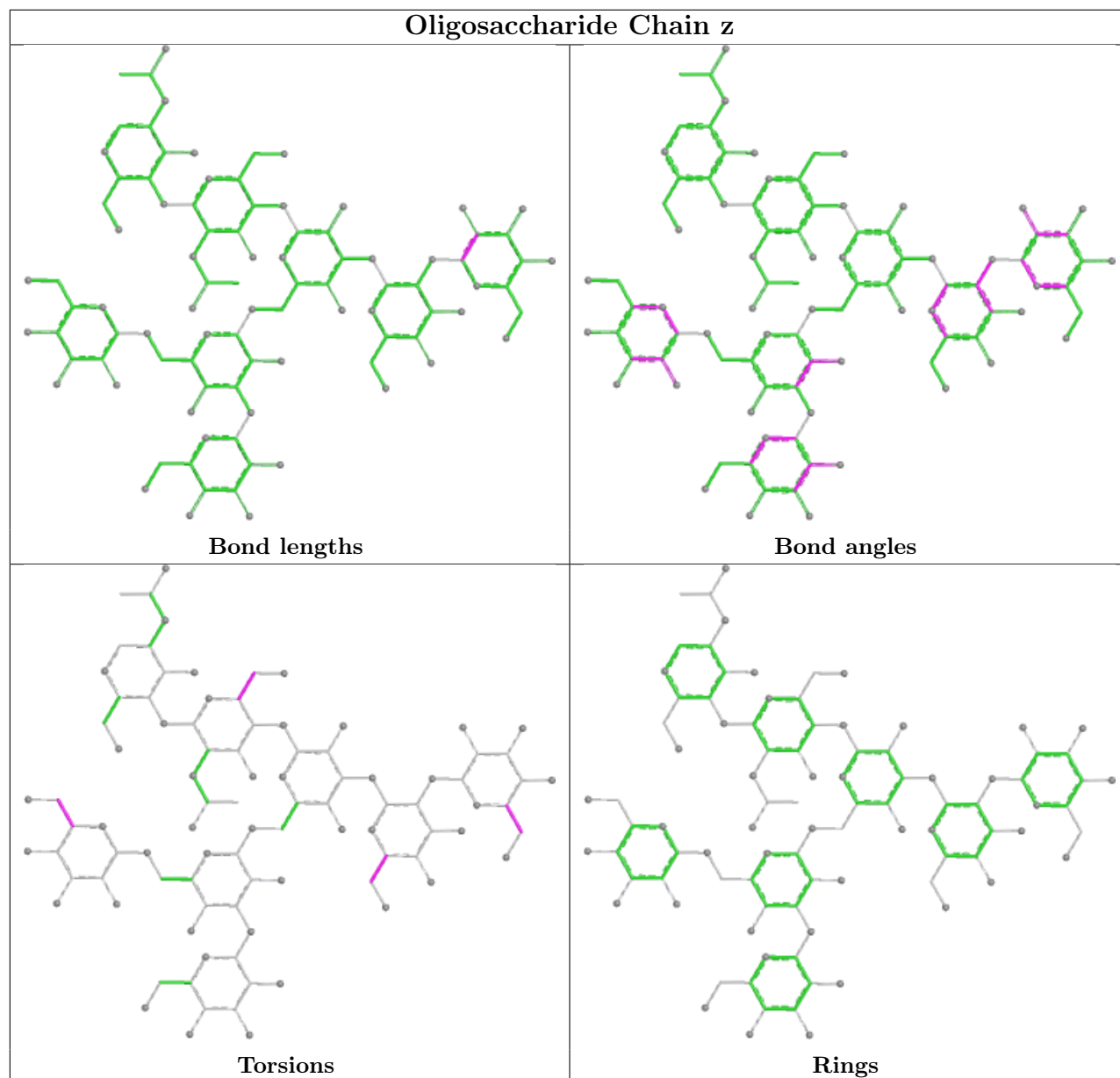


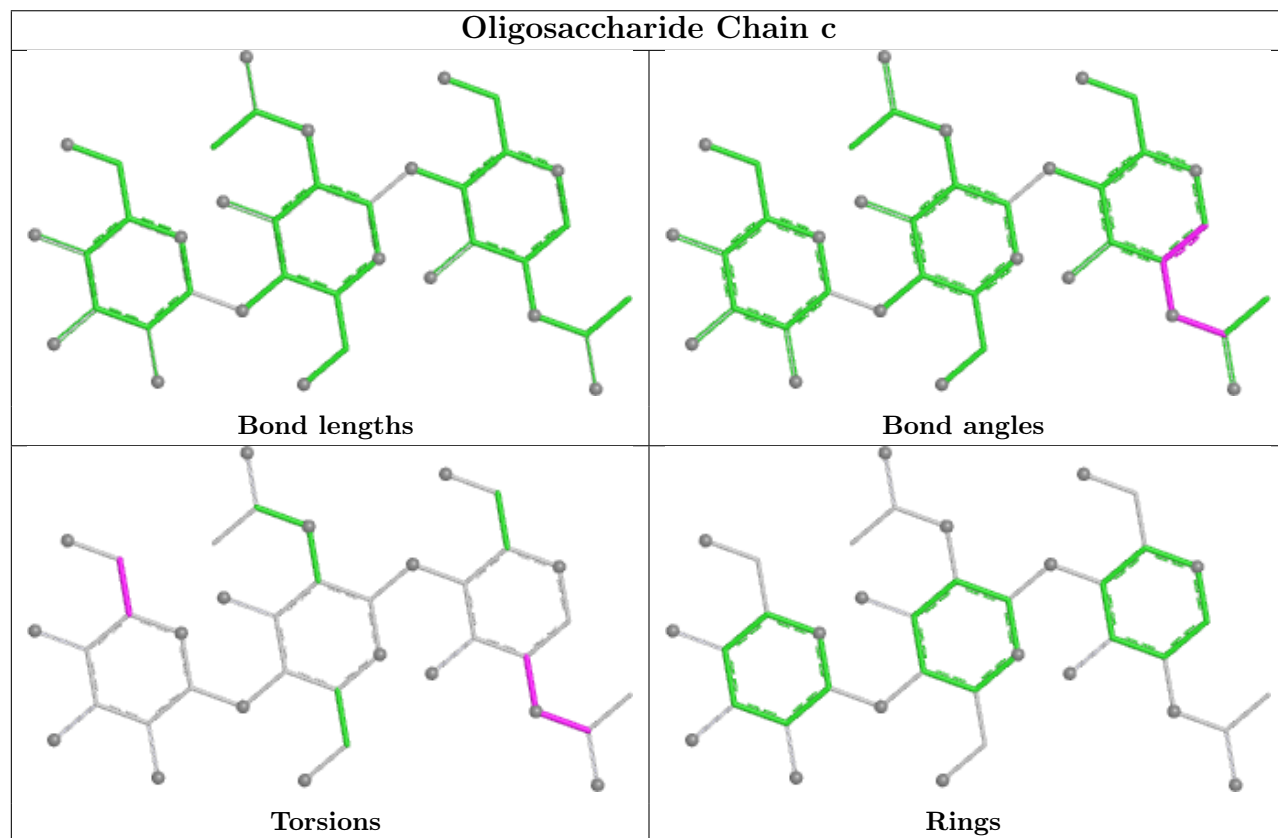
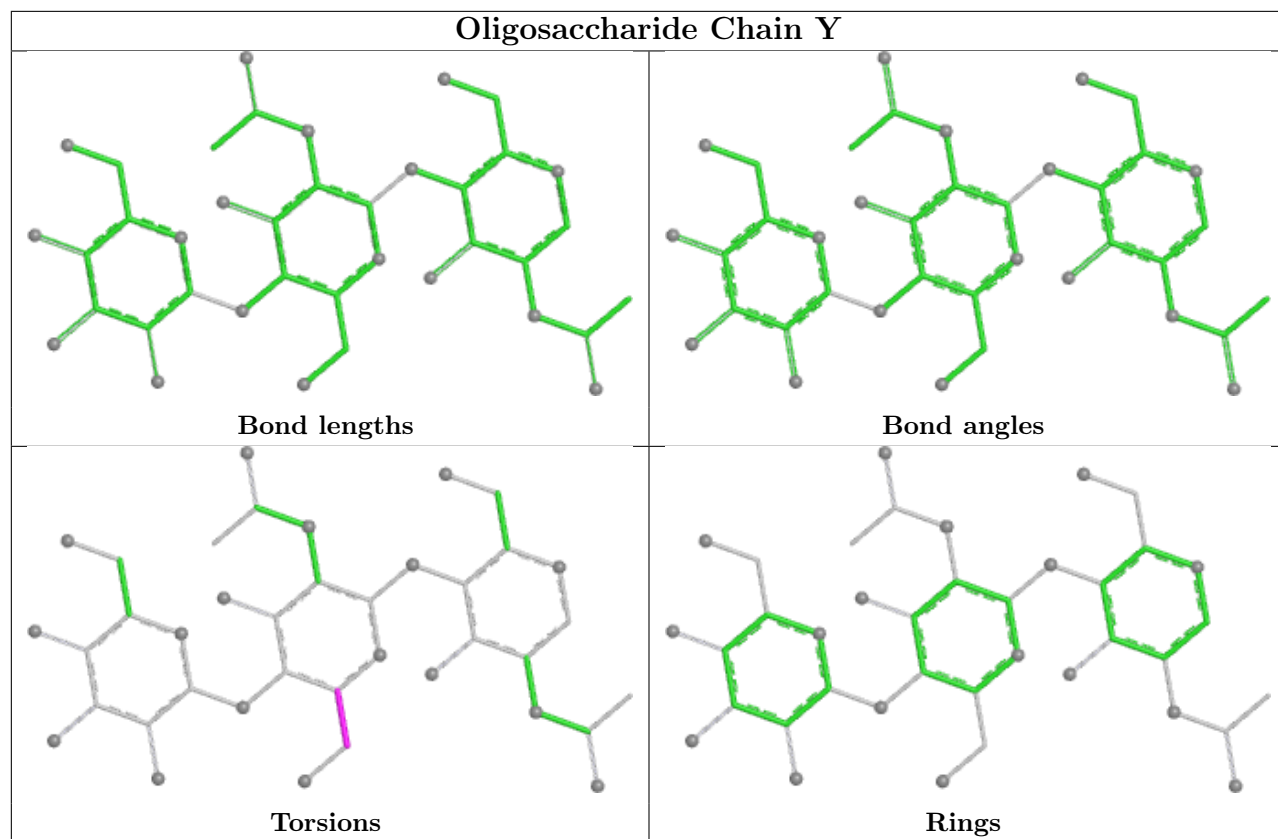


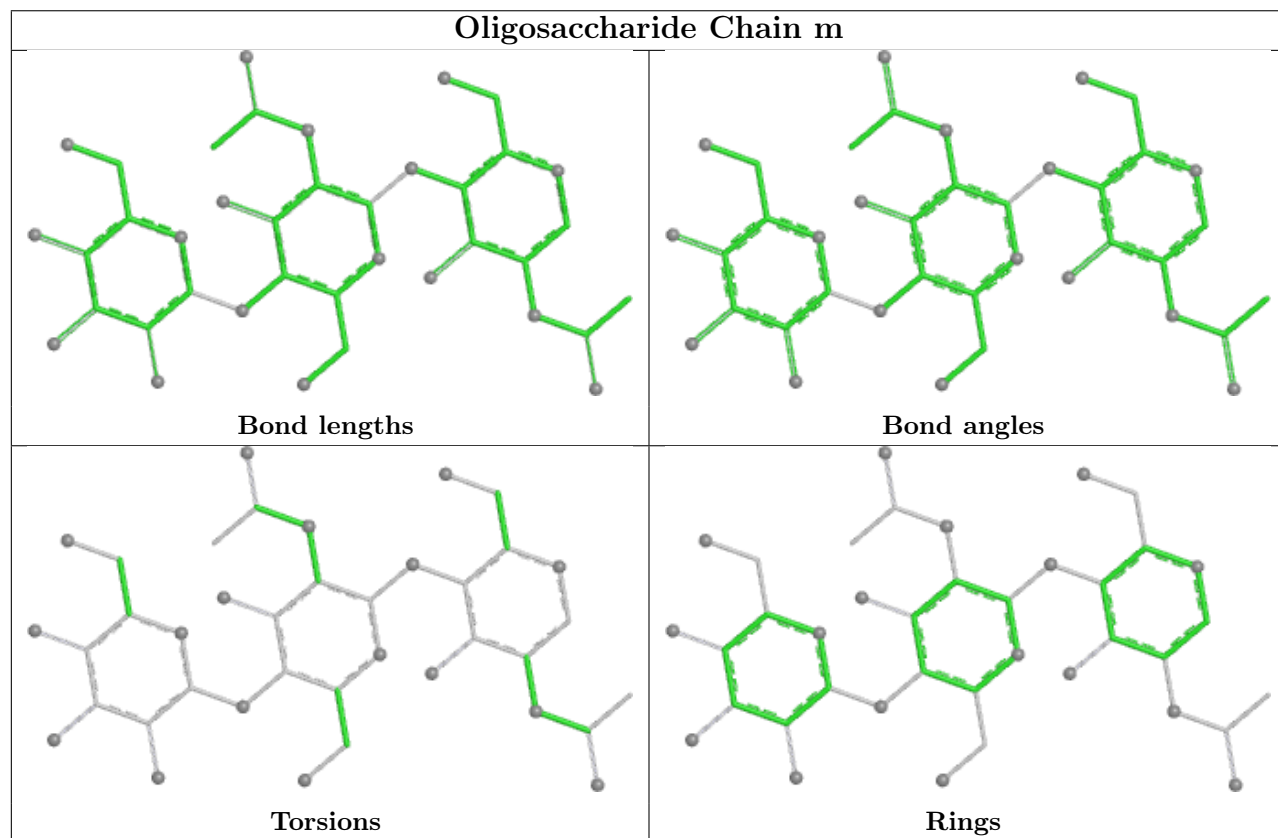
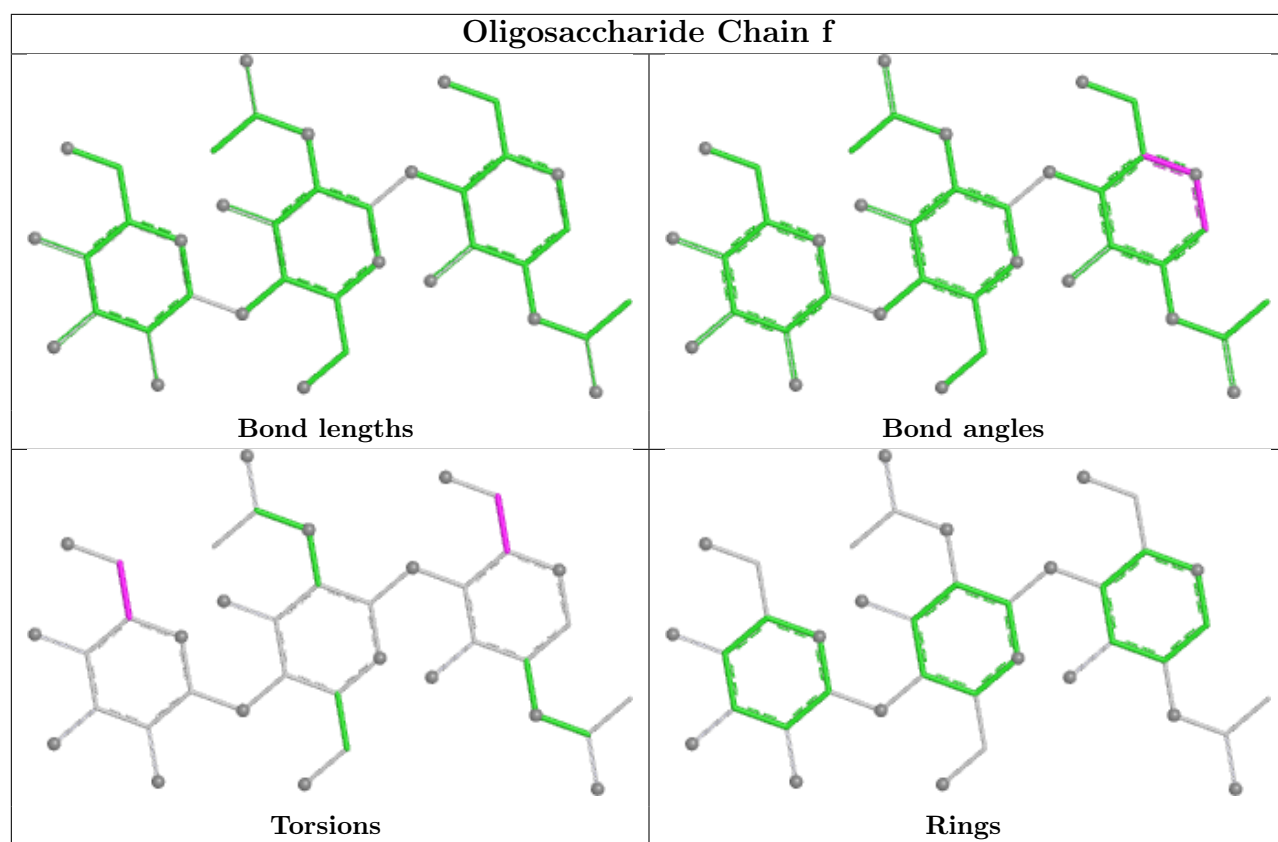


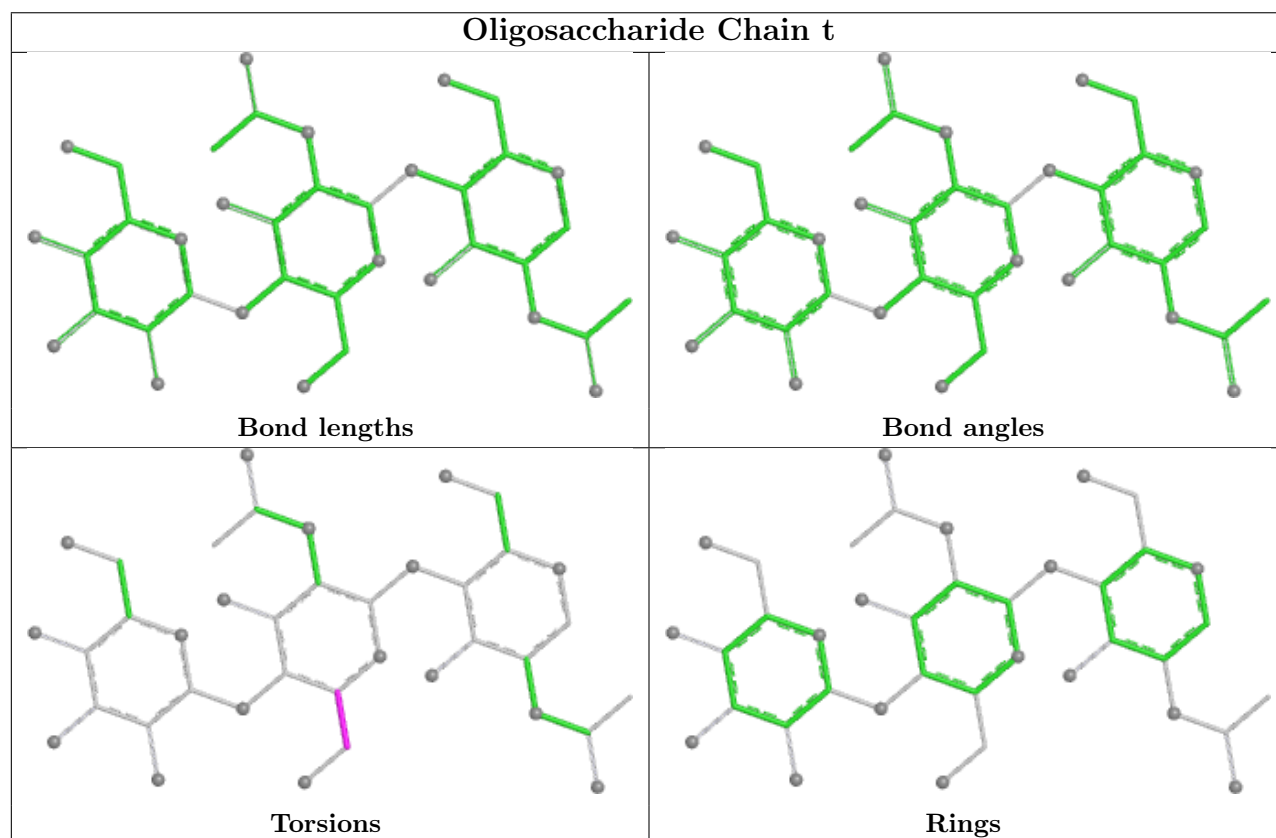
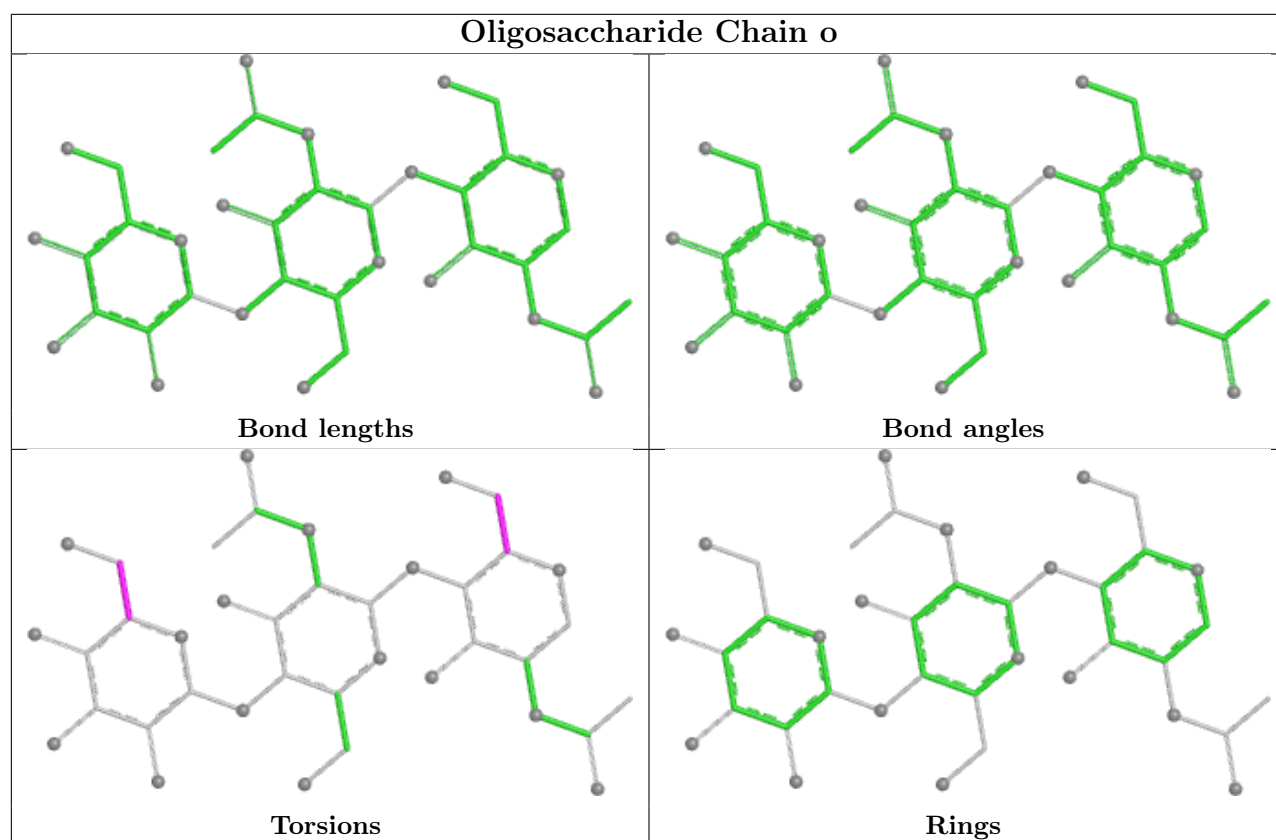


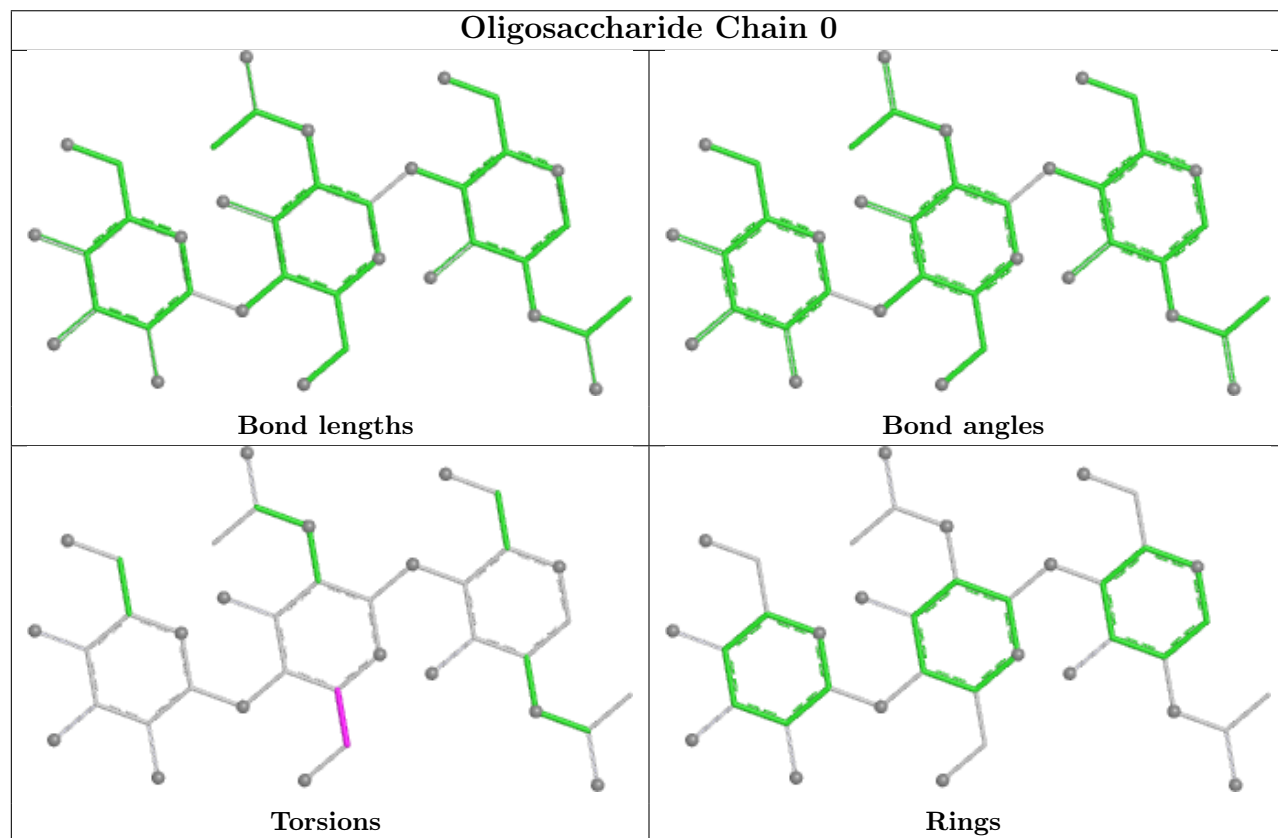
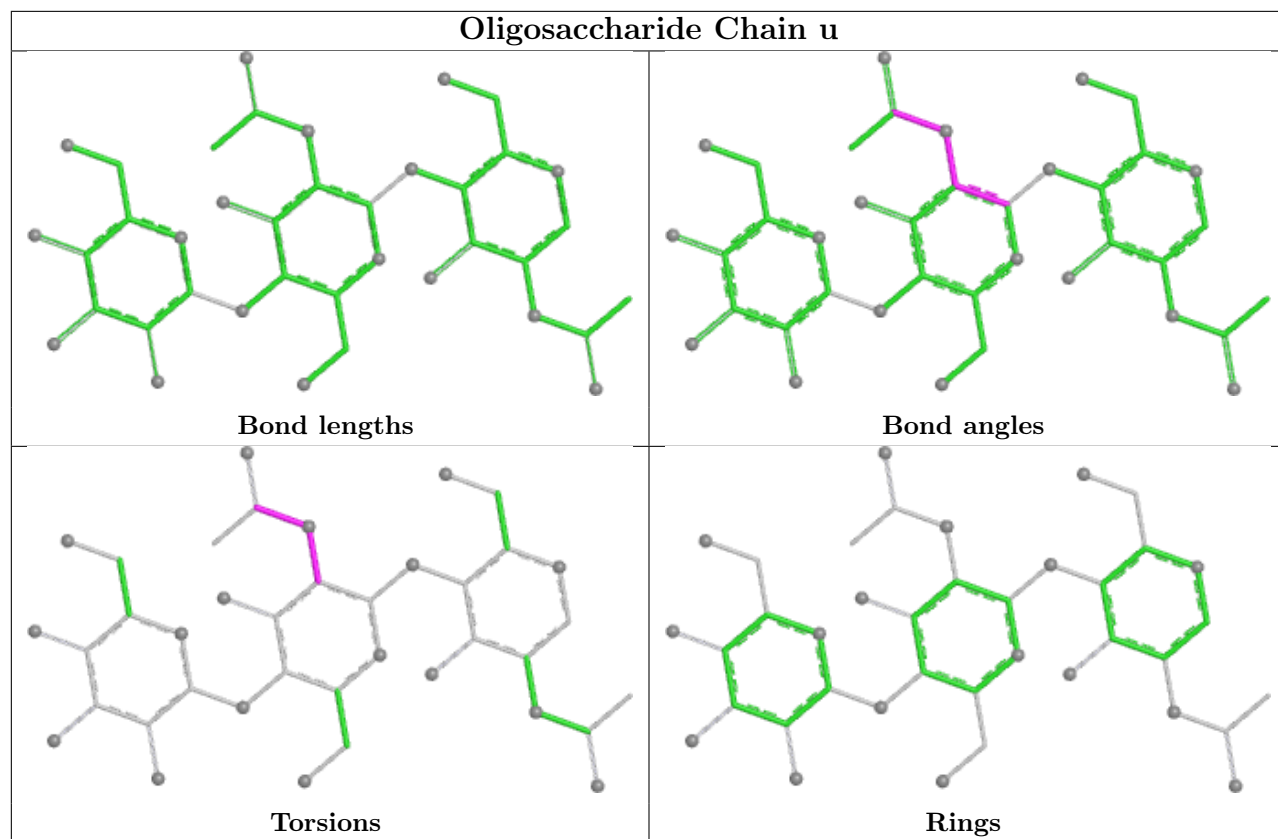


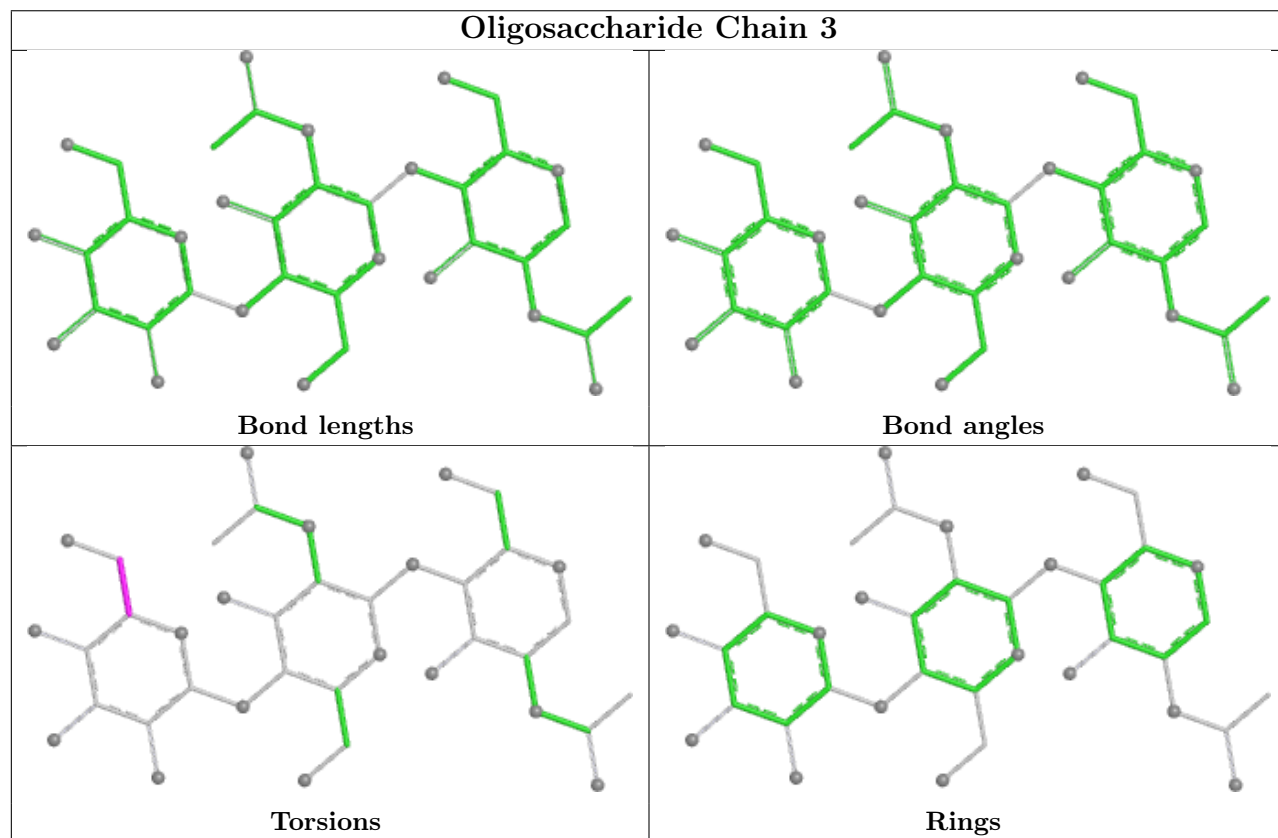
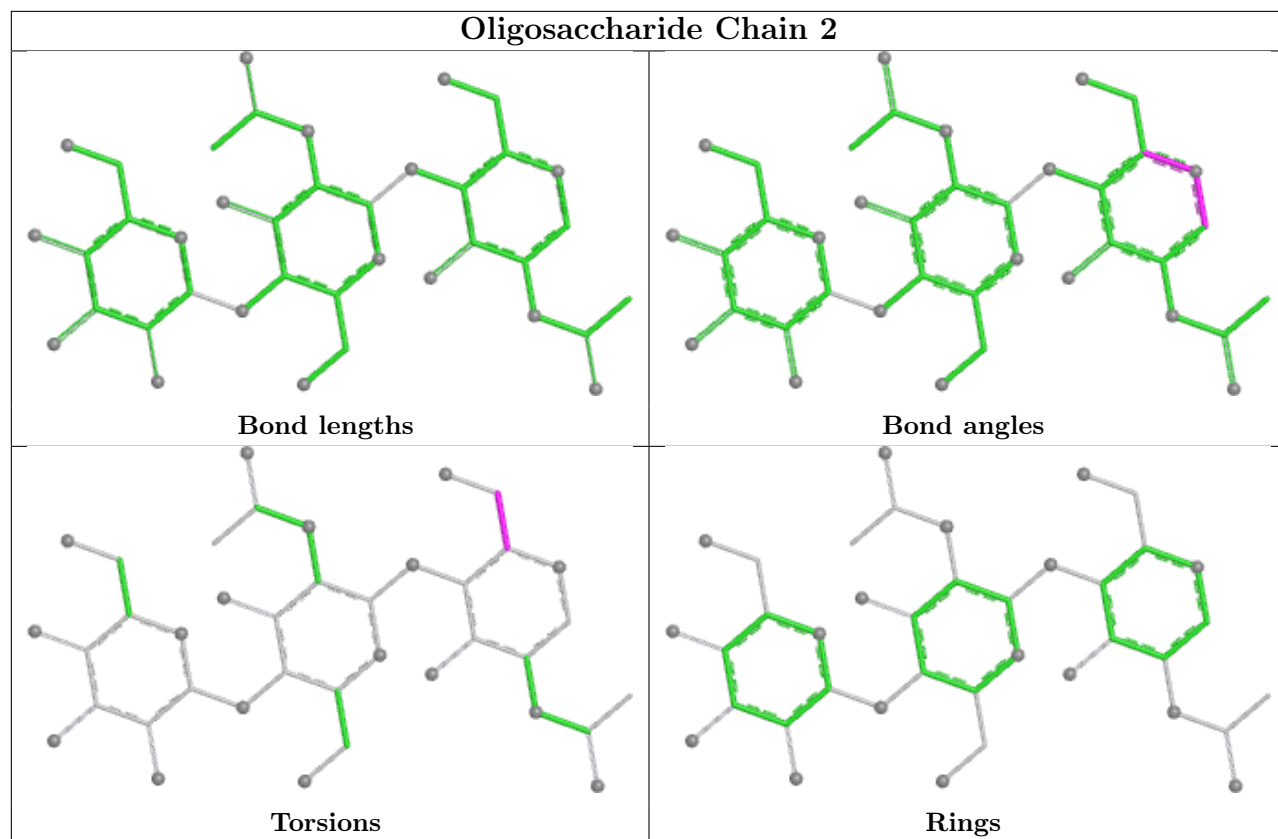


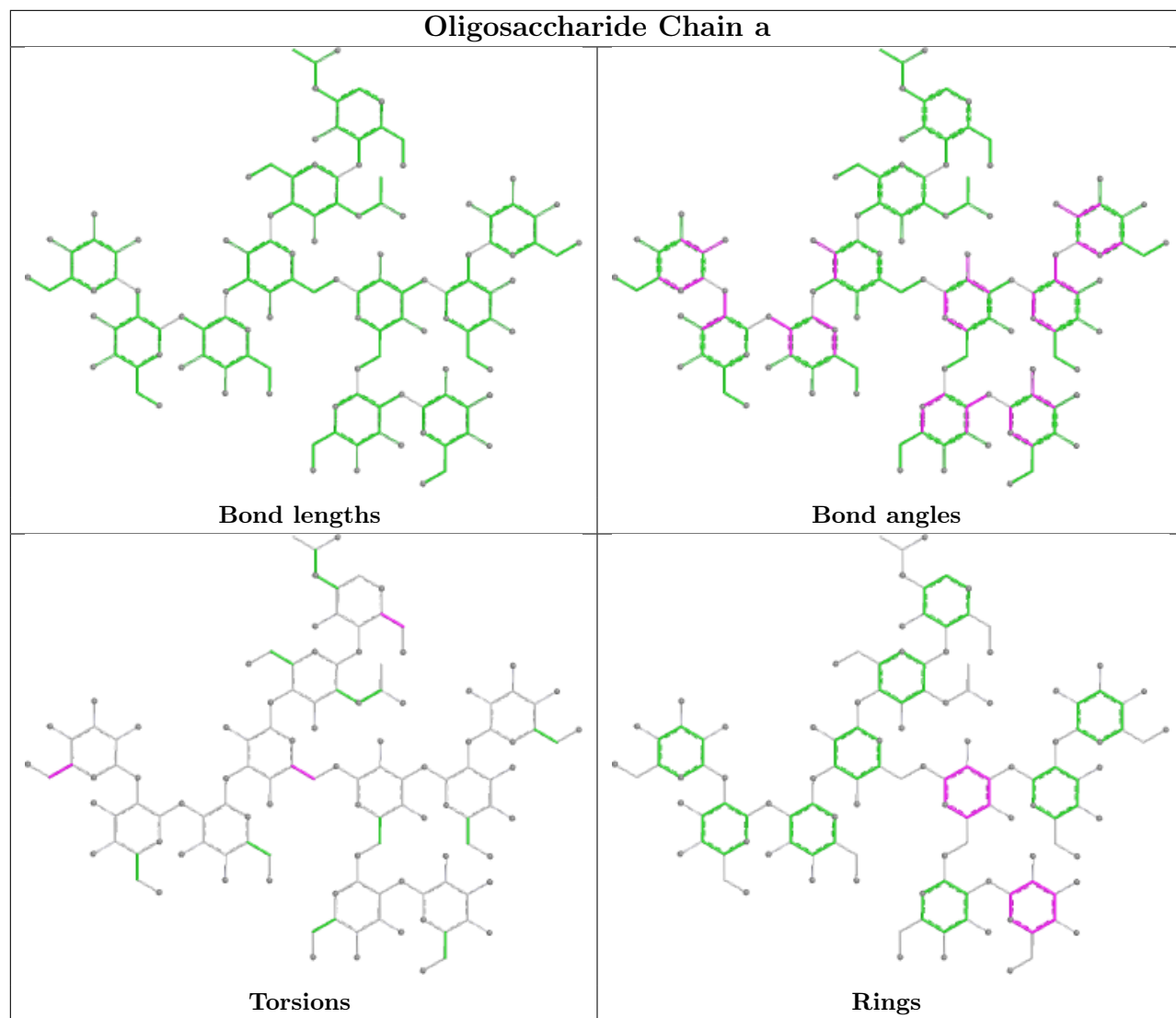


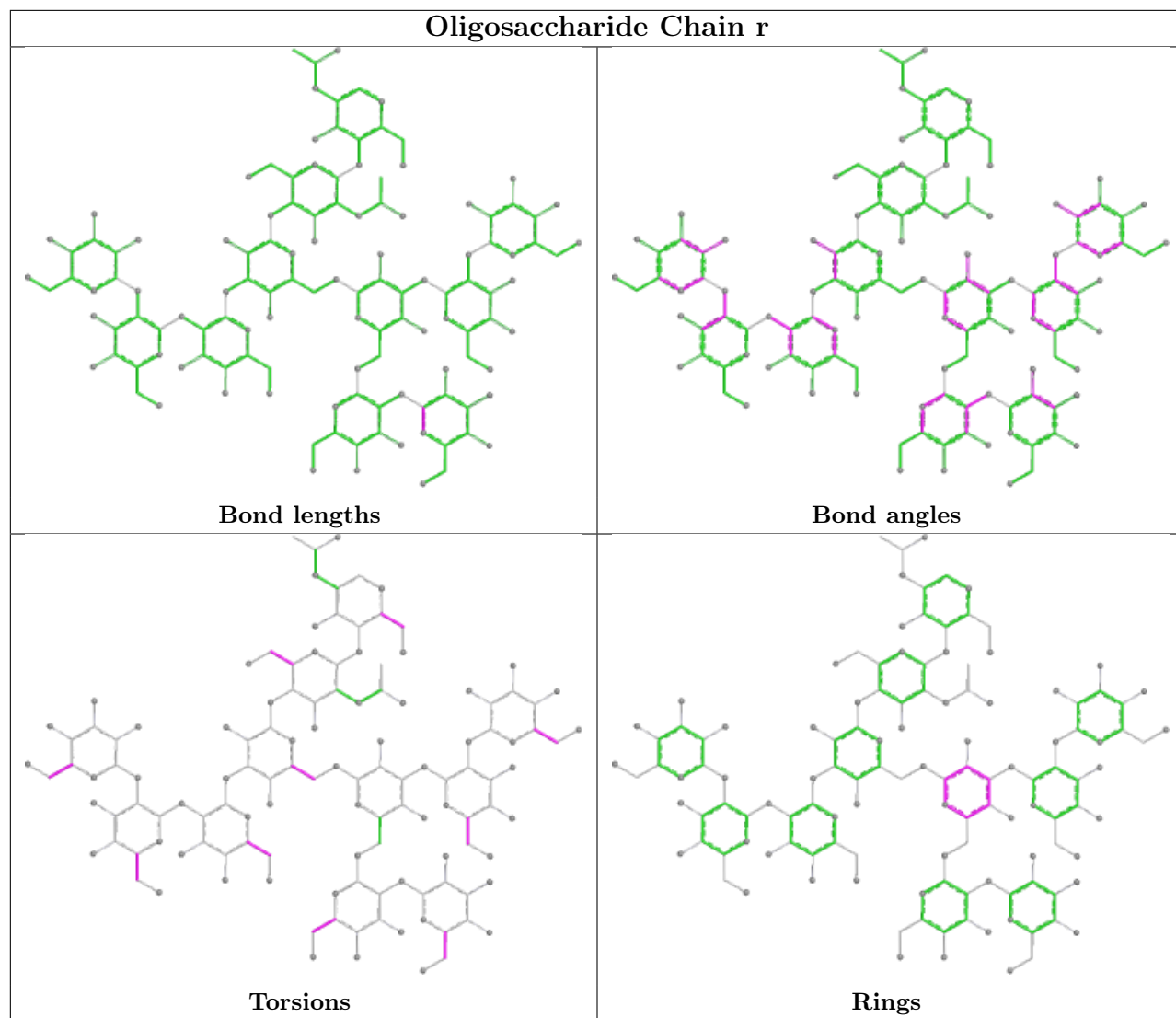




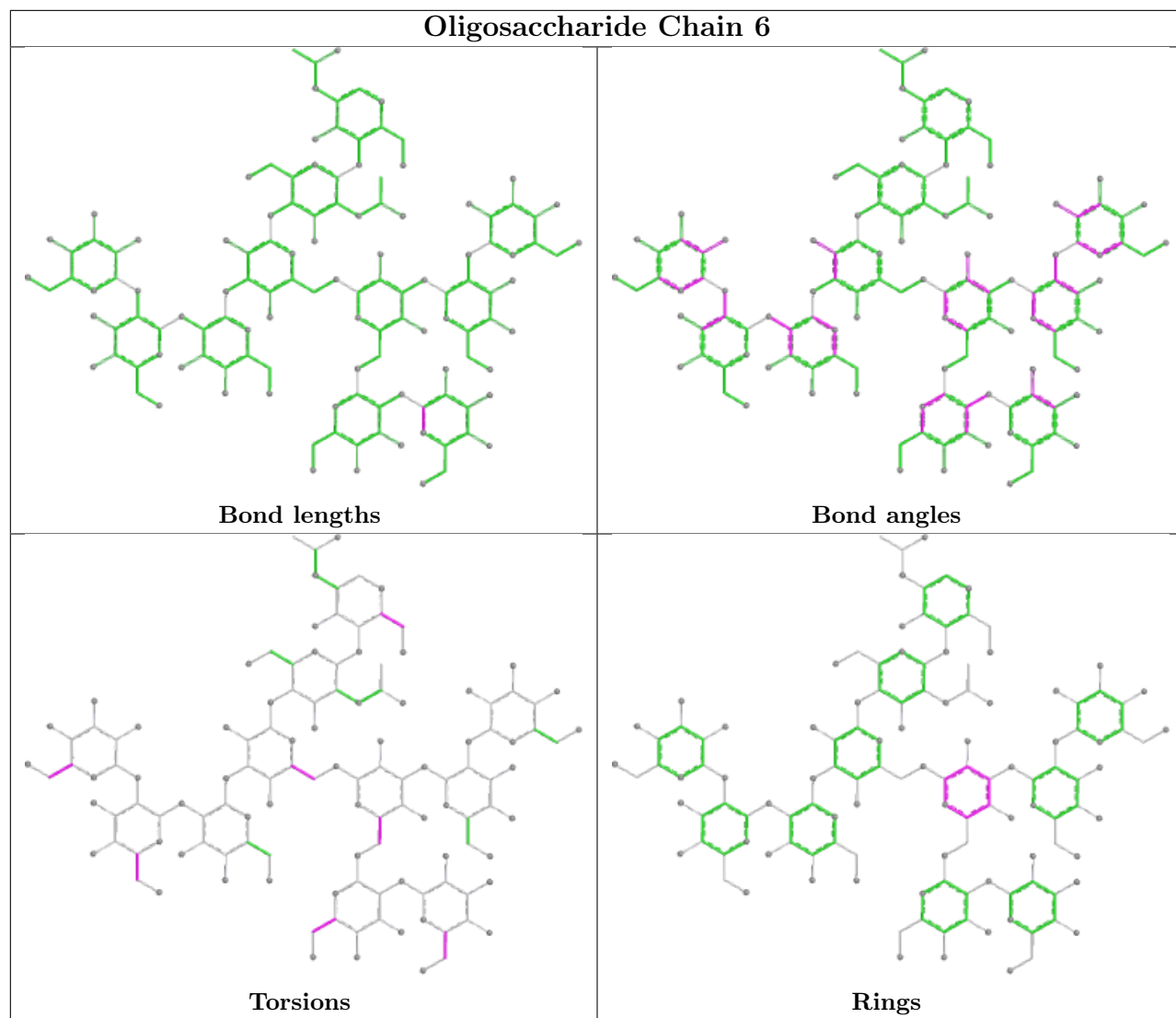


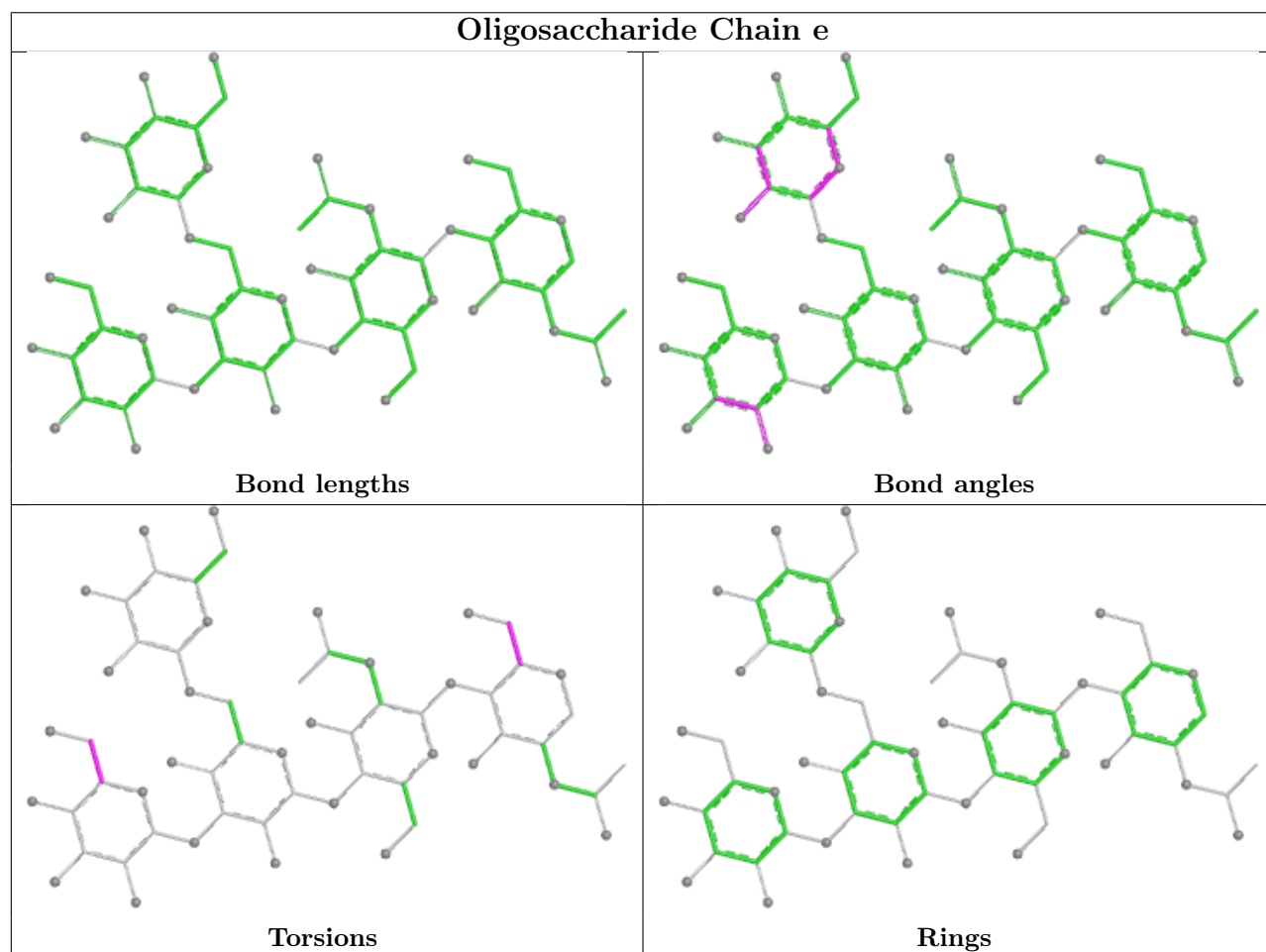
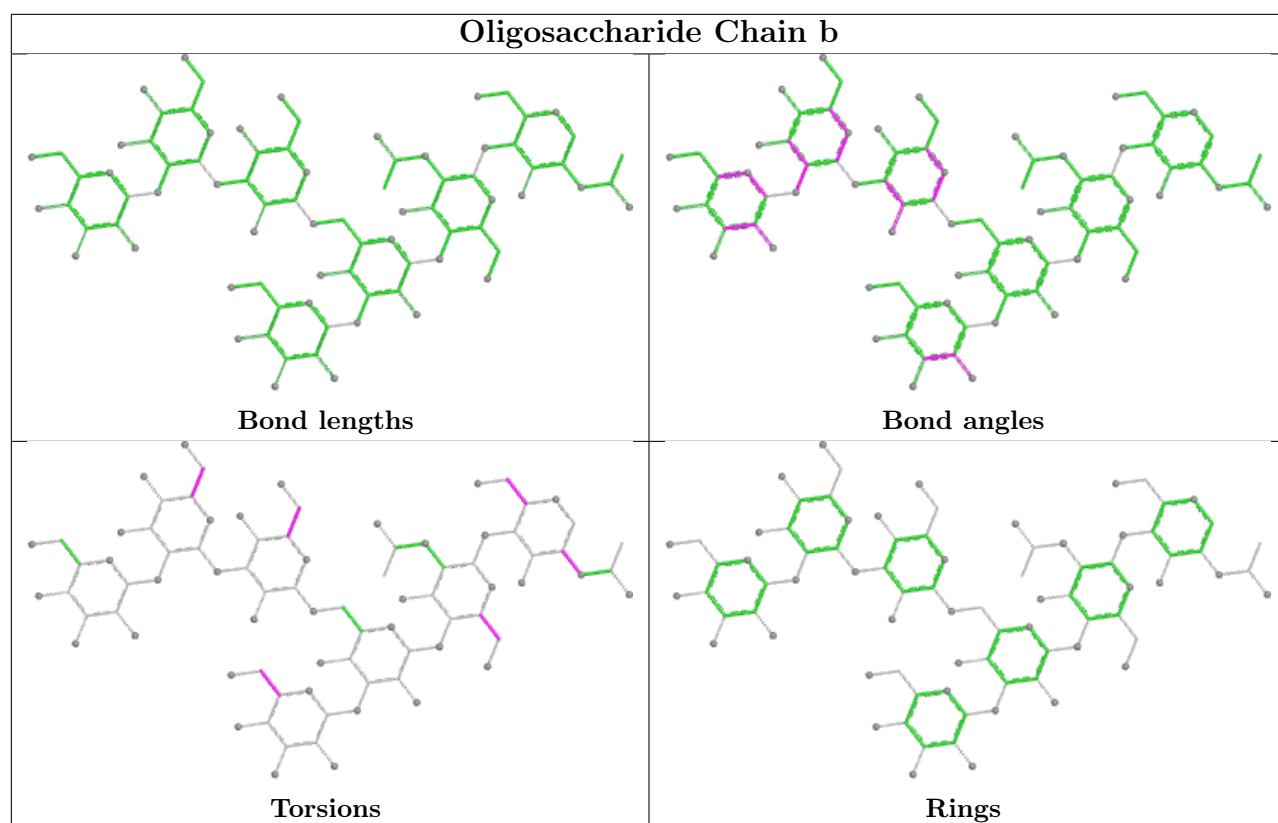


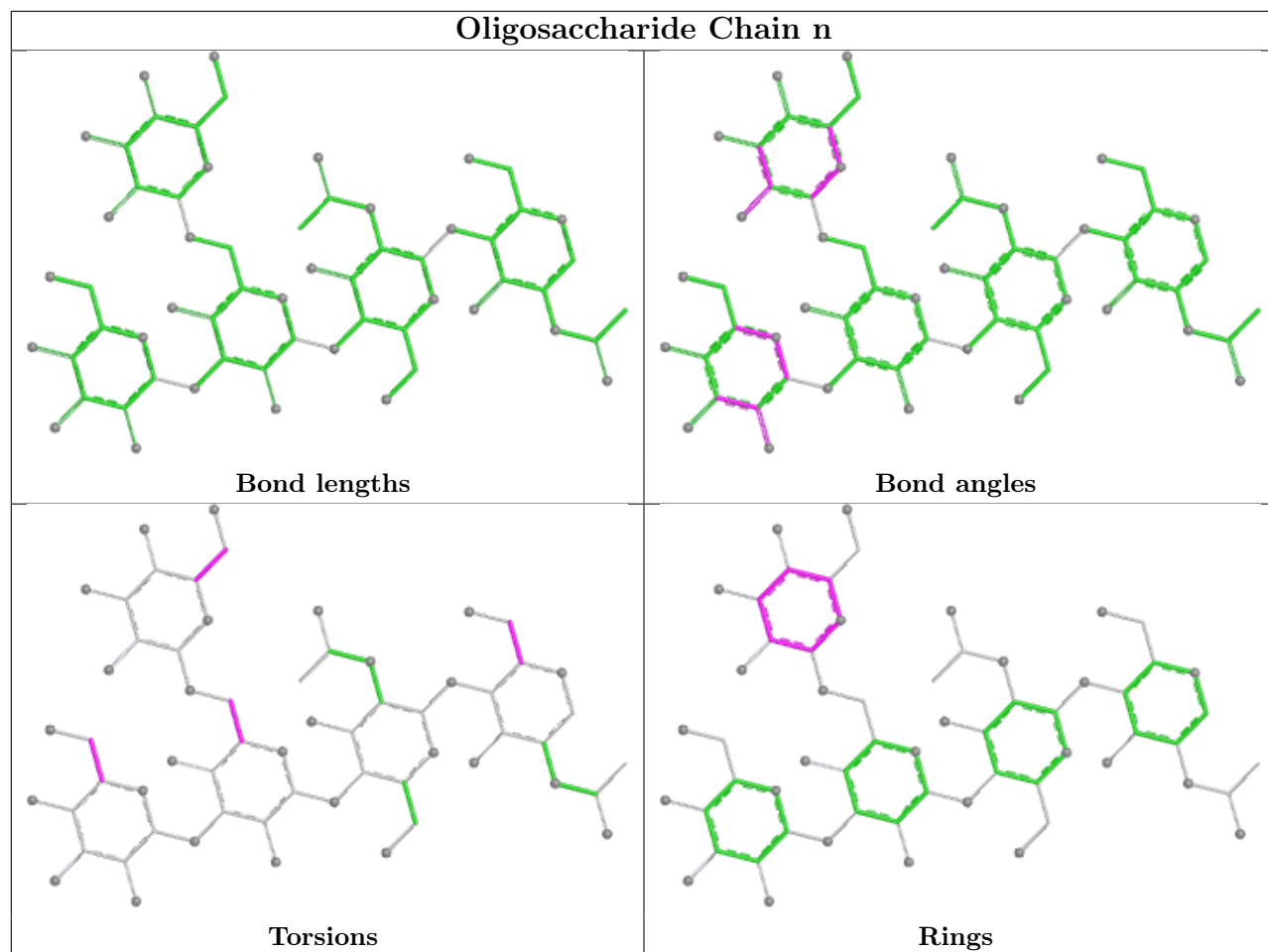


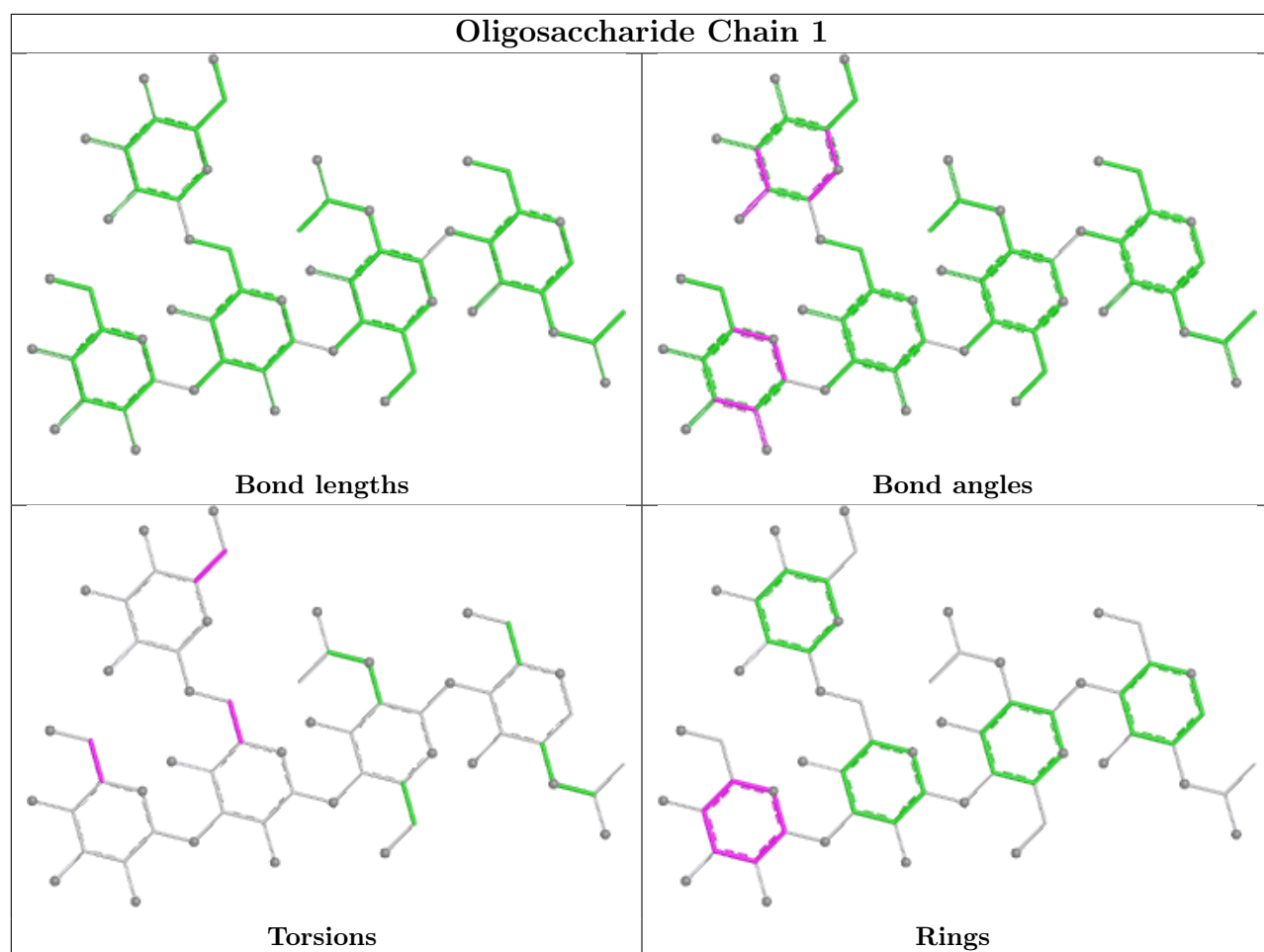


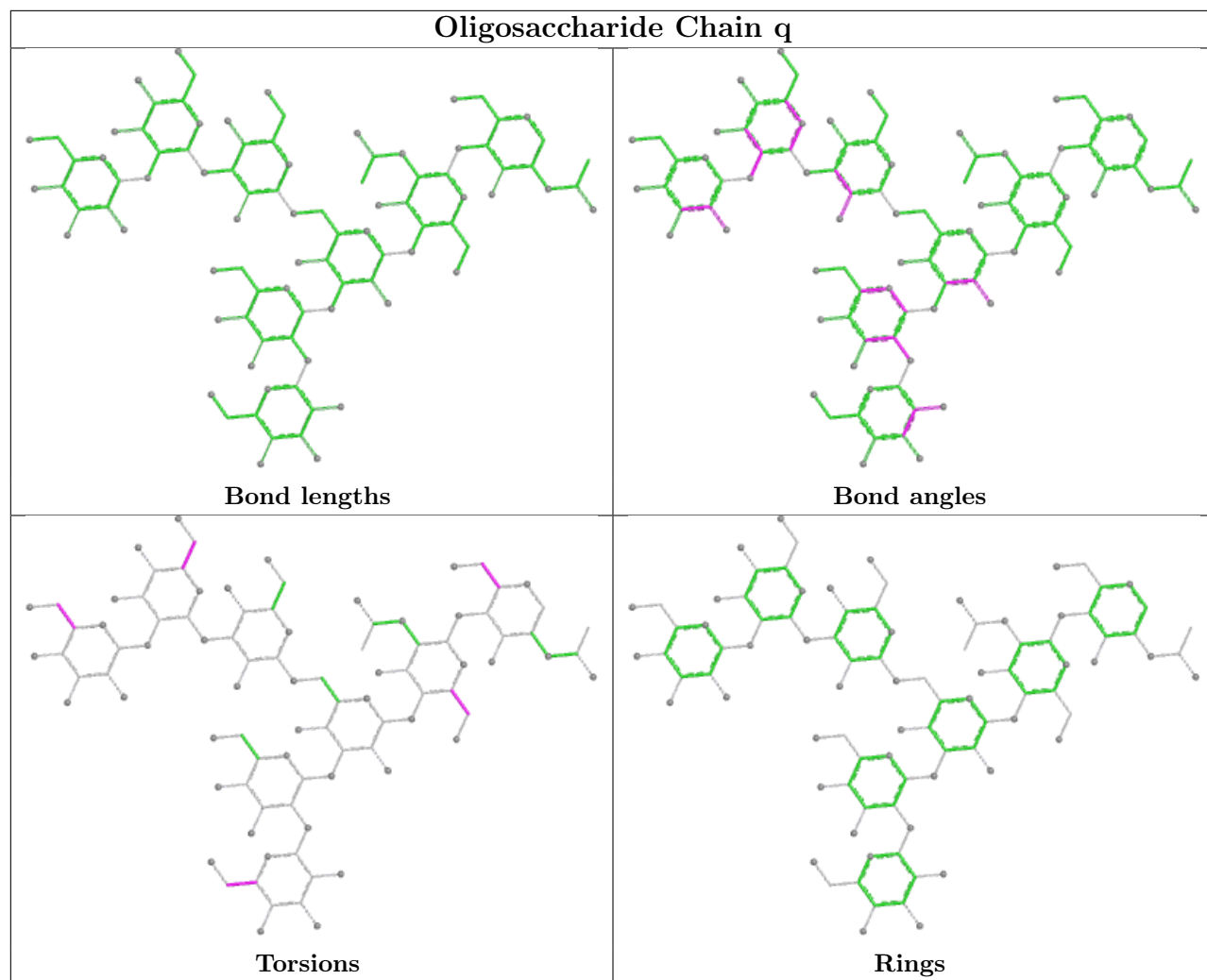


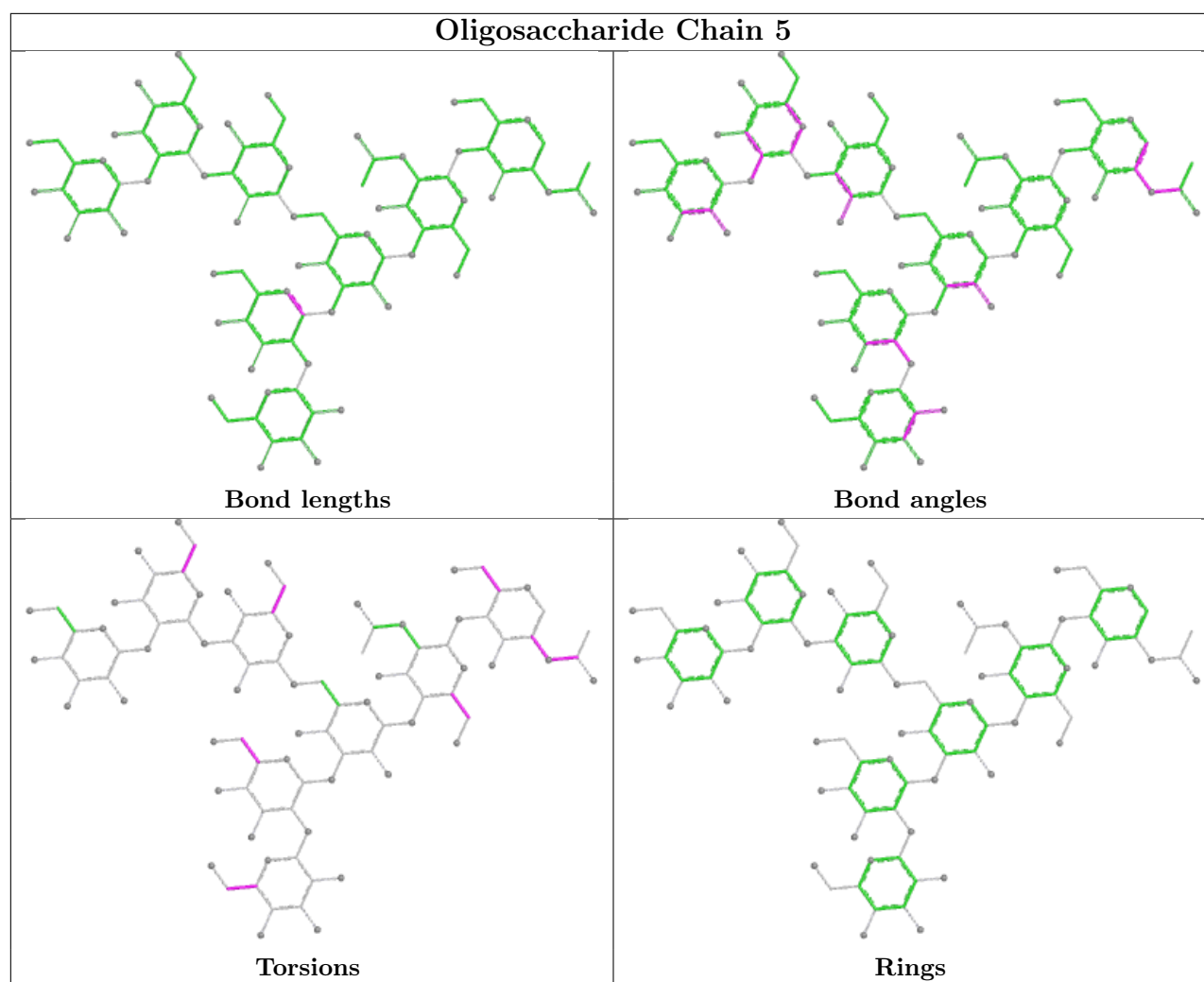












## 5.6 Ligand geometry [i](#)

20 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	$\# Z  > 2$
15	NAG	A	605	3	14,14,15	0.21	0	17,19,21	0.49	0
15	NAG	A	601	3	14,14,15	0.24	0	17,19,21	0.41	0
15	NAG	E	702	4	14,14,15	0.20	0	17,19,21	0.44	0
15	NAG	C	602	3	14,14,15	0.20	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	NAG	D	701	4	14,14,15	0.21	0	17,19,21	0.48	0
15	NAG	B	602	3	14,14,15	0.19	0	17,19,21	0.41	0
15	NAG	C	604	3	14,14,15	0.22	0	17,19,21	0.46	0
15	NAG	A	604	3	14,14,15	0.29	0	17,19,21	0.41	0
15	NAG	C	601	3	14,14,15	0.28	0	17,19,21	0.48	0
15	NAG	A	602	3	14,14,15	0.17	0	17,19,21	0.44	0
15	NAG	C	603	3	14,14,15	0.27	0	17,19,21	0.42	0
15	NAG	F	701	4	14,14,15	0.19	0	17,19,21	0.45	0
15	NAG	D	702	4	14,14,15	0.22	0	17,19,21	0.43	0
15	NAG	B	601	3	14,14,15	0.21	0	17,19,21	0.49	0
15	NAG	B	603	3	14,14,15	0.25	0	17,19,21	0.41	0
15	NAG	E	701	4	14,14,15	0.19	0	17,19,21	0.47	0
15	NAG	B	604	3	14,14,15	0.20	0	17,19,21	0.47	0
15	NAG	F	702	4	14,14,15	0.21	0	17,19,21	0.43	0
15	NAG	B	605	3	14,14,15	0.27	0	17,19,21	0.45	0
15	NAG	A	603	3	14,14,15	0.19	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	605	3	-	2/6/23/26	0/1/1/1
15	NAG	A	601	3	-	0/6/23/26	0/1/1/1
15	NAG	E	702	4	-	0/6/23/26	0/1/1/1
15	NAG	C	602	3	-	2/6/23/26	0/1/1/1
15	NAG	D	701	4	-	3/6/23/26	0/1/1/1
15	NAG	B	602	3	-	2/6/23/26	0/1/1/1
15	NAG	C	604	3	-	1/6/23/26	0/1/1/1
15	NAG	A	604	3	-	1/6/23/26	0/1/1/1
15	NAG	C	601	3	-	2/6/23/26	0/1/1/1
15	NAG	A	602	3	-	2/6/23/26	0/1/1/1
15	NAG	C	603	3	-	0/6/23/26	0/1/1/1
15	NAG	F	701	4	-	0/6/23/26	0/1/1/1
15	NAG	D	702	4	-	2/6/23/26	0/1/1/1
15	NAG	B	601	3	-	2/6/23/26	0/1/1/1
15	NAG	B	603	3	-	0/6/23/26	0/1/1/1
15	NAG	E	701	4	-	0/6/23/26	0/1/1/1
15	NAG	B	604	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	F	702	4	-	2/6/23/26	0/1/1/1
15	NAG	B	605	3	-	4/6/23/26	0/1/1/1
15	NAG	A	603	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	603	NAG	C4-C5-C6-O6
15	B	602	NAG	C4-C5-C6-O6
15	B	604	NAG	C4-C5-C6-O6
15	A	605	NAG	O5-C5-C6-O6
15	A	602	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	603	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	2
6	H	2
6	J	2
3	A	2
3	C	2
6	L	2

The worst 5 of 12 chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	141:ASP	C	150:MET	N	3.05
1	H	27:GLY	C	32:TYR	N	2.98
1	J	91:TYR	C	96:GLU	N	2.97
1	A	141:ASP	C	150:MET	N	2.96
1	B	309:ILE	C	312:GLY	N	2.95

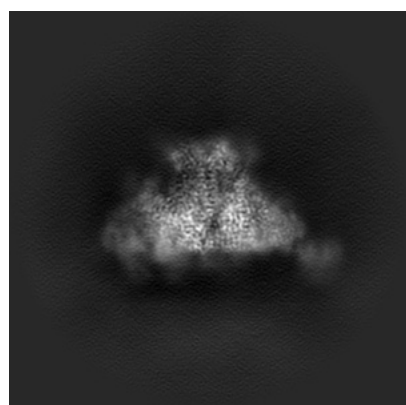
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13316. These allow visual inspection of the internal detail of the map and identification of artifacts.

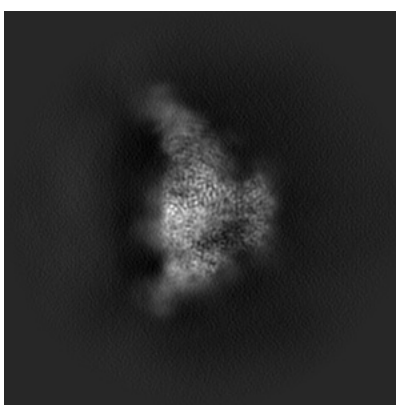
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

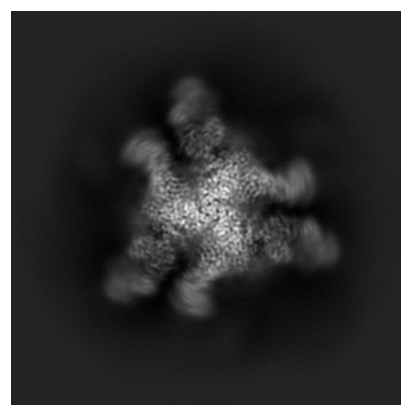
#### 6.1.1 Primary map



X



Y

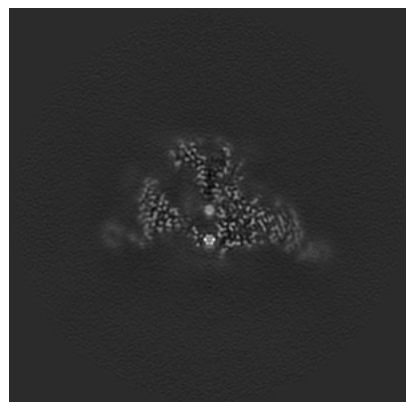


Z

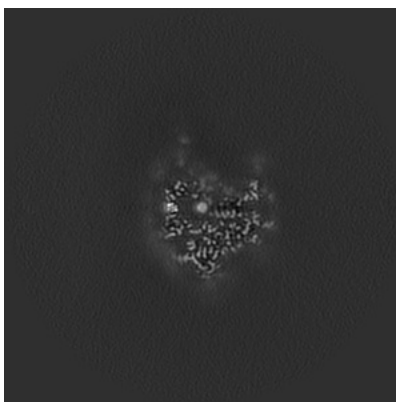
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

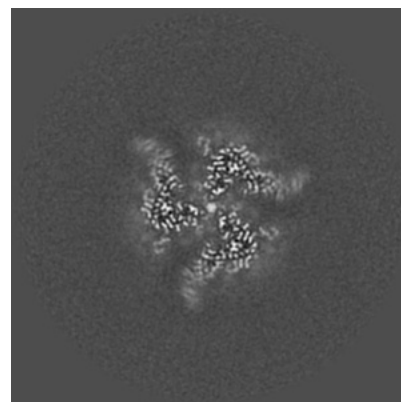
#### 6.2.1 Primary map



X Index: 210



Y Index: 210

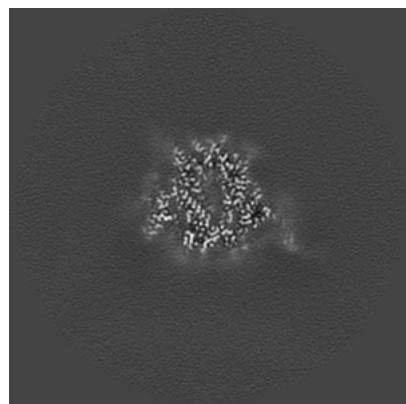


Z Index: 210

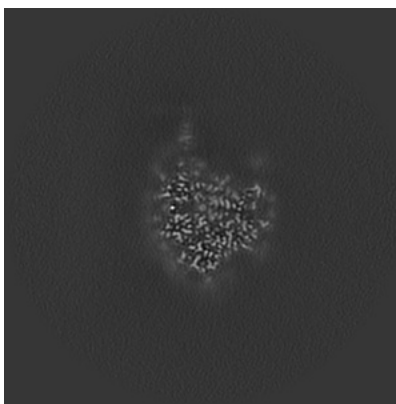
The images above show central slices of the map in three orthogonal directions.

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

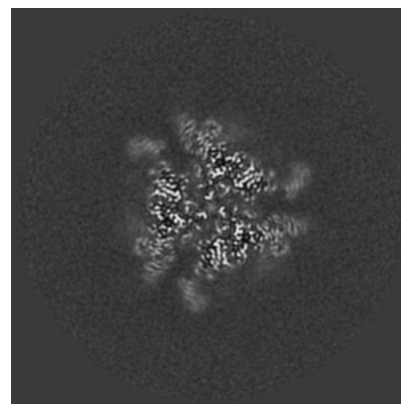
### 6.3.1 Primary map



X Index: 223



Y Index: 205

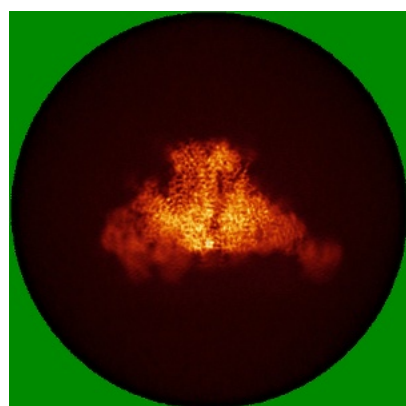


Z Index: 201

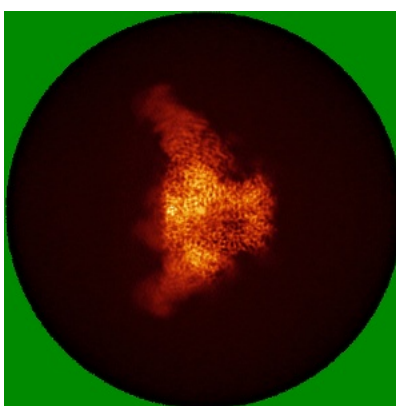
The images above show the largest variance slices of the map in three orthogonal directions.

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

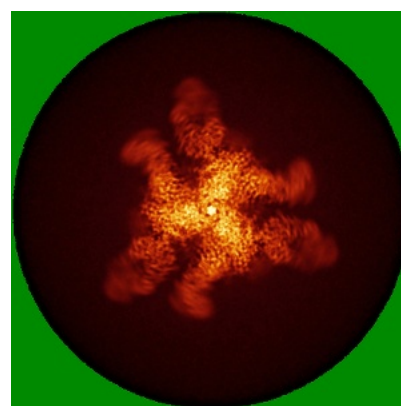
### 6.4.1 Primary map



X



Y

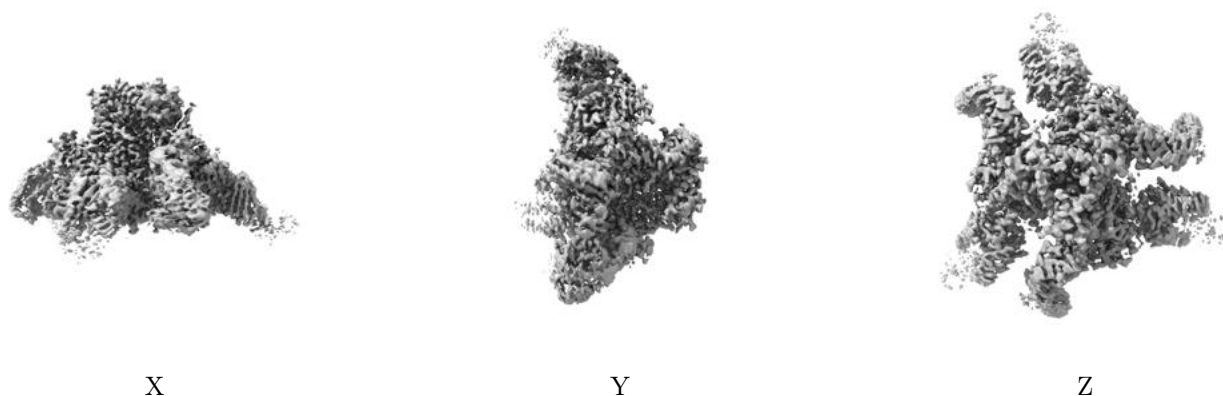


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

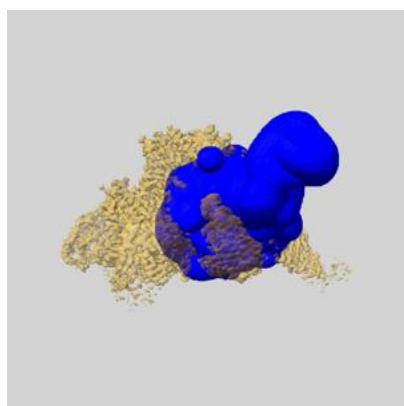
## 6.6 Mask visualisation [i](#)

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

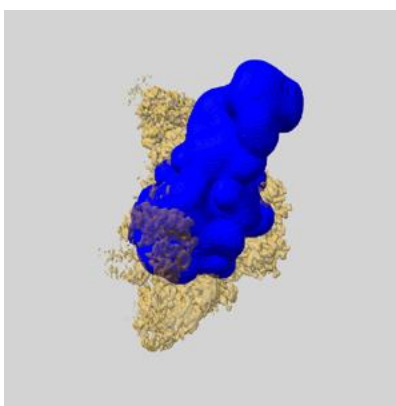
A mask typically either:

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

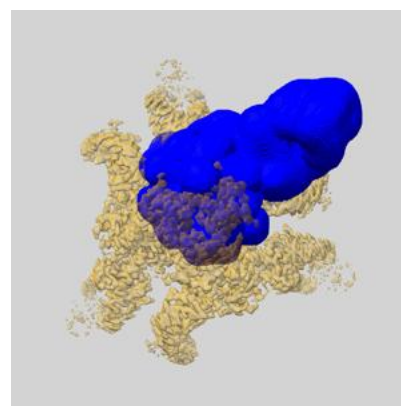
### 6.6.1 emd\_13316\_msk\_1.map [i](#)



X



Y

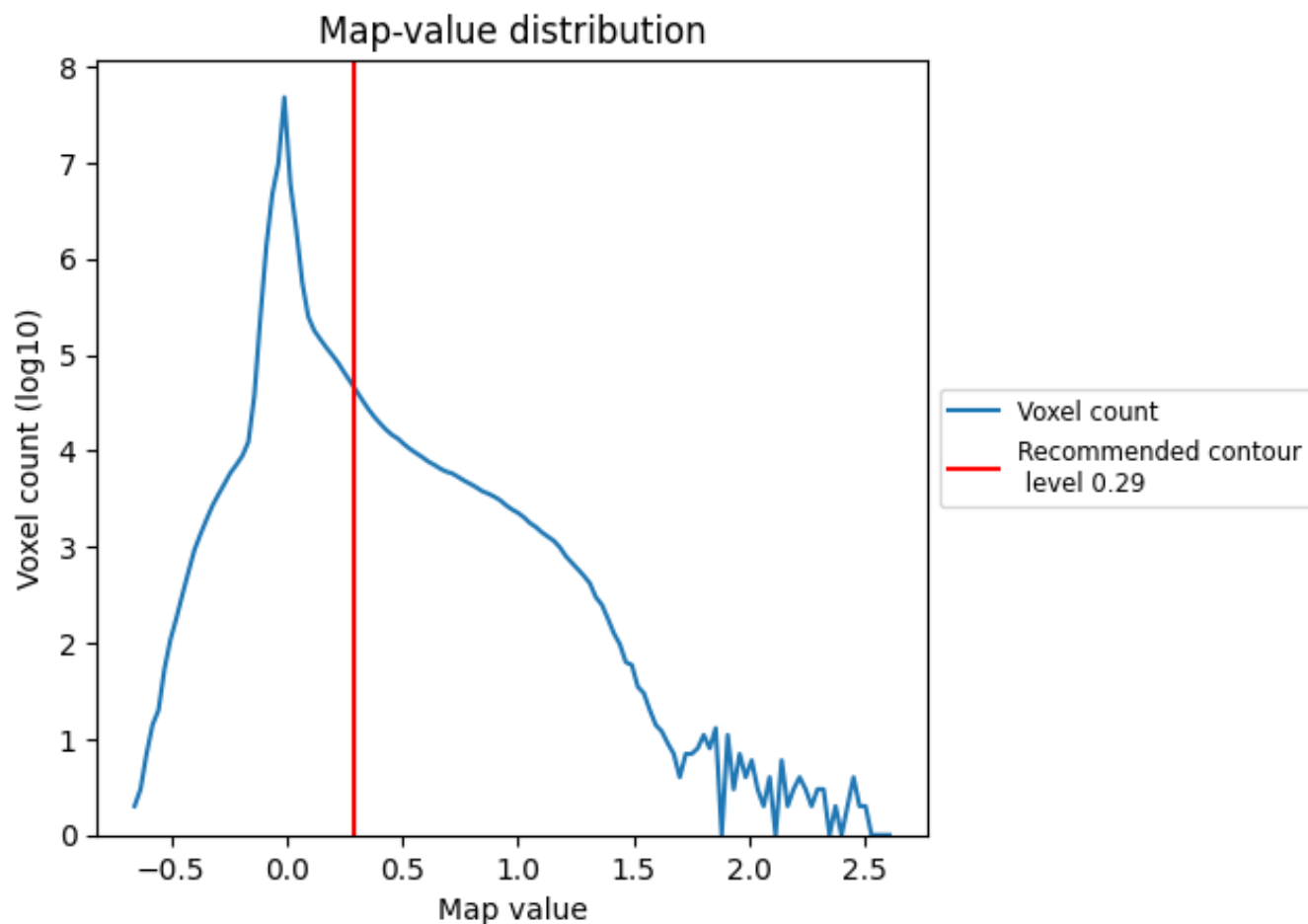


Z

## 7 Map analysis [i](#)

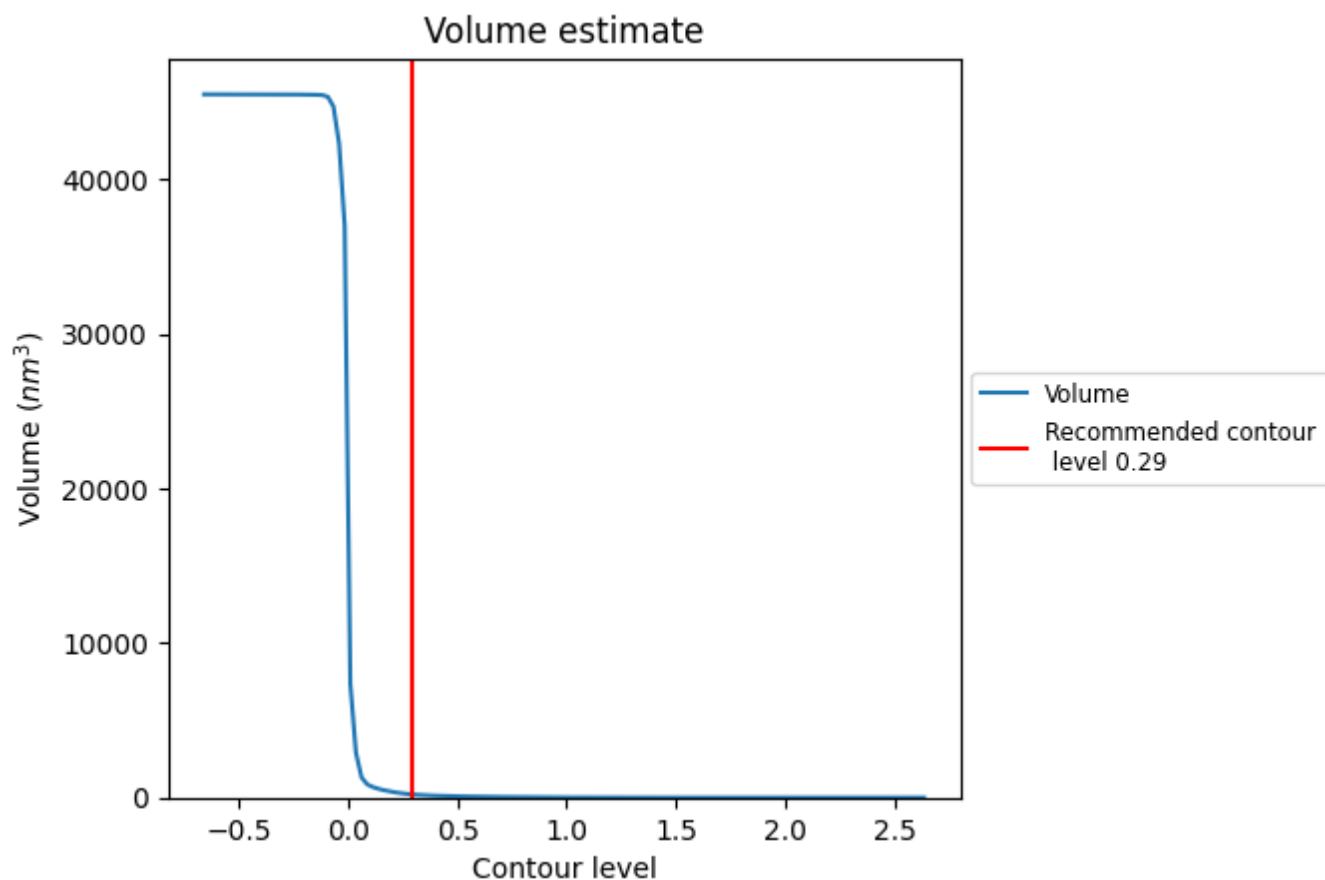
This section contains the results of statistical analysis of the map.

### 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.

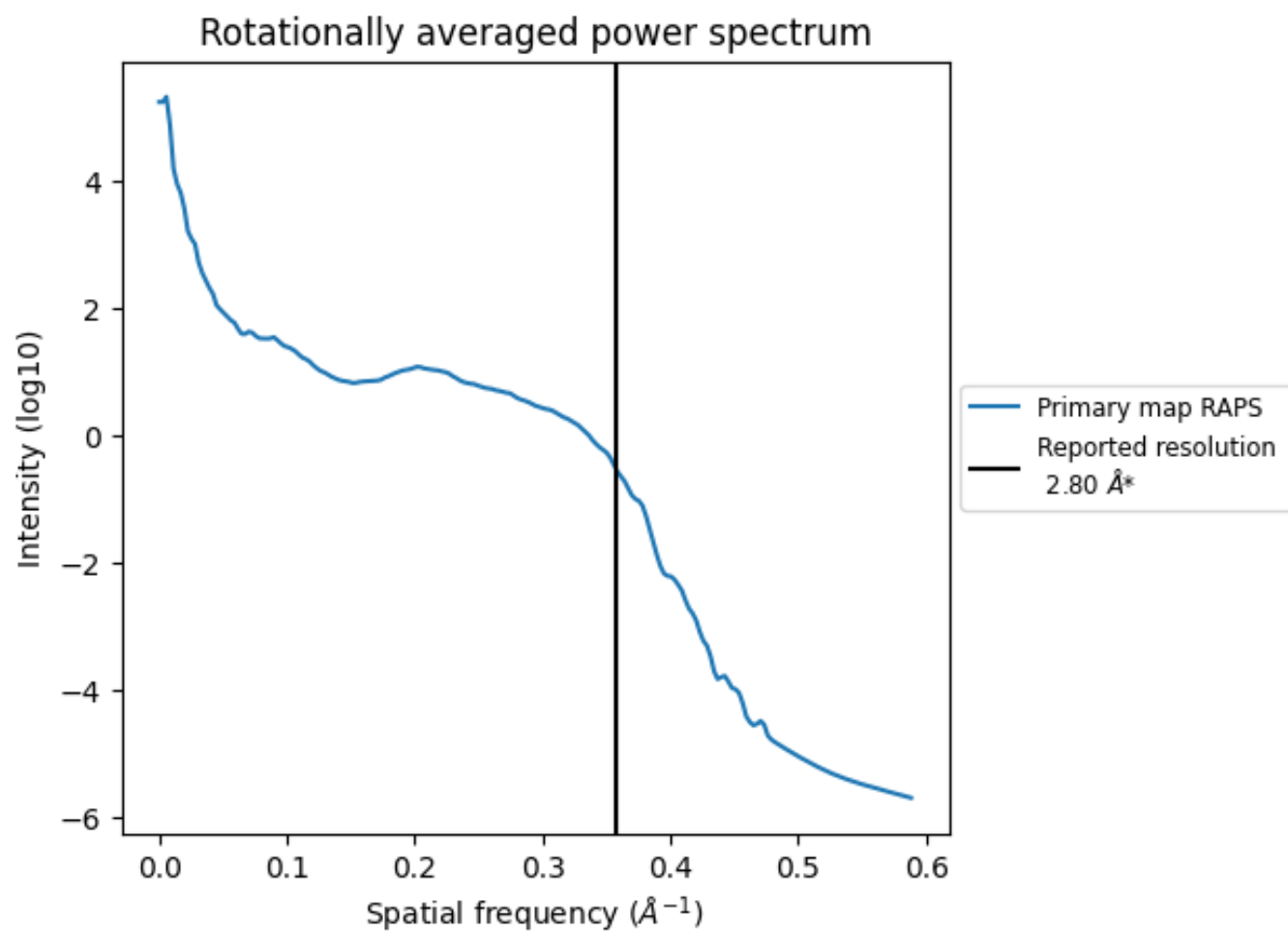
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208  $\text{nm}^3$ ; this corresponds to an approximate mass of 188 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>



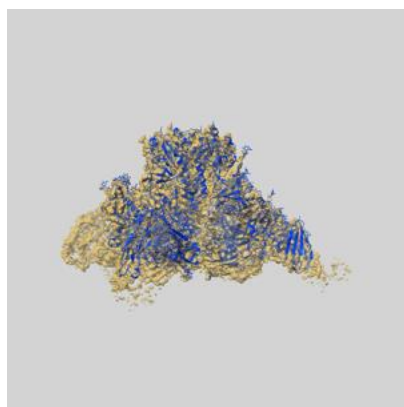
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

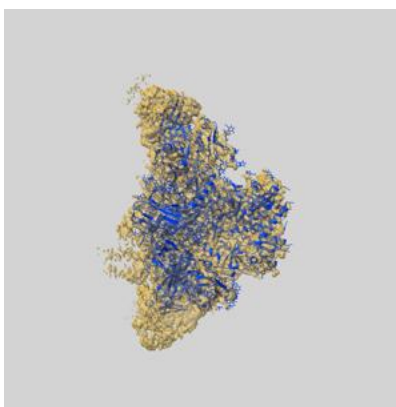
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13316 and PDB model 7PC2. Per-residue inclusion information can be found in section [3](#) on page [14](#).

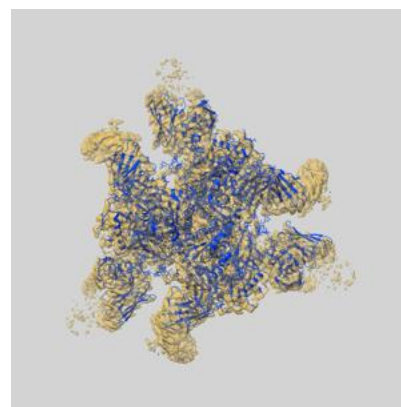
### 9.1 Map-model overlay [i](#)



X



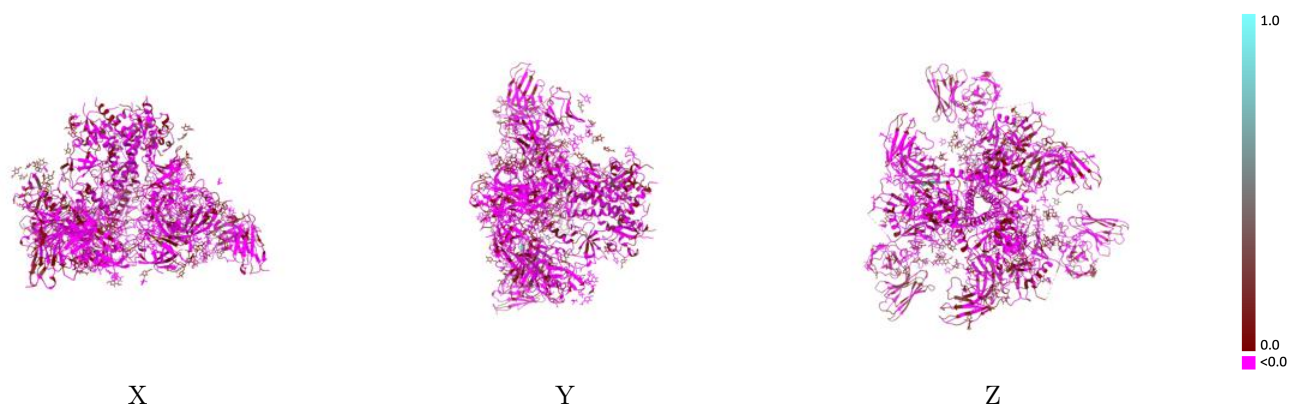
Y



Z

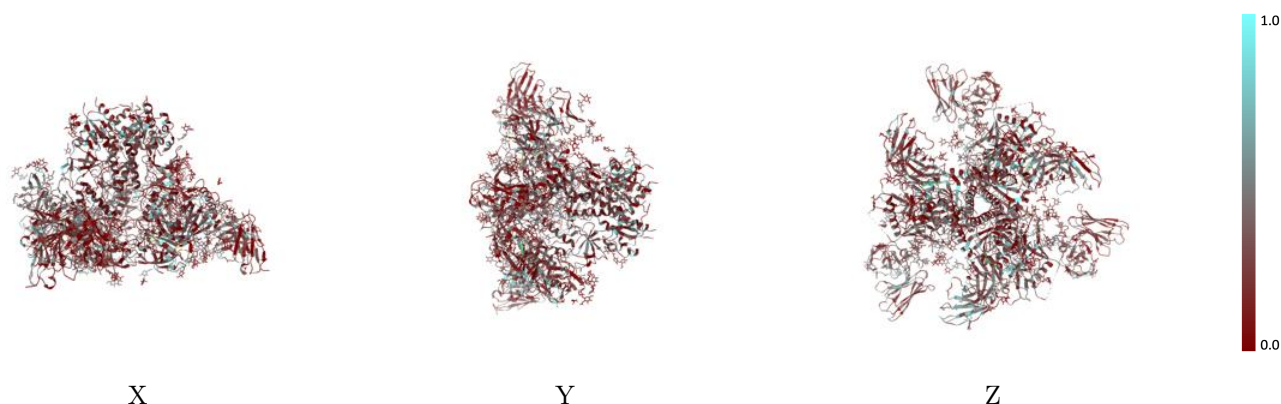
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



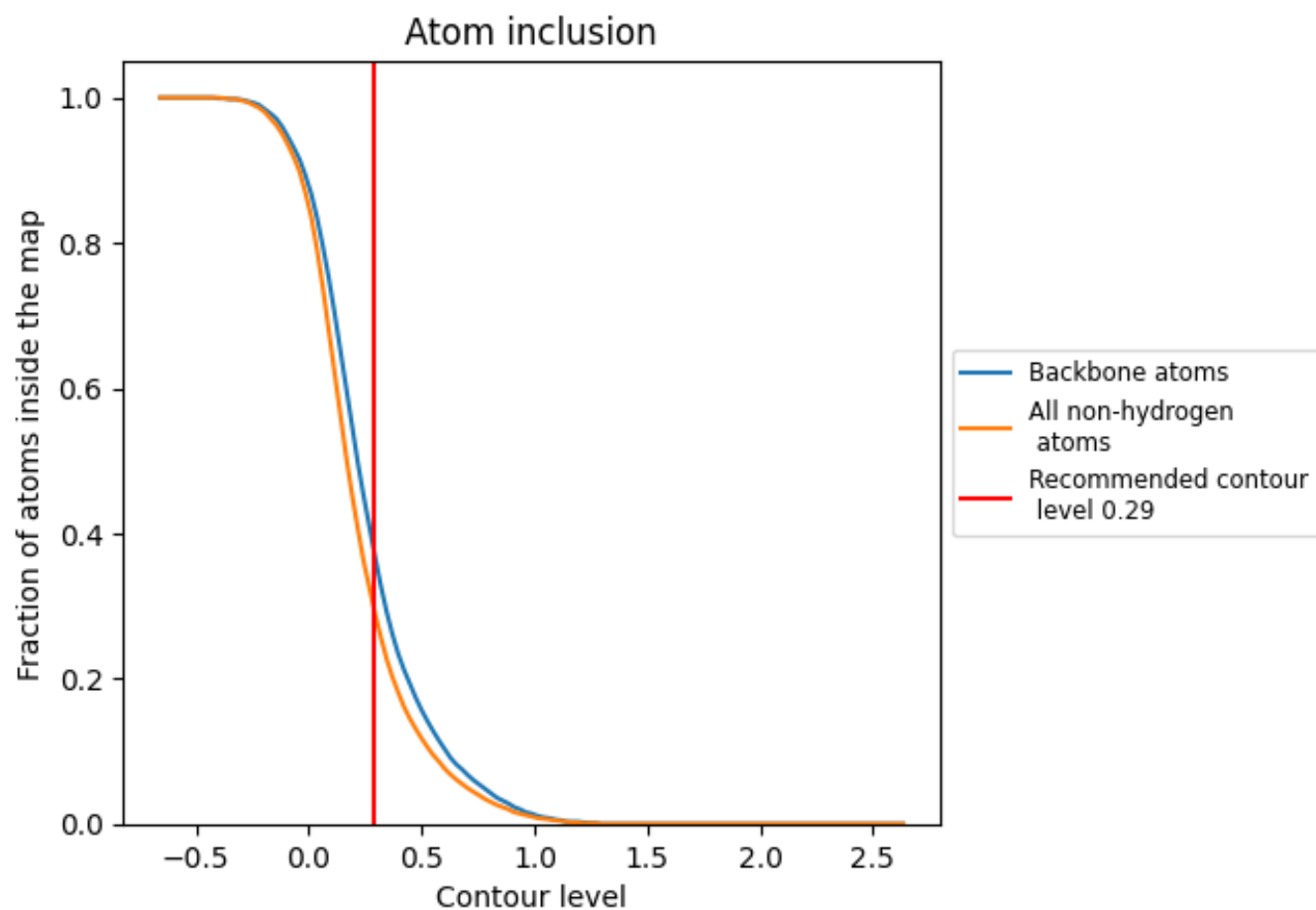
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 37% of all backbone atoms, 29% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2930	 -0.0580
0	 0.0770	 0.0660
1	 0.1310	 -0.1140
2	 0.2310	 0.0400
3	 0.0260	 0.0540
4	 0.2860	 0.0750
5	 0.3190	 0.0060
6	 0.2440	 -0.0800
7	 0.1430	 0.1100
8	 0.4290	 0.1710
9	 0.0000	 -0.0590
A	 0.2790	 -0.0950
B	 0.2990	 -0.0900
C	 0.3100	 -0.0850
D	 0.3530	 -0.0290
E	 0.3240	 -0.0480
F	 0.3340	 -0.0560
G	 0.3250	 -0.0680
H	 0.4220	 0.0490
I	 0.2920	 -0.1020
J	 0.2680	 -0.1010
K	 0.3370	 -0.0620
L	 0.3250	 -0.0470
M	 0.1660	 -0.0990
N	 0.2750	 -0.0430
O	 0.3160	 0.0550
P	 0.3310	 0.0000
Q	 0.2500	 -0.0360
R	 0.2370	 -0.0520
S	 0.2140	 0.1660
T	 0.3570	 0.2100
U	 0.4290	 0.1100
V	 0.3570	 0.0290
W	 0.2380	 0.0310
X	 0.1600	 -0.0080



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Chain	Atom inclusion	Q-score
Y	 0.2050	 0.0590
Z	 0.2500	 0.0490
a	 0.2600	 -0.1410
b	 0.3010	 -0.0140
c	 0.1280	 0.1030
d	 0.0710	 -0.1090
e	 0.4100	 0.0820
f	 0.2310	 -0.0360
g	 0.0360	 -0.0720
h	 0.1430	 0.0390
i	 0.2860	 0.0090
j	 0.1070	 -0.1380
k	 0.3210	 0.1250
l	 0.1490	 -0.0980
m	 0.1030	 -0.0570
n	 0.2130	 0.0160
o	 0.2820	 -0.1430
p	 0.1070	 -0.0180
q	 0.3080	 0.0310
r	 0.3460	 -0.0120
s	 0.1810	 0.0160
t	 0.3330	 0.0550
u	 0.0510	 0.0360
v	 0.1070	 -0.0840
w	 0.3210	 -0.0150
x	 0.1430	 -0.0930
y	 0.1520	 -0.0150
z	 0.2770	 0.1680