



## Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 08:17 AM EDT

PDB ID : 9BNP / pdb\_00009bnp  
EMDB ID : EMD-44733  
Title : Cryo-EM structure of rhesus antibody V033-a.01 in complex with HIV-1 Env BG505 DS-SOSIP  
Authors : Roark, R.S.; Shapiro, L.; Kwong, P.D.  
Deposited on : 2024-05-02  
Resolution : 3.17 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

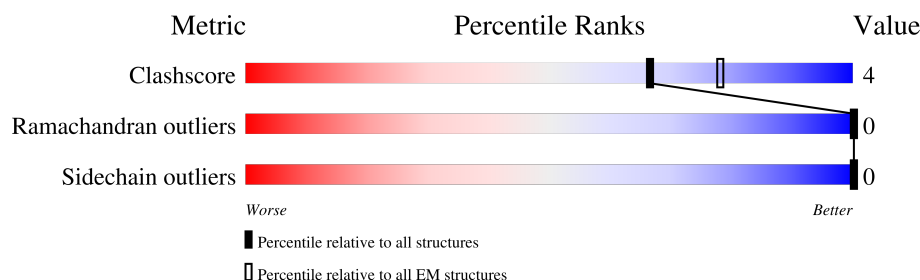
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*






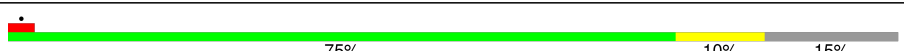
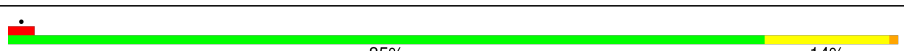
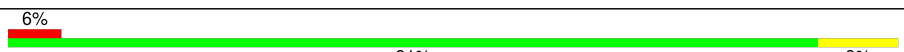
The reported resolution of this entry is 3.17 Å.

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.



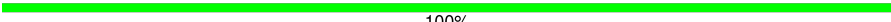



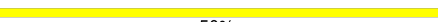


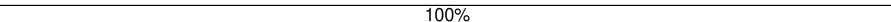







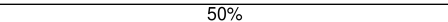
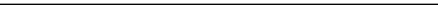




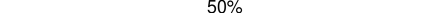
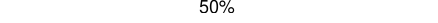
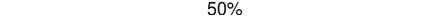
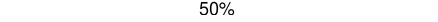
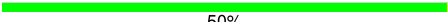
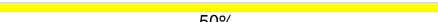



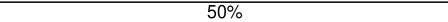


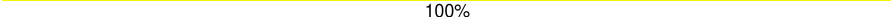






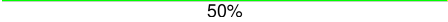
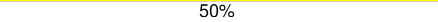


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	468	
1	E	468	
1	I	468	
2	B	145	
2	F	145	
2	J	145	
3	H	132	
4	L	107	

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Mol	Chain	Length	Quality of chain
5	C	2	 100%
5	D	2	 50%  100%
5	G	2	 50%  50%
5	M	2	 50%  50%
5	N	2	 100%  50%  50%
5	O	2	 100%
5	P	2	 50%  50%
5	Q	2	 50%  50%
5	R	2	 50%  50%
5	S	2	 50%  50%
5	T	2	 50%  50%
5	U	2	 50%  50%
5	V	2	 50%  50%
5	X	2	 50%  50%
5	Y	2	 100%
5	b	2	 50%  50%
5	c	2	 50%  100%
5	d	2	 100%
5	e	2	 100%
5	f	2	 50%  50%
5	g	2	 50%  50%
5	h	2	 100%
5	i	2	 100%
5	k	2	 50%  50%
5	n	2	 50%  100%

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Mol	Chain	Length	Quality of chain
5	o	2	
5	p	2	
5	q	2	
5	r	2	
6	K	4	
6	W	4	
7	Z	6	
8	a	7	
9	j	3	
9	m	3	
10	l	4	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16537 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein Gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	437	Total	C	N	O	S	0	0
			3434	2157	606	642	29		
1	E	436	Total	C	N	O	S	0	0
			3428	2154	605	640	29		
1	I	439	Total	C	N	O	S	0	0
			3450	2165	610	646	29		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q2N0S6
A	?	-	MET	deletion	UNP Q2N0S6
A	?	-	ARG	deletion	UNP Q2N0S6
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
E	?	-	ASP	deletion	UNP Q2N0S6
E	?	-	MET	deletion	UNP Q2N0S6
E	?	-	ARG	deletion	UNP Q2N0S6
E	201	CYS	ILE	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	433	CYS	ALA	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
I	?	-	ASP	deletion	UNP Q2N0S6
I	?	-	MET	deletion	UNP Q2N0S6
I	?	-	ARG	deletion	UNP Q2N0S6
I	201	CYS	ILE	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	433	CYS	ALA	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein Gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	123	Total	C	N	O	S	0	0
			981	620	169	186	6		
2	F	123	Total	C	N	O	S	0	0
			981	620	169	186	6		
2	J	123	Total	C	N	O	S	0	0
			981	620	169	186	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6
J	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called V033-a.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	132	Total	C	N	O	S	4	0
			1016	646	171	195	4		

- Molecule 4 is a protein called V033-a.01 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			819	518	133	165	3		

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	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	V	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	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
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		

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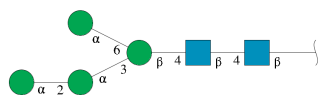
Mol	Chain	Residues	Atoms				AltConf	Trace
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	q	2	Total	C	N	O	0	0
			28	16	2	10		
5	r	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	4	Total	C	N	O	0	0
			50	28	2	20		
6	W	4	Total	C	N	O	0	0
			50	28	2	20		

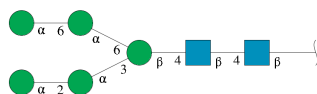
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

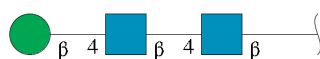
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

- Molecule 9 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
9	j	3	Total	C	N	O	0	0
			39	22	2	15		
9	m	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 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
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	F	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	

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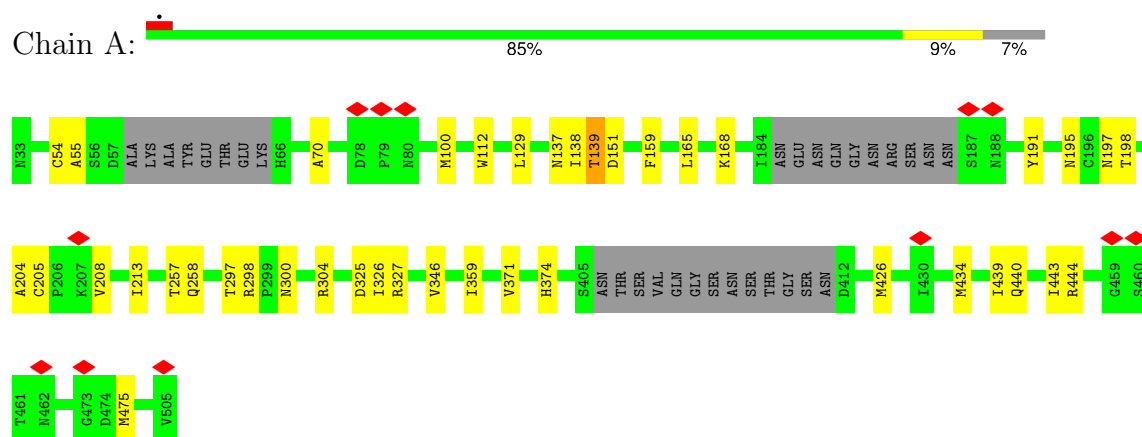
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Mol	Chain	Residues	Atoms				AltConf
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	I	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	
11	J	1	Total	C	N	O	0
			14	8	1	5	

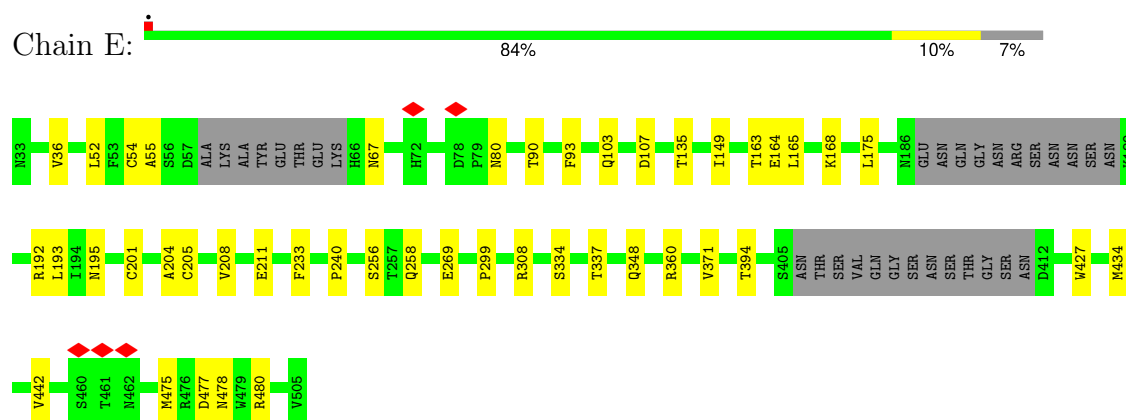
### 3 Residue-property plots

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.

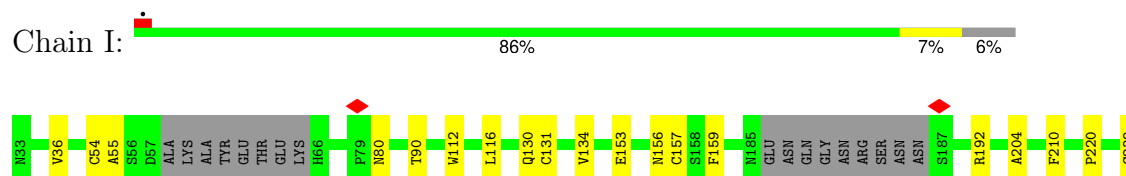
#### • Molecule 1: Envelope glycoprotein Gp120

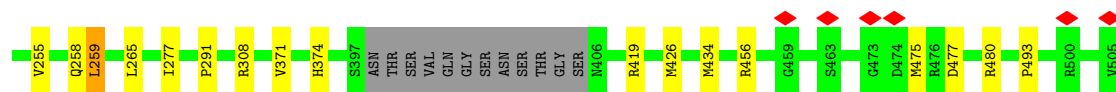


#### • Molecule 1: Envelope glycoprotein Gp120

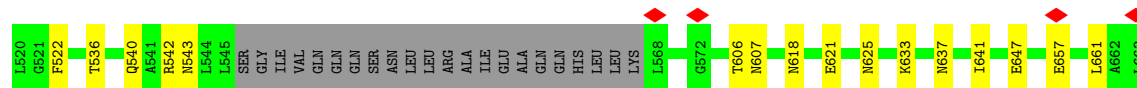
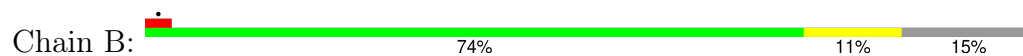


#### • Molecule 1: Envelope glycoprotein Gp120

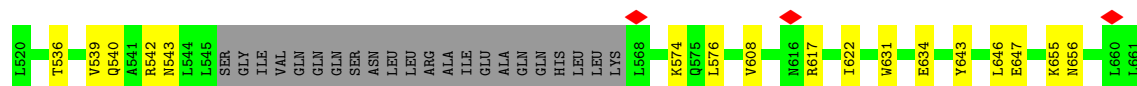




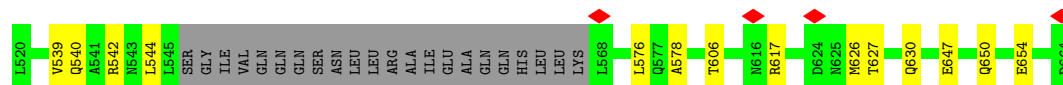
• Molecule 2: Envelope glycoprotein Gp41



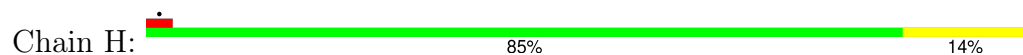
• Molecule 2: Envelope glycoprotein Gp41



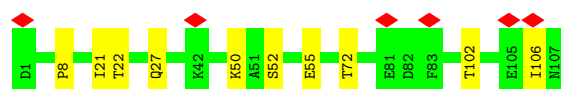
• Molecule 2: Envelope glycoprotein Gp41



• Molecule 3: V033-a.01 heavy chain



• Molecule 4: V033-a.01 light chain



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

Chain C:  100%



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

Chain D:  50% 100%



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

Chain G:  50% 50%



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

Chain M:  50% 50% 50%



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

Chain N:  100% 50% 50%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  50% 50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 50% 50%



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

Chain V:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  100%



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

Chain b:  50% 50% 50%



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

Chain c:  50% 100% 50%



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

Chain d:  100%



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

Chain e:  100%





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

Chain f: 50%50%



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

Chain g: 50%50%

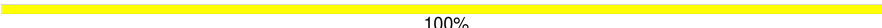


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 100%



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

Chain i: 100%



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

Chain k: 50%50%



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

Chain n: 50%100%




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

Chain o: 



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

Chain p: 



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

Chain q: 



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

Chain r: 



- Molecule 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

Chain K: 



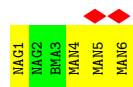
- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 



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

Chain Z: 



- Molecule 8:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -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

Chain a: 



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

Chain j: 



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

Chain m: 



- Molecule 10:  $\alpha$ -D-mannopyranose-(1-6)- $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain l: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.518	Depositor
Minimum map value	-0.217	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, 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	0.25	0/3506	0.67	3/4761 (0.1%)
1	E	0.27	0/3500	0.64	2/4753 (0.0%)
1	I	0.24	0/3522	0.59	1/4783 (0.0%)
2	B	0.30	0/998	0.67	1/1354 (0.1%)
2	F	0.28	0/998	0.66	0/1354
2	J	0.33	0/998	0.67	0/1354
3	H	0.28	0/1043	0.72	1/1411 (0.1%)
4	L	0.31	0/839	0.80	2/1138 (0.2%)
All	All	0.27	0/15404	0.66	10/20908 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	CA-C-N	10.97	140.72	122.07
1	A	139	THR	C-N-CA	10.97	140.72	122.07
1	A	475	MET	CB-CG-SD	5.95	130.54	112.70
3	H	34	MET	CA-CB-CG	5.81	125.73	114.10
1	E	80	ASN	CB-CA-C	5.78	120.16	111.14
1	I	259	LEU	CA-CB-CG	5.71	136.28	116.30
2	B	633	LYS	CA-CB-CG	5.50	125.11	114.10
4	L	27	GLN	CA-CB-CG	5.39	124.87	114.10
1	E	80	ASN	CA-CB-CG	5.14	117.74	112.60
4	L	106	ILE	CA-CB-CG1	5.05	118.99	110.40

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	A	3434	0	3368	26	0
1	E	3428	0	3363	26	0
1	I	3450	0	3380	28	0
2	B	981	0	963	11	0
2	F	981	0	962	13	0
2	J	981	0	961	13	0
3	H	1016	0	956	11	0
4	L	819	0	790	5	0
5	C	28	0	25	0	0
5	D	28	0	25	0	0
5	G	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	1	0
5	P	28	0	25	1	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
5	f	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
5	i	28	0	25	0	0
5	k	28	0	25	0	0
5	n	28	0	25	0	0
5	o	28	0	25	0	0
5	p	28	0	25	0	0
5	q	28	0	25	0	0
5	r	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	50	0	43	0	0
6	W	50	0	43	0	0
7	Z	72	0	61	0	0
8	a	83	0	70	1	0
9	j	39	0	34	0	0
9	m	39	0	34	0	0
10	l	50	0	43	2	0
11	A	84	0	78	0	0
11	E	56	0	52	0	0
11	F	14	0	13	0	0
11	I	70	0	65	0	0
11	J	28	0	26	0	0
All	All	16537	0	16030	121	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 4.

All (121) 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)
4:L:22:THR:HG22	4:L:72:THR:OG1	1.86	0.74
1:E:195:ASN:ND2	1:E:201:CYS:SG	2.62	0.72
1:I:204:ALA:HB2	1:I:434:MET:CE	2.24	0.67
2:J:617:ARG:HH12	2:J:626:MET:HE1	1.59	0.67
1:E:165:LEU:HD21	1:I:192:ARG:HG3	1.76	0.65
1:I:204:ALA:HB2	1:I:434:MET:HE3	1.78	0.64
1:A:258:GLN:NE2	1:A:371:VAL:O	2.29	0.63
1:A:204:ALA:HB2	1:A:434:MET:HE3	1.81	0.62
3:H:96:ASP:OD1	3:H:97:GLY:N	2.34	0.61
4:L:8:PRO:HD2	4:L:21:ILE:HD13	1.84	0.60
2:B:657:GLU:O	2:B:661:LEU:HD13	2.01	0.59
1:I:36:VAL:O	2:J:606:THR:OG1	2.21	0.59
1:A:444:ARG:NH2	5:O:1:NAG:O6	2.37	0.58
1:E:192:ARG:NH1	1:E:193:LEU:O	2.37	0.57
2:B:536:THR:O	2:B:540:GLN:NE2	2.38	0.57
1:E:269:GLU:OE1	1:E:348:GLN:NE2	2.37	0.57
1:A:137:ASN:O	1:A:138:ILE:HD13	2.05	0.57
1:A:300:ASN:ND2	1:A:327:ARG:O	2.39	0.56
1:A:112:TRP:CH2	1:A:426:MET:HE1	2.41	0.56
1:E:258:GLN:NE2	1:E:371:VAL:O	2.38	0.55
1:I:54:CYS:SG	1:I:55:ALA:N	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:CYS:SG	1:E:55:ALA:N	2.80	0.55
1:E:135:THR:HA	1:E:149:ILE:HG12	1.88	0.55
1:E:163:THR:HG23	1:E:165:LEU:H	1.71	0.55
1:A:138:ILE:HG23	1:A:151:ASP:O	2.07	0.54
2:F:536:THR:O	2:F:540:GLN:NE2	2.40	0.54
1:A:257:THR:O	1:A:374:HIS:ND1	2.41	0.54
1:A:298:ARG:NH1	1:A:300:ASN:O	2.41	0.53
2:B:647:GLU:OE1	2:J:542:ARG:NH1	2.41	0.53
3:H:87:THR:HA	3:H:109:VAL:O	2.09	0.53
2:F:655:LYS:NZ	2:F:656:ASN:OD1	2.42	0.52
1:I:134:VAL:HG22	1:I:156:ASN:HB2	1.89	0.52
3:H:34:MET:HG3	3:H:78:LEU:HD13	1.91	0.52
3:H:52:ASN:O	3:H:71:ARG:NH1	2.42	0.52
1:I:159:PHE:HA	10:I:1:NAG:H83	1.92	0.52
1:A:325:ASP:OD2	1:A:327:ARG:NH1	2.43	0.51
1:A:205:CYS:HB2	1:A:208:VAL:HG22	1.93	0.51
3:H:11:LEU:HD13	3:H:110:THR:HG23	1.91	0.51
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.44	0.50
1:E:299:PRO:HA	1:E:442:VAL:HG13	1.93	0.50
1:E:67:ASN:ND2	1:E:211:GLU:O	2.45	0.50
3:H:29:PHE:O	3:H:71:ARG:NH2	2.45	0.50
2:B:542:ARG:NH1	2:F:647:GLU:OE1	2.44	0.50
1:E:205:CYS:HB2	1:E:208:VAL:HG22	1.94	0.49
2:F:542:ARG:NH2	2:J:647:GLU:OE2	2.45	0.49
1:A:195:ASN:ND2	1:A:198:THR:OG1	2.33	0.49
2:J:617:ARG:NH1	2:J:626:MET:HE1	2.27	0.49
1:E:93:PHE:HB2	1:E:233:PHE:HZ	1.78	0.49
1:I:116:LEU:HD21	1:I:434:MET:SD	2.53	0.49
1:E:164:GLU:OE2	1:E:308:ARG:NH1	2.45	0.49
1:E:427:TRP:HE3	1:E:475:MET:HE3	1.78	0.49
2:B:621:GLU:HA	2:B:625:ASN:HB2	1.94	0.48
4:L:21:ILE:HD12	4:L:102:THR:HG21	1.94	0.48
3:H:93:ALA:HB1	3:H:100(O):PHE:HB3	1.95	0.48
1:I:493:PRO:HB3	2:J:544:LEU:HD11	1.96	0.48
1:A:54:CYS:SG	1:A:55:ALA:N	2.87	0.47
1:A:138:ILE:HD11	1:A:326:ILE:HD12	1.97	0.47
1:E:52:LEU:N	1:E:103:GLN:HE22	2.12	0.47
1:E:90:THR:HG22	1:E:240:PRO:HA	1.97	0.47
1:I:204:ALA:HB2	1:I:434:MET:HE2	1.94	0.47
1:I:220:PRO:HB3	2:J:578:ALA:HB1	1.97	0.47
1:I:116:LEU:HD21	1:I:434:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:539:VAL:O	2:F:543:ASN:ND2	2.48	0.46
1:I:130:GLN:HG3	10:I:1:NAG:H82	1.98	0.46
1:I:116:LEU:HD21	1:I:434:MET:CE	2.46	0.46
1:I:258:GLN:NE2	1:I:371:VAL:O	2.37	0.46
2:B:522:PHE:HB2	2:B:543:ASN:ND2	2.31	0.45
1:I:210:PHE:CE1	1:I:434:MET:HE1	2.50	0.45
1:E:360:ARG:HG2	1:E:394:THR:HG23	1.99	0.45
1:E:204:ALA:HB2	1:E:434:MET:HE3	1.99	0.45
1:E:475:MET:SD	1:E:475:MET:N	2.82	0.45
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.49	0.45
3:H:1:GLU:HB3	3:H:2:VAL:H	1.64	0.45
2:F:576:LEU:HD21	2:J:576:LEU:HD12	1.98	0.45
2:J:626:MET:HB2	2:J:626:MET:HE3	1.56	0.45
3:H:100(N):TYR:OH	4:L:55:GLU:OE1	2.34	0.45
1:I:90:THR:HA	1:I:239:CYS:O	2.17	0.44
1:I:204:ALA:CB	1:I:434:MET:HE3	2.46	0.44
1:A:129:LEU:O	1:A:191:TYR:N	2.49	0.44
1:E:107:ASP:OD2	2:F:574:LYS:NZ	2.50	0.44
1:A:197:ASN:O	1:I:308:ARG:NH2	2.51	0.44
2:F:643:TYR:HA	2:F:646:LEU:HD12	1.99	0.44
1:A:304:ARG:N	1:A:440:GLN:OE1	2.50	0.44
1:I:112:TRP:CZ2	1:I:426:MET:HE1	2.53	0.44
2:B:657:GLU:HG3	2:B:661:LEU:HD13	2.00	0.43
1:E:163:THR:HG22	1:E:168:LYS:O	2.17	0.43
1:I:255:VAL:HA	1:I:475:MET:HE1	2.00	0.43
1:E:256:SER:O	1:E:478:ASN:ND2	2.50	0.43
1:A:159:PHE:HA	5:P:1:NAG:H83	1.99	0.43
1:I:259:LEU:HD22	1:I:374:HIS:CE1	2.54	0.43
1:A:297:THR:OG1	1:A:443:ILE:O	2.34	0.42
1:E:175:LEU:HD21	8:a:1:NAG:H82	2.00	0.42
1:I:153:GLU:OE2	1:I:419:ARG:NH1	2.52	0.42
1:A:439:ILE:HD11	1:A:443:ILE:HD13	2.02	0.42
3:H:12:ALA:HB3	3:H:111:VAL:HG22	2.02	0.42
1:A:139:THR:OG1	1:A:151:ASP:OD1	2.37	0.42
2:J:650:GLN:NE2	2:J:654:GLU:OE1	2.52	0.42
2:B:606:THR:HG22	2:B:607:ASN:H	1.84	0.42
1:I:265:LEU:HD11	1:I:291:PRO:HD3	2.01	0.42
2:B:641:ILE:H	2:B:641:ILE:HD12	1.85	0.42
1:I:277:ILE:O	1:I:456:ARG:NH1	2.52	0.42
2:J:540:GLN:O	2:J:544:LEU:HG	2.20	0.42
1:A:165:LEU:HD12	1:A:168:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:622:ILE:HD11	2:F:631:TRP:CZ3	2.55	0.41
1:I:131:CYS:HA	1:I:157:CYS:HA	2.02	0.41
1:E:334:SER:OG	1:E:337:THR:OG1	2.31	0.41
1:I:80:ASN:OD1	1:I:80:ASN:N	2.54	0.41
2:F:617:ARG:NH1	2:F:634:GLU:OE1	2.54	0.41
2:F:655:LYS:HE2	2:F:655:LYS:HB2	1.94	0.41
2:B:637:ASN:OD1	2:B:637:ASN:N	2.50	0.41
4:L:50:LYS:C	4:L:52:SER:H	2.28	0.41
1:A:346:VAL:HG13	1:A:359:ILE:HD13	2.03	0.41
2:B:618:ASN:HB2	2:B:621:GLU:HG2	2.03	0.41
3:H:90:TYR:O	3:H:106:GLY:HA2	2.20	0.41
2:F:622:ILE:HD13	2:F:622:ILE:HG21	1.90	0.41
2:J:539:VAL:HG12	2:J:542:ARG:HH22	1.85	0.41
1:A:112:TRP:CH2	1:A:426:MET:CE	3.03	0.40
1:E:36:VAL:HG12	2:F:608:VAL:HB	2.01	0.40
1:A:70:ALA:HB3	1:A:213:ILE:HD11	2.02	0.40
2:J:627:THR:OG1	2:J:630:GLN:OE1	2.39	0.40
1:A:100:MET:HE2	1:A:100:MET:HB3	1.93	0.40

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	A	429/468 (92%)	412 (96%)	17 (4%)	0	100	100
1	E	428/468 (92%)	408 (95%)	20 (5%)	0	100	100
1	I	431/468 (92%)	411 (95%)	20 (5%)	0	100	100
2	B	119/145 (82%)	116 (98%)	3 (2%)	0	100	100
2	F	119/145 (82%)	116 (98%)	3 (2%)	0	100	100
2	J	119/145 (82%)	115 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
4	L	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
All	All	1880/2078 (90%)	1802 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	392/418 (94%)	392 (100%)	0	100	100
1	E	391/418 (94%)	391 (100%)	0	100	100
1	I	394/418 (94%)	394 (100%)	0	100	100
2	B	106/125 (85%)	106 (100%)	0	100	100
2	F	106/125 (85%)	106 (100%)	0	100	100
2	J	106/125 (85%)	106 (100%)	0	100	100
3	H	106/107 (99%)	106 (100%)	0	100	100
4	L	92/92 (100%)	92 (100%)	0	100	100
All	All	1693/1828 (93%)	1693 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	330	HIS
1	A	425	ASN
1	A	462	ASN
2	B	590	GLN
1	E	94	ASN
1	E	103	GLN

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Mol	Chain	Res	Type
1	E	105	HIS
2	F	590	GLN
2	F	658	GLN
3	H	81	GLN
3	H	82(A)	ASN
1	I	67	ASN
1	I	246	GLN
2	J	590	GLN

### 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](#)

89 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	$\# Z  > 2$
5	NAG	C	1	1,5	14,14,15	0.68	0	17,19,21	0.66	0
5	NAG	C	2	5	14,14,15	0.70	0	17,19,21	0.76	0
5	NAG	D	1	1,5	14,14,15	0.69	0	17,19,21	0.64	0
5	NAG	D	2	5	14,14,15	0.70	0	17,19,21	0.75	0
5	NAG	G	1	1,5	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
5	NAG	G	2	5	14,14,15	0.67	0	17,19,21	0.63	0
6	NAG	K	1	1,6	14,14,15	0.68	0	17,19,21	0.80	1 (5%)
6	NAG	K	2	6	14,14,15	0.69	0	17,19,21	0.60	0
6	BMA	K	3	6	11,11,12	0.83	0	15,15,17	0.77	0
6	MAN	K	4	6	11,11,12	0.67	0	15,15,17	1.38	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	M	1	1,5	14,14,15	0.65	0	17,19,21	1.63	2 (11%)
5	NAG	M	2	5	14,14,15	0.68	0	17,19,21	0.76	0
5	NAG	N	1	1,5	14,14,15	0.69	0	17,19,21	0.75	1 (5%)
5	NAG	N	2	5	14,14,15	0.74	0	17,19,21	0.77	0
5	NAG	O	1	1,5	14,14,15	0.66	0	17,19,21	0.73	0
5	NAG	O	2	5	14,14,15	0.73	0	17,19,21	0.81	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.65	0	17,19,21	1.55	3 (17%)
5	NAG	P	2	5	14,14,15	0.68	0	17,19,21	0.74	0
5	NAG	Q	1	1,5	14,14,15	0.73	0	17,19,21	0.54	0
5	NAG	Q	2	5	14,14,15	0.70	0	17,19,21	1.60	2 (11%)
5	NAG	R	1	1,5	14,14,15	0.71	0	17,19,21	0.68	0
5	NAG	R	2	5	14,14,15	0.68	0	17,19,21	1.60	2 (11%)
5	NAG	S	1	1,5	14,14,15	0.72	0	17,19,21	0.57	0
5	NAG	S	2	5	14,14,15	0.71	0	17,19,21	0.79	1 (5%)
5	NAG	T	1	1,5	14,14,15	0.67	0	17,19,21	0.58	0
5	NAG	T	2	5	14,14,15	0.68	0	17,19,21	1.58	2 (11%)
5	NAG	U	1	1,5	14,14,15	0.70	0	17,19,21	0.48	0
5	NAG	U	2	5	14,14,15	0.71	0	17,19,21	0.85	1 (5%)
5	NAG	V	1	1,5	14,14,15	0.74	0	17,19,21	0.83	1 (5%)
5	NAG	V	2	5	14,14,15	0.69	0	17,19,21	0.67	0
6	NAG	W	1	1,6	14,14,15	0.71	0	17,19,21	0.77	0
6	NAG	W	2	6	14,14,15	0.71	0	17,19,21	1.61	2 (11%)
6	BMA	W	3	6	11,11,12	0.83	0	15,15,17	0.82	1 (6%)
6	MAN	W	4	6	11,11,12	0.66	0	15,15,17	1.40	1 (6%)
5	NAG	X	1	1,5	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
5	NAG	X	2	5	14,14,15	0.67	0	17,19,21	0.69	0
5	NAG	Y	1	1,5	14,14,15	0.71	0	17,19,21	0.80	1 (5%)
5	NAG	Y	2	5	14,14,15	0.66	0	17,19,21	1.58	2 (11%)
7	NAG	Z	1	7,1	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
7	NAG	Z	2	7	14,14,15	0.74	0	17,19,21	0.59	0
7	BMA	Z	3	7	11,11,12	0.95	0	15,15,17	0.86	0
7	MAN	Z	4	7	11,11,12	0.68	0	15,15,17	1.44	1 (6%)
7	MAN	Z	5	7	11,11,12	0.57	0	15,15,17	2.94	1 (6%)
7	MAN	Z	6	7	11,11,12	0.74	0	15,15,17	1.12	1 (6%)
8	NAG	a	1	8,1	14,14,15	0.74	0	17,19,21	0.76	0
8	NAG	a	2	8	14,14,15	0.72	0	17,19,21	1.54	1 (5%)
8	BMA	a	3	8	11,11,12	0.69	0	15,15,17	0.67	1 (6%)
8	MAN	a	4	8	11,11,12	0.62	0	15,15,17	1.60	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	a	5	8	11,11,12	0.78	0	15,15,17	0.98	1 (6%)
8	MAN	a	6	8	11,11,12	0.68	0	15,15,17	1.16	1 (6%)
8	MAN	a	7	8	11,11,12	0.67	0	15,15,17	1.48	1 (6%)
5	NAG	b	1	1,5	14,14,15	0.73	0	17,19,21	1.17	1 (5%)
5	NAG	b	2	5	14,14,15	0.71	0	17,19,21	0.79	0
5	NAG	c	1	1,5	14,14,15	0.76	0	17,19,21	1.59	2 (11%)
5	NAG	c	2	5	14,14,15	0.77	1 (7%)	17,19,21	1.64	2 (11%)
5	NAG	d	1	1,5	14,14,15	0.70	0	17,19,21	0.64	0
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	0.78	0
5	NAG	e	1	1,5	14,14,15	0.67	0	17,19,21	0.72	0
5	NAG	e	2	5	14,14,15	0.69	0	17,19,21	0.71	0
5	NAG	f	1	1,5	14,14,15	0.70	0	17,19,21	0.81	1 (5%)
5	NAG	f	2	5	14,14,15	0.71	0	17,19,21	0.69	0
5	NAG	g	1	1,5	14,14,15	0.68	0	17,19,21	0.64	0
5	NAG	g	2	5	14,14,15	0.66	0	17,19,21	1.58	2 (11%)
5	NAG	h	1	1,5	14,14,15	0.68	0	17,19,21	0.64	0
5	NAG	h	2	5	14,14,15	0.71	0	17,19,21	0.73	0
5	NAG	i	1	1,5	14,14,15	0.74	0	17,19,21	0.78	1 (5%)
5	NAG	i	2	5	14,14,15	0.67	0	17,19,21	1.58	2 (11%)
9	NAG	j	1	9,1	14,14,15	0.69	0	17,19,21	0.85	1 (5%)
9	NAG	j	2	9	14,14,15	0.76	1 (7%)	17,19,21	0.60	0
9	BMA	j	3	9	11,11,12	0.78	0	15,15,17	0.88	1 (6%)
5	NAG	k	1	1,5	14,14,15	0.70	0	17,19,21	0.75	0
5	NAG	k	2	5	14,14,15	0.67	0	17,19,21	1.58	2 (11%)
10	NAG	l	1	1,10	14,14,15	0.66	0	17,19,21	1.42	3 (17%)
10	NAG	l	2	10	14,14,15	0.73	0	17,19,21	0.72	0
10	BMA	l	3	10	11,11,12	0.84	0	15,15,17	0.87	1 (6%)
10	MAN	l	4	10	11,11,12	0.68	0	15,15,17	1.31	1 (6%)
9	NAG	m	1	9,1	14,14,15	0.68	0	17,19,21	0.95	1 (5%)
9	NAG	m	2	9	14,14,15	0.75	0	17,19,21	3.51	5 (29%)
9	BMA	m	3	9	11,11,12	0.78	0	15,15,17	0.92	1 (6%)
5	NAG	n	1	1,5	14,14,15	0.71	0	17,19,21	0.84	1 (5%)
5	NAG	n	2	5	14,14,15	0.68	0	17,19,21	1.57	2 (11%)
5	NAG	o	1	1,5	14,14,15	0.67	0	17,19,21	0.66	0
5	NAG	o	2	5	14,14,15	0.67	0	17,19,21	1.58	2 (11%)
5	NAG	p	1	1,5	14,14,15	0.71	0	17,19,21	0.53	0
5	NAG	p	2	5	14,14,15	0.70	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	q	1	1,5	14,14,15	0.67	0	17,19,21	1.58	2 (11%)
5	NAG	q	2	5	14,14,15	0.70	0	17,19,21	0.76	0
5	NAG	r	1	1,5	14,14,15	0.68	0	17,19,21	0.56	0
5	NAG	r	2	5	14,14,15	0.70	0	17,19,21	0.79	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
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2	NAG	C1-C2	2.21	1.55	1.52
9	j	2	NAG	C1-C2	2.04	1.55	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	2	NAG	C2-N2-C7	12.88	140.16	122.90
7	Z	5	MAN	C1-O5-C5	10.56	126.33	112.19
6	W	2	NAG	C2-N2-C7	5.52	130.29	122.90
8	a	4	MAN	C1-O5-C5	5.50	119.56	112.19
8	a	2	NAG	C2-N2-C7	5.46	130.22	122.90
5	c	2	NAG	C2-N2-C7	5.46	130.21	122.90
5	Q	2	NAG	C2-N2-C7	5.43	130.18	122.90
5	M	1	NAG	C2-N2-C7	5.42	130.17	122.90
5	q	1	NAG	C2-N2-C7	5.36	130.09	122.90
5	R	2	NAG	C2-N2-C7	5.35	130.07	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	n	2	NAG	C2-N2-C7	5.35	130.07	122.90
5	c	1	NAG	C2-N2-C7	5.32	130.03	122.90
5	k	2	NAG	C2-N2-C7	5.31	130.02	122.90
5	o	2	NAG	C2-N2-C7	5.26	129.95	122.90
5	Y	2	NAG	C2-N2-C7	5.25	129.94	122.90
5	i	2	NAG	C2-N2-C7	5.23	129.91	122.90
5	T	2	NAG	C2-N2-C7	5.19	129.86	122.90
5	g	2	NAG	C2-N2-C7	5.17	129.83	122.90
8	a	7	MAN	C1-O5-C5	4.85	118.69	112.19
5	P	1	NAG	C2-N2-C7	4.73	129.24	122.90
6	W	4	MAN	C1-O5-C5	4.68	118.46	112.19
9	m	2	NAG	C8-C7-N2	4.62	123.78	116.12
6	K	4	MAN	C1-O5-C5	4.42	118.12	112.19
10	l	4	MAN	C1-O5-C5	4.16	117.76	112.19
7	Z	4	MAN	C1-O5-C5	3.97	117.51	112.19
10	l	1	NAG	C2-N2-C7	3.80	128.00	122.90
5	b	1	NAG	C1-O5-C5	3.51	116.89	112.19
8	a	6	MAN	C1-O5-C5	3.23	116.51	112.19
7	Z	6	MAN	C1-O5-C5	3.14	116.39	112.19
9	m	3	BMA	C1-O5-C5	2.98	116.18	112.19
10	l	3	BMA	C1-O5-C5	2.78	115.91	112.19
9	j	3	BMA	C1-O5-C5	2.76	115.88	112.19
9	m	1	NAG	C2-N2-C7	2.71	126.54	122.90
10	l	1	NAG	O7-C7-N2	2.71	126.76	121.98
9	m	2	NAG	O7-C7-C8	-2.70	117.24	122.05
5	X	1	NAG	C1-O5-C5	2.69	115.79	112.19
5	P	1	NAG	O7-C7-N2	2.61	126.60	121.98
5	f	1	NAG	C1-O5-C5	2.57	115.64	112.19
5	V	1	NAG	C1-O5-C5	2.43	115.44	112.19
5	G	1	NAG	C1-O5-C5	2.40	115.41	112.19
9	m	2	NAG	C1-O5-C5	2.40	115.40	112.19
5	M	1	NAG	O7-C7-N2	2.39	126.20	121.98
5	i	2	NAG	O7-C7-N2	2.39	126.20	121.98
5	g	2	NAG	O7-C7-N2	2.38	126.19	121.98
5	q	1	NAG	O7-C7-N2	2.38	126.19	121.98
5	c	1	NAG	O7-C7-N2	2.37	126.18	121.98
5	i	1	NAG	C1-O5-C5	2.37	115.36	112.19
7	Z	1	NAG	C1-O5-C5	2.37	115.36	112.19
5	Y	2	NAG	O7-C7-N2	2.37	126.17	121.98
5	T	2	NAG	O7-C7-N2	2.35	126.14	121.98
5	o	2	NAG	O7-C7-N2	2.35	126.14	121.98
5	k	2	NAG	O7-C7-N2	2.34	126.11	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	NAG	C2-N2-C7	2.34	126.03	122.90
5	n	2	NAG	O7-C7-N2	2.32	126.08	121.98
5	R	2	NAG	O7-C7-N2	2.30	126.05	121.98
5	Q	2	NAG	O7-C7-N2	2.28	126.02	121.98
5	c	2	NAG	O7-C7-N2	2.28	126.02	121.98
5	Y	1	NAG	C2-N2-C7	2.28	125.95	122.90
5	P	1	NAG	C1-O5-C5	2.27	115.22	112.19
6	W	2	NAG	O7-C7-N2	2.26	125.97	121.98
6	W	3	BMA	C1-O5-C5	2.21	115.15	112.19
5	O	2	NAG	C2-N2-C7	2.20	125.85	122.90
5	n	1	NAG	C2-N2-C7	2.19	125.84	122.90
9	j	1	NAG	C1-O5-C5	2.16	115.08	112.19
9	m	2	NAG	C1-C2-N2	2.13	113.79	110.43
5	U	2	NAG	C2-N2-C7	2.11	125.73	122.90
10	l	1	NAG	C1-O5-C5	2.10	115.00	112.19
8	a	5	MAN	C1-O5-C5	2.10	115.00	112.19
6	K	1	NAG	C1-O5-C5	2.08	114.97	112.19
5	S	2	NAG	C2-N2-C7	2.07	125.68	122.90
8	a	3	BMA	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	l	3	BMA	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	n	1	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	W	4	MAN	O5-C5-C6-O6
8	a	7	MAN	O5-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
8	a	6	MAN	O5-C5-C6-O6
5	o	1	NAG	C4-C5-C6-O6
9	m	2	NAG	C8-C7-N2-C2
9	m	2	NAG	O7-C7-N2-C2
10	l	3	BMA	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	i	2	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	o	1	NAG	O5-C5-C6-O6
7	Z	3	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	n	1	NAG	C4-C5-C6-O6
9	m	3	BMA	O5-C5-C6-O6
10	l	2	NAG	O5-C5-C6-O6
10	l	4	MAN	O5-C5-C6-O6
7	Z	4	MAN	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
5	q	1	NAG	O5-C5-C6-O6
9	m	2	NAG	O5-C5-C6-O6
8	a	4	MAN	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
8	a	7	MAN	C4-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C1-C2-N2-C7
5	T	2	NAG	C1-C2-N2-C7
5	Y	2	NAG	C1-C2-N2-C7
5	c	1	NAG	C1-C2-N2-C7
5	c	2	NAG	C1-C2-N2-C7
5	g	2	NAG	C1-C2-N2-C7
5	i	2	NAG	C1-C2-N2-C7
5	k	2	NAG	C1-C2-N2-C7
5	n	2	NAG	C1-C2-N2-C7
5	o	2	NAG	C1-C2-N2-C7
5	q	1	NAG	C1-C2-N2-C7
6	W	2	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
9	m	2	NAG	C1-C2-N2-C7
7	Z	6	MAN	C4-C5-C6-O6
6	W	4	MAN	C4-C5-C6-O6
7	Z	6	MAN	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	P	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7

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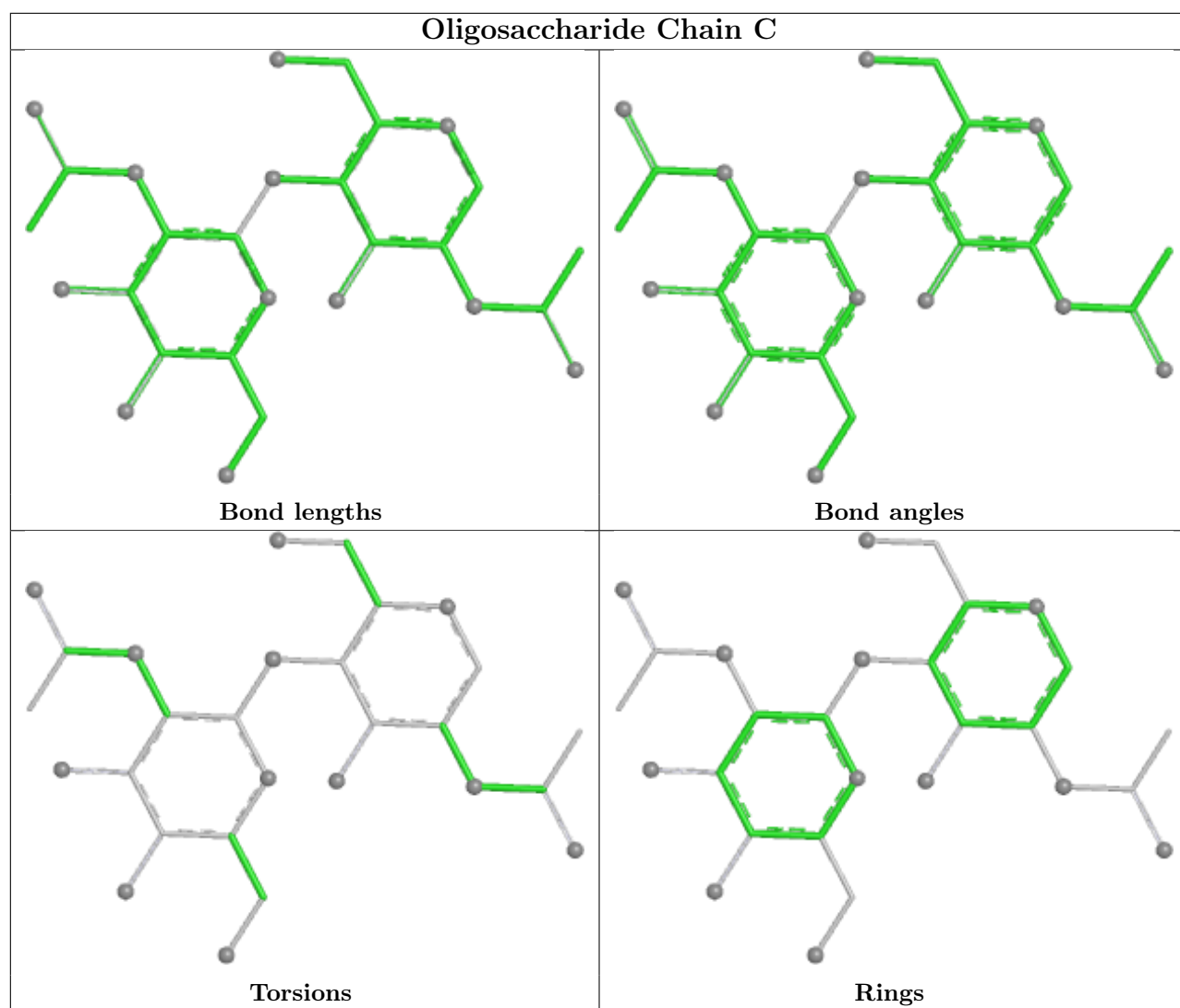
Mol	Chain	Res	Type	Atoms
5	R	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	c	1	NAG	C3-C2-N2-C7
5	c	2	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7
5	i	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
5	n	2	NAG	C3-C2-N2-C7
5	o	2	NAG	C3-C2-N2-C7
5	q	1	NAG	C3-C2-N2-C7
6	W	2	NAG	C3-C2-N2-C7
10	l	1	NAG	C3-C2-N2-C7
5	f	1	NAG	C4-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
8	a	6	MAN	C4-C5-C6-O6
7	Z	3	BMA	C4-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
5	O	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7
5	q	2	NAG	C1-C2-N2-C7
8	a	1	NAG	C1-C2-N2-C7
10	l	1	NAG	C1-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
9	m	2	NAG	C3-C2-N2-C7

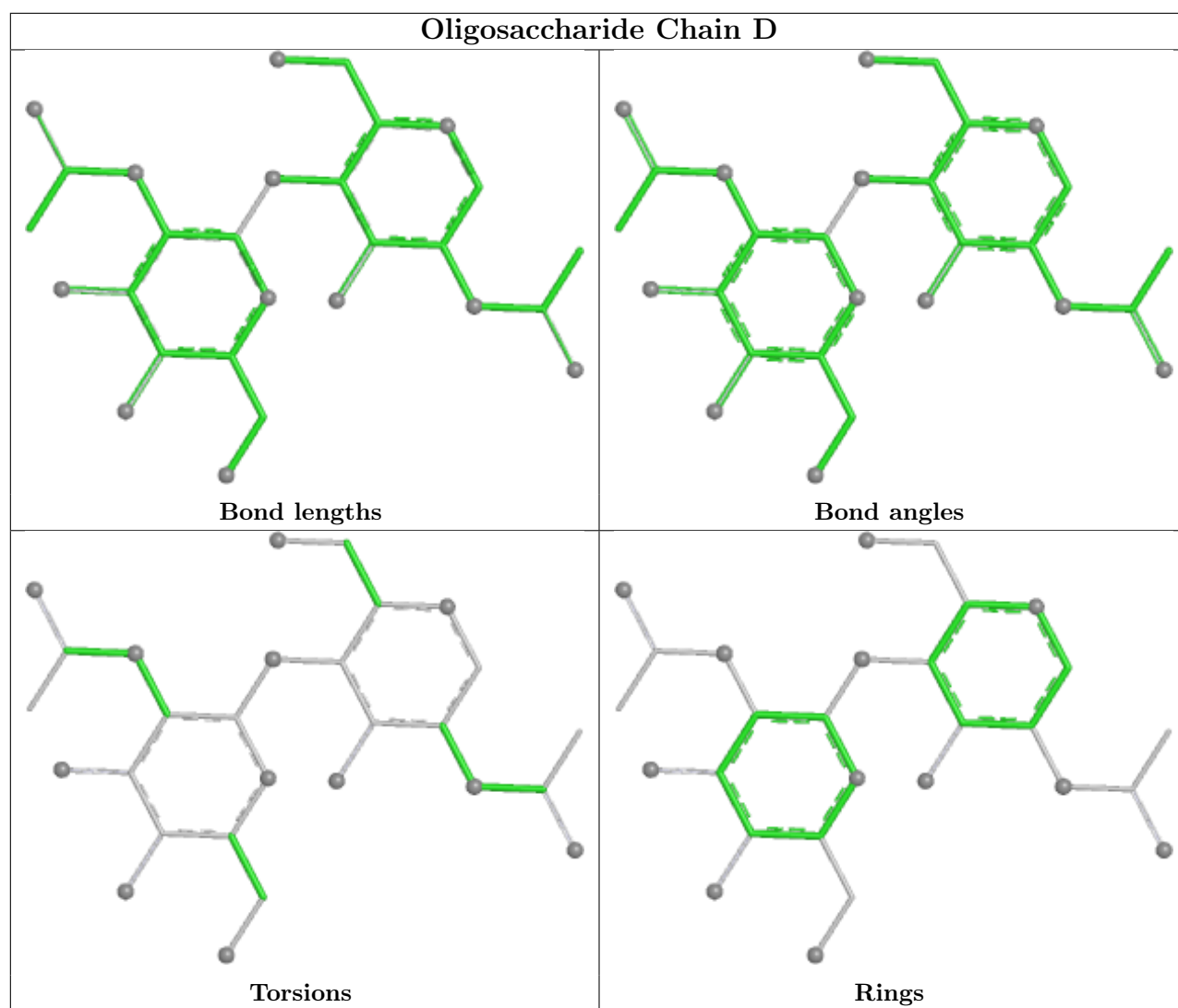
There are no ring outliers.

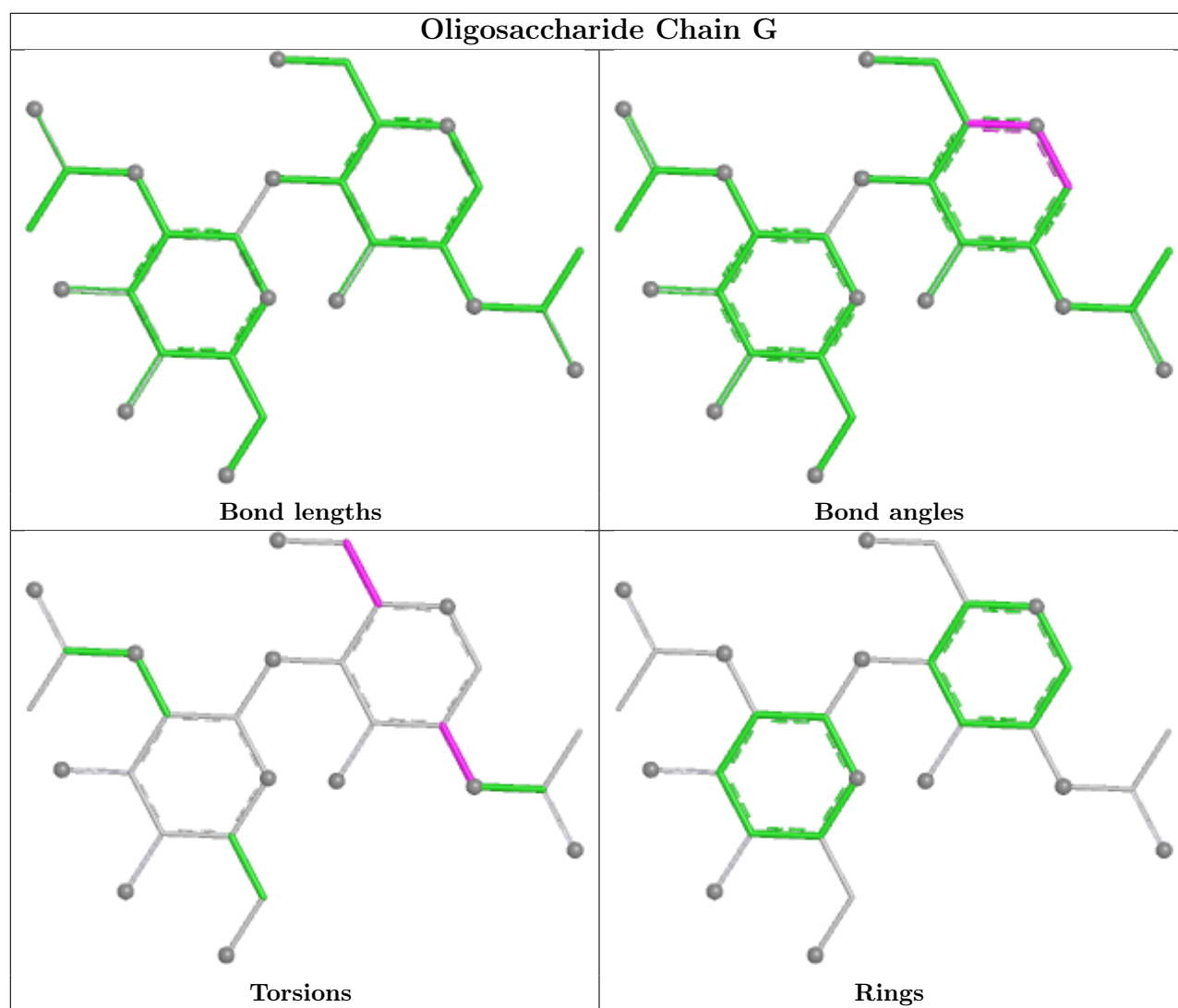
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1	NAG	1	0
10	l	1	NAG	2	0
5	O	1	NAG	1	0
8	a	1	NAG	1	0

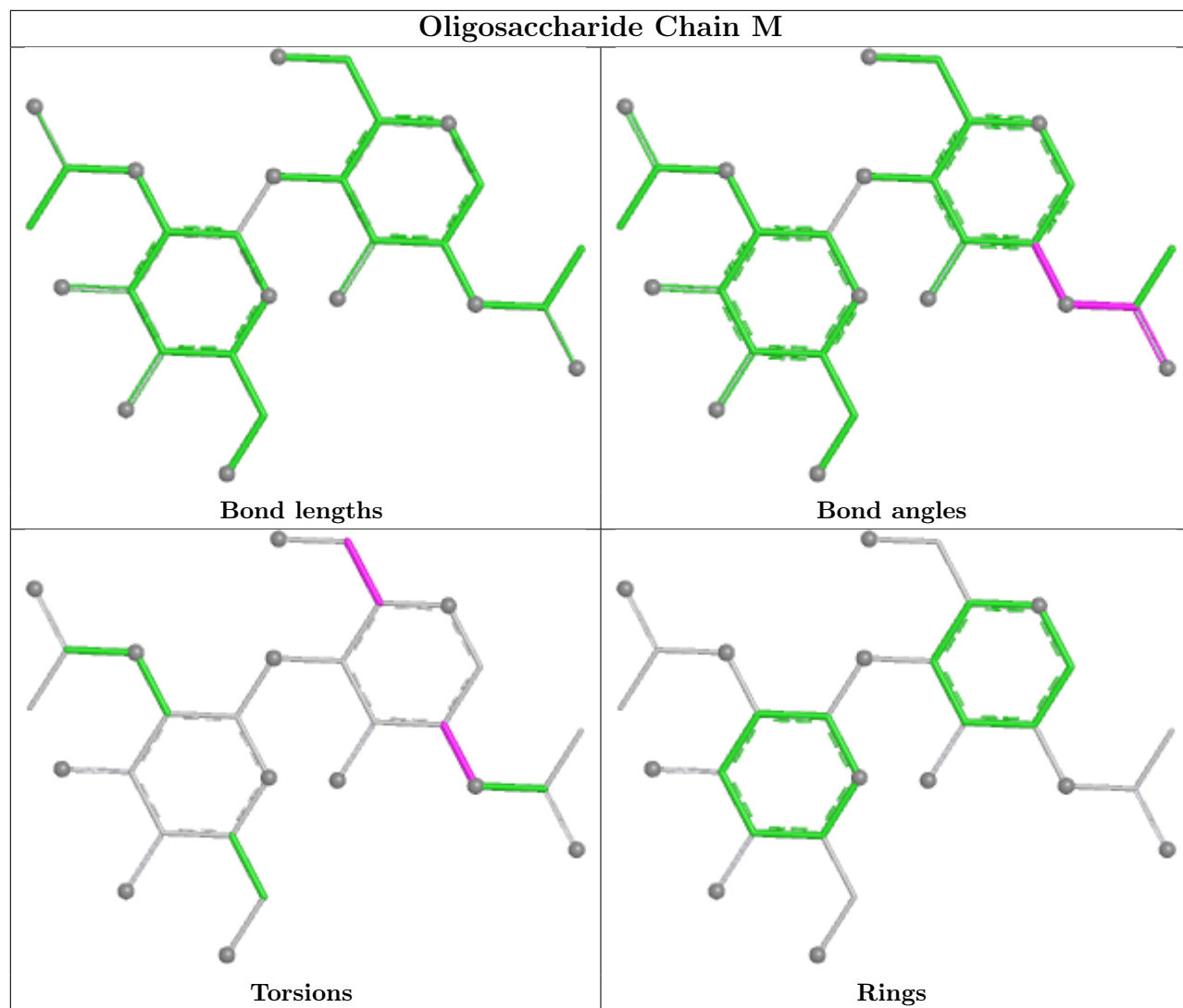
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

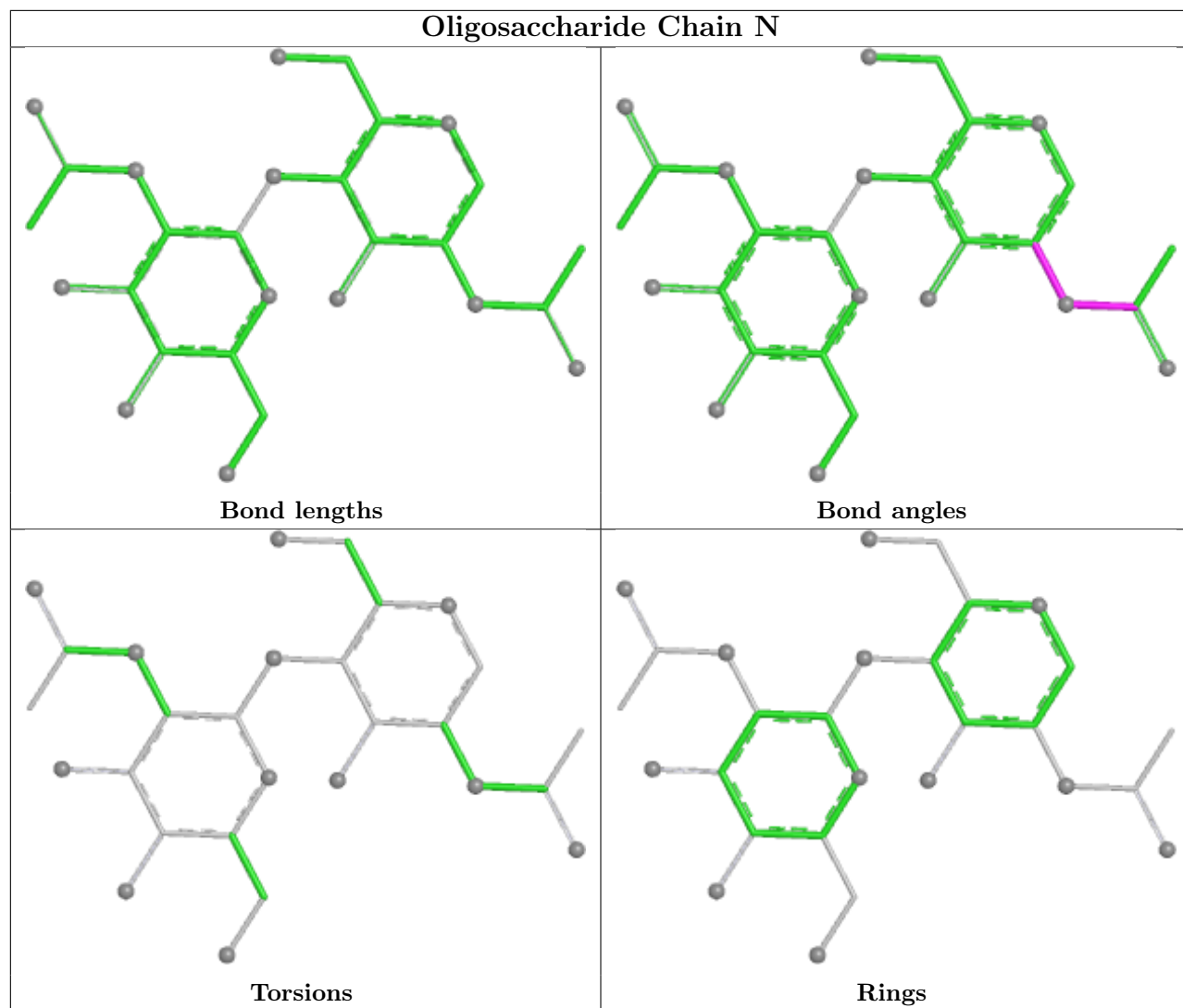


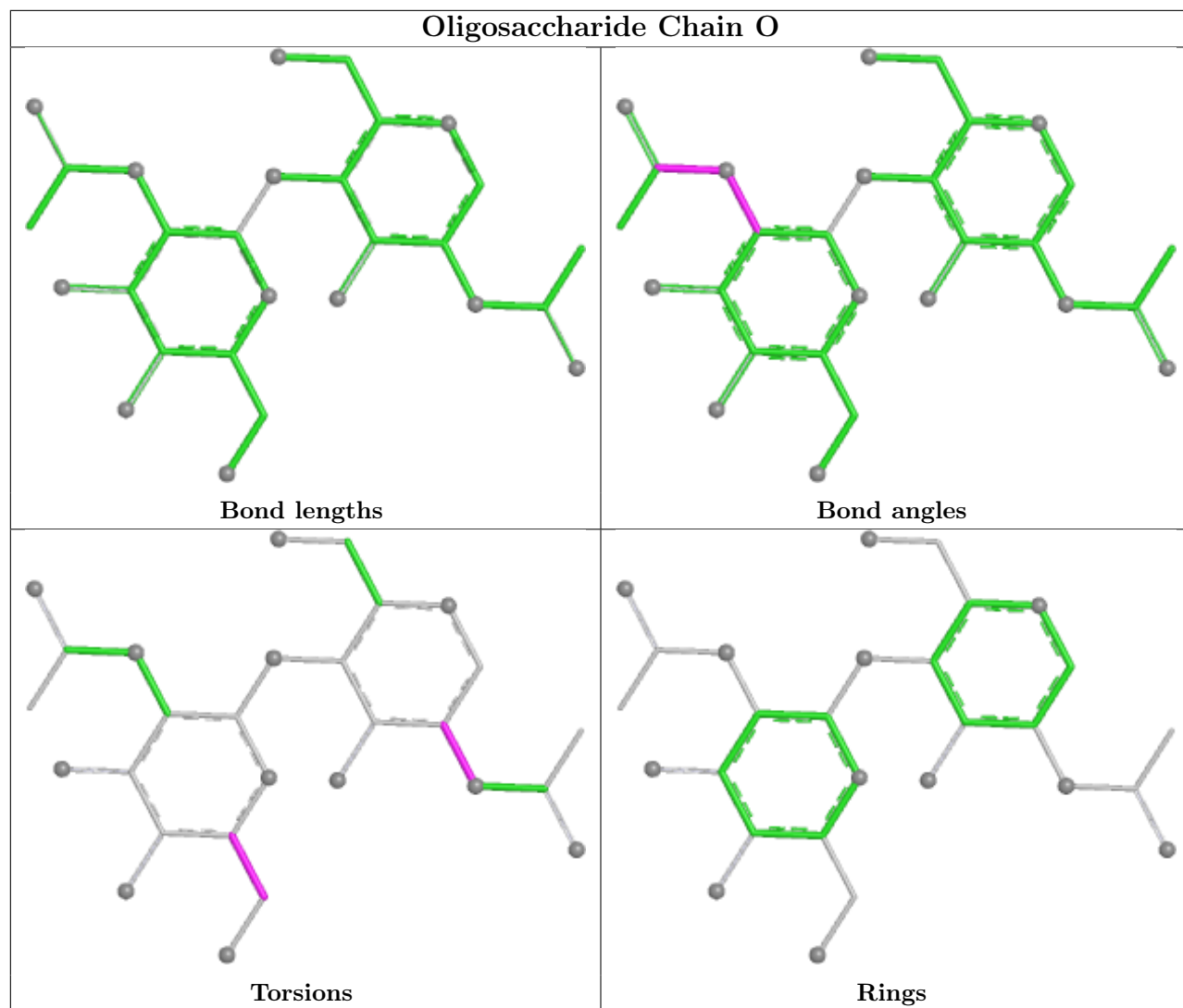


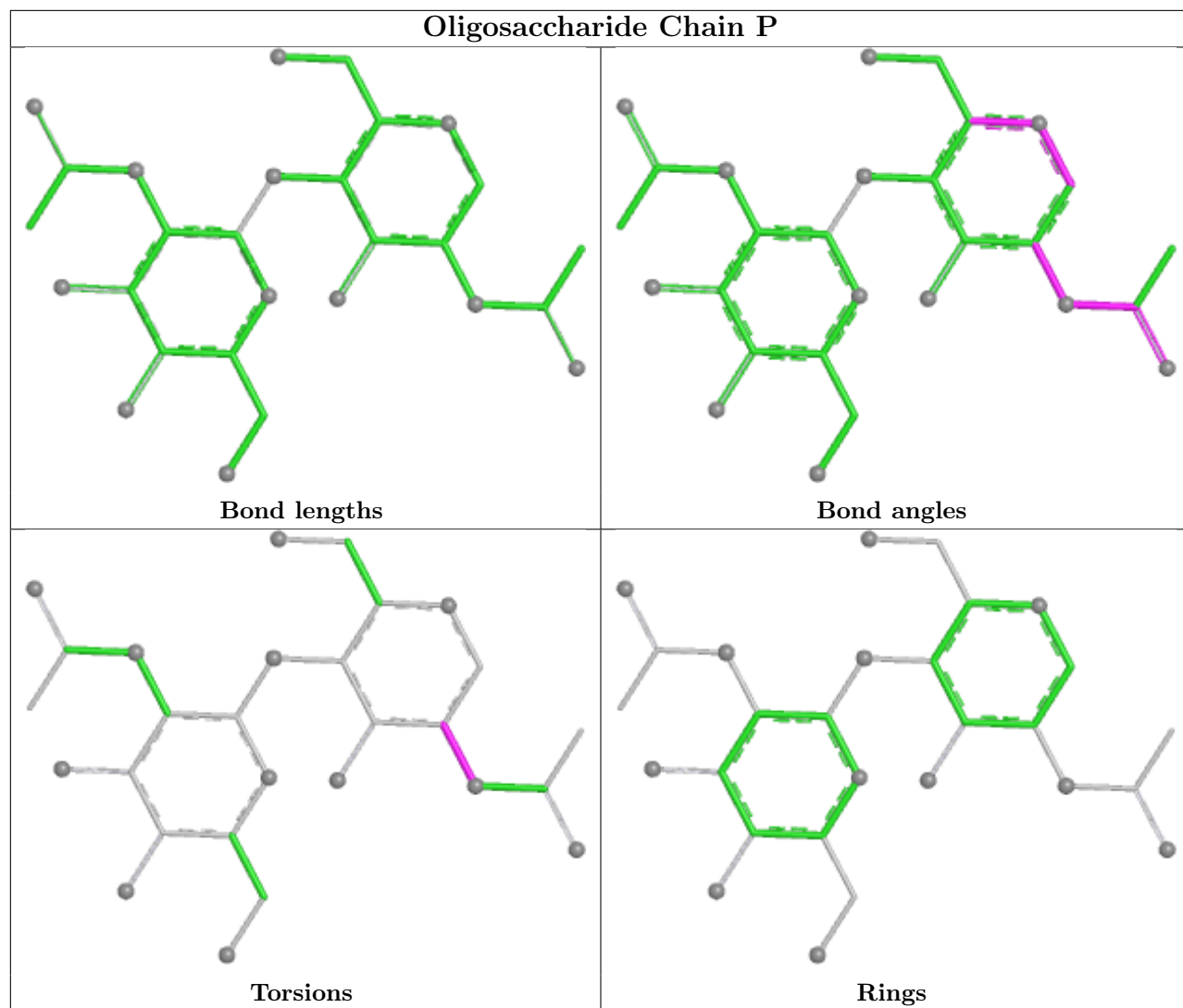


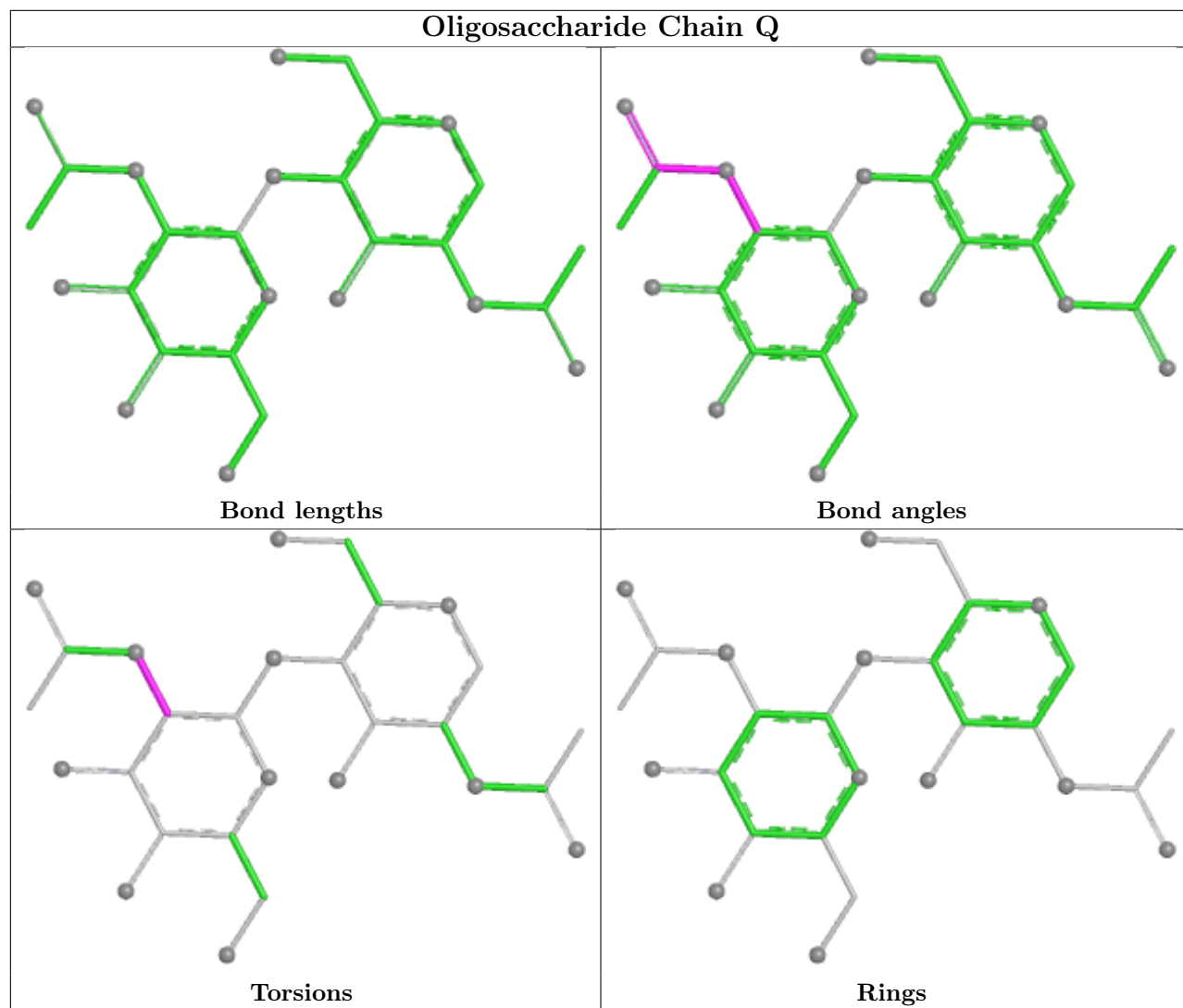


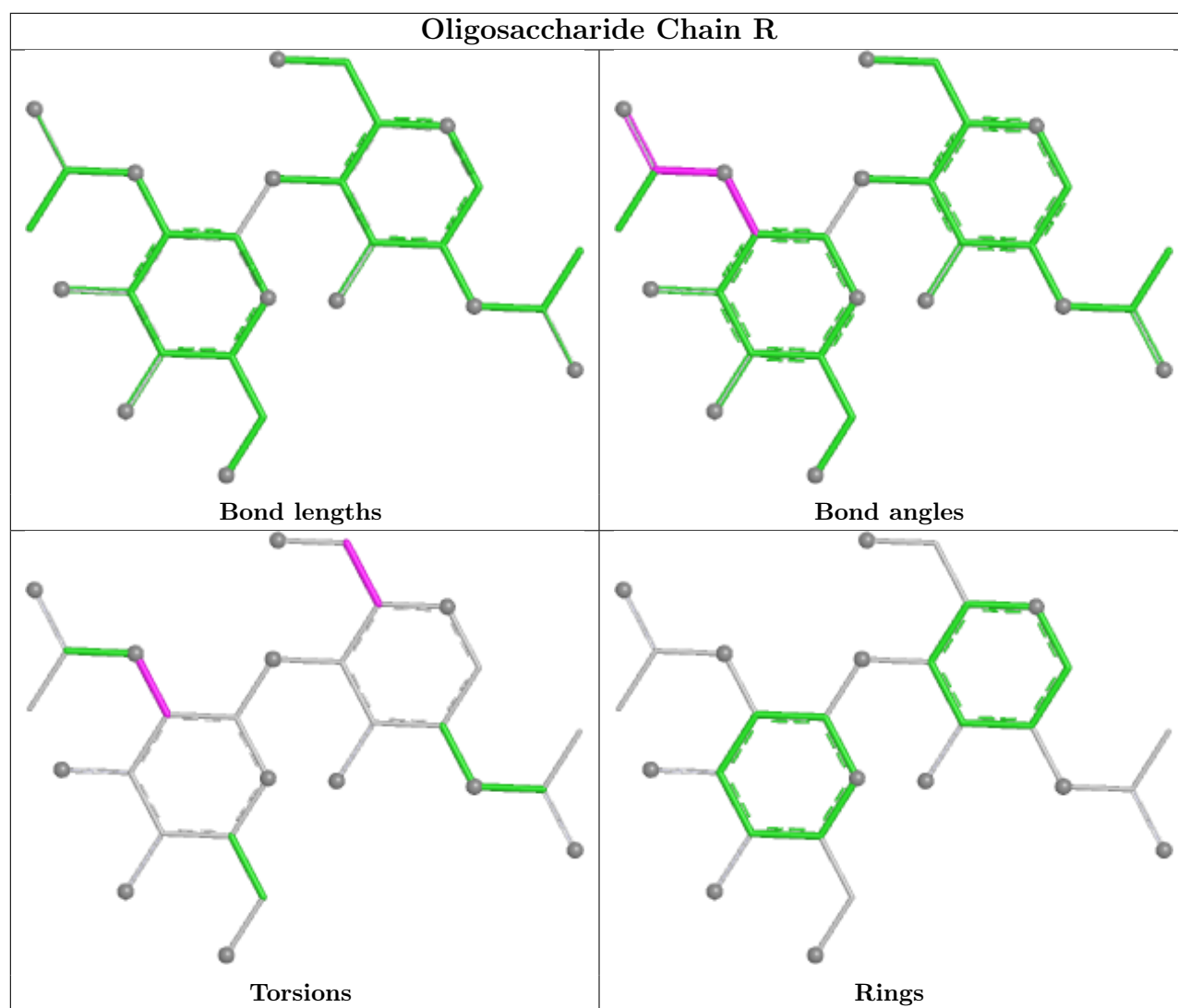


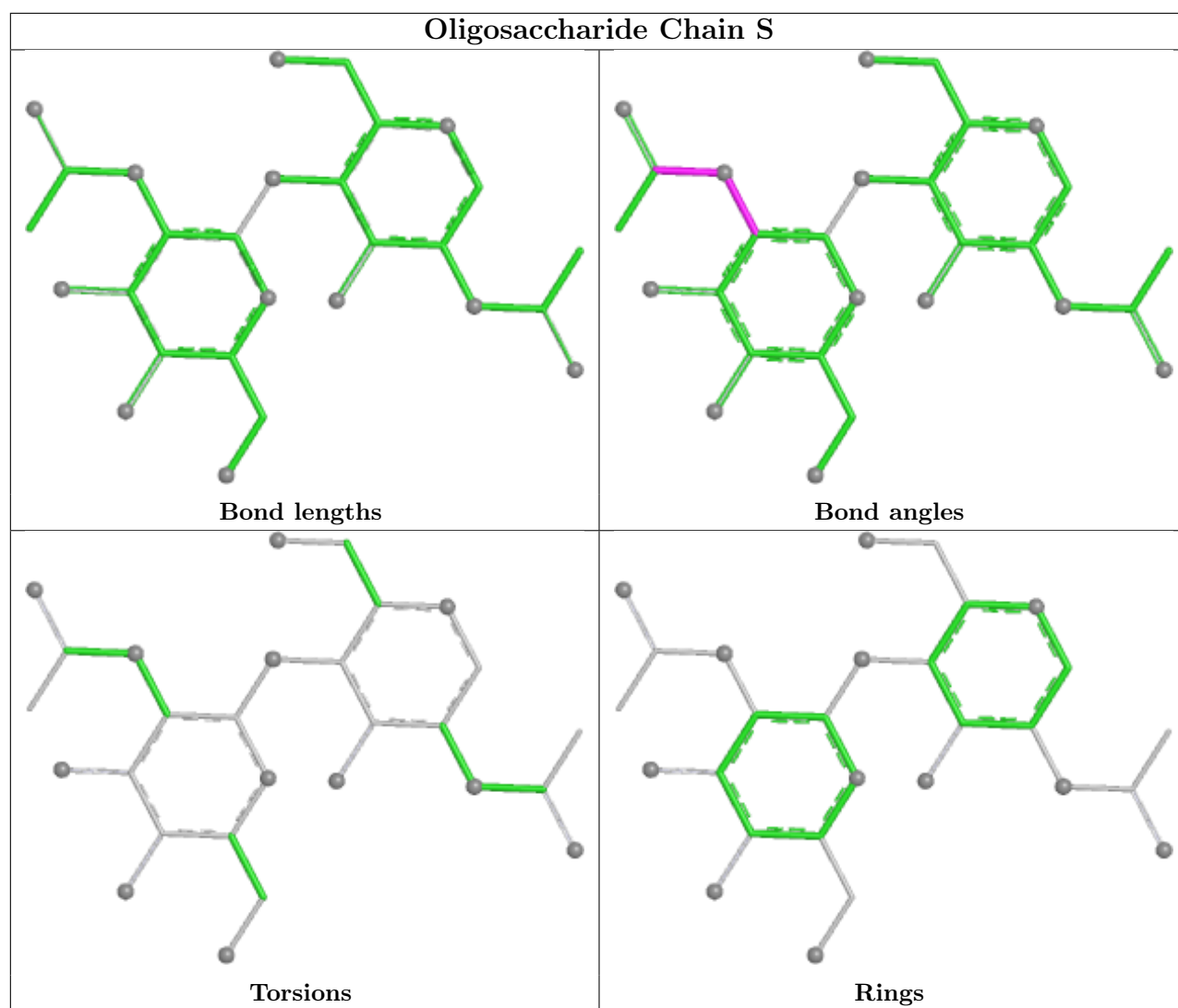


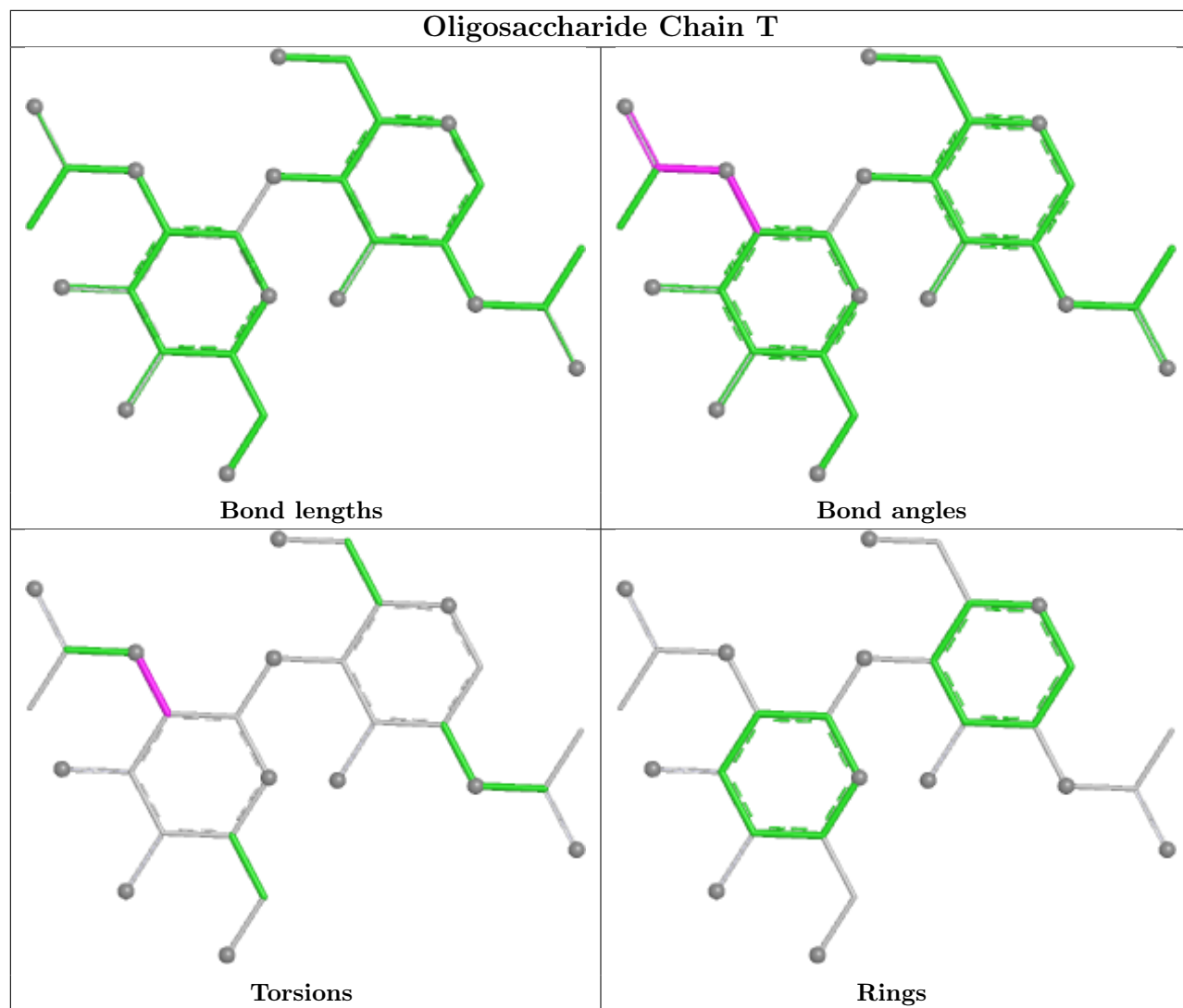




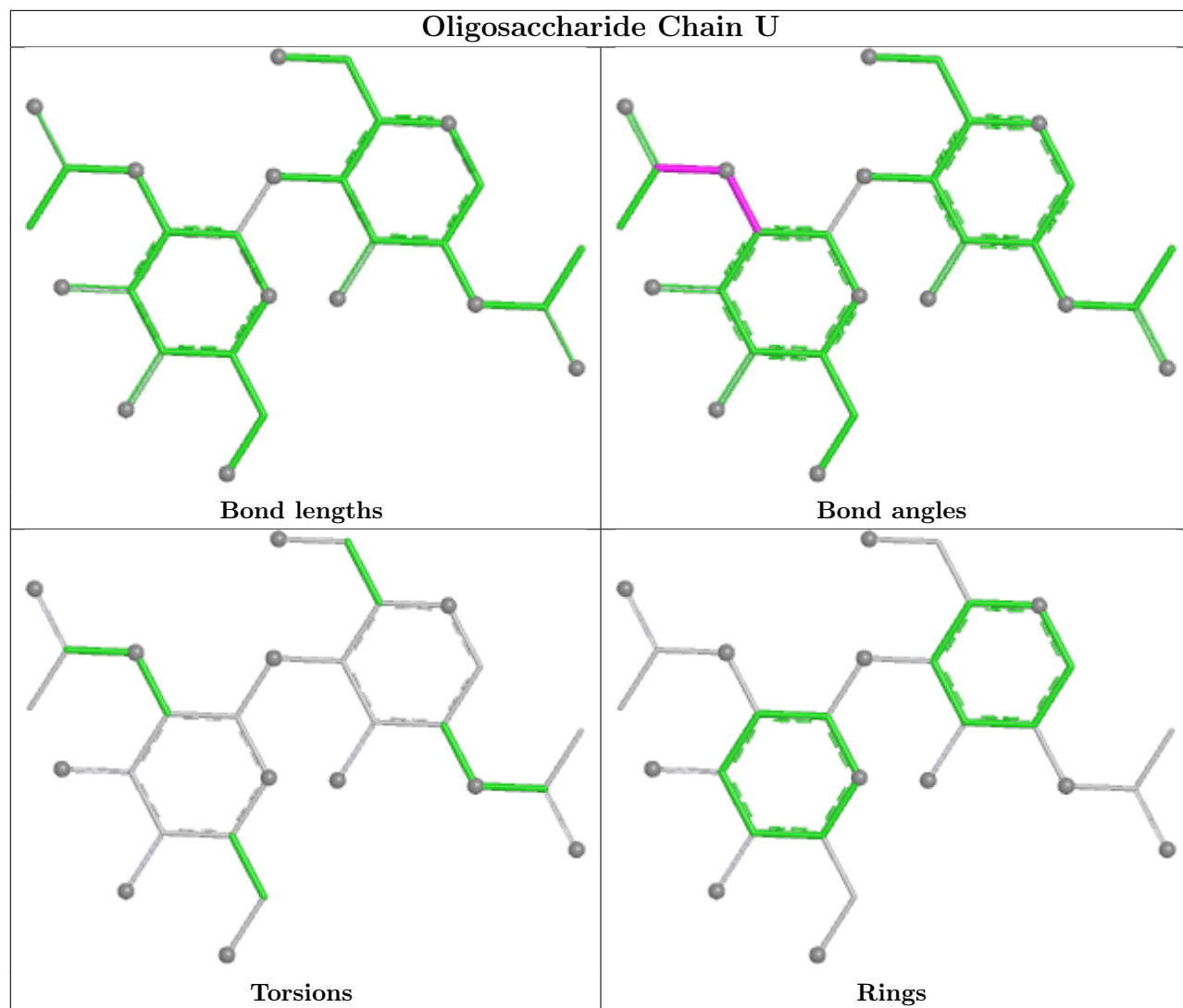


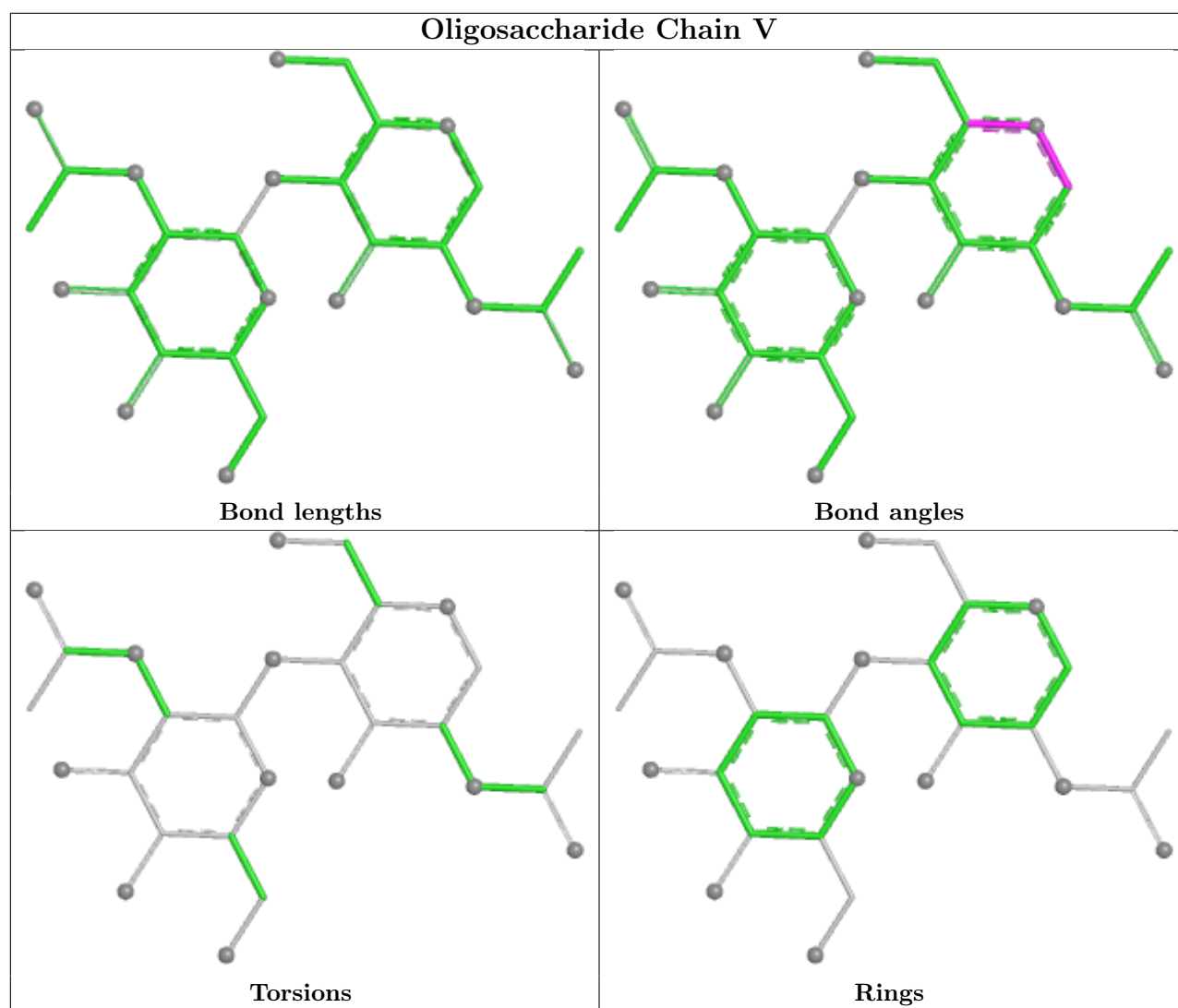


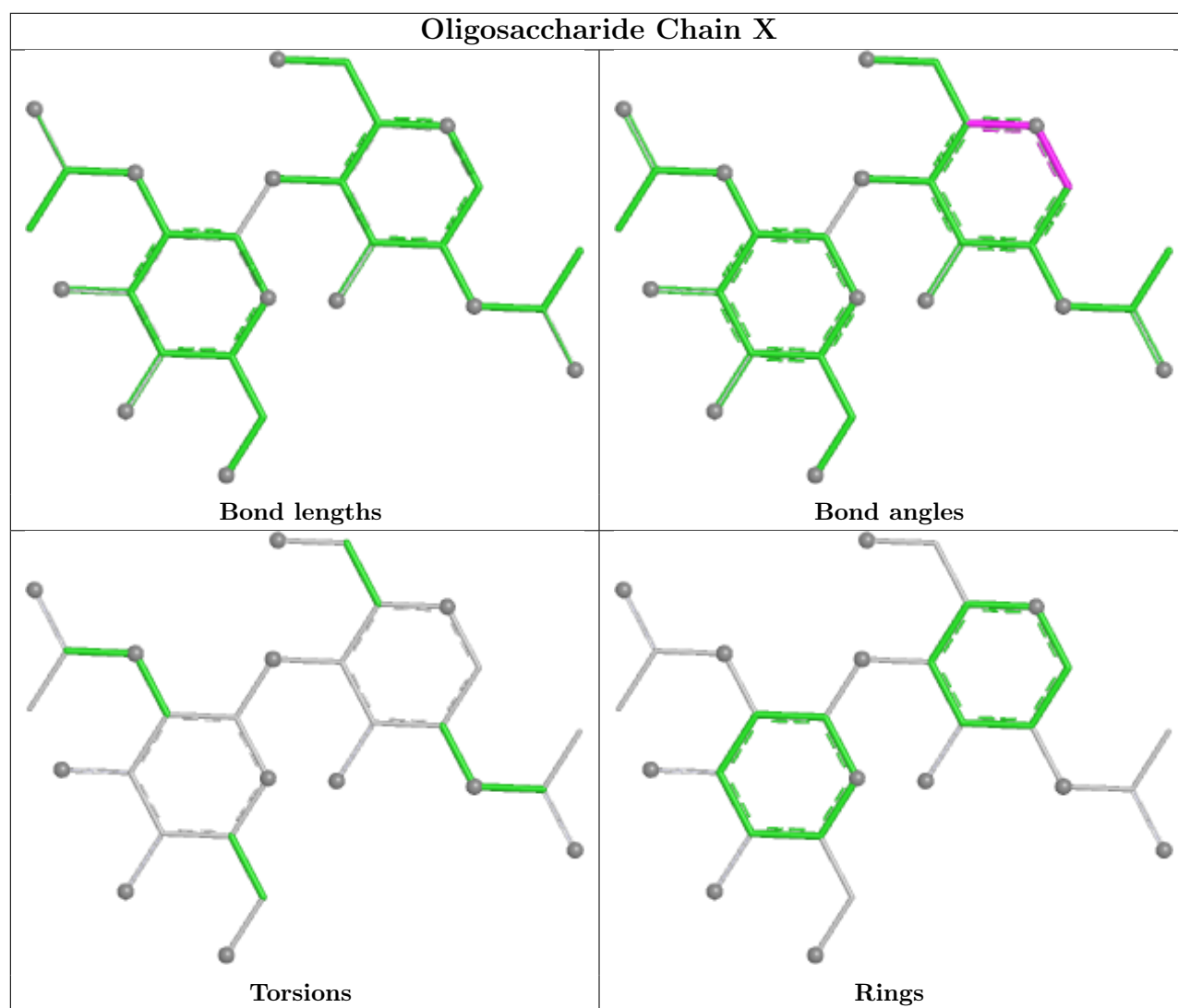


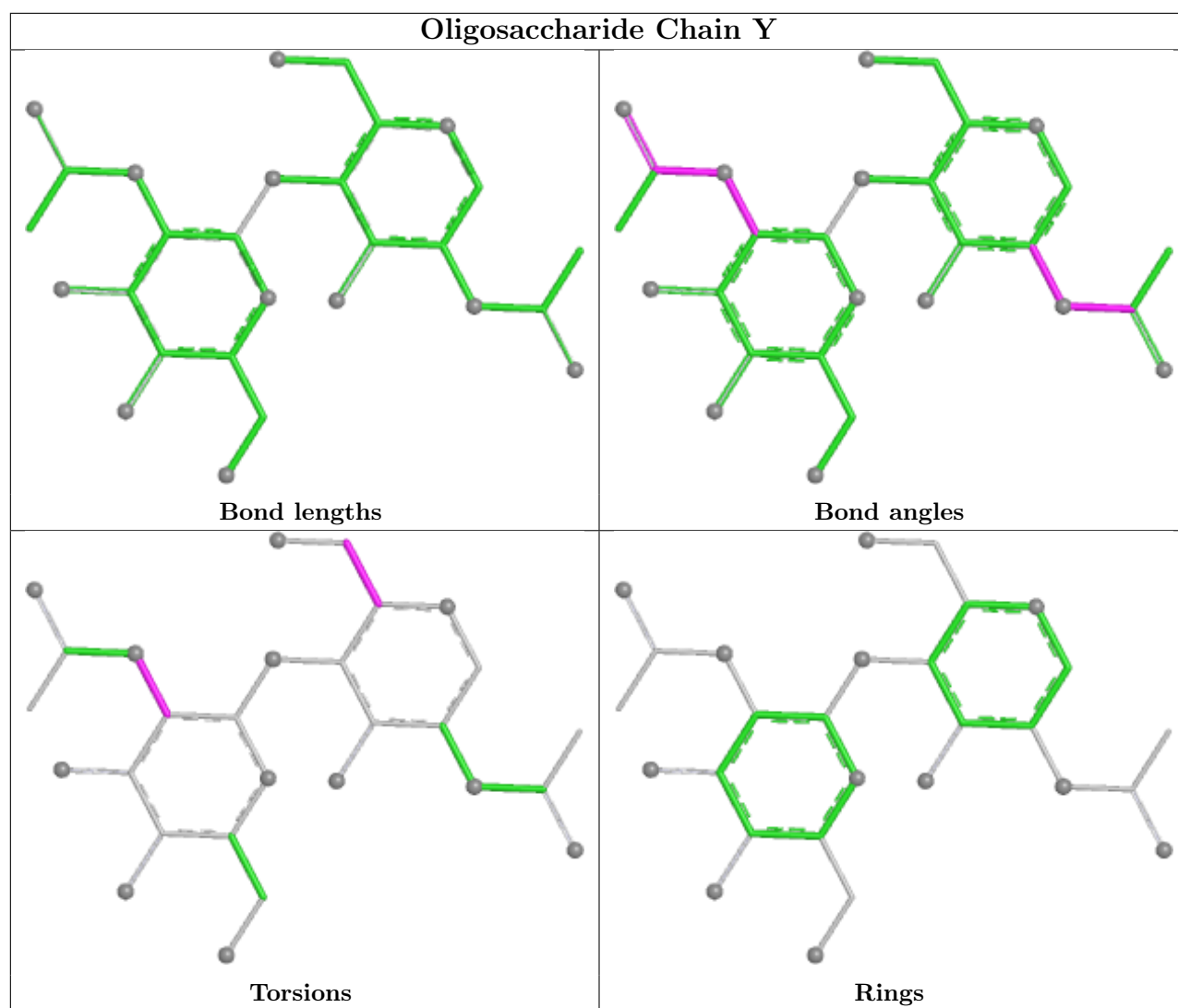


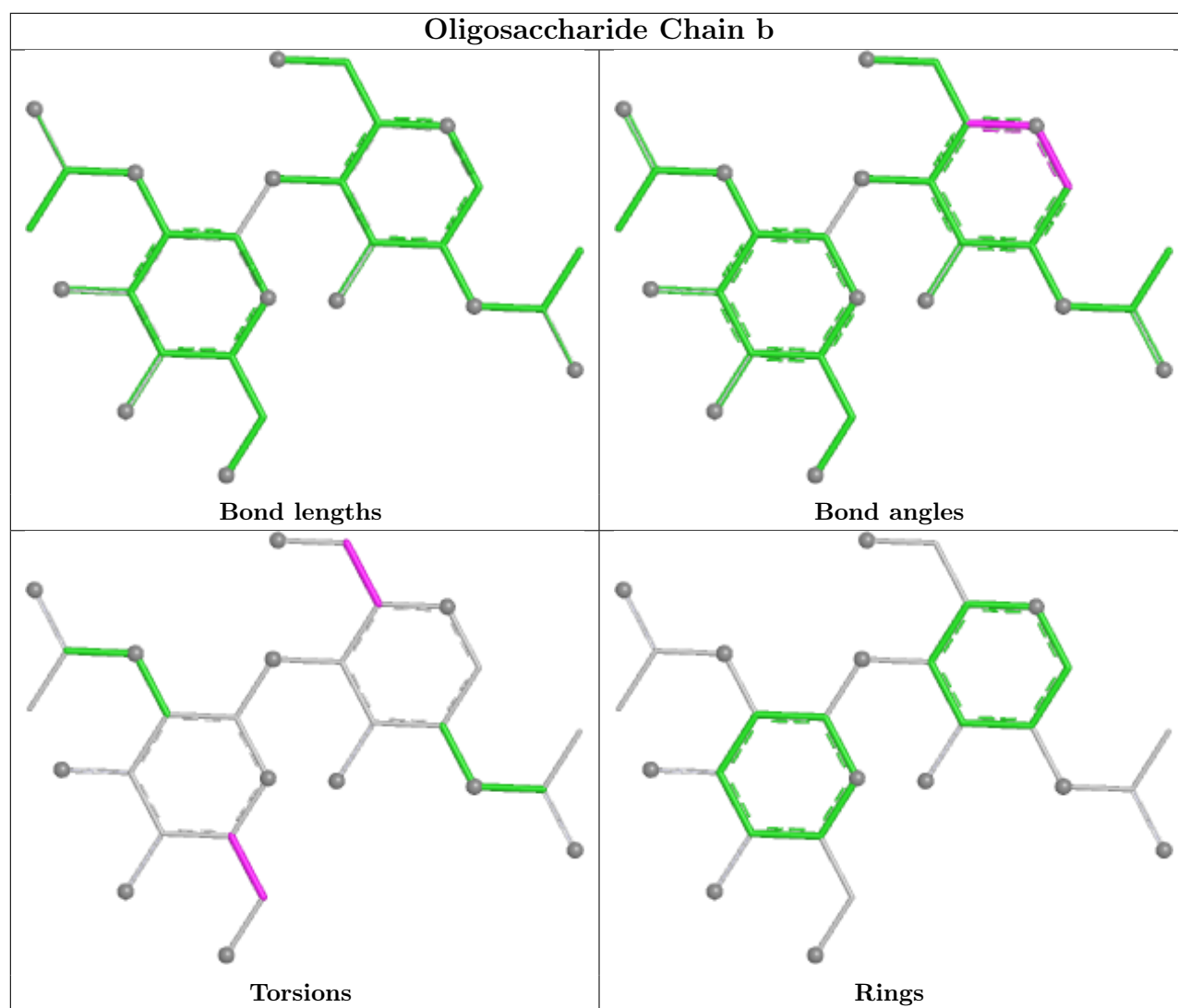


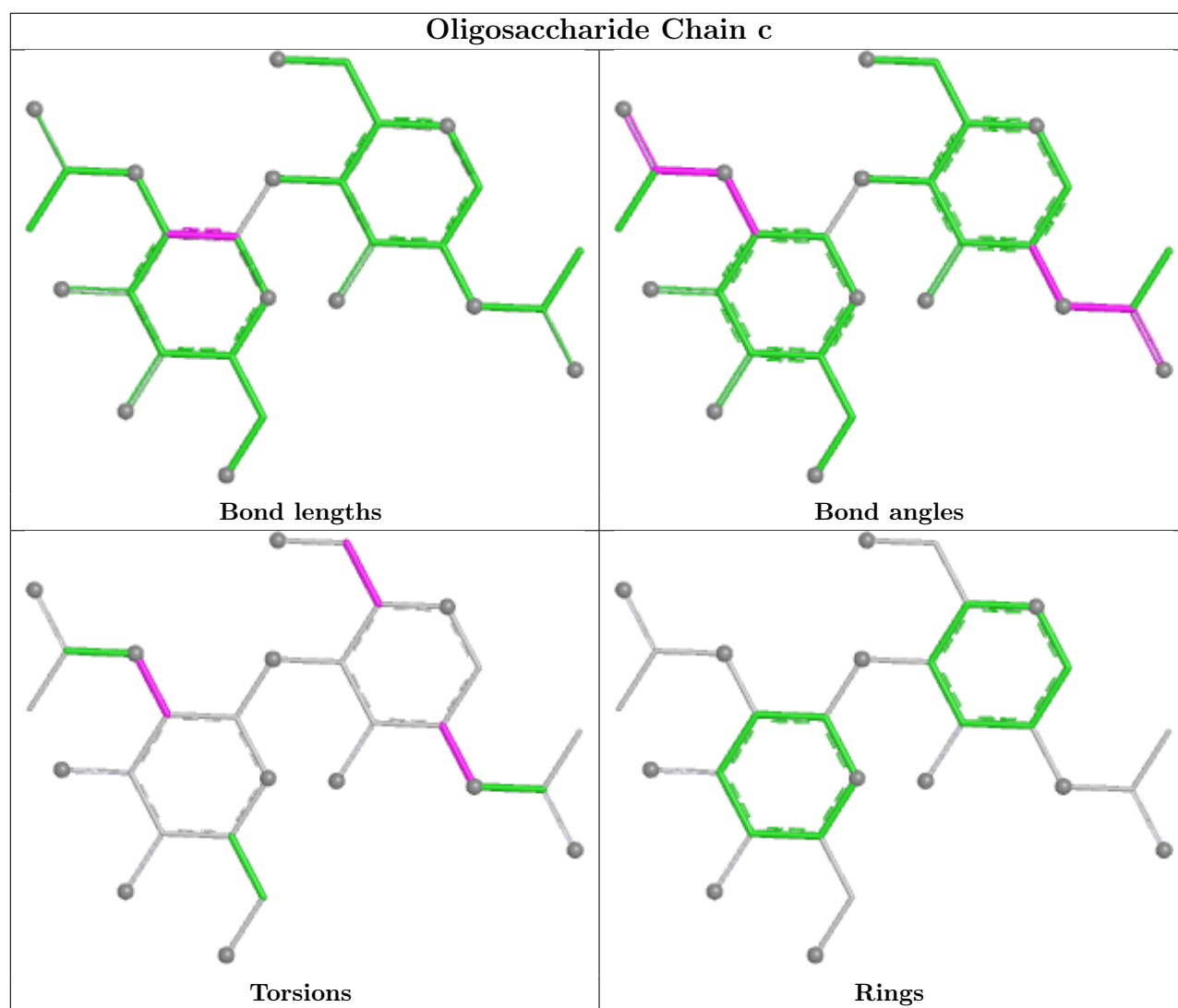


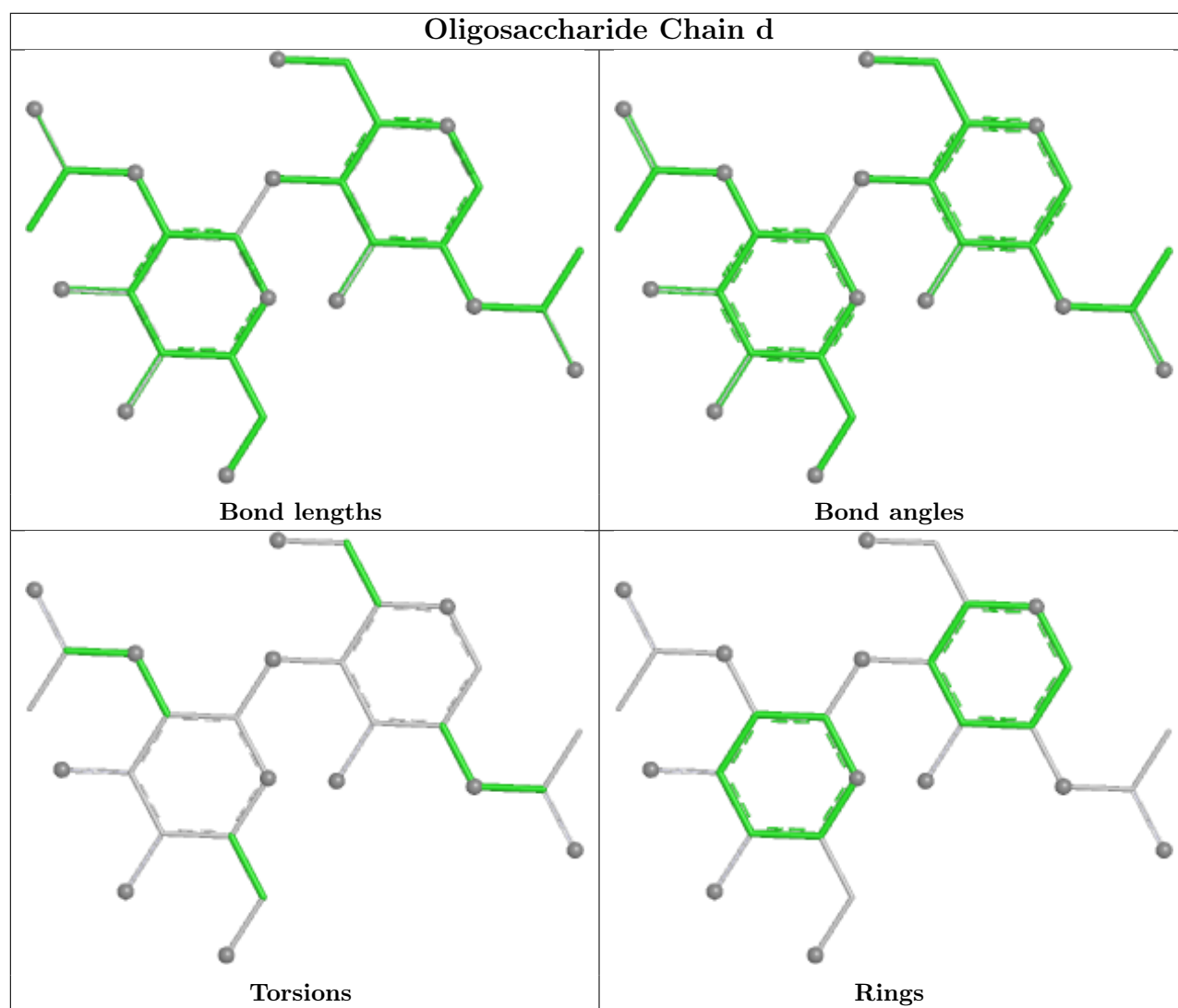


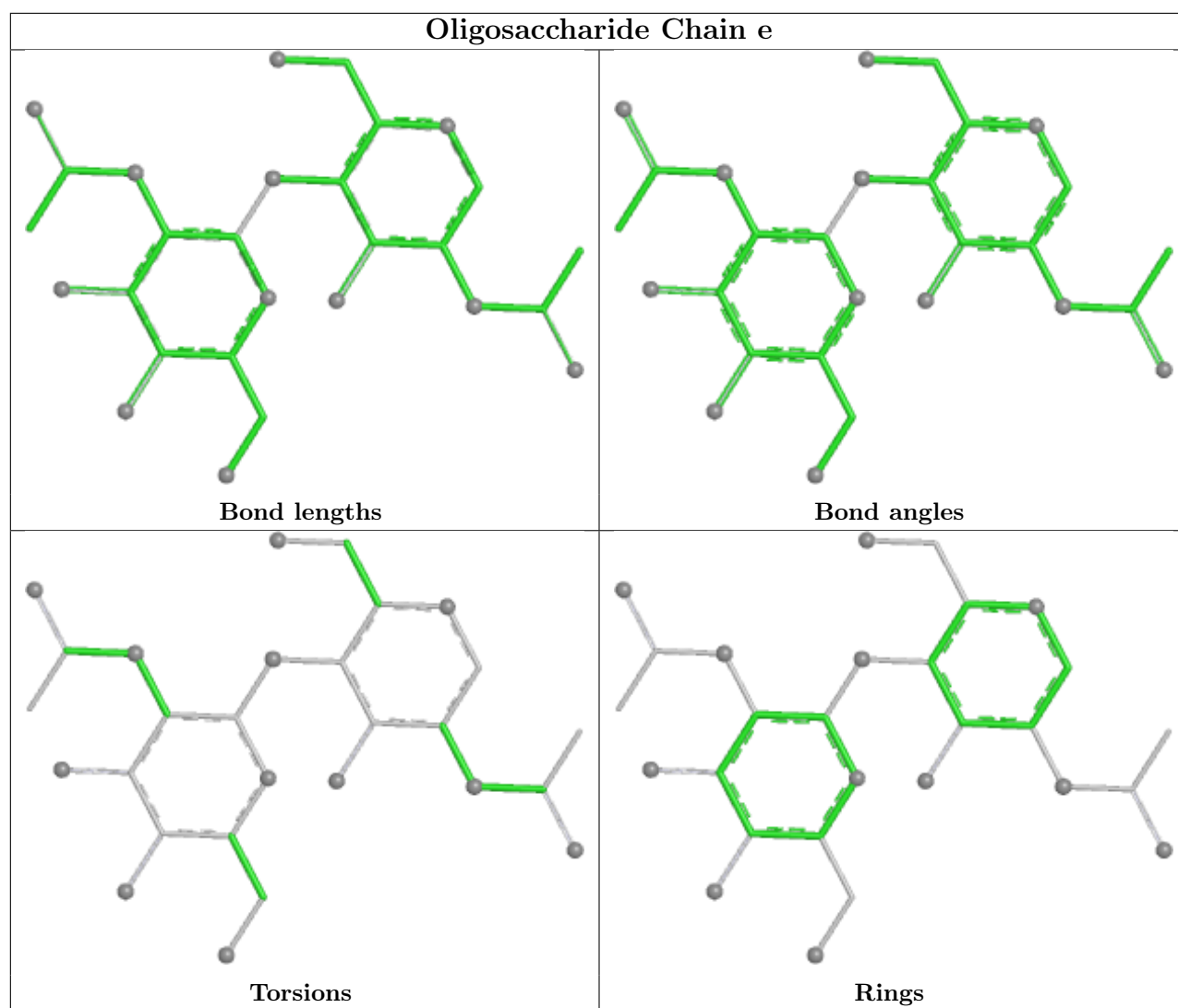




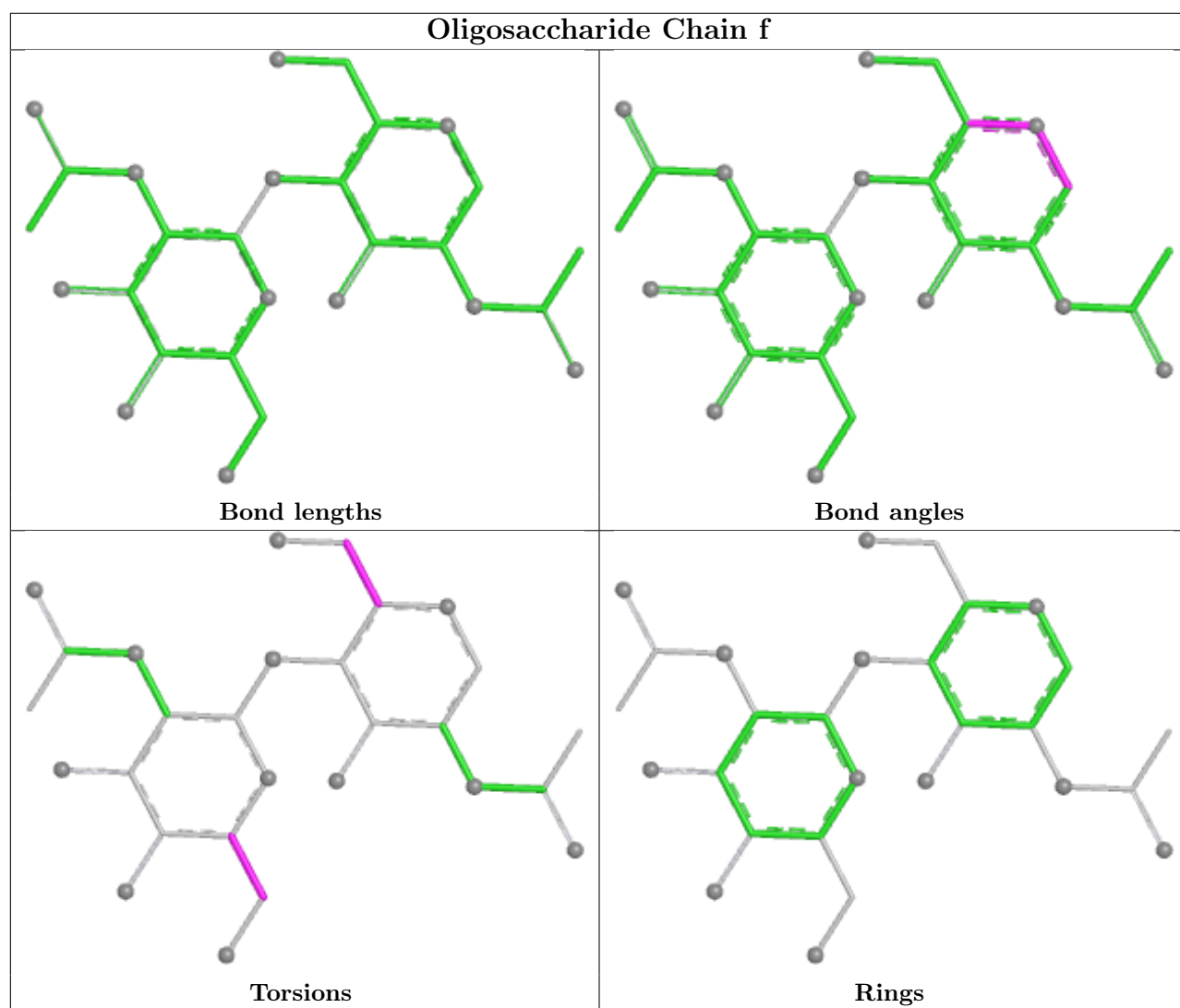


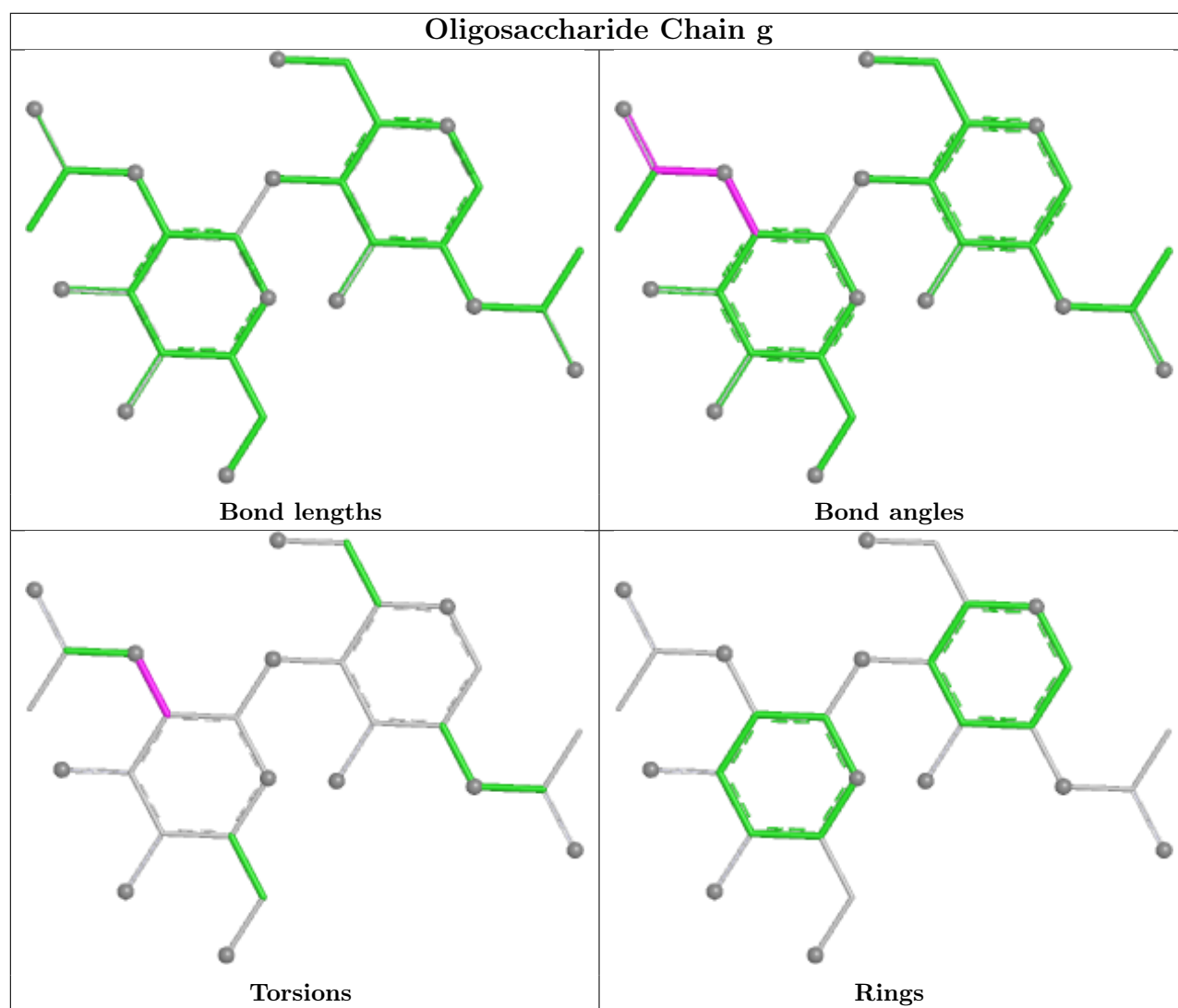


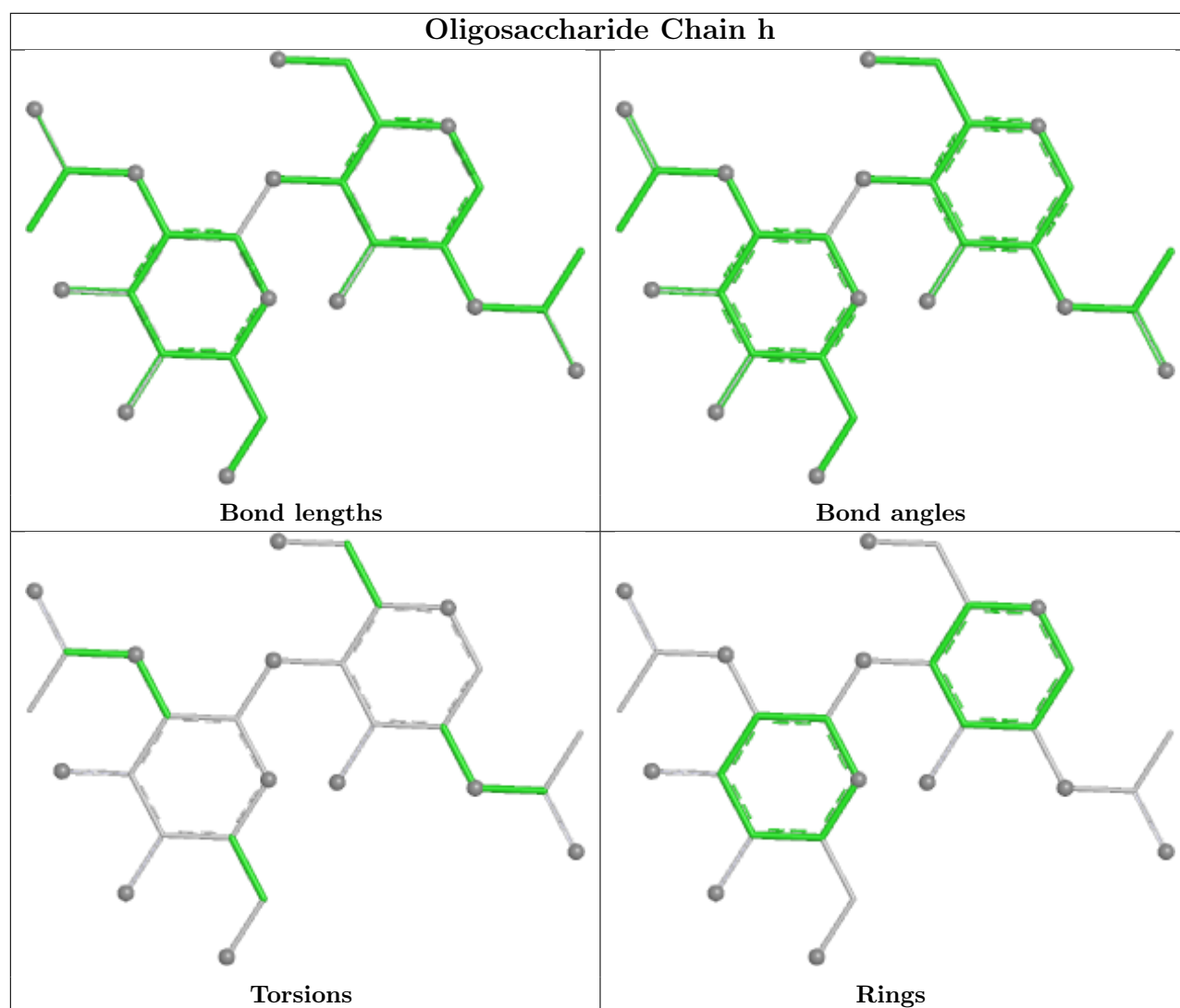


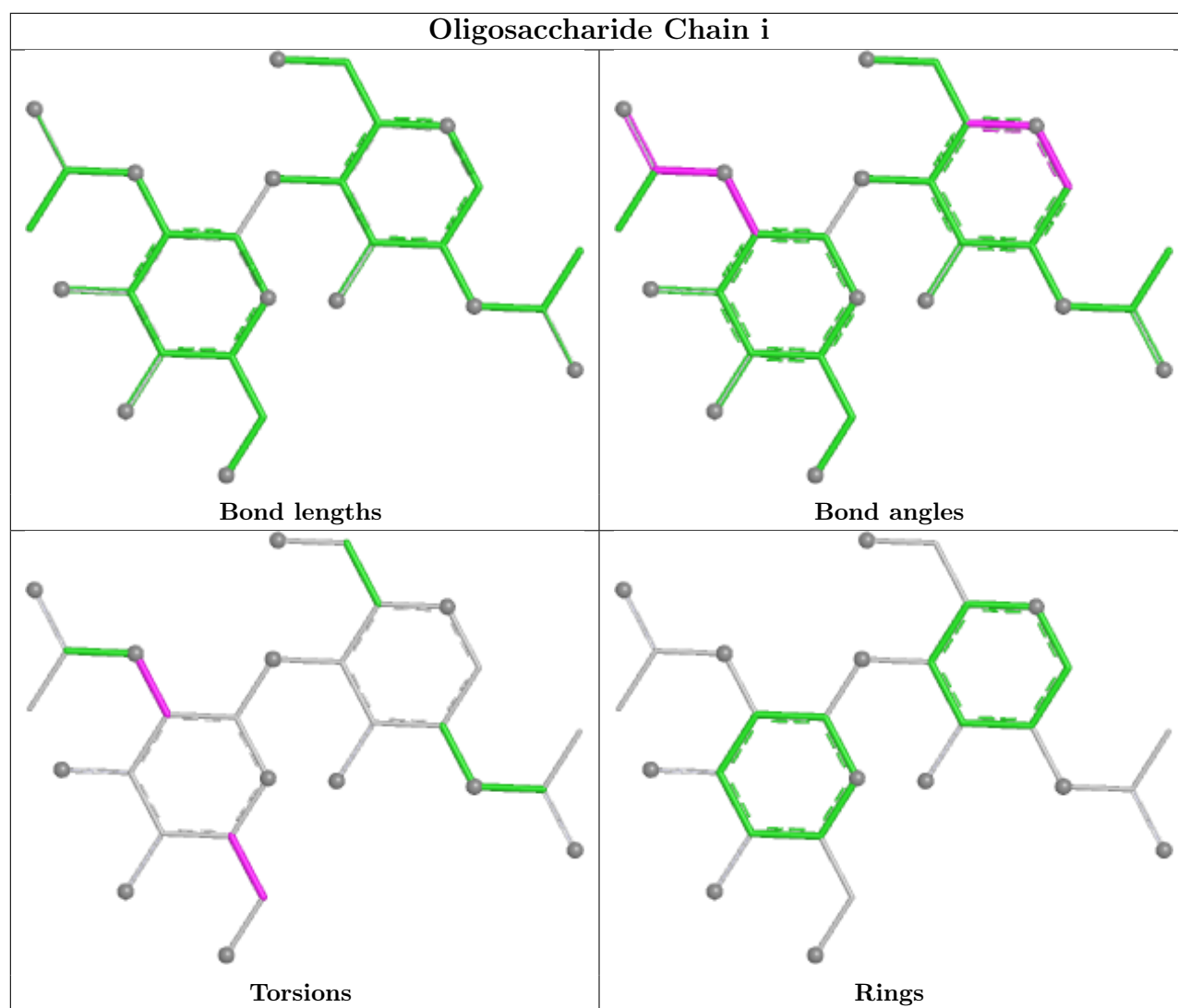


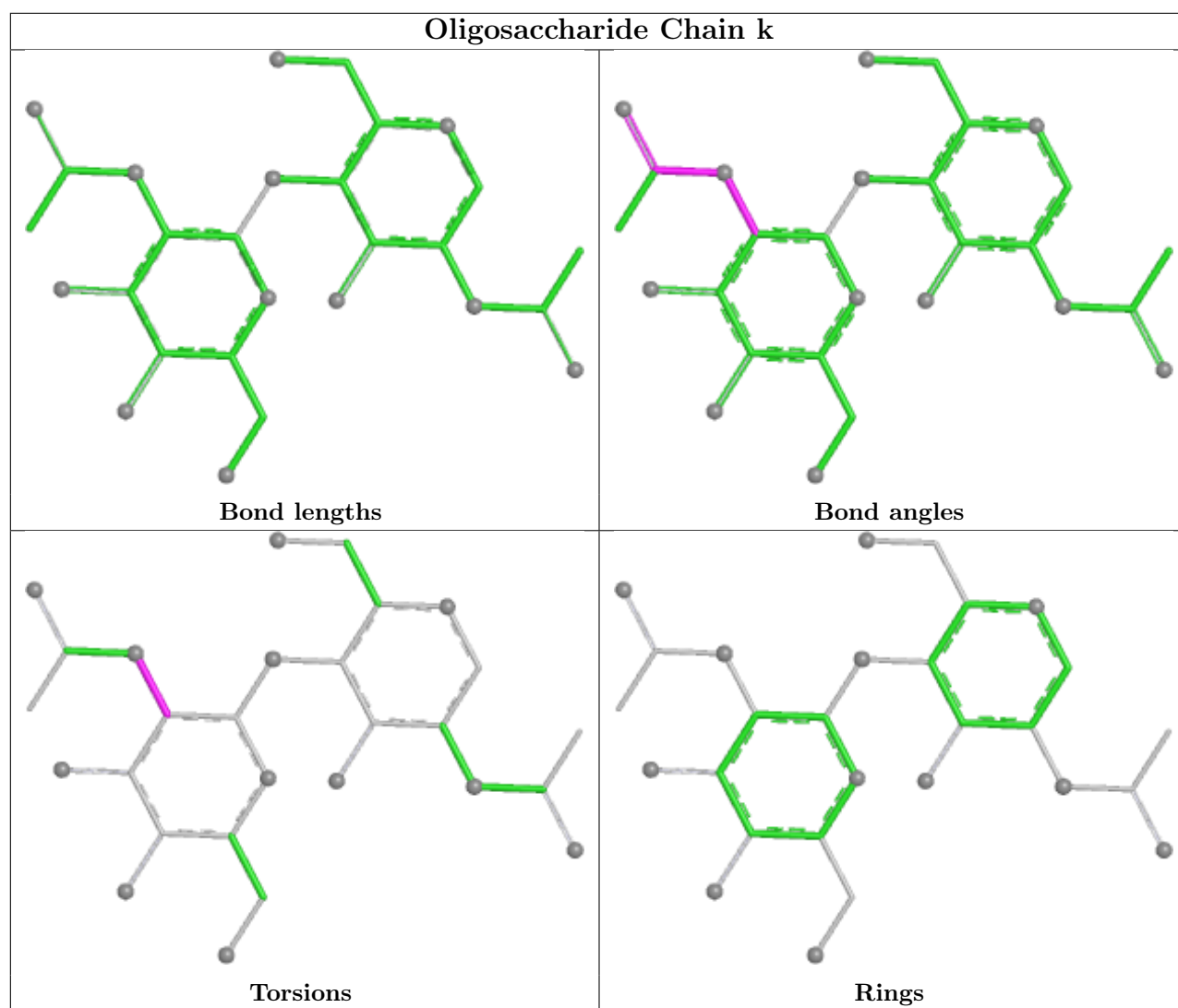


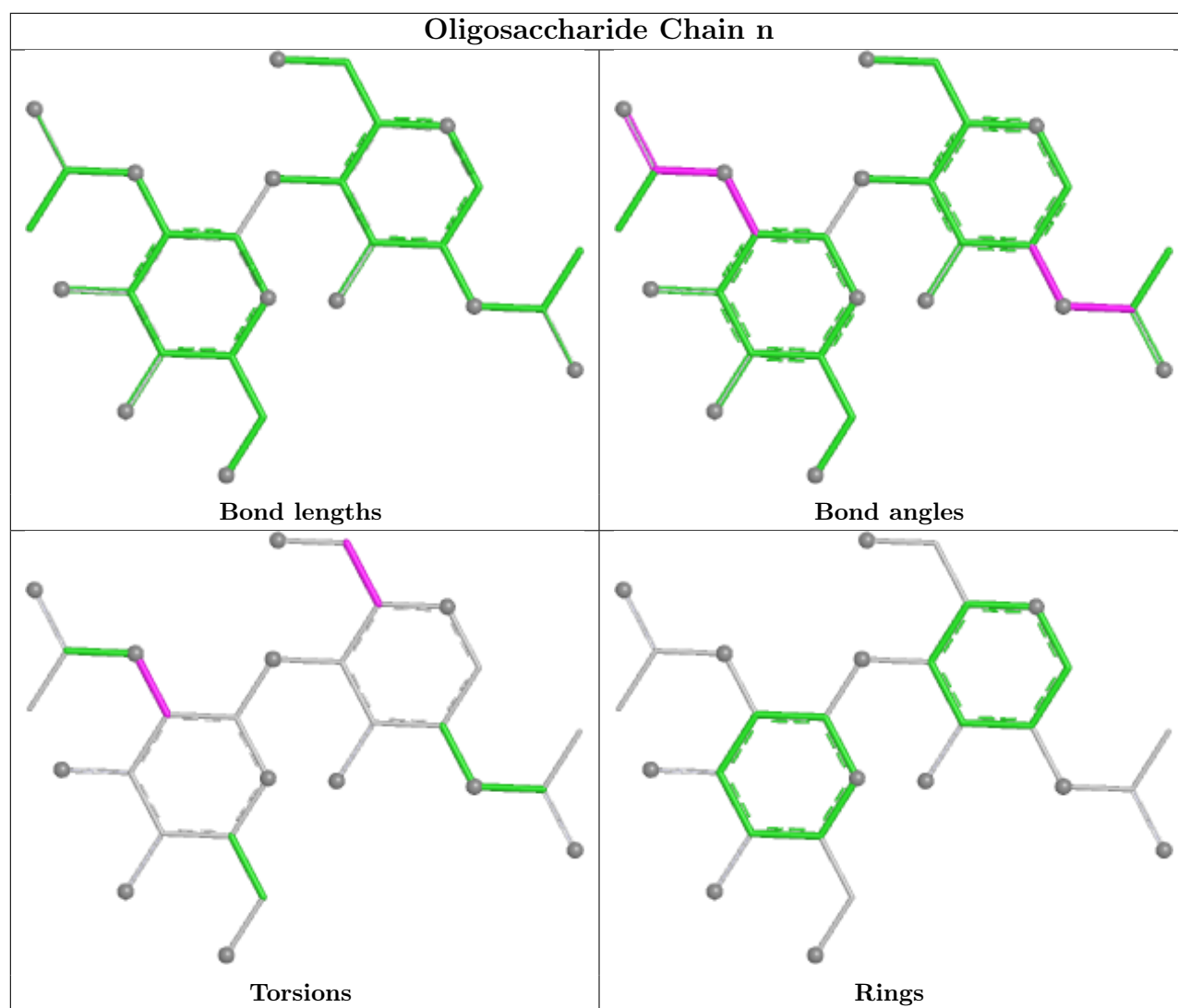


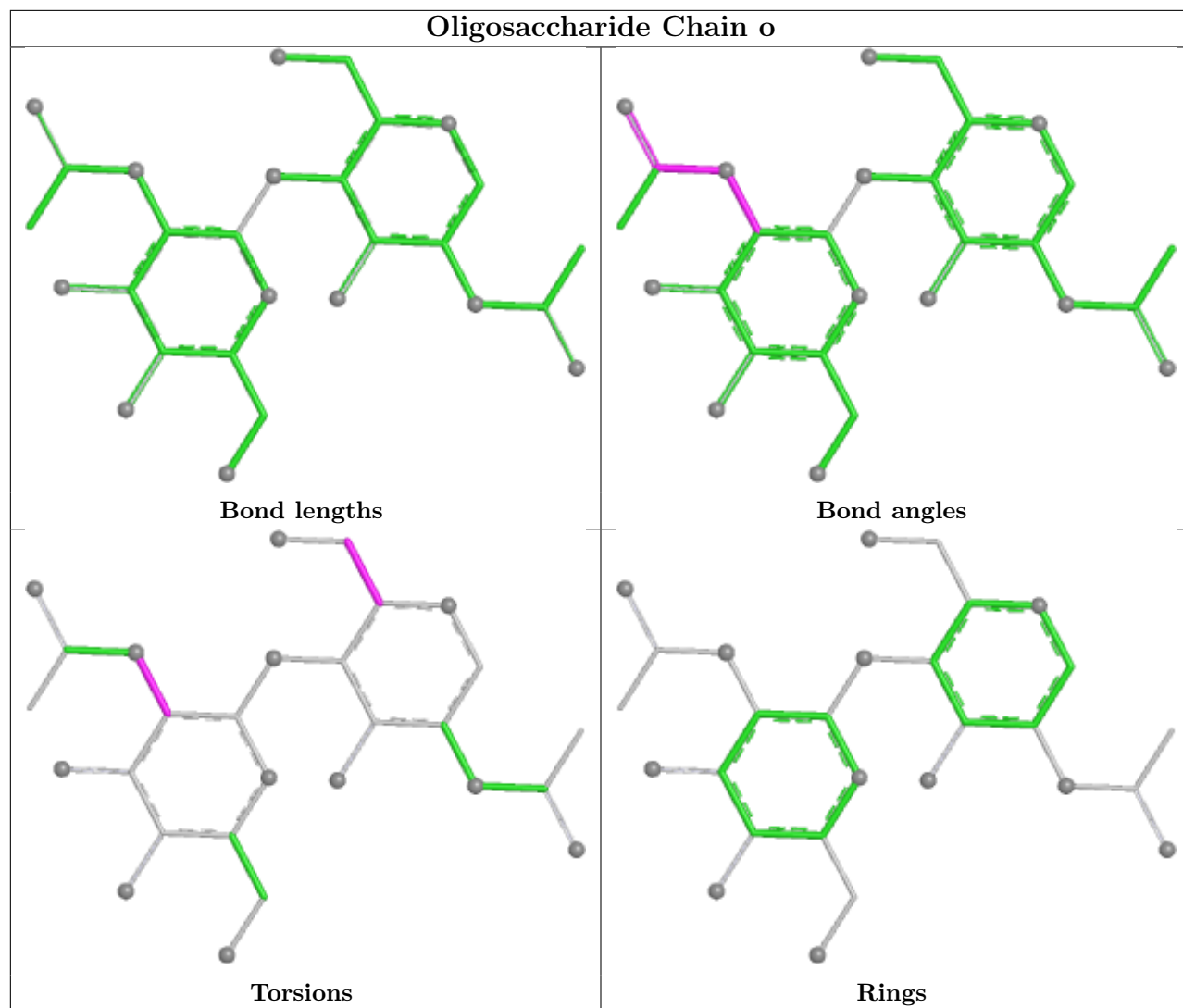


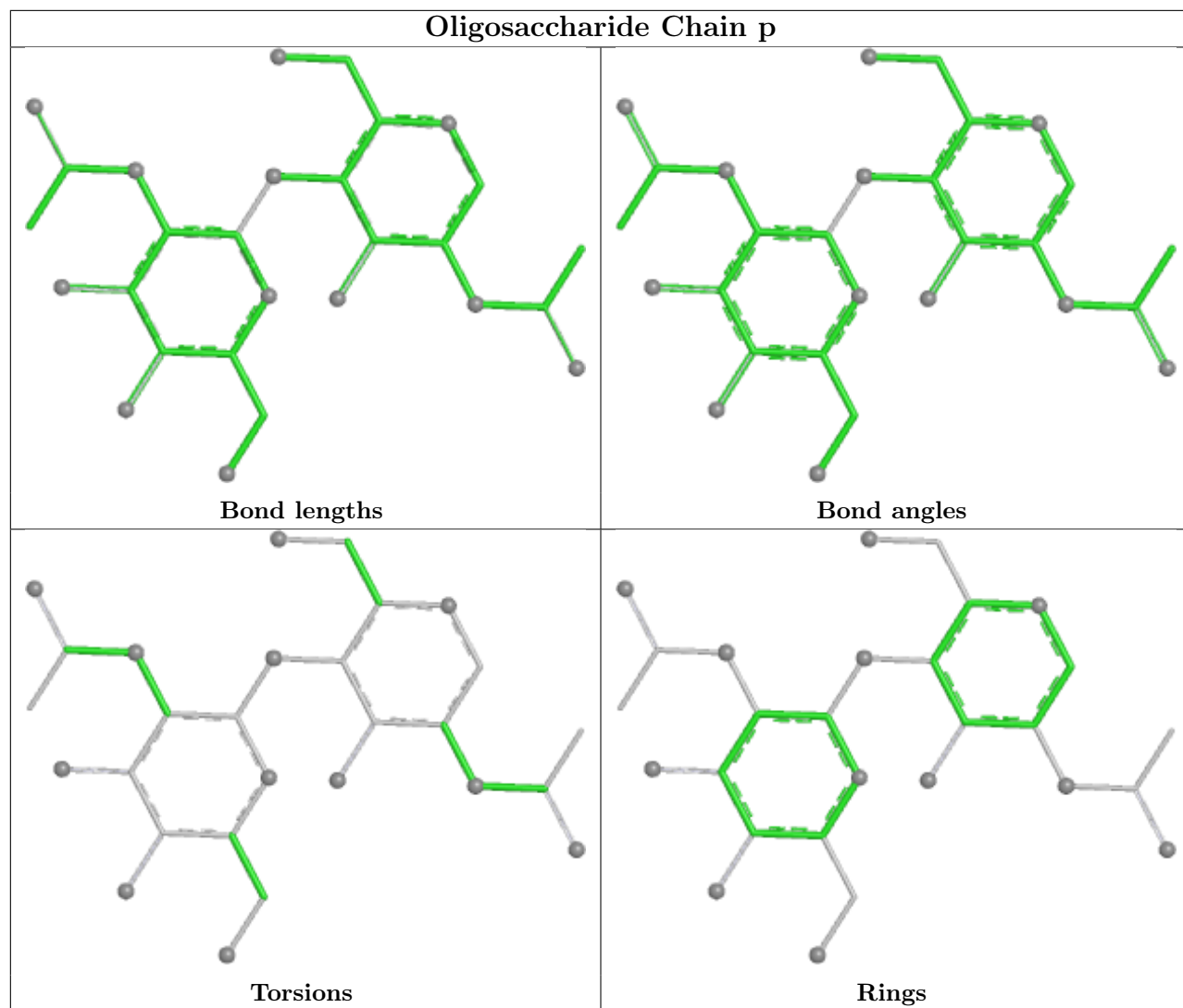




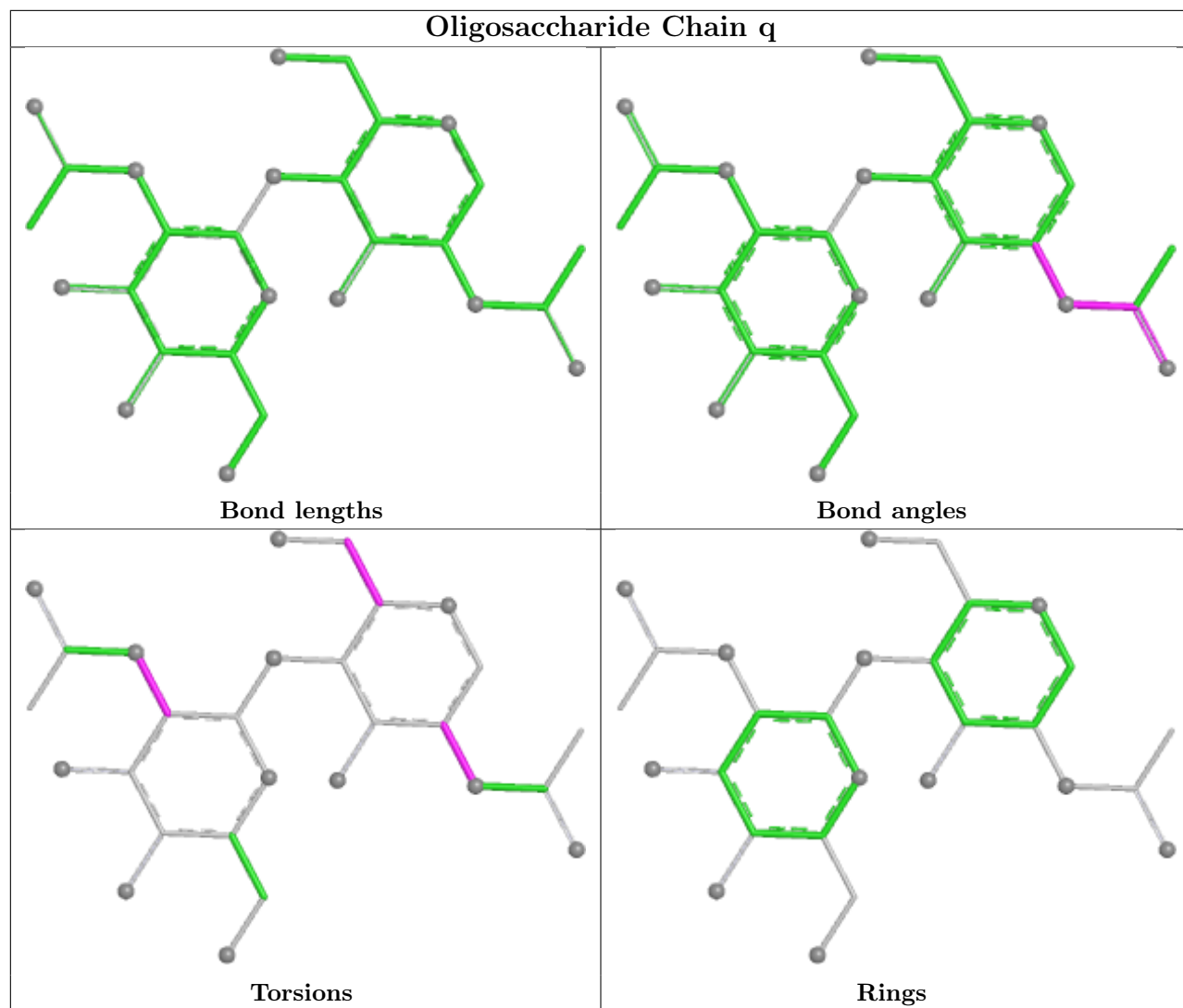


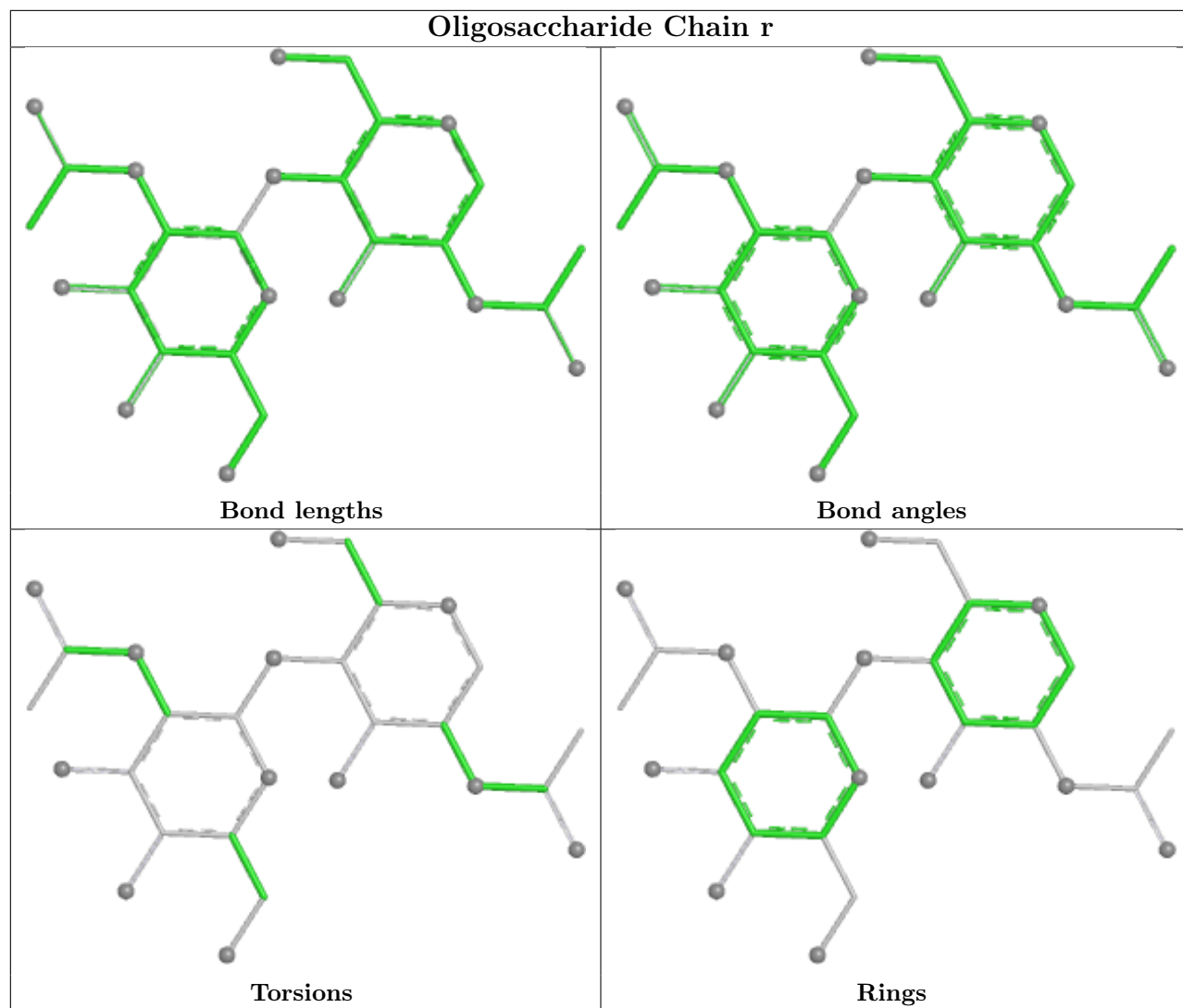


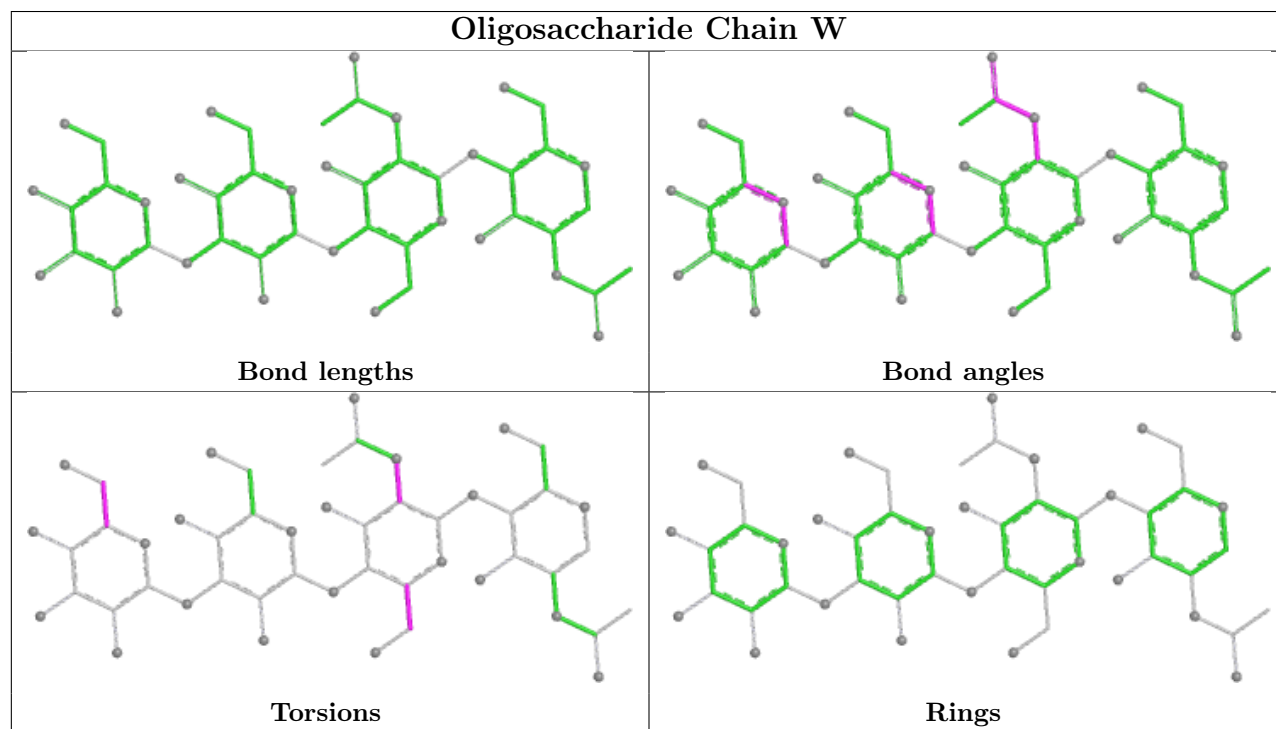
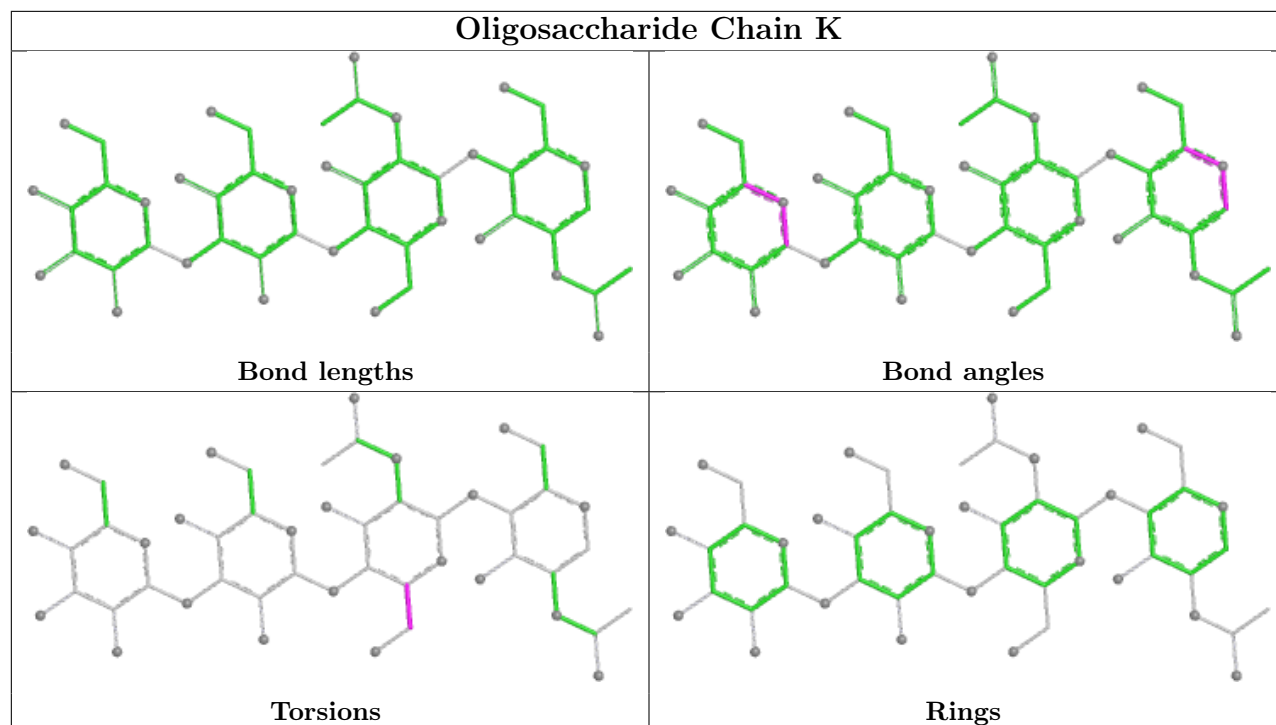


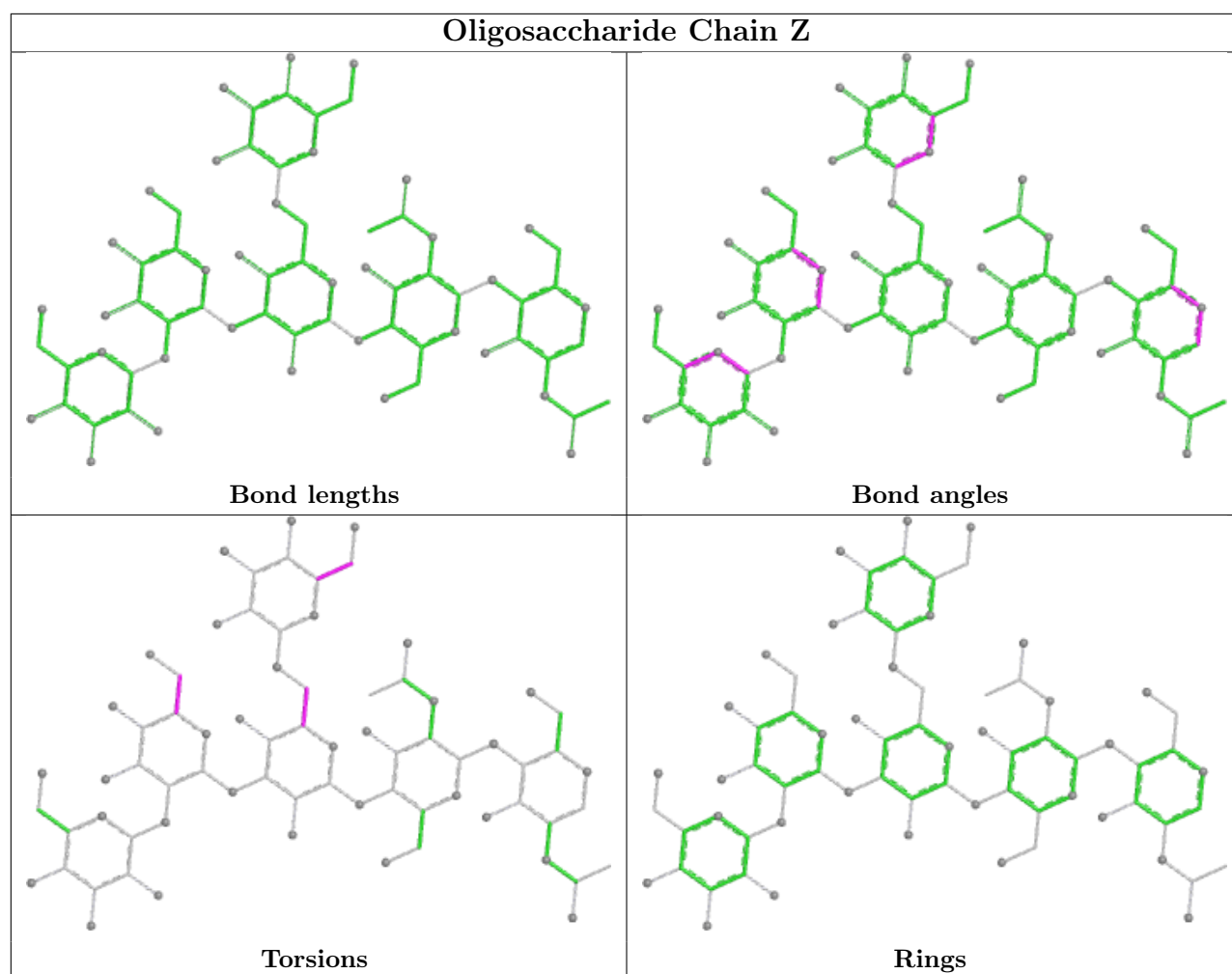


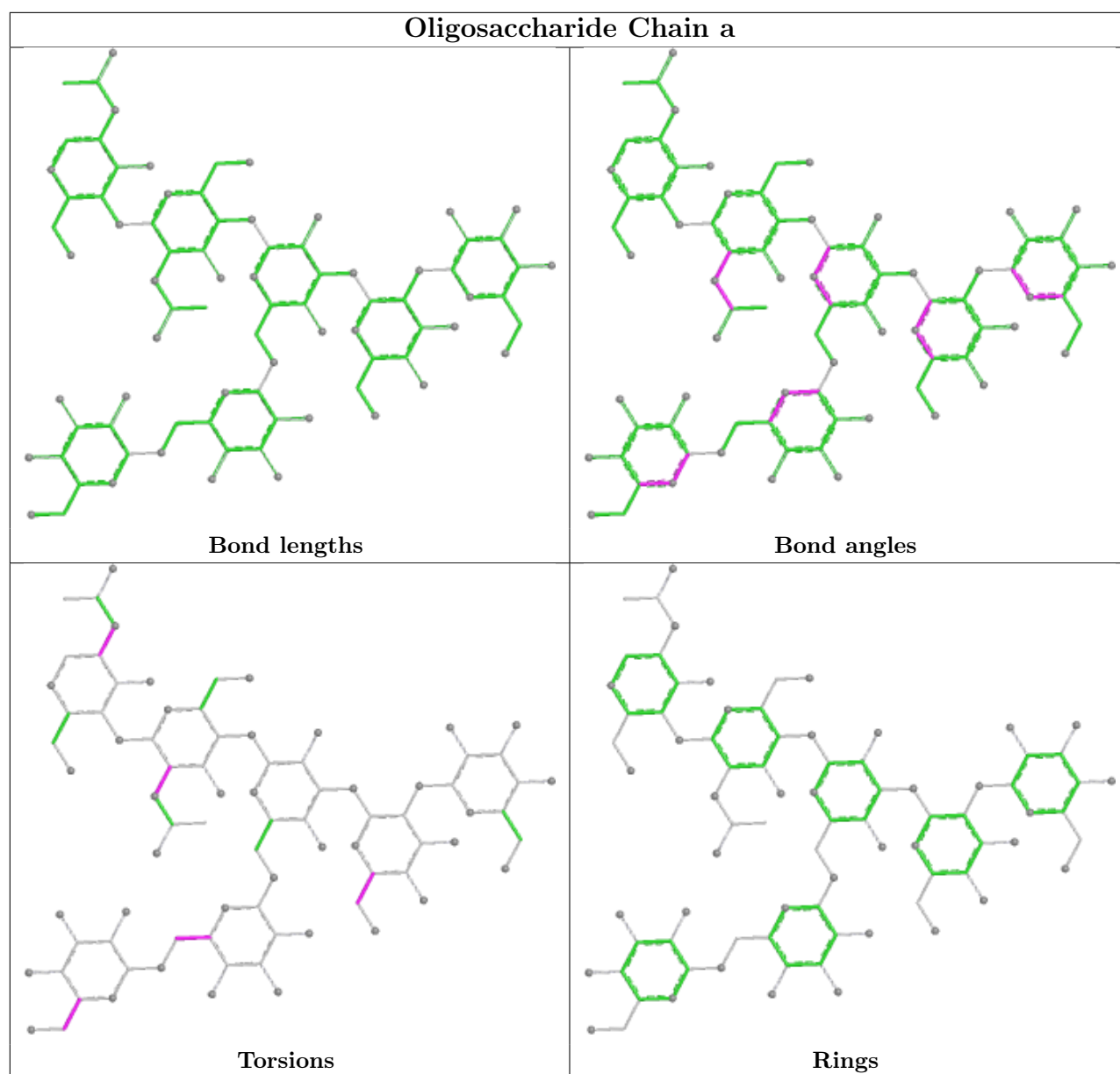


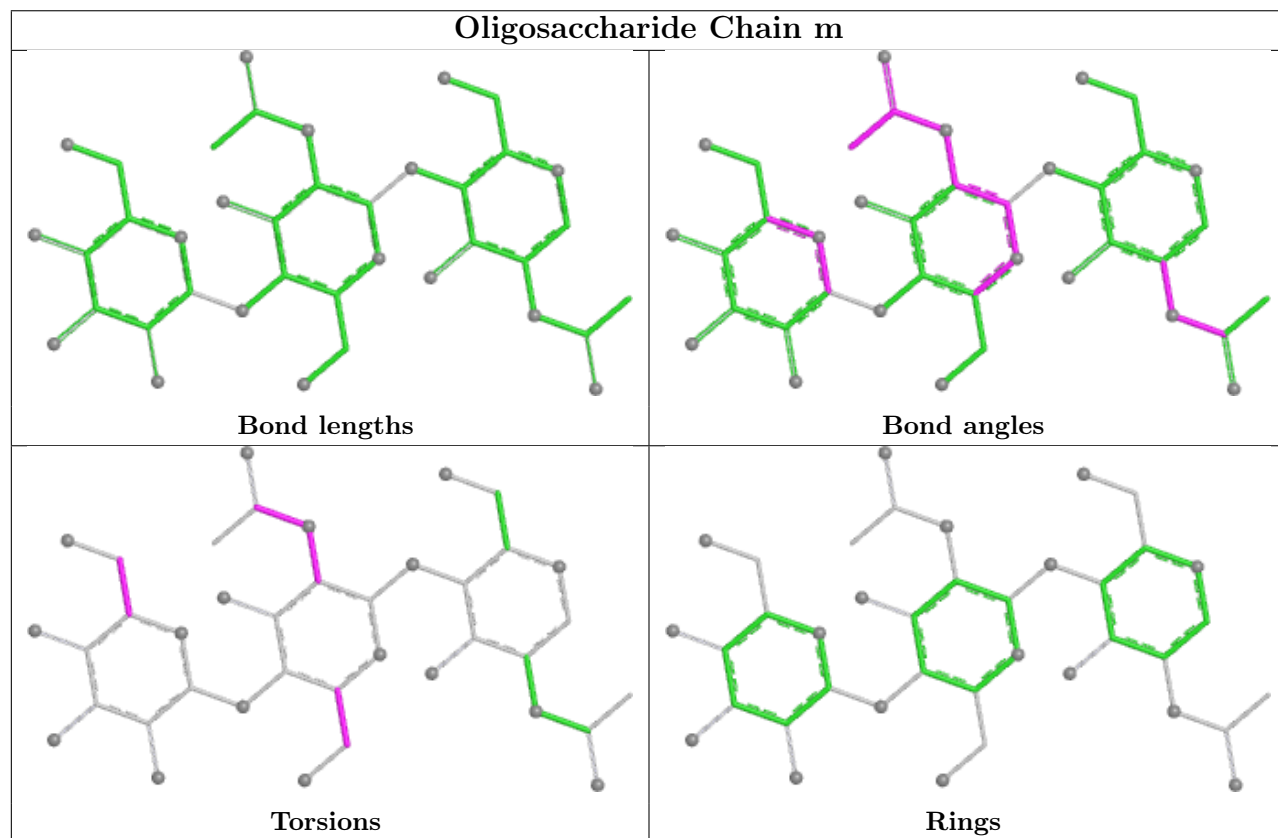
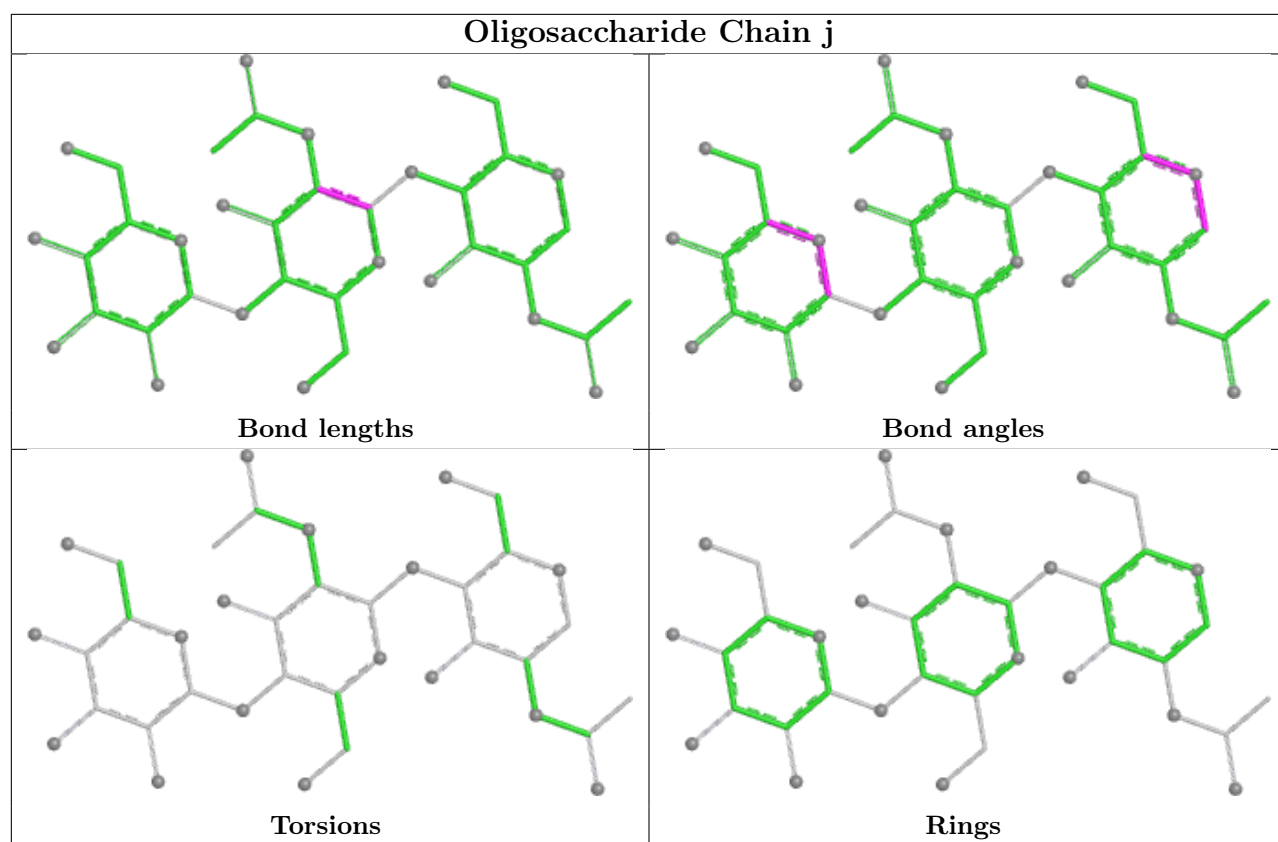


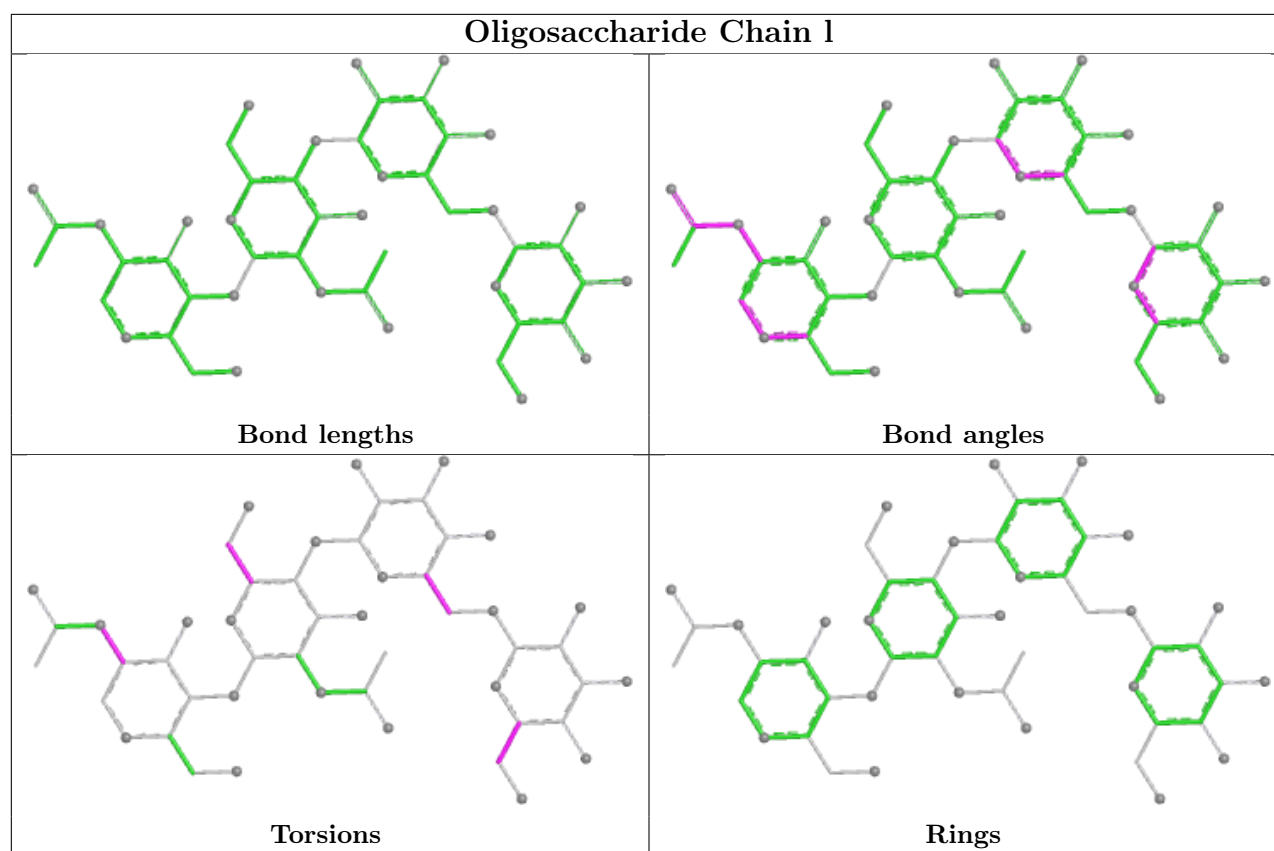












## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	NAG	E	603	1	14,14,15	0.68	0	17,19,21	0.64	0
11	NAG	I	604	1	14,14,15	0.70	0	17,19,21	1.62	3 (17%)
11	NAG	A	605	1	14,14,15	0.75	0	17,19,21	0.80	1 (5%)
11	NAG	I	603	1	14,14,15	0.69	0	17,19,21	0.74	0
11	NAG	A	604	1	14,14,15	0.69	0	17,19,21	0.68	0
11	NAG	A	602	1	14,14,15	0.69	0	17,19,21	0.71	0
11	NAG	I	601	1	14,14,15	0.72	0	17,19,21	0.67	0
11	NAG	J	701	2	14,14,15	0.72	0	17,19,21	1.58	3 (17%)
11	NAG	A	606	1	14,14,15	0.71	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	E	604	1	14,14,15	0.39	0	17,19,21	0.48	0
11	NAG	A	603	1	14,14,15	0.67	0	17,19,21	1.59	2 (11%)
11	NAG	E	602	1	14,14,15	0.70	0	17,19,21	0.78	0
11	NAG	F	701	2	14,14,15	0.69	0	17,19,21	0.74	1 (5%)
11	NAG	E	601	1	14,14,15	0.69	0	17,19,21	0.78	0
11	NAG	J	702	2	14,14,15	0.74	0	17,19,21	0.76	0
11	NAG	I	602	1	14,14,15	0.75	0	17,19,21	1.66	2 (11%)
11	NAG	I	605	1	14,14,15	0.69	0	17,19,21	0.70	0
11	NAG	A	601	1	14,14,15	0.70	0	17,19,21	0.60	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
11	NAG	E	603	1	-	1/6/23/26	0/1/1/1
11	NAG	I	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	605	1	-	2/6/23/26	0/1/1/1
11	NAG	I	603	1	-	0/6/23/26	0/1/1/1
11	NAG	A	604	1	-	0/6/23/26	0/1/1/1
11	NAG	A	602	1	-	1/6/23/26	0/1/1/1
11	NAG	I	601	1	-	0/6/23/26	0/1/1/1
11	NAG	J	701	2	-	4/6/23/26	0/1/1/1
11	NAG	A	606	1	-	0/6/23/26	0/1/1/1
11	NAG	E	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	603	1	-	3/6/23/26	0/1/1/1
11	NAG	E	602	1	-	0/6/23/26	0/1/1/1
11	NAG	F	701	2	-	1/6/23/26	0/1/1/1
11	NAG	E	601	1	-	1/6/23/26	0/1/1/1
11	NAG	J	702	2	-	0/6/23/26	0/1/1/1
11	NAG	I	602	1	-	1/6/23/26	0/1/1/1
11	NAG	I	605	1	-	1/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	604	NAG	C2-N2-C7	5.40	130.13	122.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	603	NAG	C2-N2-C7	5.26	129.95	122.90
11	I	602	NAG	C2-N2-C7	5.00	129.59	122.90
11	J	701	NAG	C2-N2-C7	4.92	129.49	122.90
11	I	602	NAG	C1-O5-C5	3.92	117.44	112.19
11	A	605	NAG	C2-N2-C7	2.62	126.41	122.90
11	J	701	NAG	O7-C7-N2	2.48	126.37	121.98
11	A	603	NAG	O7-C7-N2	2.33	126.11	121.98
11	I	604	NAG	O7-C7-N2	2.30	126.05	121.98
11	J	701	NAG	C1-O5-C5	2.28	115.24	112.19
11	F	701	NAG	C1-O5-C5	2.05	114.93	112.19
11	I	604	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	604	NAG	C8-C7-N2-C2
11	A	605	NAG	O5-C5-C6-O6
11	E	604	NAG	O7-C7-N2-C2
11	E	603	NAG	O5-C5-C6-O6
11	A	605	NAG	C4-C5-C6-O6
11	A	603	NAG	O5-C5-C6-O6
11	E	601	NAG	O5-C5-C6-O6
11	A	601	NAG	C4-C5-C6-O6
11	A	601	NAG	O5-C5-C6-O6
11	A	603	NAG	C1-C2-N2-C7
11	I	604	NAG	C1-C2-N2-C7
11	J	701	NAG	C1-C2-N2-C7
11	J	701	NAG	C4-C5-C6-O6
11	A	603	NAG	C3-C2-N2-C7
11	I	602	NAG	C3-C2-N2-C7
11	I	604	NAG	C3-C2-N2-C7
11	J	701	NAG	C3-C2-N2-C7
11	J	701	NAG	O5-C5-C6-O6
11	A	602	NAG	C1-C2-N2-C7
11	F	701	NAG	C1-C2-N2-C7
11	I	605	NAG	C1-C2-N2-C7

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 [i](#)

There are no chain breaks in this entry.

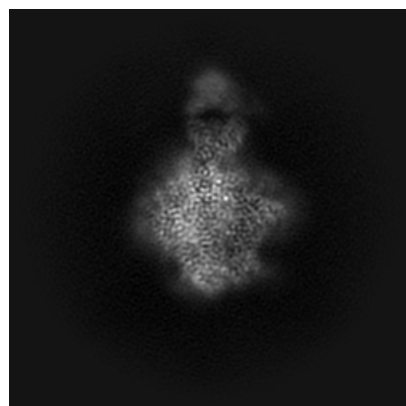
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44733. These allow visual inspection of the internal detail of the map and identification of artifacts.

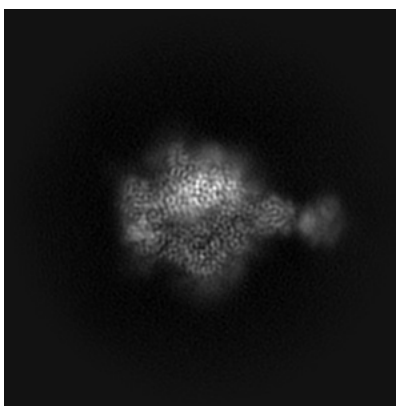
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

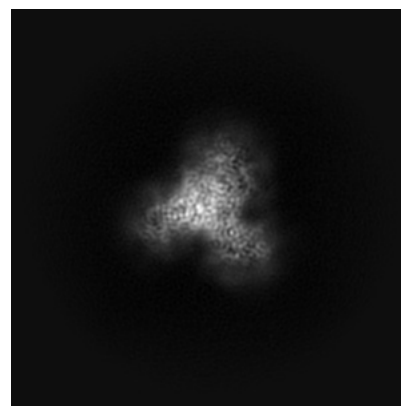
#### 6.1.1 Primary map



X

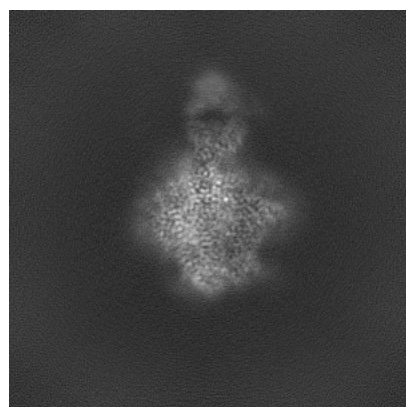


Y

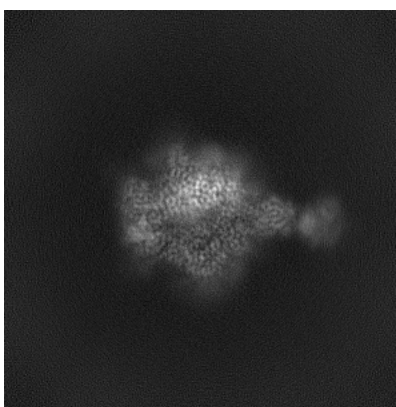


Z

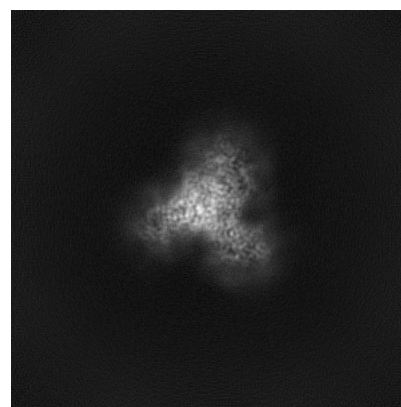
#### 6.1.2 Raw map



X



Y

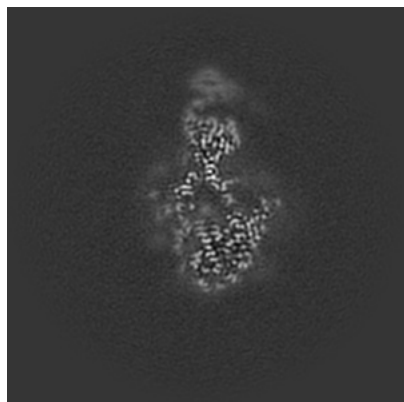


Z

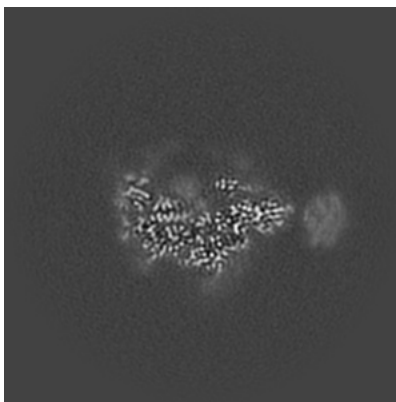
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

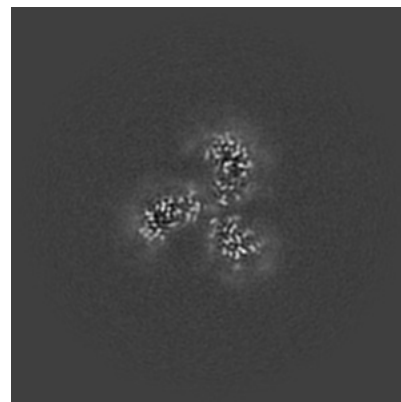
### 6.2.1 Primary map



X Index: 192

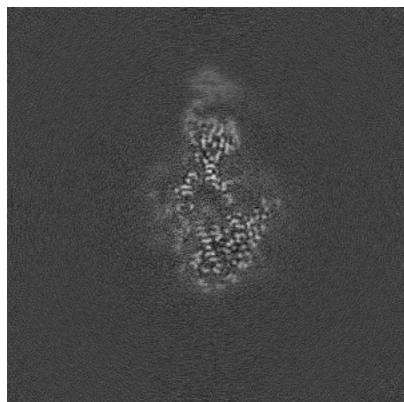


Y Index: 192

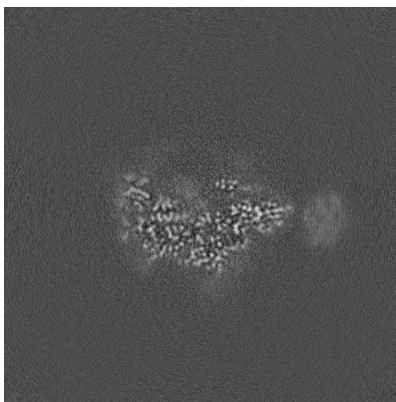


Z Index: 192

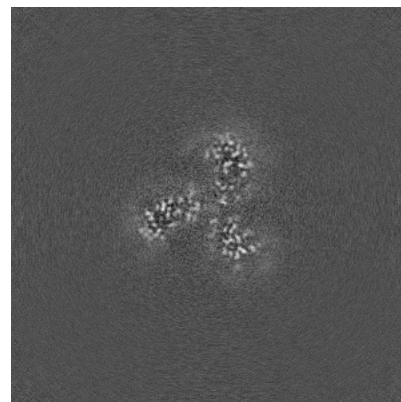
### 6.2.2 Raw map



X Index: 192



Y Index: 192

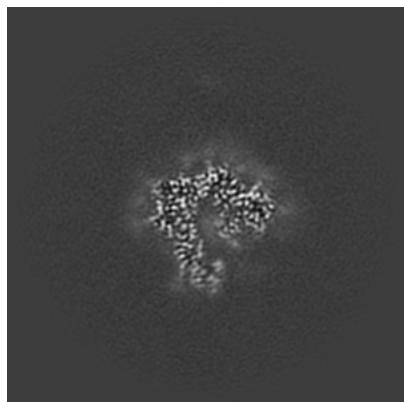


Z Index: 192

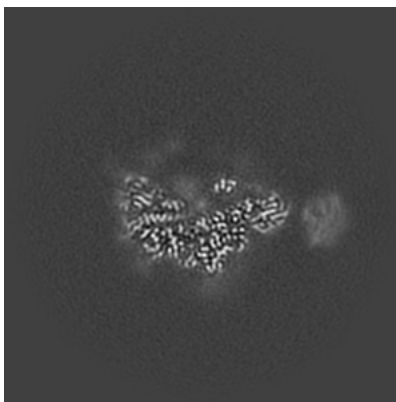
The images above show central slices of the map in three orthogonal directions.

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

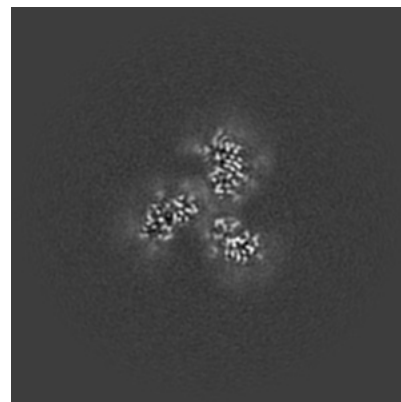
### 6.3.1 Primary map



X Index: 211

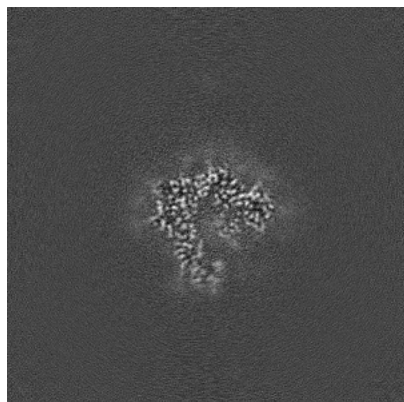


Y Index: 190

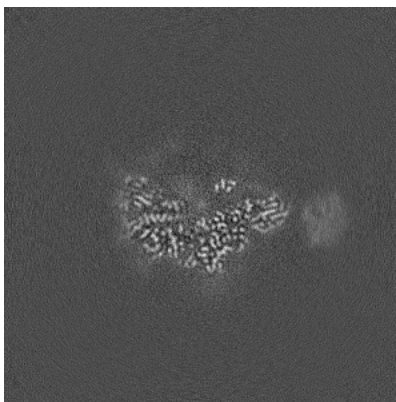


Z Index: 185

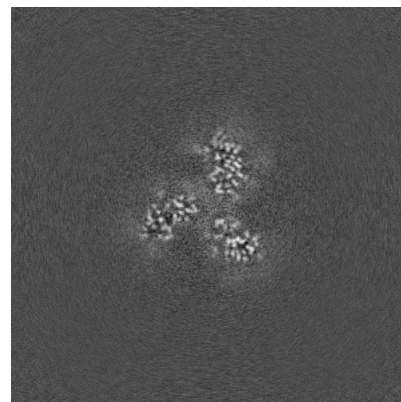
### 6.3.2 Raw map



X Index: 211



Y Index: 190

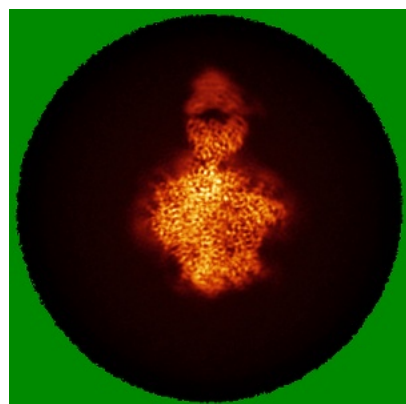


Z Index: 185

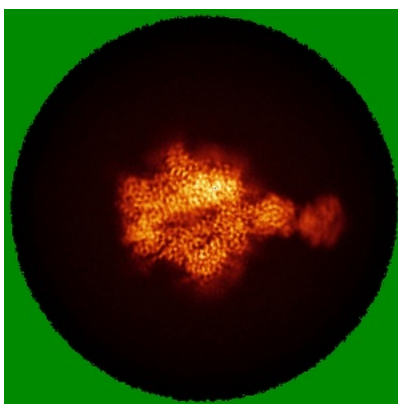
The images above show the largest variance slices of the map in three orthogonal directions.

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

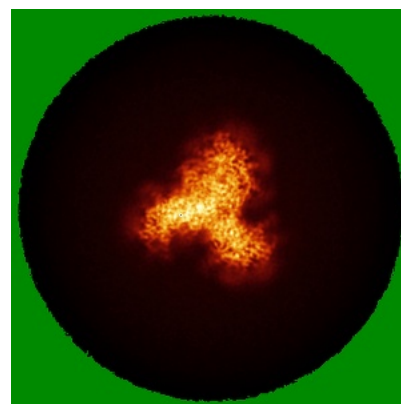
### 6.4.1 Primary map



X

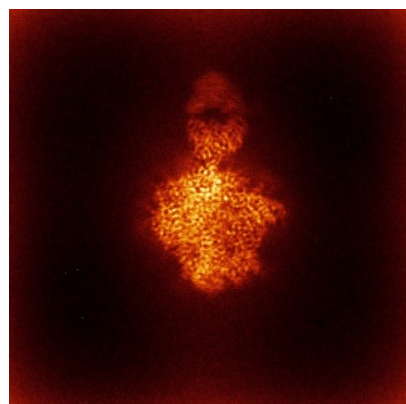


Y

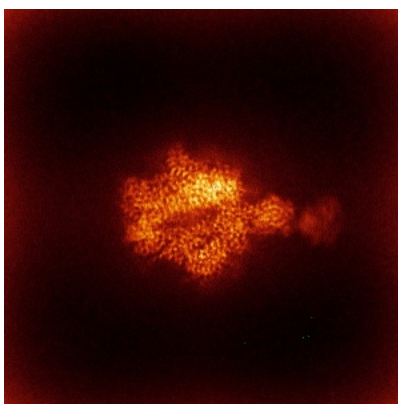


Z

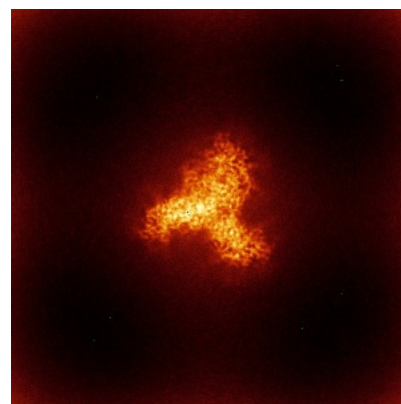
### 6.4.2 Raw map



X



Y



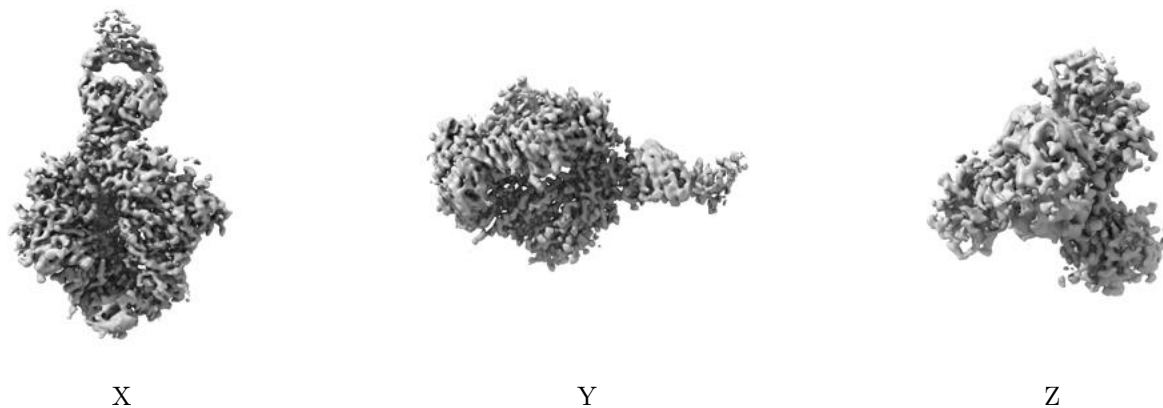
Z

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



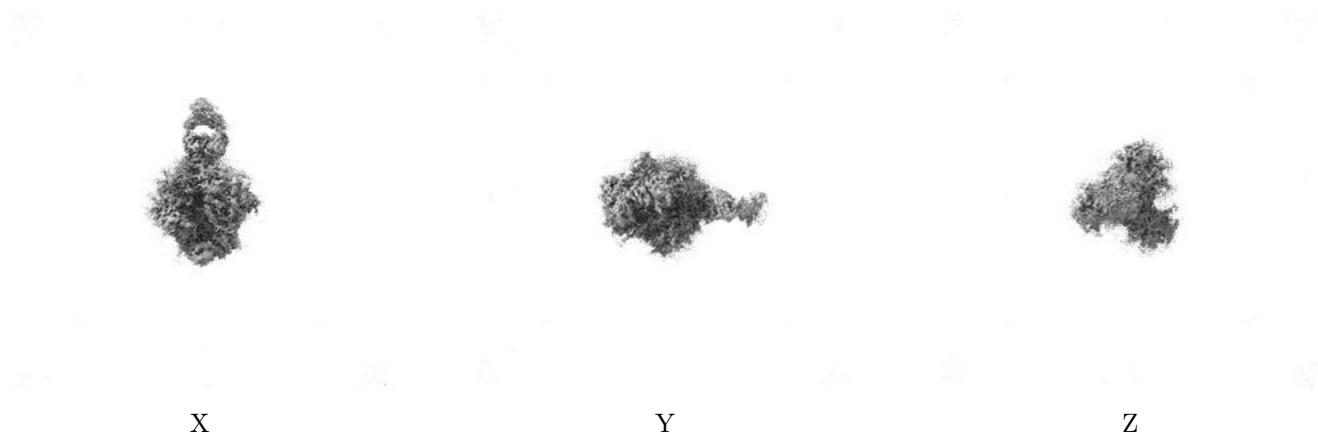
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

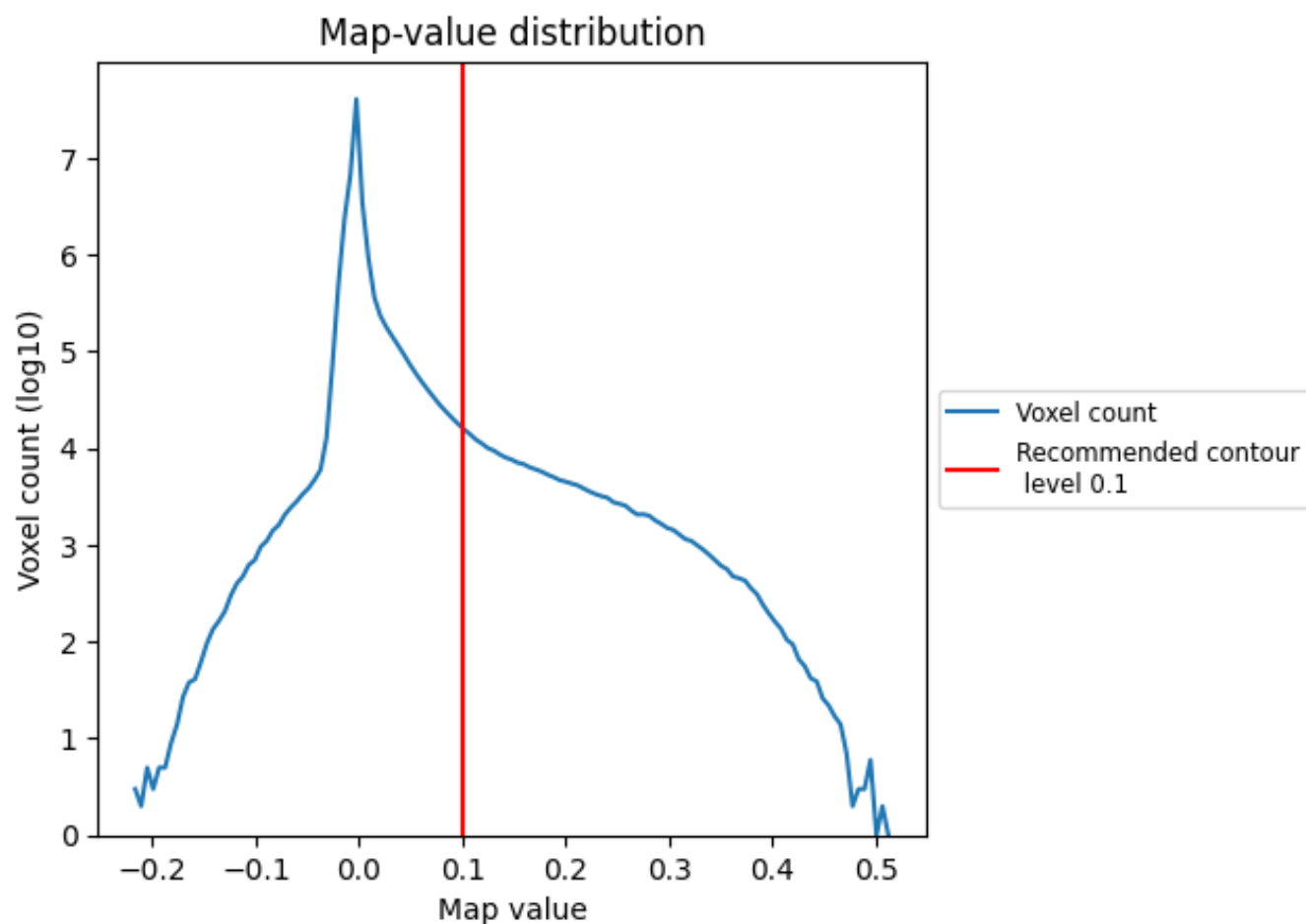
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

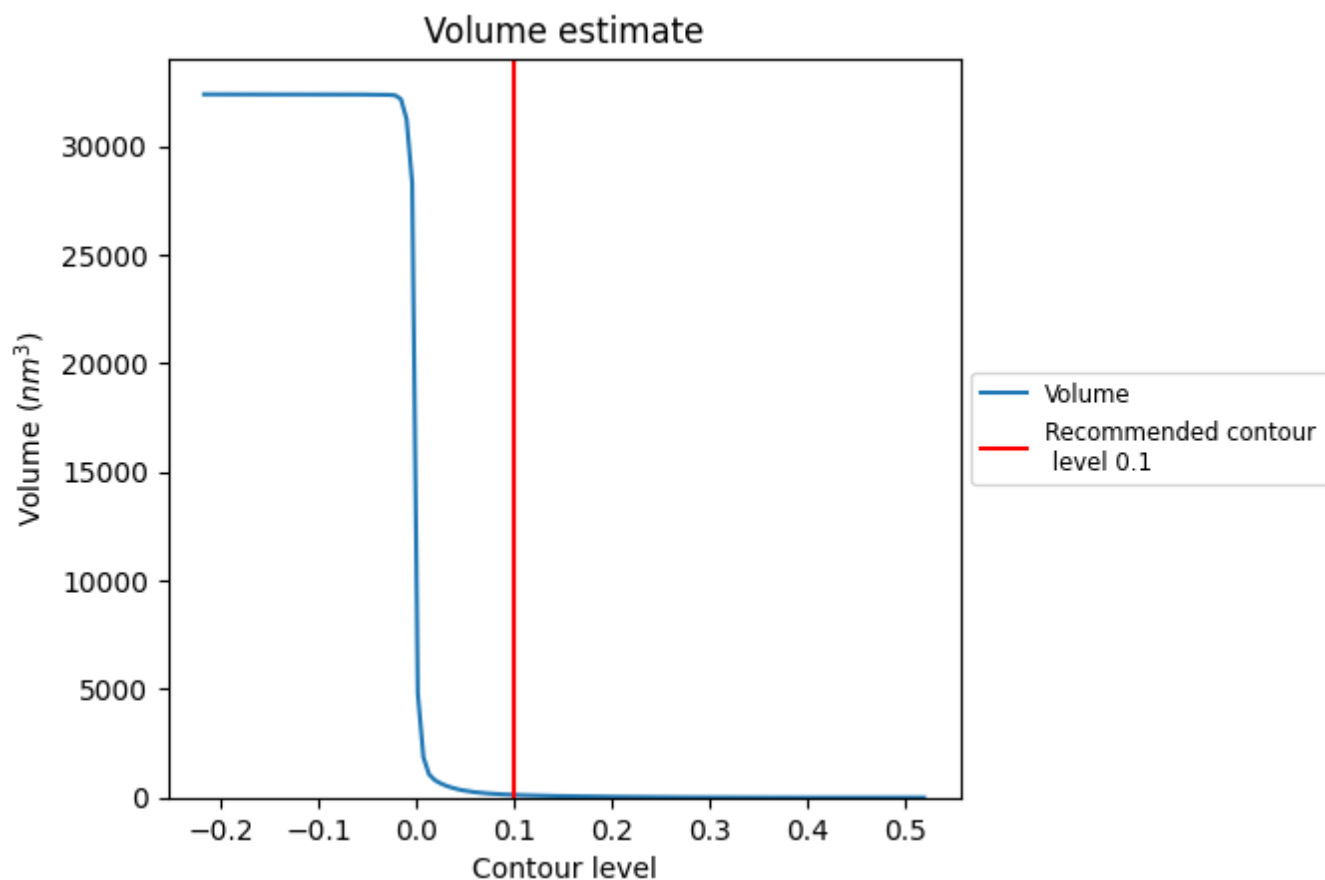
### 7.1 Map-value distribution [i](#)



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



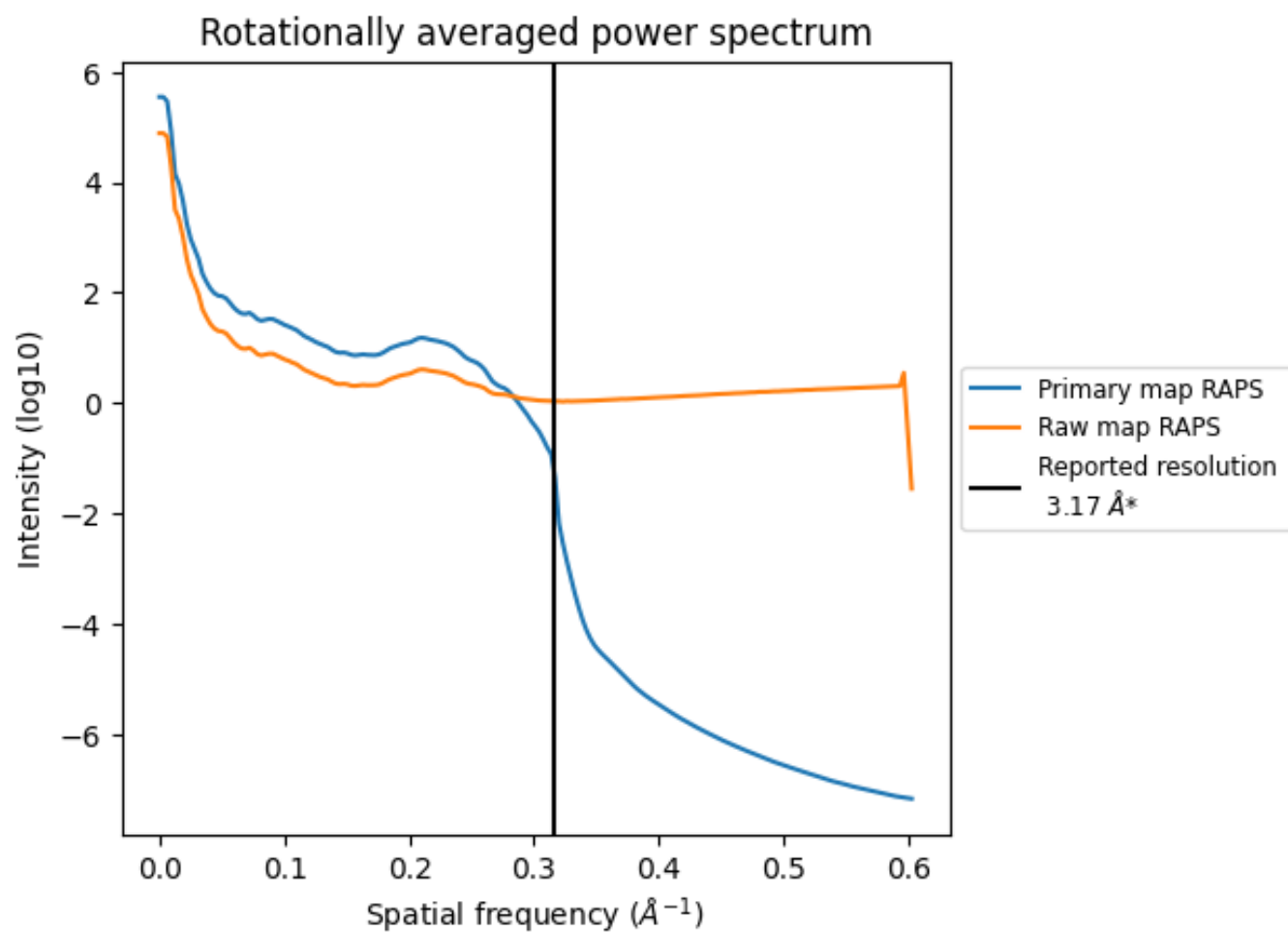
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm<sup>3</sup>; this corresponds to an approximate mass of 110 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 ⓘ

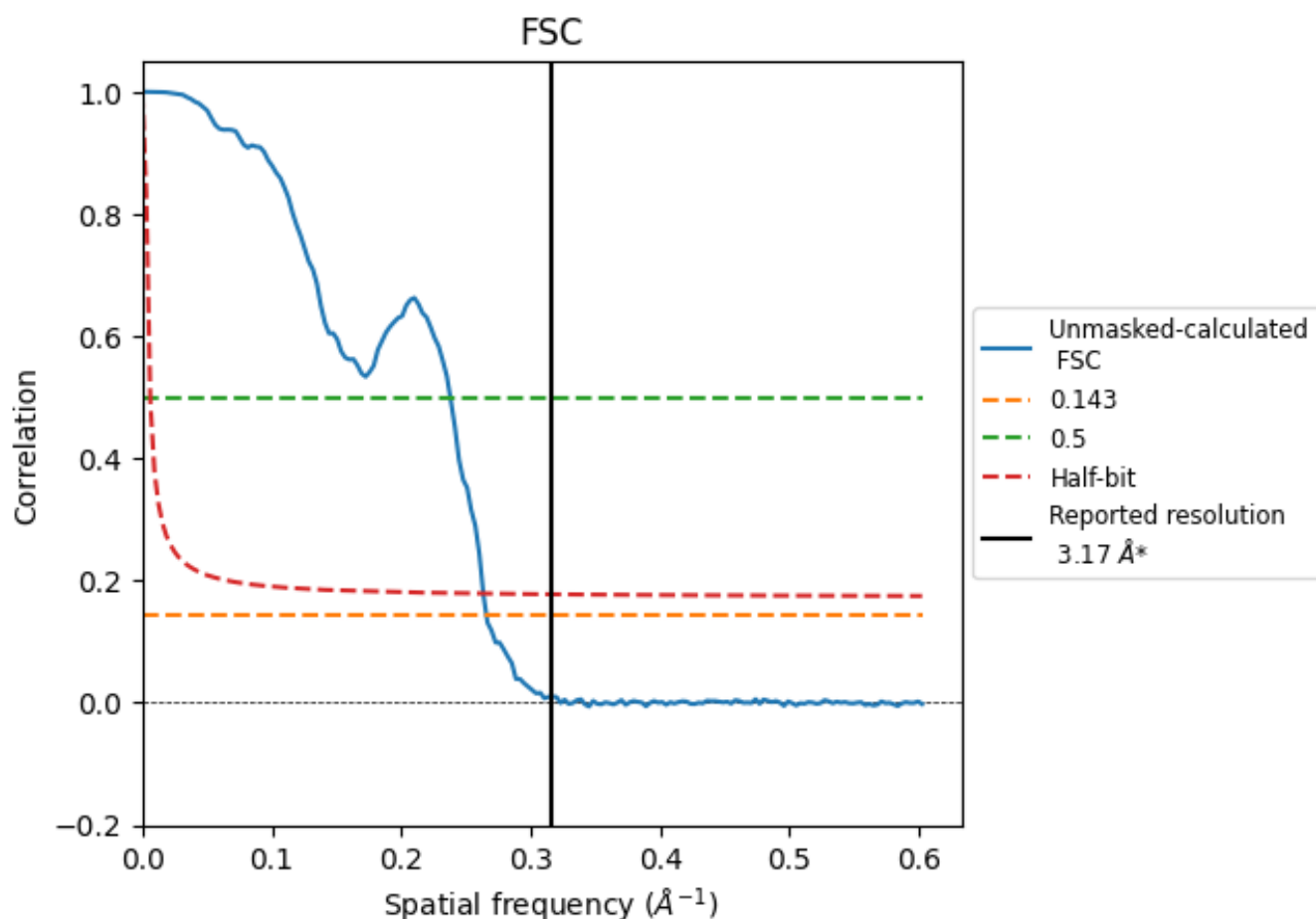


\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.315 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

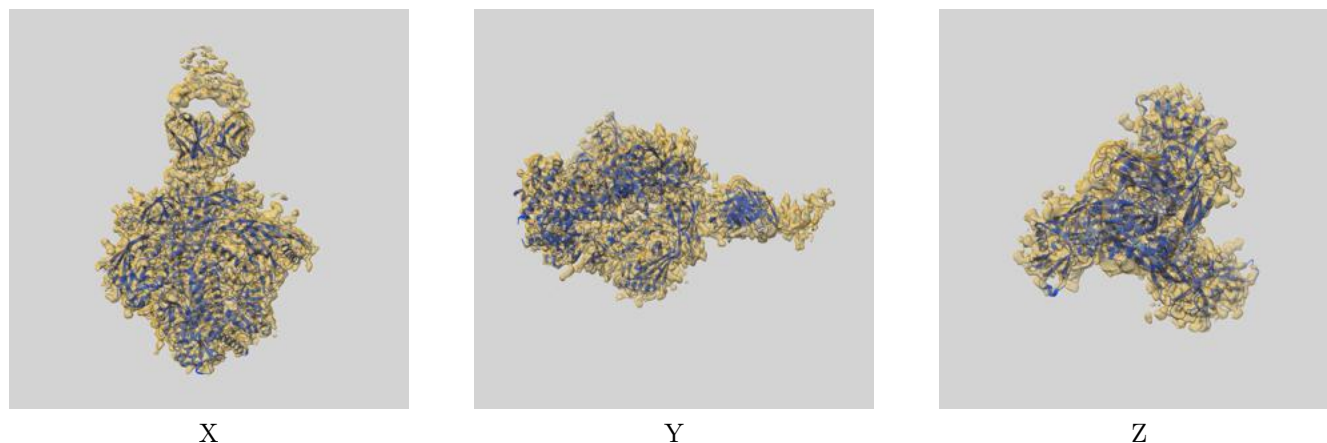
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.20	3.80

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.17 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-44733 and PDB model 9BNP. Per-residue inclusion information can be found in section 3 on page 12.

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



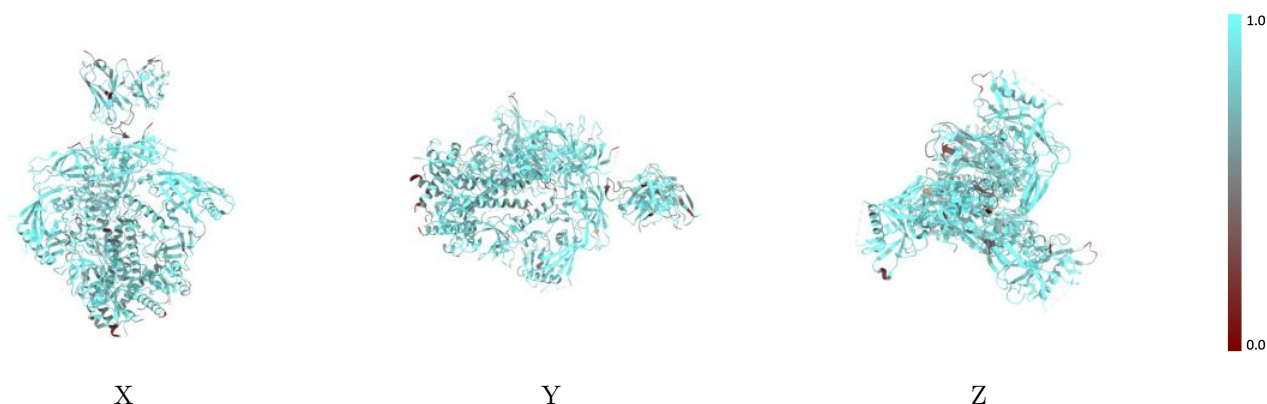
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



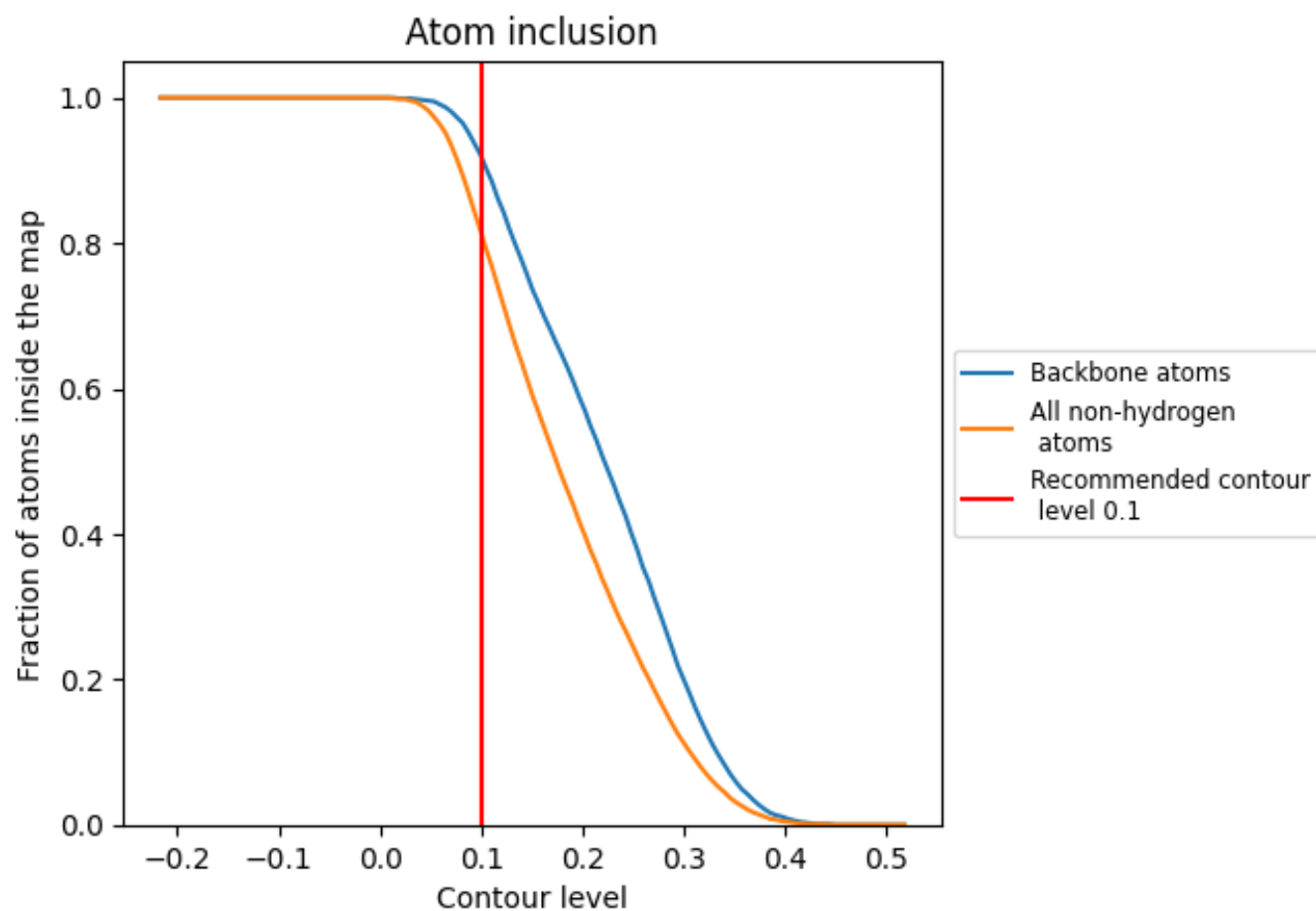
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.1) and Q-score for the entire model and for each chain.





















Chain	Atom inclusion	Q-score
All	 0.8150	 0.4870
A	 0.8340	 0.4970
B	 0.7840	 0.4480
C	 0.6070	 0.4250
D	 0.4290	 0.4400
E	 0.8620	 0.5110
F	 0.7940	 0.4660
G	 0.7500	 0.4620
H	 0.8540	 0.5050
I	 0.8360	 0.4980
J	 0.7940	 0.4560
K	 0.7800	 0.5090
L	 0.7650	 0.4530
M	 0.5000	 0.3650
N	 0.1430	 0.2630
O	 0.6070	 0.4130
P	 0.6070	 0.4410
Q	 0.7860	 0.4740
R	 0.4290	 0.4010
S	 0.7500	 0.5050
T	 0.7140	 0.3720
U	 0.4290	 0.4570
V	 0.6790	 0.4320
W	 0.8800	 0.4830
X	 0.5710	 0.3670
Y	 0.6430	 0.4300
Z	 0.5830	 0.4220
a	 0.8430	 0.4840
b	 0.3930	 0.4460
c	 0.5710	 0.3840
d	 0.8570	 0.5360
e	 0.5710	 0.4590
f	 0.6430	 0.4190
g	 0.6790	 0.3600
h	 0.5710	 0.4530



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Chain	Atom inclusion	Q-score
i	 0.7140	 0.4400
j	 0.8970	 0.5300
k	 0.6790	 0.4800
l	 0.5800	 0.3760
m	 0.5640	 0.4510
n	 0.3210	 0.4340
o	 0.3570	 0.3670
p	 0.7860	 0.4870
q	 0.5360	 0.4180
r	 0.4640	 0.3730