



## wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 12:00 AM JST

PDB ID : 7CT5  
EMDB ID : EMD-30460  
Title : S protein of SARS-CoV-2 in complex bound with T-ACE2  
Authors : Guo, L.; Bi, W.W.; Zhang, Y.Y.; Yan, R.H.; Li, Y.N.; Zhou, Q.; Dang, B.B.  
Deposited on : 2020-08-18  
Resolution : 4.00 Å (reported)

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

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

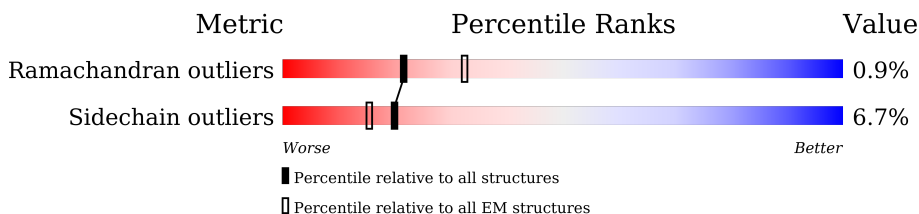
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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







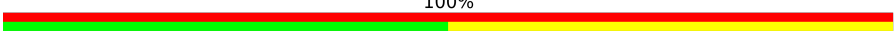

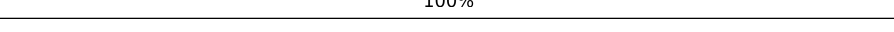




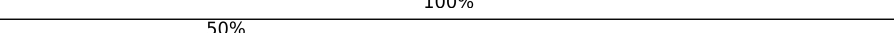




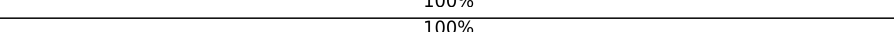

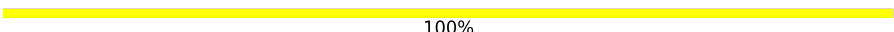

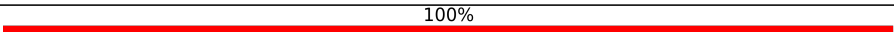
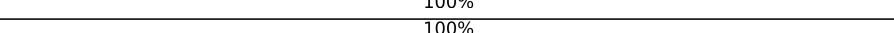
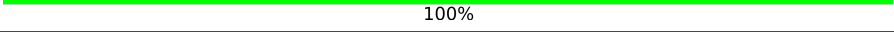


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1283	
1	B	1283	
1	C	1283	
2	D	655	
2	E	655	
2	F	655	
3	G	2	
3	H	2	
3	I	2	


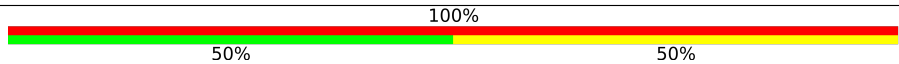
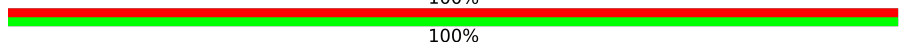
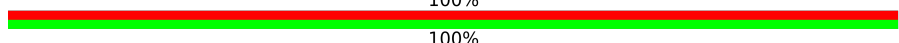
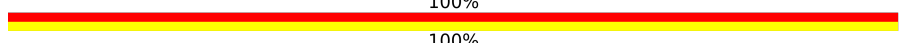
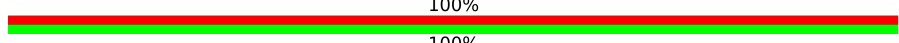

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Mol	Chain	Length	Quality of chain
3	J	2	 50% 50%
3	K	2	 50% 100%
3	L	2	 50% 50%
3	M	2	 50% 50%
3	N	2	 100% 50%
3	O	2	 50% 100%
3	P	2	 50% 50%
3	Q	2	 50% 50%
3	R	2	 50% 50%
3	S	2	 100%
3	T	2	 50% 50%
3	U	2	 50% 50%
3	V	2	 50% 50%
3	W	2	 100%
3	X	2	 100% 50%
3	Y	2	 100%
3	Z	2	 100%
3	a	2	 100% 100%
3	b	2	 100% 100%
3	c	2	 100% 100%
3	d	2	 100% 100%
3	e	2	 50% 100% 50%
3	f	2	 100% 100%
3	g	2	 100% 100%
3	h	2	 100% 100%

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Mol	Chain	Length	Quality of chain
3	i	2	100% 
3	j	2	100% 
3	k	2	100% 
3	l	2	100% 
3	m	2	100% 
3	n	2	100% 
3	o	2	100% 

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 39626 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1006	7863	5019	1308	1500	36	0	0
1	B	1007	7870	5023	1310	1501	36	0	0
1	C	1006	7866	5022	1309	1499	36	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	595	4857	3108	804	916	29	0	0
2	E	595	4857	3108	804	916	29	0	0
2	F	595	4857	3108	804	916	29	0	0

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	GLY	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	GLU	-	expression tag	UNP Q9BYF1
D	619	ALA	-	expression tag	UNP Q9BYF1
D	620	ALA	-	expression tag	UNP Q9BYF1
D	621	ALA	-	expression tag	UNP Q9BYF1
D	622	LYS	-	expression tag	UNP Q9BYF1
D	623	GLU	-	expression tag	UNP Q9BYF1
D	624	ALA	-	expression tag	UNP Q9BYF1
D	625	ALA	-	expression tag	UNP Q9BYF1
D	626	ALA	-	expression tag	UNP Q9BYF1
D	627	LYS	-	expression tag	UNP Q9BYF1
D	628	GLU	-	expression tag	UNP Q9BYF1
D	629	ALA	-	expression tag	UNP Q9BYF1
D	630	ALA	-	expression tag	UNP Q9BYF1
D	631	ALA	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	632	LYS	-	expression tag	UNP Q9BYF1
D	633	GLU	-	expression tag	UNP Q9BYF1
D	634	ALA	-	expression tag	UNP Q9BYF1
D	635	ALA	-	expression tag	UNP Q9BYF1
D	636	ALA	-	expression tag	UNP Q9BYF1
D	637	LYS	-	expression tag	UNP Q9BYF1
D	638	GLU	-	expression tag	UNP Q9BYF1
D	639	ALA	-	expression tag	UNP Q9BYF1
D	640	ALA	-	expression tag	UNP Q9BYF1
D	641	ALA	-	expression tag	UNP Q9BYF1
D	642	LYS	-	expression tag	UNP Q9BYF1
D	643	GLY	-	expression tag	UNP Q9BYF1
D	644	SER	-	expression tag	UNP Q9BYF1
D	645	GLY	-	expression tag	UNP Q9BYF1
D	646	TYR	-	expression tag	UNP Q9BYF1
D	647	ILE	-	expression tag	UNP Q9BYF1
D	648	PRO	-	expression tag	UNP Q9BYF1
D	649	GLU	-	expression tag	UNP Q9BYF1
D	650	ALA	-	expression tag	UNP Q9BYF1
D	651	PRO	-	expression tag	UNP Q9BYF1
D	652	ARG	-	expression tag	UNP Q9BYF1
D	653	ASP	-	expression tag	UNP Q9BYF1
D	654	GLY	-	expression tag	UNP Q9BYF1
D	655	GLN	-	expression tag	UNP Q9BYF1
D	656	ALA	-	expression tag	UNP Q9BYF1
D	657	TYR	-	expression tag	UNP Q9BYF1
D	658	VAL	-	expression tag	UNP Q9BYF1
D	659	ARG	-	expression tag	UNP Q9BYF1
D	660	LYS	-	expression tag	UNP Q9BYF1
D	661	ASP	-	expression tag	UNP Q9BYF1
D	662	GLY	-	expression tag	UNP Q9BYF1
D	663	GLU	-	expression tag	UNP Q9BYF1
D	664	TRP	-	expression tag	UNP Q9BYF1
D	665	VAL	-	expression tag	UNP Q9BYF1
D	666	LEU	-	expression tag	UNP Q9BYF1
D	667	LEU	-	expression tag	UNP Q9BYF1
D	668	SER	-	expression tag	UNP Q9BYF1
D	669	THR	-	expression tag	UNP Q9BYF1
D	670	PHE	-	expression tag	UNP Q9BYF1
D	671	LEU	-	expression tag	UNP Q9BYF1
D	672	GLY	-	expression tag	UNP Q9BYF1
D	673	SER	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	616	GLY	-	expression tag	UNP Q9BYF1
E	617	SER	-	expression tag	UNP Q9BYF1
E	618	GLU	-	expression tag	UNP Q9BYF1
E	619	ALA	-	expression tag	UNP Q9BYF1
E	620	ALA	-	expression tag	UNP Q9BYF1
E	621	ALA	-	expression tag	UNP Q9BYF1
E	622	LYS	-	expression tag	UNP Q9BYF1
E	623	GLU	-	expression tag	UNP Q9BYF1
E	624	ALA	-	expression tag	UNP Q9BYF1
E	625	ALA	-	expression tag	UNP Q9BYF1
E	626	ALA	-	expression tag	UNP Q9BYF1
E	627	LYS	-	expression tag	UNP Q9BYF1
E	628	GLU	-	expression tag	UNP Q9BYF1
E	629	ALA	-	expression tag	UNP Q9BYF1
E	630	ALA	-	expression tag	UNP Q9BYF1
E	631	ALA	-	expression tag	UNP Q9BYF1
E	632	LYS	-	expression tag	UNP Q9BYF1
E	633	GLU	-	expression tag	UNP Q9BYF1
E	634	ALA	-	expression tag	UNP Q9BYF1
E	635	ALA	-	expression tag	UNP Q9BYF1
E	636	ALA	-	expression tag	UNP Q9BYF1
E	637	LYS	-	expression tag	UNP Q9BYF1
E	638	GLU	-	expression tag	UNP Q9BYF1
E	639	ALA	-	expression tag	UNP Q9BYF1
E	640	ALA	-	expression tag	UNP Q9BYF1
E	641	ALA	-	expression tag	UNP Q9BYF1
E	642	LYS	-	expression tag	UNP Q9BYF1
E	643	GLY	-	expression tag	UNP Q9BYF1
E	644	SER	-	expression tag	UNP Q9BYF1
E	645	GLY	-	expression tag	UNP Q9BYF1
E	646	TYR	-	expression tag	UNP Q9BYF1
E	647	ILE	-	expression tag	UNP Q9BYF1
E	648	PRO	-	expression tag	UNP Q9BYF1
E	649	GLU	-	expression tag	UNP Q9BYF1
E	650	ALA	-	expression tag	UNP Q9BYF1
E	651	PRO	-	expression tag	UNP Q9BYF1
E	652	ARG	-	expression tag	UNP Q9BYF1
E	653	ASP	-	expression tag	UNP Q9BYF1
E	654	GLY	-	expression tag	UNP Q9BYF1
E	655	GLN	-	expression tag	UNP Q9BYF1
E	656	ALA	-	expression tag	UNP Q9BYF1
E	657	TYR	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	658	VAL	-	expression tag	UNP Q9BYF1
E	659	ARG	-	expression tag	UNP Q9BYF1
E	660	LYS	-	expression tag	UNP Q9BYF1
E	661	ASP	-	expression tag	UNP Q9BYF1
E	662	GLY	-	expression tag	UNP Q9BYF1
E	663	GLU	-	expression tag	UNP Q9BYF1
E	664	TRP	-	expression tag	UNP Q9BYF1
E	665	VAL	-	expression tag	UNP Q9BYF1
E	666	LEU	-	expression tag	UNP Q9BYF1
E	667	LEU	-	expression tag	UNP Q9BYF1
E	668	SER	-	expression tag	UNP Q9BYF1
E	669	THR	-	expression tag	UNP Q9BYF1
E	670	PHE	-	expression tag	UNP Q9BYF1
E	671	LEU	-	expression tag	UNP Q9BYF1
E	672	GLY	-	expression tag	UNP Q9BYF1
E	673	SER	-	expression tag	UNP Q9BYF1
F	616	GLY	-	expression tag	UNP Q9BYF1
F	617	SER	-	expression tag	UNP Q9BYF1
F	618	GLU	-	expression tag	UNP Q9BYF1
F	619	ALA	-	expression tag	UNP Q9BYF1
F	620	ALA	-	expression tag	UNP Q9BYF1
F	621	ALA	-	expression tag	UNP Q9BYF1
F	622	LYS	-	expression tag	UNP Q9BYF1
F	623	GLU	-	expression tag	UNP Q9BYF1
F	624	ALA	-	expression tag	UNP Q9BYF1
F	625	ALA	-	expression tag	UNP Q9BYF1
F	626	ALA	-	expression tag	UNP Q9BYF1
F	627	LYS	-	expression tag	UNP Q9BYF1
F	628	GLU	-	expression tag	UNP Q9BYF1
F	629	ALA	-	expression tag	UNP Q9BYF1
F	630	ALA	-	expression tag	UNP Q9BYF1
F	631	ALA	-	expression tag	UNP Q9BYF1
F	632	LYS	-	expression tag	UNP Q9BYF1
F	633	GLU	-	expression tag	UNP Q9BYF1
F	634	ALA	-	expression tag	UNP Q9BYF1
F	635	ALA	-	expression tag	UNP Q9BYF1
F	636	ALA	-	expression tag	UNP Q9BYF1
F	637	LYS	-	expression tag	UNP Q9BYF1
F	638	GLU	-	expression tag	UNP Q9BYF1
F	639	ALA	-	expression tag	UNP Q9BYF1
F	640	ALA	-	expression tag	UNP Q9BYF1
F	641	ALA	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	642	LYS	-	expression tag	UNP Q9BYF1
F	643	GLY	-	expression tag	UNP Q9BYF1
F	644	SER	-	expression tag	UNP Q9BYF1
F	645	GLY	-	expression tag	UNP Q9BYF1
F	646	TYR	-	expression tag	UNP Q9BYF1
F	647	ILE	-	expression tag	UNP Q9BYF1
F	648	PRO	-	expression tag	UNP Q9BYF1
F	649	GLU	-	expression tag	UNP Q9BYF1
F	650	ALA	-	expression tag	UNP Q9BYF1
F	651	PRO	-	expression tag	UNP Q9BYF1
F	652	ARG	-	expression tag	UNP Q9BYF1
F	653	ASP	-	expression tag	UNP Q9BYF1
F	654	GLY	-	expression tag	UNP Q9BYF1
F	655	GLN	-	expression tag	UNP Q9BYF1
F	656	ALA	-	expression tag	UNP Q9BYF1
F	657	TYR	-	expression tag	UNP Q9BYF1
F	658	VAL	-	expression tag	UNP Q9BYF1
F	659	ARG	-	expression tag	UNP Q9BYF1
F	660	LYS	-	expression tag	UNP Q9BYF1
F	661	ASP	-	expression tag	UNP Q9BYF1
F	662	GLY	-	expression tag	UNP Q9BYF1
F	663	GLU	-	expression tag	UNP Q9BYF1
F	664	TRP	-	expression tag	UNP Q9BYF1
F	665	VAL	-	expression tag	UNP Q9BYF1
F	666	LEU	-	expression tag	UNP Q9BYF1
F	667	LEU	-	expression tag	UNP Q9BYF1
F	668	SER	-	expression tag	UNP Q9BYF1
F	669	THR	-	expression tag	UNP Q9BYF1
F	670	PHE	-	expression tag	UNP Q9BYF1
F	671	LEU	-	expression tag	UNP Q9BYF1
F	672	GLY	-	expression tag	UNP Q9BYF1
F	673	SER	-	expression tag	UNP Q9BYF1

- Molecule 3 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
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0
3	J	2	Total 28	C 16	N 2	O 10	0	0
3	K	2	Total 28	C 16	N 2	O 10	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0
3	M	2	Total 28	C 16	N 2	O 10	0	0
3	N	2	Total 28	C 16	N 2	O 10	0	0
3	O	2	Total 28	C 16	N 2	O 10	0	0
3	P	2	Total 28	C 16	N 2	O 10	0	0
3	Q	2	Total 28	C 16	N 2	O 10	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0
3	S	2	Total 28	C 16	N 2	O 10	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0
3	U	2	Total 28	C 16	N 2	O 10	0	0
3	V	2	Total 28	C 16	N 2	O 10	0	0
3	W	2	Total 28	C 16	N 2	O 10	0	0
3	X	2	Total 28	C 16	N 2	O 10	0	0
3	Y	2	Total 28	C 16	N 2	O 10	0	0
3	Z	2	Total 28	C 16	N 2	O 10	0	0
3	a	2	Total 28	C 16	N 2	O 10	0	0
3	b	2	Total 28	C 16	N 2	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	A	1	Total	C	N	O	0
			126	72	9	45	
4	B	1	Total	C	N	O	0
			168	96	12	60	
4	B	1	Total	C	N	O	0
			168	96	12	60	
4	B	1	Total	C	N	O	0
			168	96	12	60	
4	B	1	Total	C	N	O	0
			168	96	12	60	
4	B	1	Total	C	N	O	0
			168	96	12	60	

*Continued on next page...*

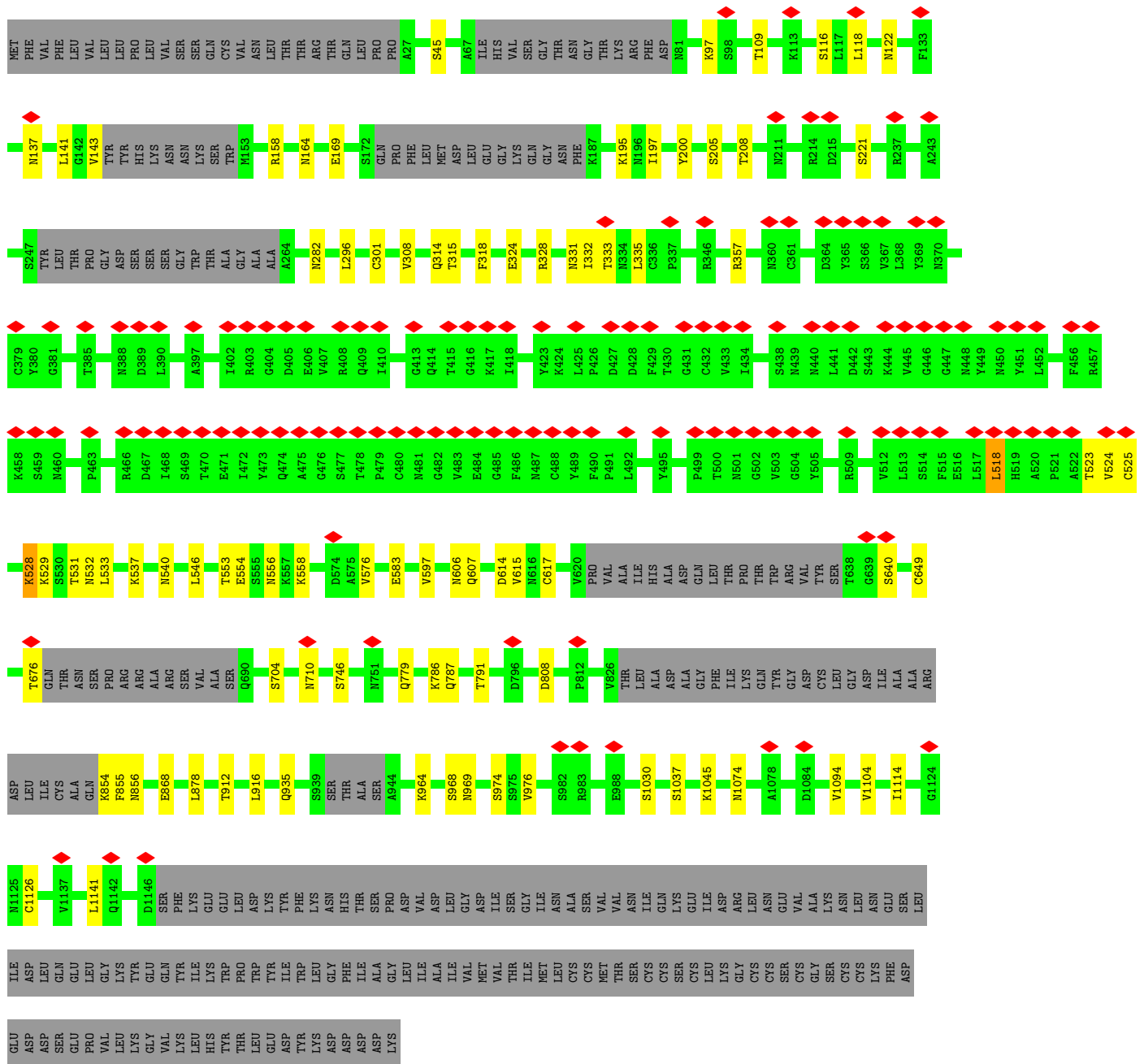
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	E	1	Total 14	C 8	N 1	O 5	0
4	F	1	Total 14	C 8	N 1	O 5	0



ASP  
ASP  
LYS

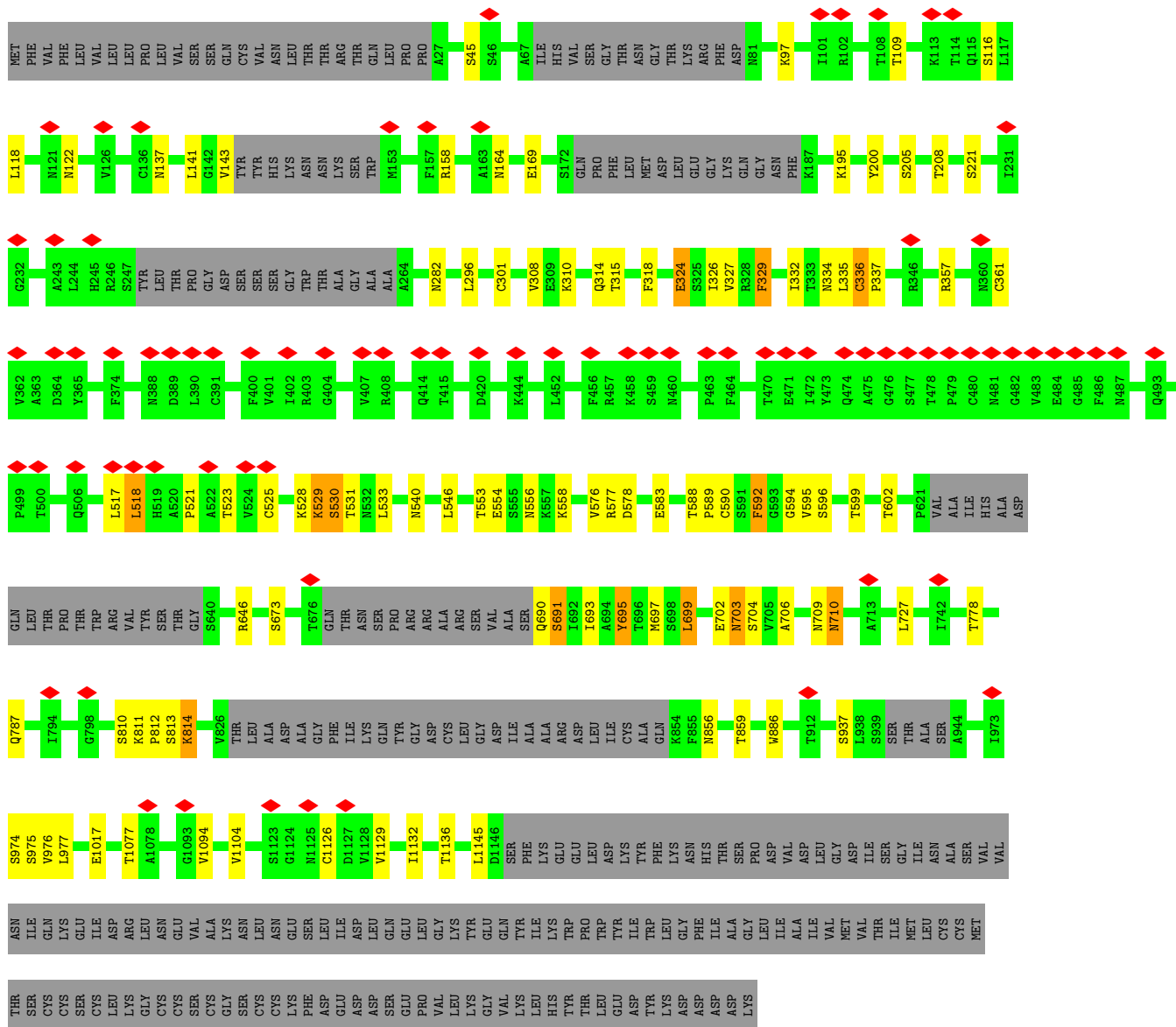
• Molecule 1: Spike glycoprotein



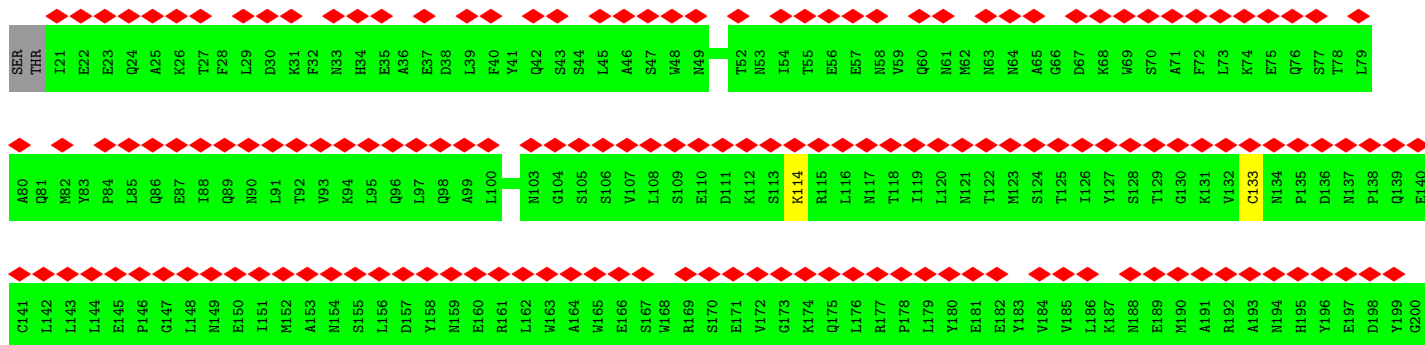
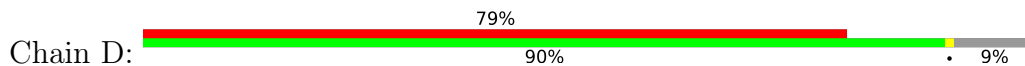
• Molecule 1: Spike glycoprotein

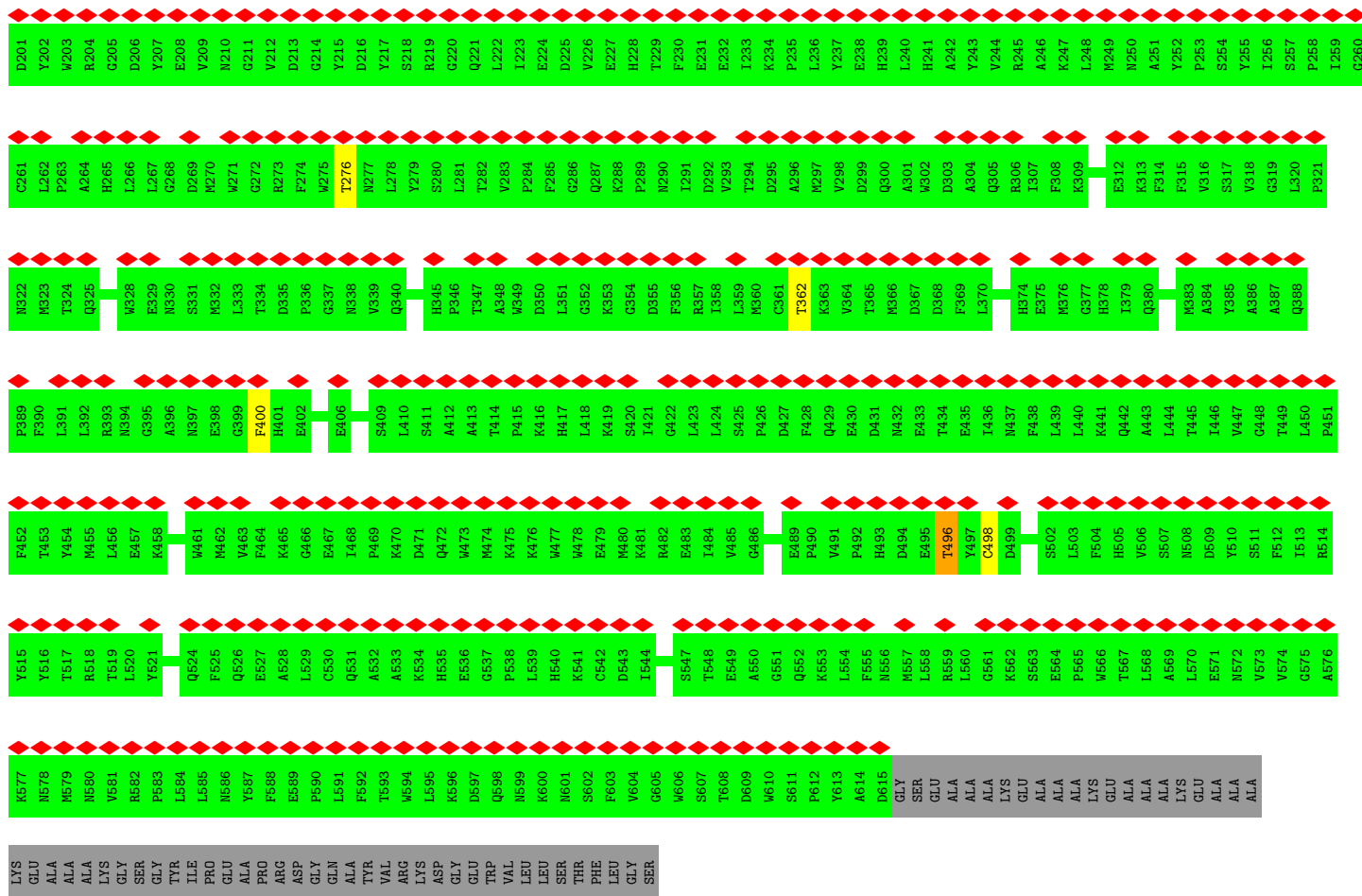




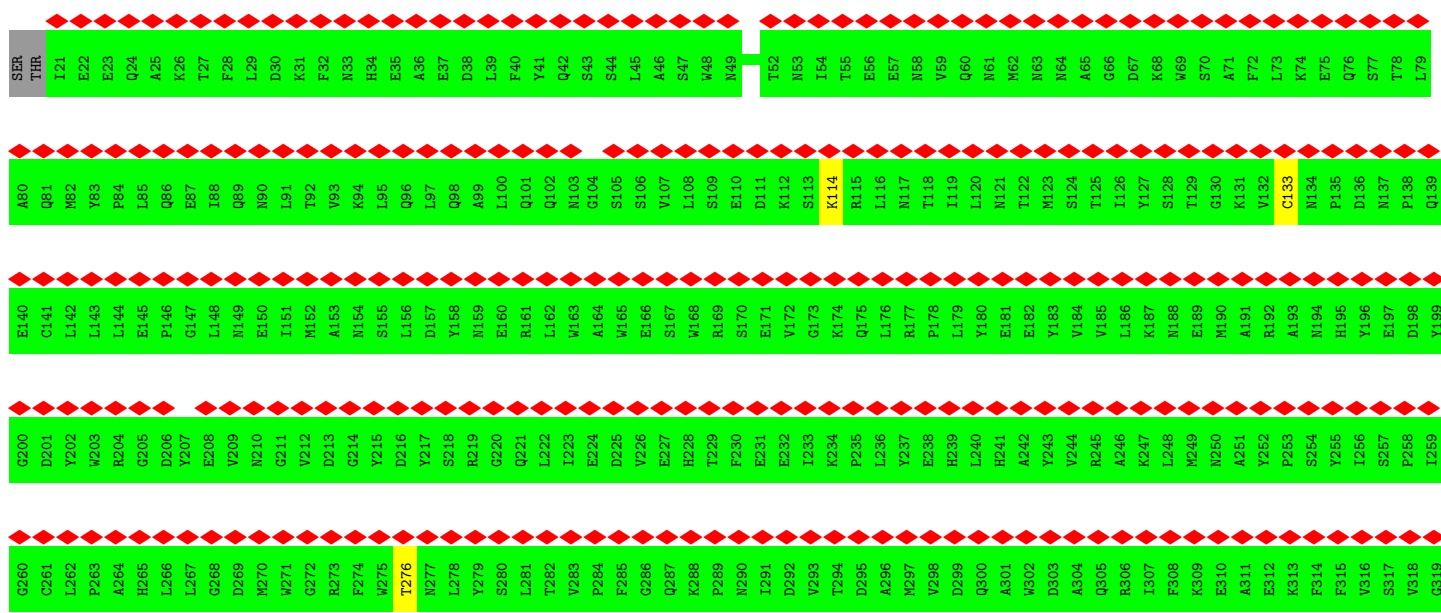
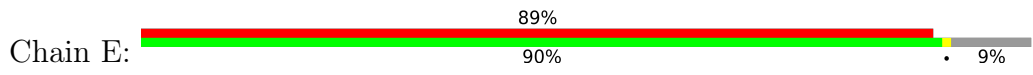


● Molecule 2: Angiotensin-converting enzyme 2

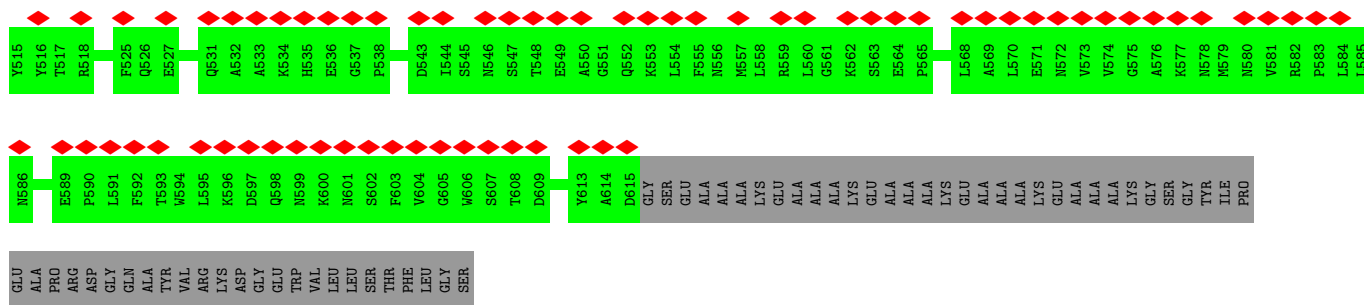




• Molecule 2: Angiotensin-converting enzyme 2







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



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



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



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



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



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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  50% 100% 50%



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

Chain O:  50% 100%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain T:  50% 50% 50%



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

Chain U:  50% 50% 50%



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

Chain V:  50% 50%



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

Chain W:  100%



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

Chain X:  50% 50% 100%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain a:  100%  
 100%



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

Chain b:  100%  
 100%



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

Chain c:  100%  
 100%



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

Chain d:  100%  
 100%



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



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



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



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



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



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





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



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



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



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



- Molecule 3: 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, Not provided	
Number of particles used	57404	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 ( $e^-/\text{\AA}^2$ )	50	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	0.088	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [i](#)

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

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

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	0.52	0/8039	0.56	0/10936
1	B	0.51	0/8045	0.56	0/10942
1	C	0.50	0/8042	0.54	0/10939
2	D	0.39	0/4994	0.54	0/6785
2	E	0.39	0/4994	0.54	0/6785
2	F	0.39	0/4994	0.54	0/6785
All	All	0.47	0/39108	0.55	0/53172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

### 5.3 Torsion angles [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	988/1283 (77%)	874 (88%)	108 (11%)	6 (1%)	25	63
1	B	989/1283 (77%)	874 (88%)	109 (11%)	6 (1%)	25	63
1	C	988/1283 (77%)	849 (86%)	109 (11%)	30 (3%)	4	32
2	D	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	47	79
2	E	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	47	79
2	F	593/655 (90%)	560 (94%)	32 (5%)	1 (0%)	47	79
All	All	4744/5814 (82%)	4277 (90%)	422 (9%)	45 (1%)	21	55

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	983	ARG
1	C	332	ILE
1	C	518	LEU
1	C	529	LYS
1	C	530	SER

### 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	881/1122 (78%)	793 (90%)	88 (10%)	7	29
1	B	881/1122 (78%)	796 (90%)	85 (10%)	8	30
1	C	881/1122 (78%)	794 (90%)	87 (10%)	8	29
2	D	525/562 (93%)	518 (99%)	7 (1%)	69	82
2	E	525/562 (93%)	518 (99%)	7 (1%)	69	82
2	F	525/562 (93%)	518 (99%)	7 (1%)	69	82
All	All	4218/5052 (84%)	3937 (93%)	281 (7%)	20	44

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	690	GLN

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Mol	Chain	Res	Type
1	C	710	ASN
2	D	114	LYS
1	B	158	ARG
1	B	137	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	ASN
2	E	586	ASN
1	C	690	GLN
2	E	556	ASN
2	F	417	HIS

### 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](#)

70 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	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	H	2	3	14,14,15	0.51	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	1,3	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
3	NAG	I	2	3	14,14,15	0.52	0	17,19,21	0.46	0
3	NAG	J	1	1,3	14,14,15	0.38	0	17,19,21	0.74	0
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	1.31	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
3	NAG	K	2	3	14,14,15	0.39	0	17,19,21	1.38	3 (17%)
3	NAG	L	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.67	0
3	NAG	L	2	3	14,14,15	0.28	0	17,19,21	0.64	0
3	NAG	M	1	1,3	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
3	NAG	M	2	3	14,14,15	0.16	0	17,19,21	0.45	0
3	NAG	N	1	1,3	14,14,15	0.31	0	17,19,21	0.71	0
3	NAG	N	2	3	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.33	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.39	0	17,19,21	0.36	0
3	NAG	P	1	1,3	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	R	1	1,3	14,14,15	0.77	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	R	2	3	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	S	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	S	2	3	14,14,15	0.28	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.30	0	17,19,21	0.72	0
3	NAG	T	2	3	14,14,15	0.52	0	17,19,21	0.64	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
3	NAG	U	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	V	1	1,3	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
3	NAG	V	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	W	1	1,3	14,14,15	0.38	0	17,19,21	0.42	0
3	NAG	W	2	3	14,14,15	0.26	0	17,19,21	0.72	0
3	NAG	X	1	1,3	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	X	2	3	14,14,15	0.55	0	17,19,21	1.32	1 (5%)
3	NAG	Y	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.44	0
3	NAG	Y	2	3	14,14,15	0.30	0	17,19,21	1.35	2 (11%)
3	NAG	Z	1	1,3	14,14,15	0.43	0	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	a	1	2,3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	a	2	3	14,14,15	0.59	0	17,19,21	0.45	0
3	NAG	b	1	2,3	14,14,15	0.47	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	b	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	c	1	2,3	14,14,15	0.60	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	c	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	d	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	e	1	2,3	14,14,15	0.66	1 (7%)	17,19,21	0.83	0
3	NAG	e	2	3	14,14,15	0.25	0	17,19,21	0.55	0
3	NAG	f	1	2,3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	f	2	3	14,14,15	0.59	0	17,19,21	0.46	0
3	NAG	g	1	2,3	14,14,15	0.48	0	17,19,21	0.60	0
3	NAG	g	2	3	14,14,15	0.27	0	17,19,21	0.58	0
3	NAG	h	1	2,3	14,14,15	0.61	1 (7%)	17,19,21	1.29	2 (11%)
3	NAG	h	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	j	1	2,3	14,14,15	0.66	1 (7%)	17,19,21	0.83	0
3	NAG	j	2	3	14,14,15	0.24	0	17,19,21	0.55	0
3	NAG	k	1	2,3	14,14,15	0.34	0	17,19,21	0.61	0
3	NAG	k	2	3	14,14,15	0.57	0	17,19,21	0.44	0
3	NAG	l	1	2,3	14,14,15	0.47	0	17,19,21	0.61	0
3	NAG	l	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	m	1	2,3	14,14,15	0.61	1 (7%)	17,19,21	1.28	2 (11%)
3	NAG	m	2	3	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	n	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	n	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	o	1	2,3	14,14,15	0.65	1 (7%)	17,19,21	0.83	0
3	NAG	o	2	3	14,14,15	0.23	0	17,19,21	0.55	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	5/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	2,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	k	2	3	-	2/6/23/26	0/1/1/1
3	NAG	l	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	NAG	m	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	NAG	n	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	2/6/23/26	0/1/1/1
3	NAG	o	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.80	1.39	1.43
3	L	1	NAG	O5-C1	-2.51	1.39	1.43
3	K	1	NAG	O5-C1	-2.35	1.40	1.43
3	Y	1	NAG	O5-C1	-2.27	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	1	NAG	O5-C1	-2.25	1.40	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C2-N2-C7	4.61	129.47	122.90
3	h	1	NAG	C1-O5-C5	4.43	118.19	112.19
3	c	1	NAG	C1-O5-C5	4.42	118.19	112.19
3	m	1	NAG	C1-O5-C5	4.41	118.16	112.19
3	Y	2	NAG	C2-N2-C7	4.36	129.11	122.90

There are no chirality outliers.

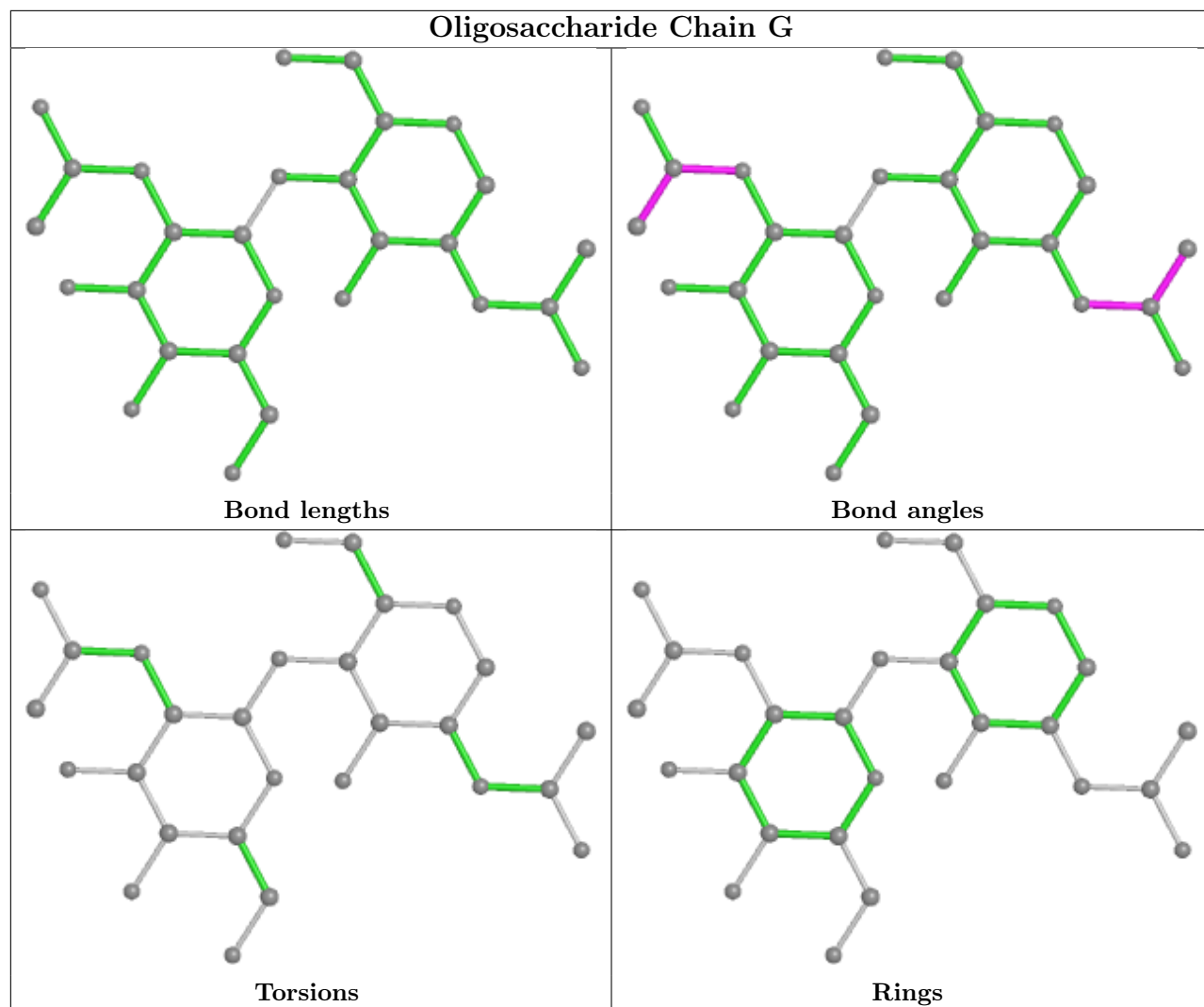
5 of 130 torsion outliers are listed below:

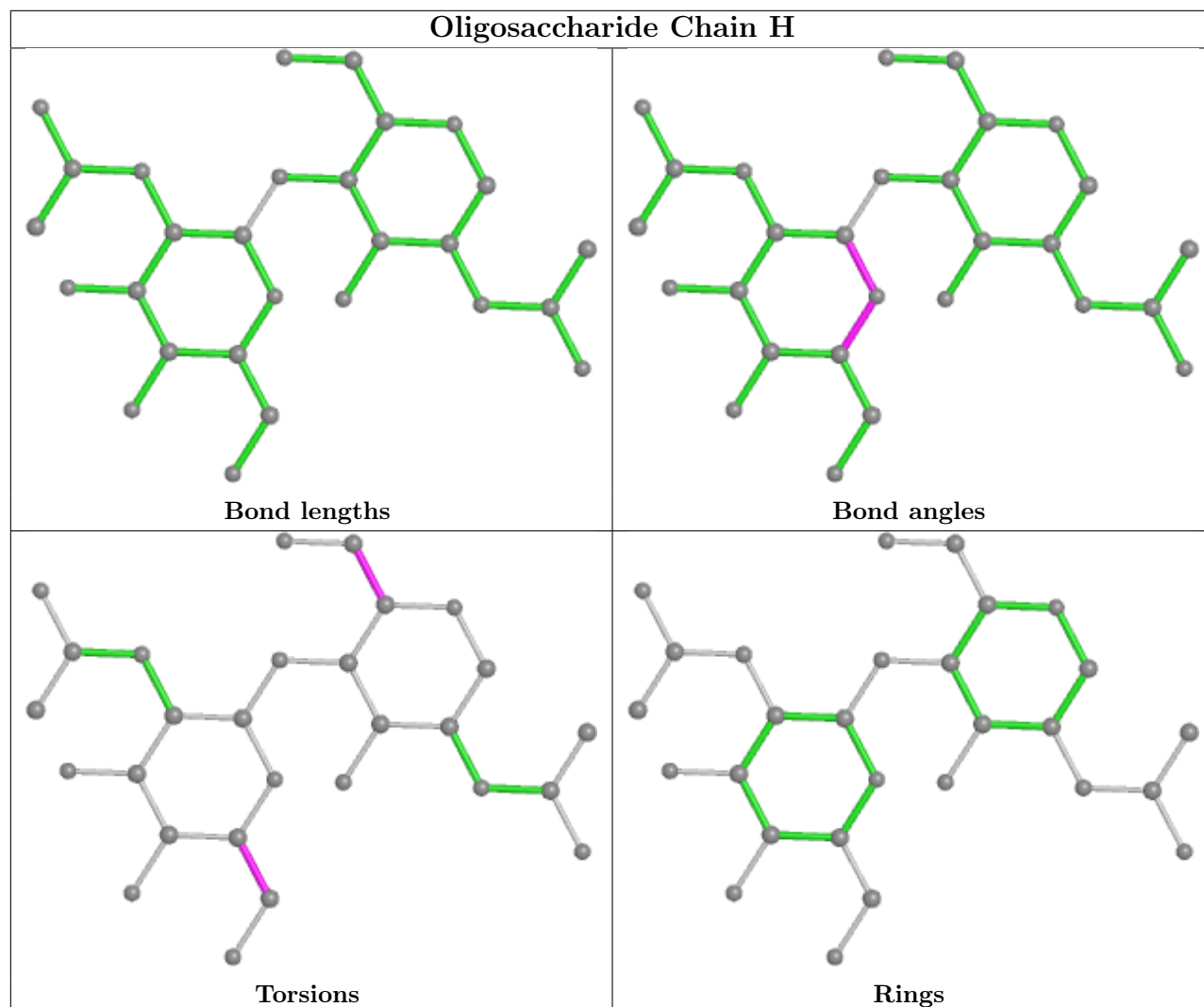
Mol	Chain	Res	Type	Atoms
3	U	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6

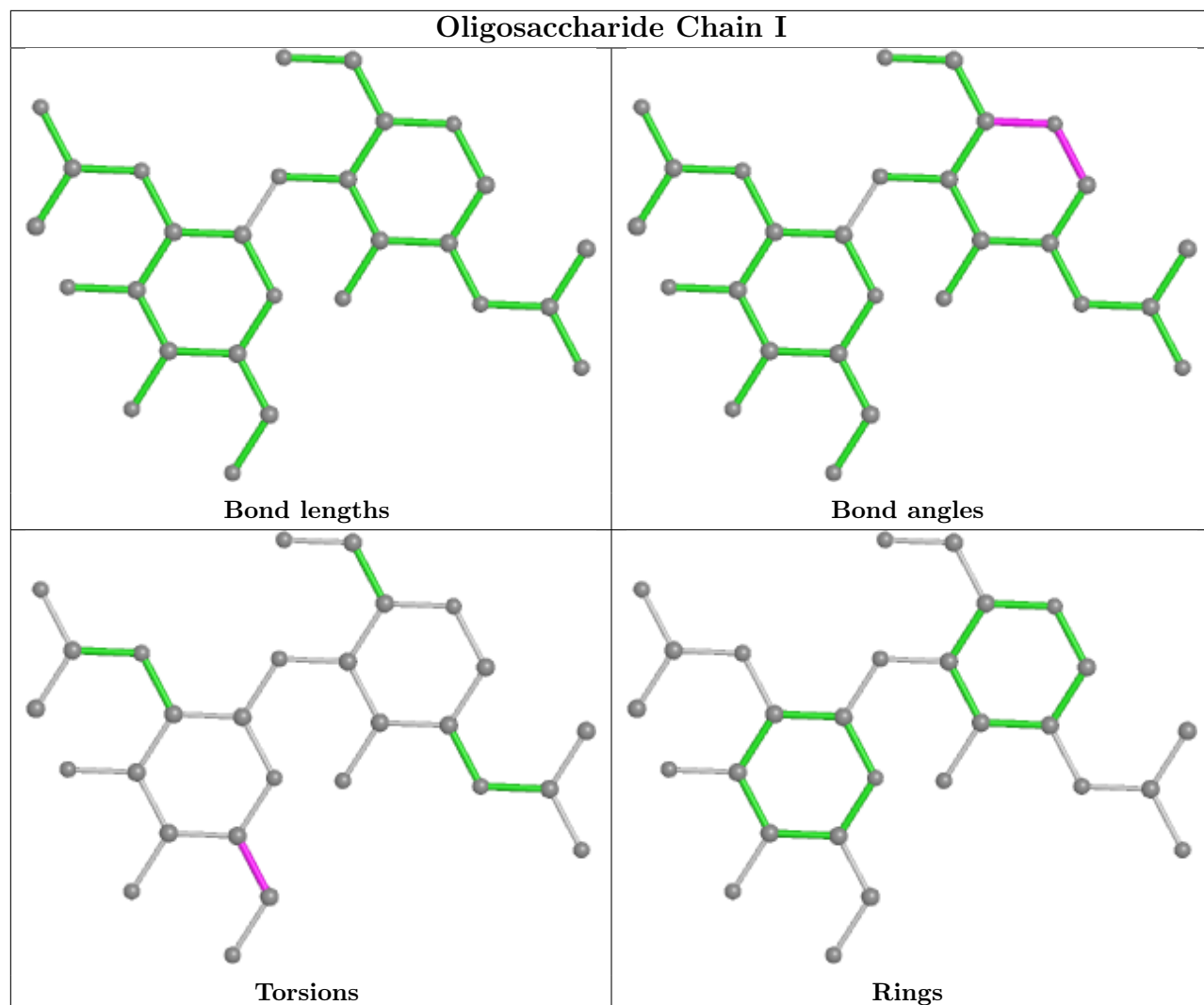
There are no ring outliers.

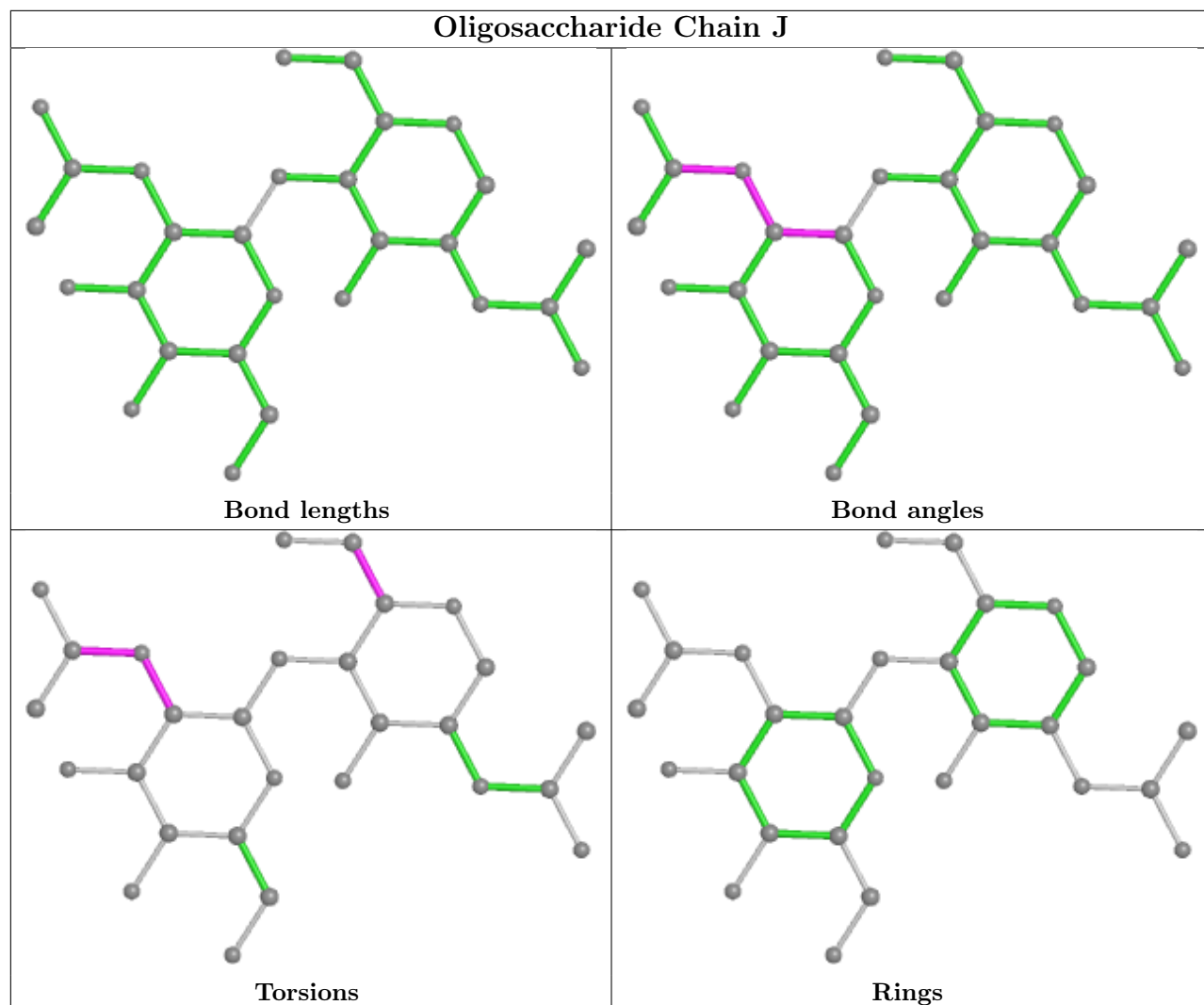
No monomer is involved in short contacts.

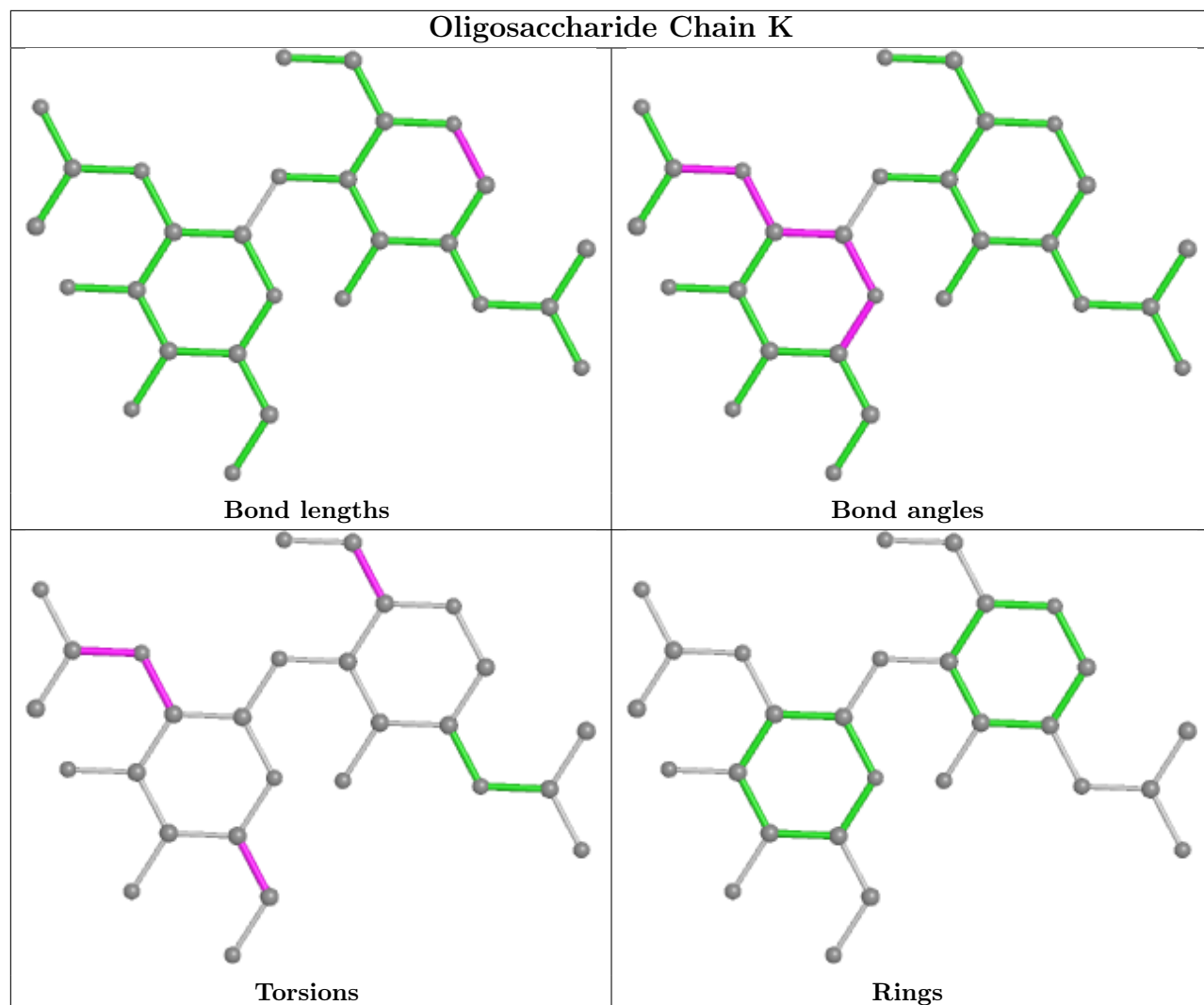
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

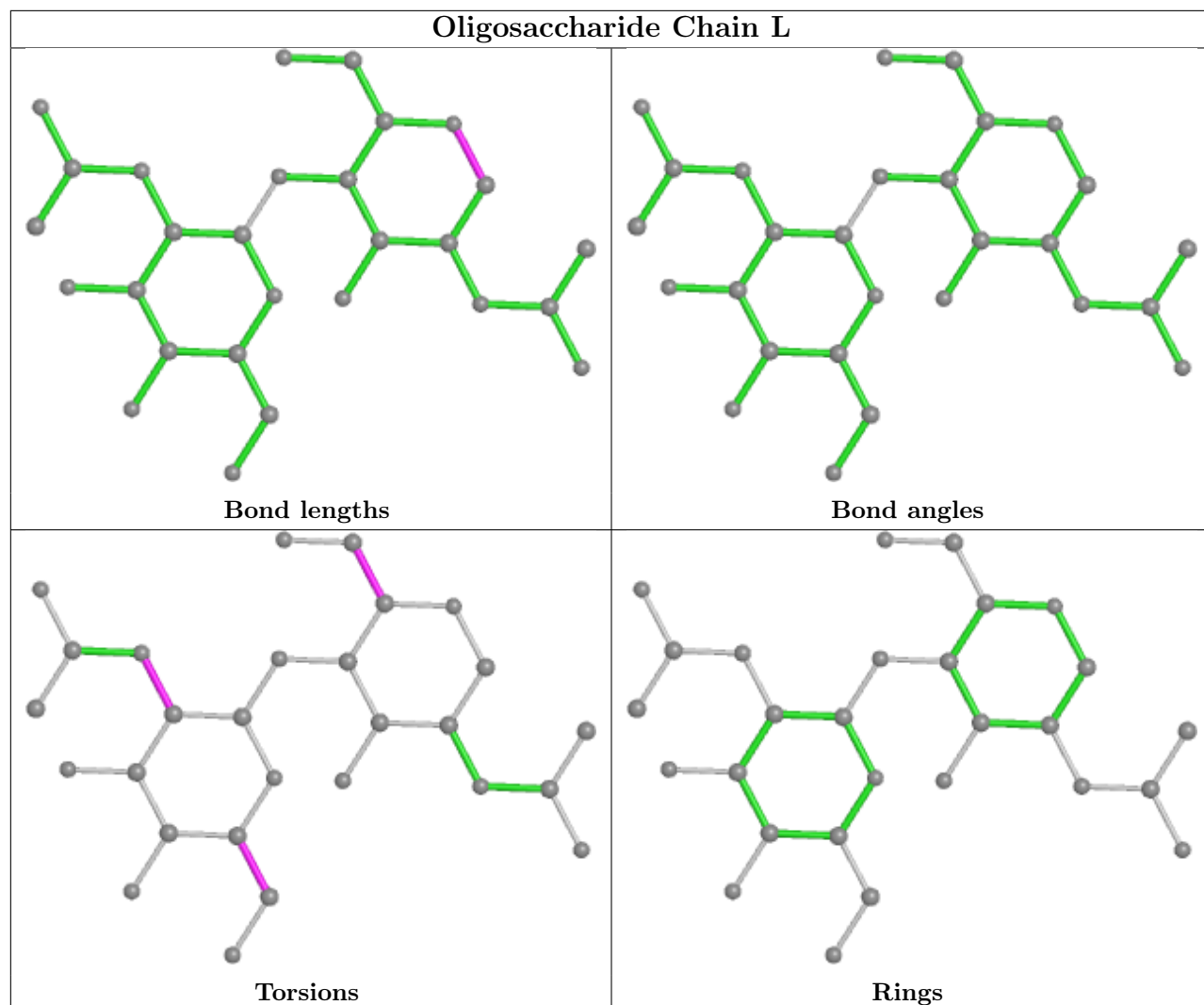




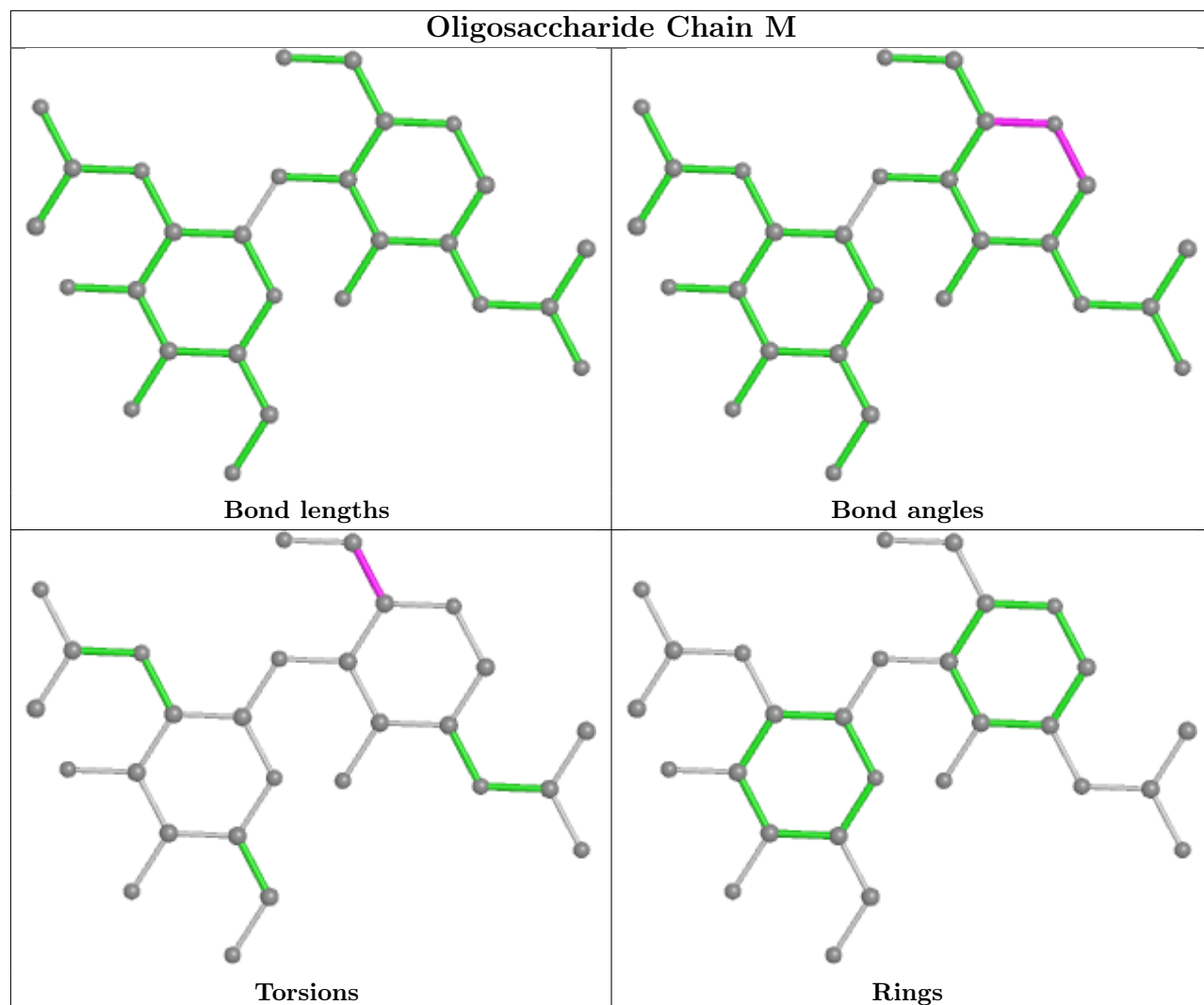


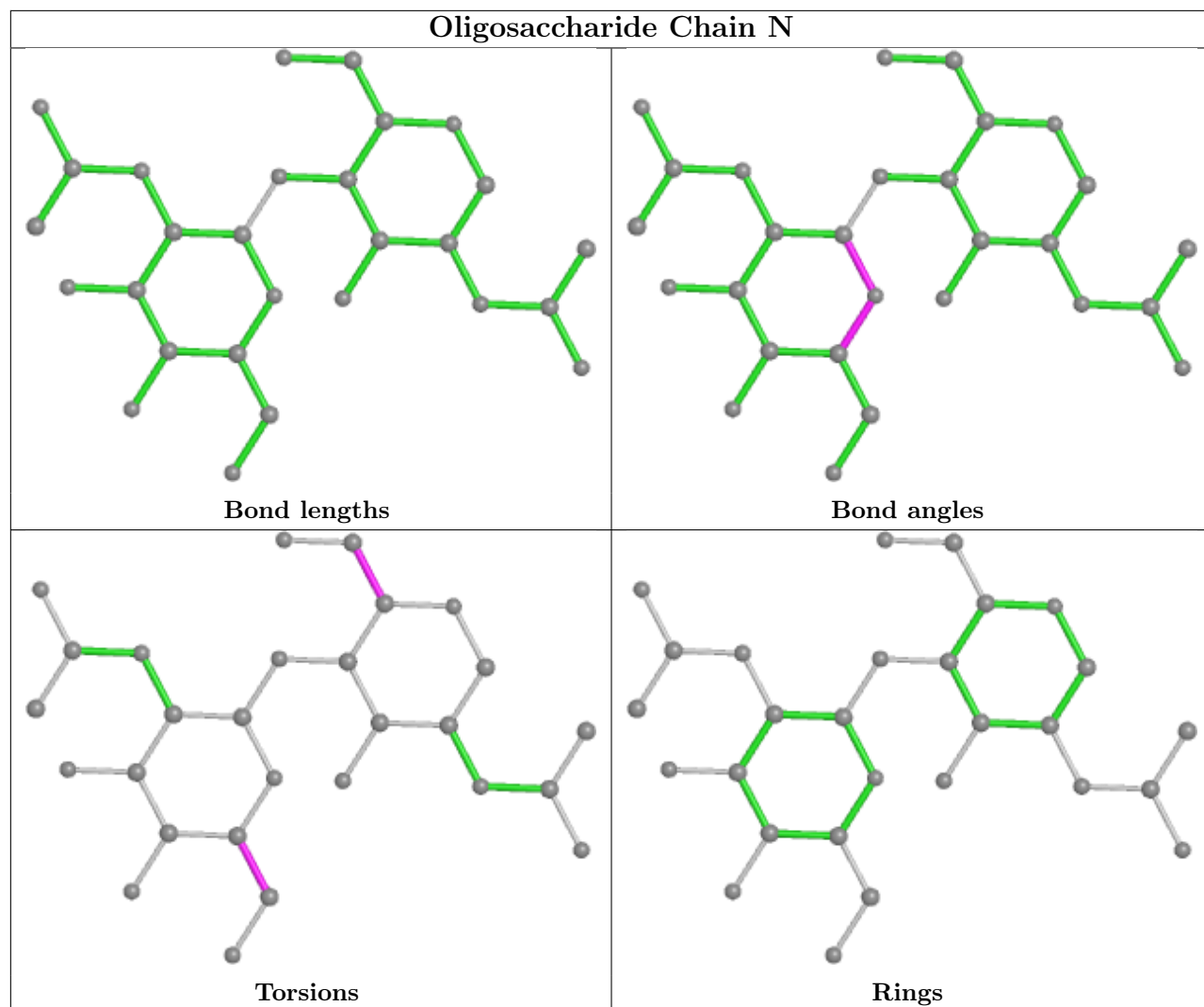


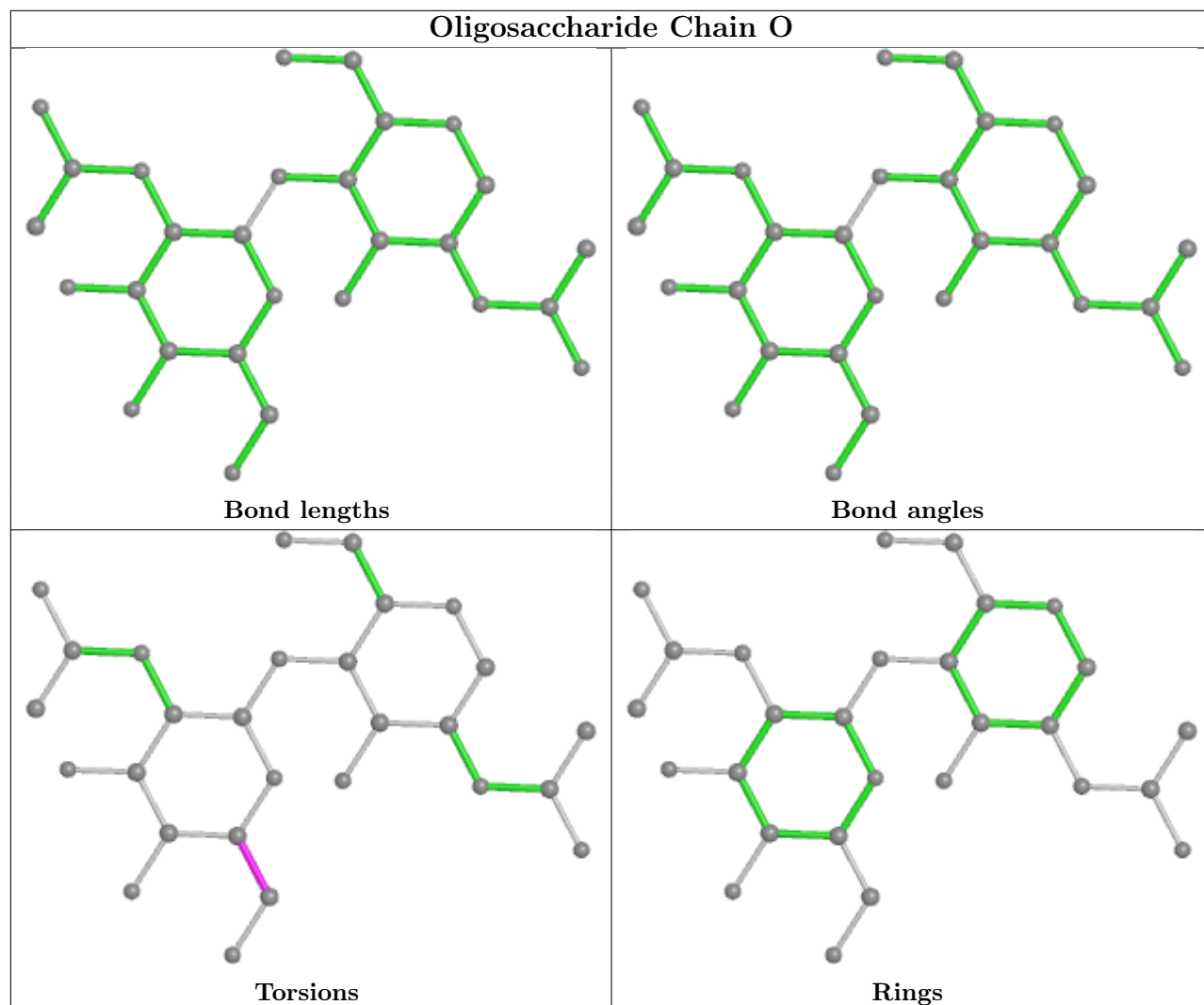


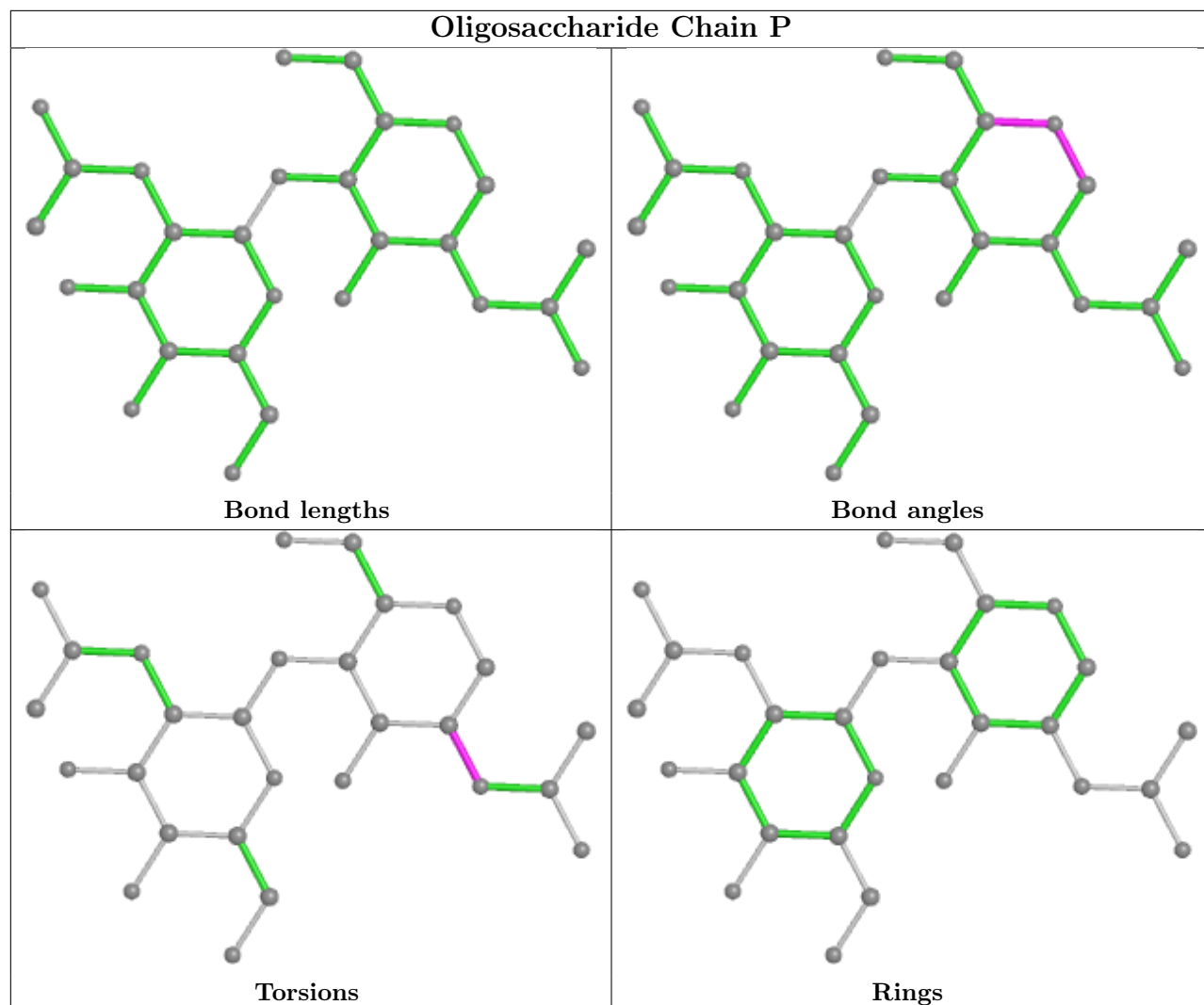


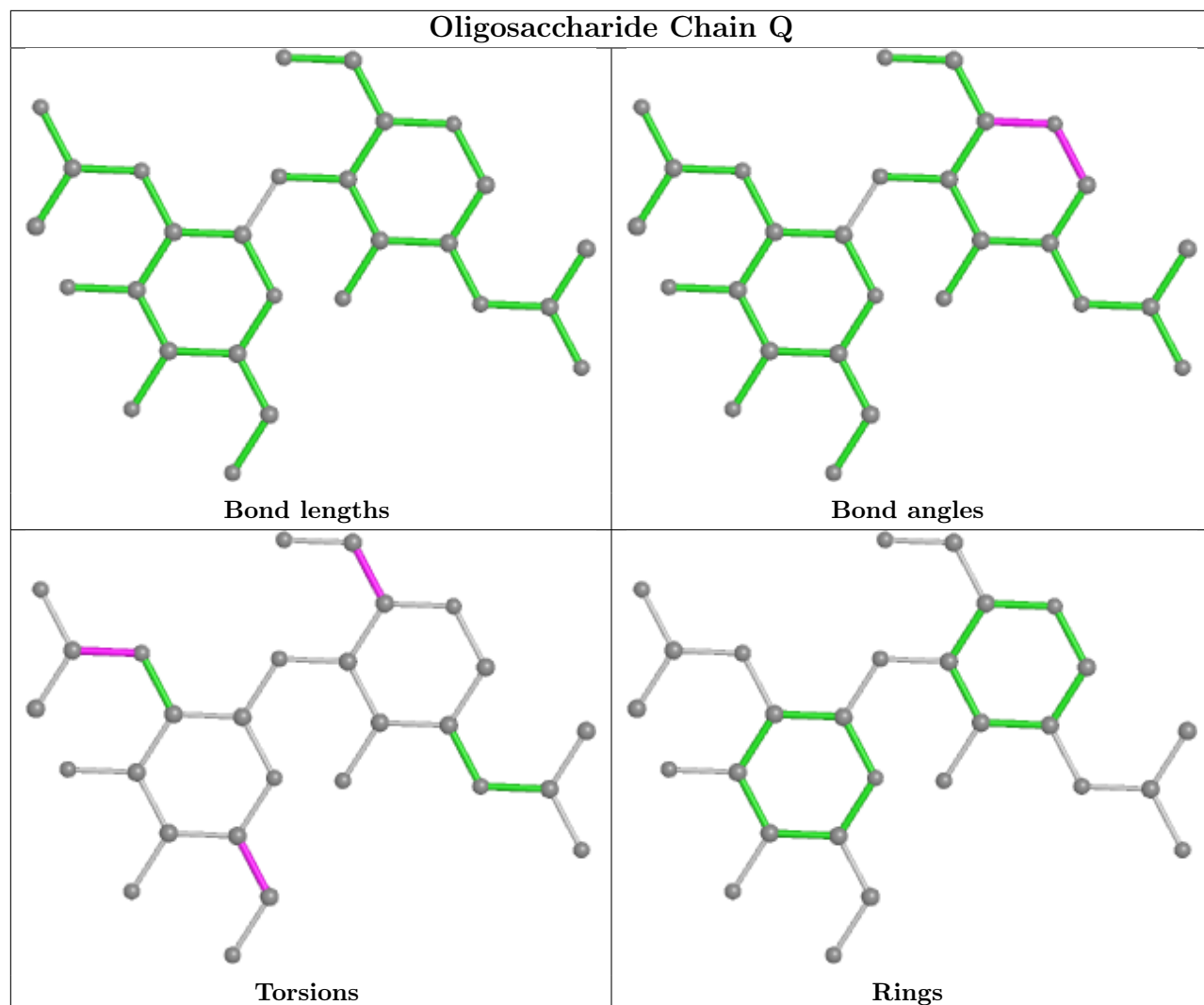


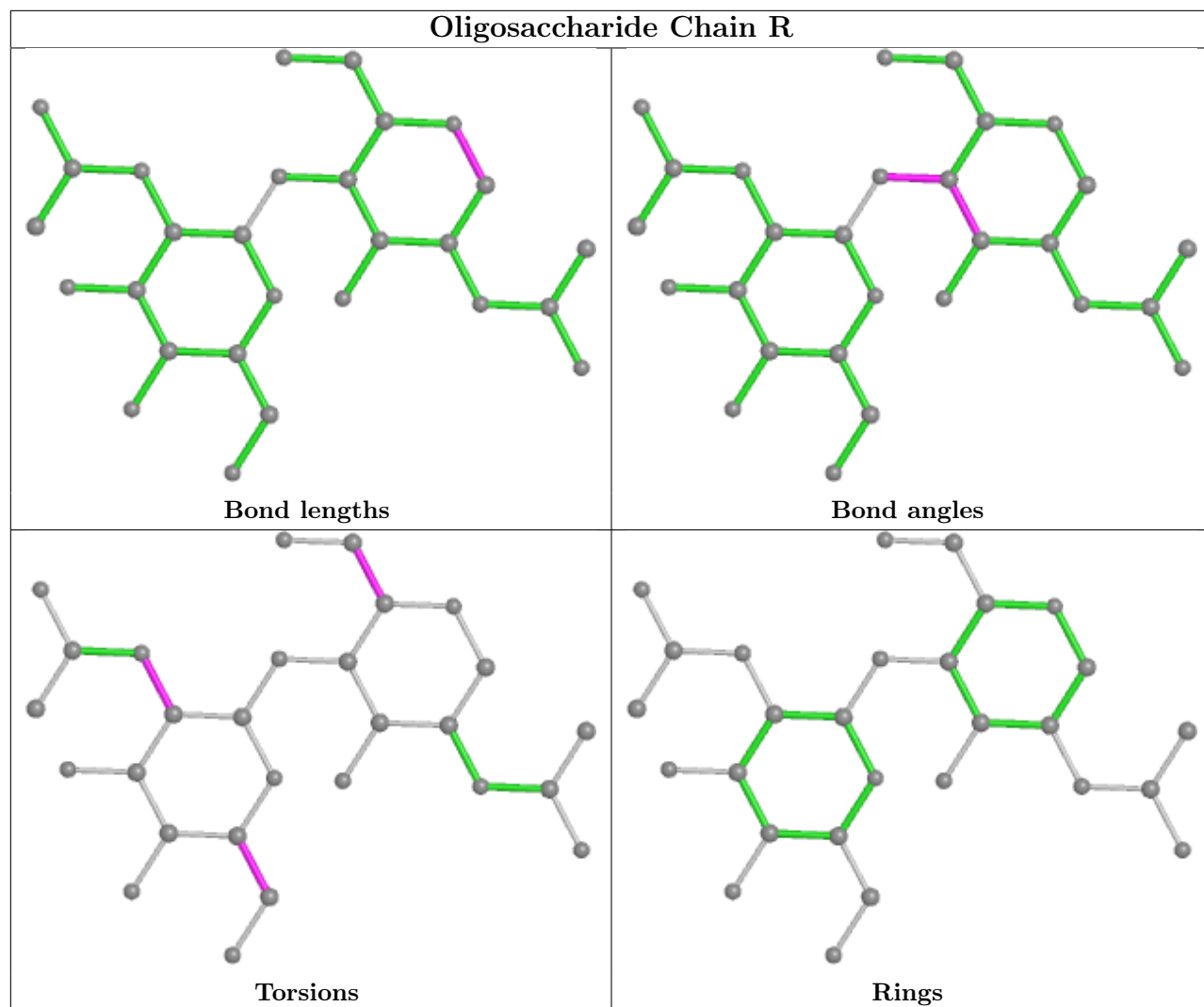


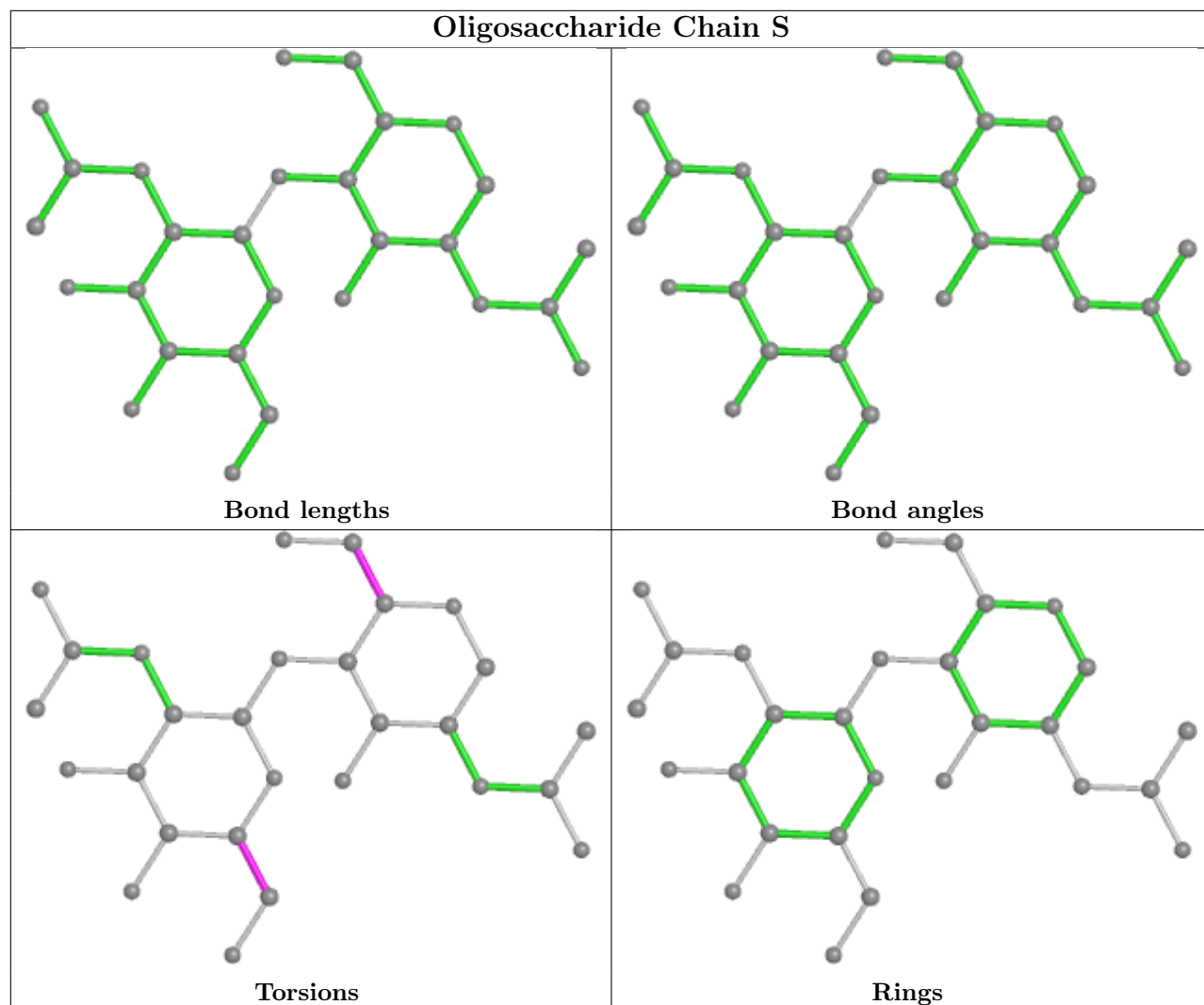


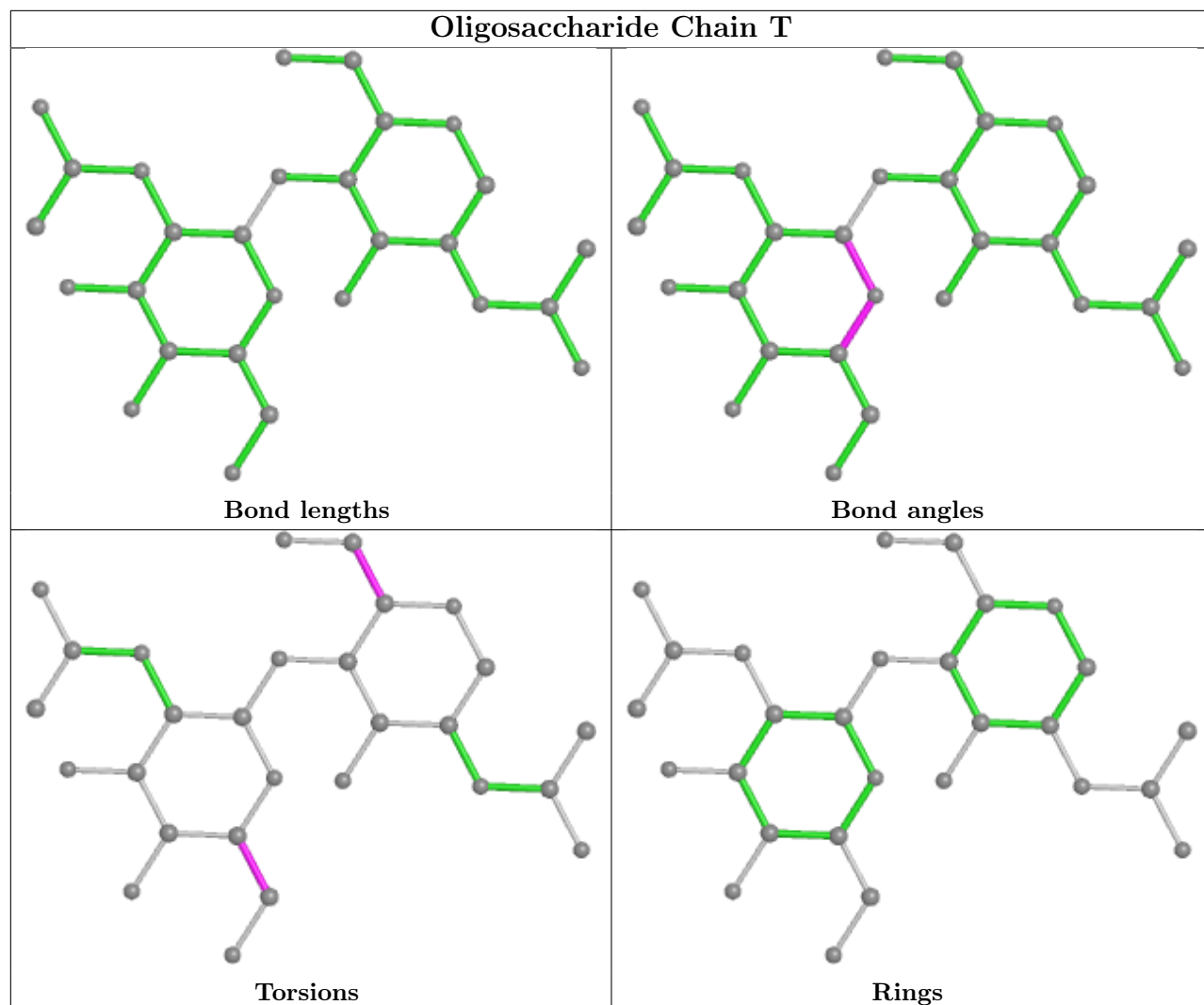




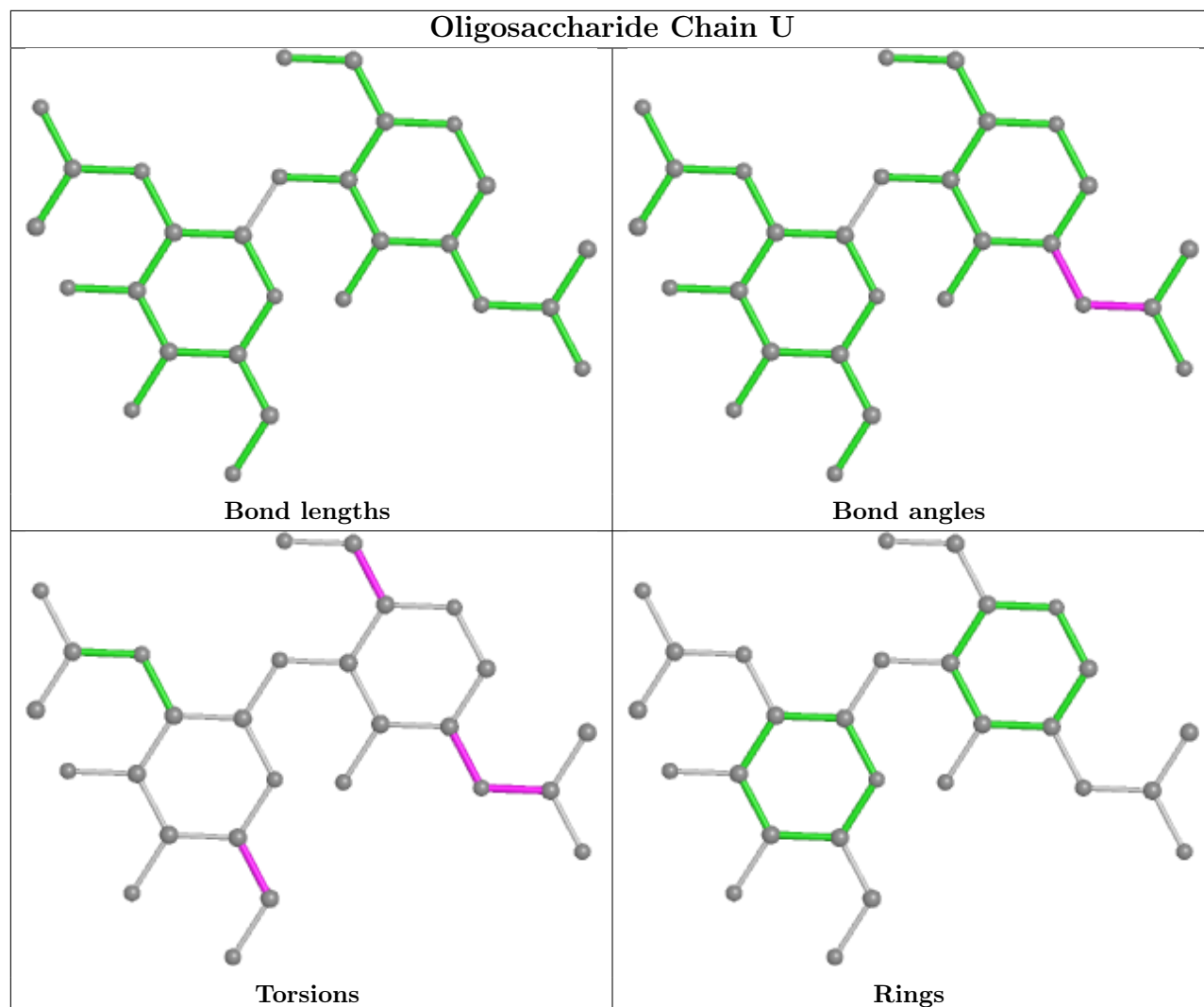


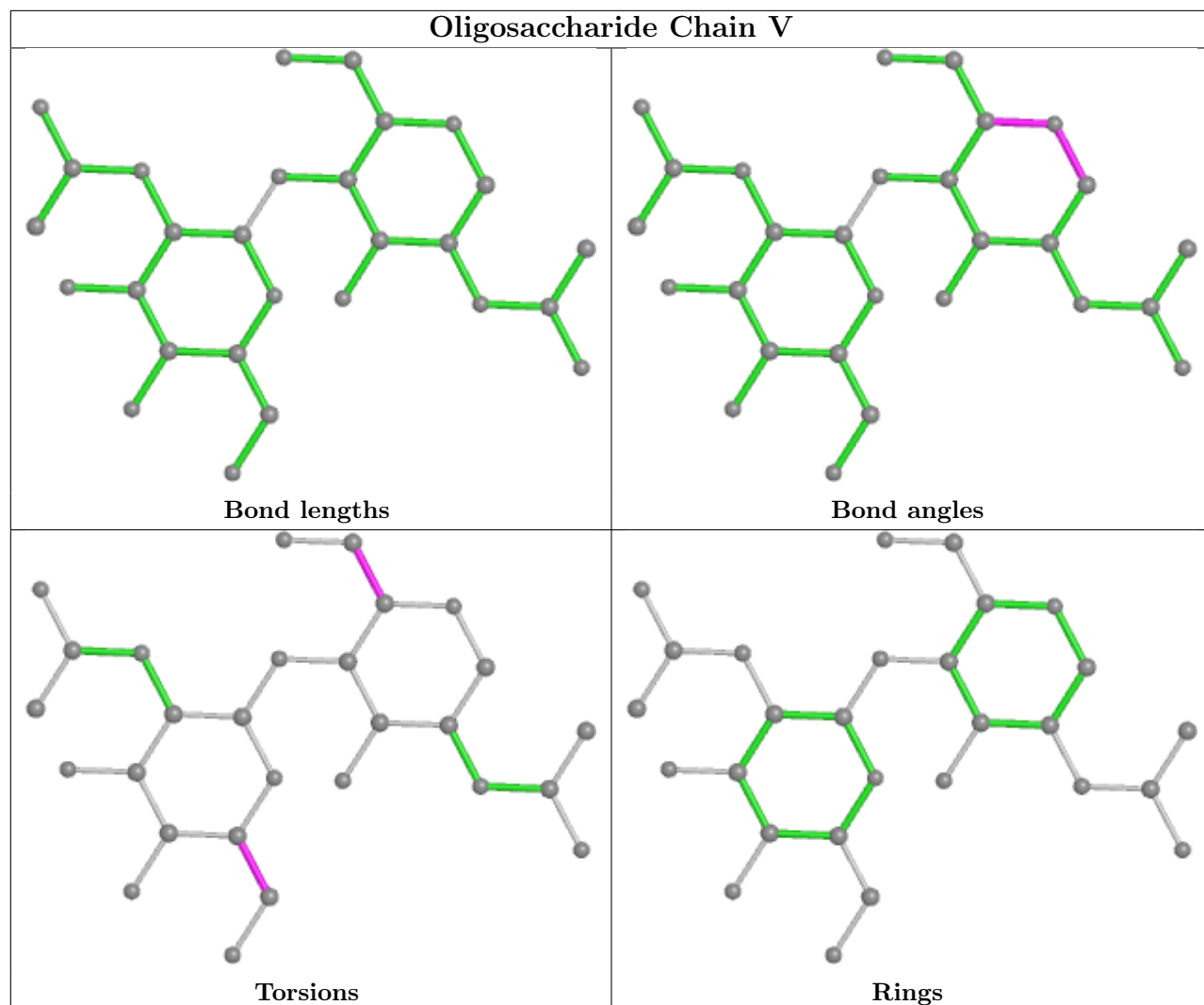


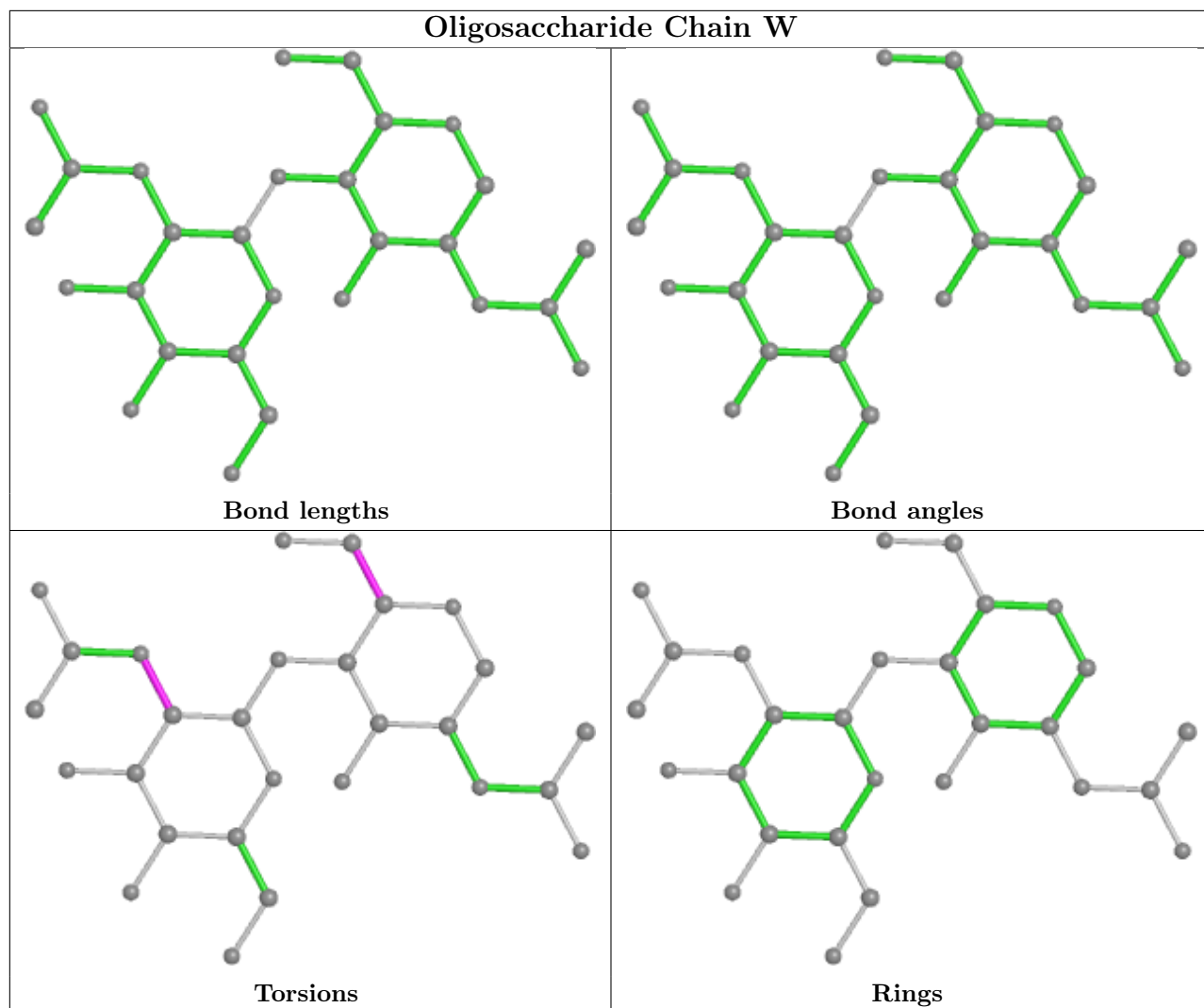


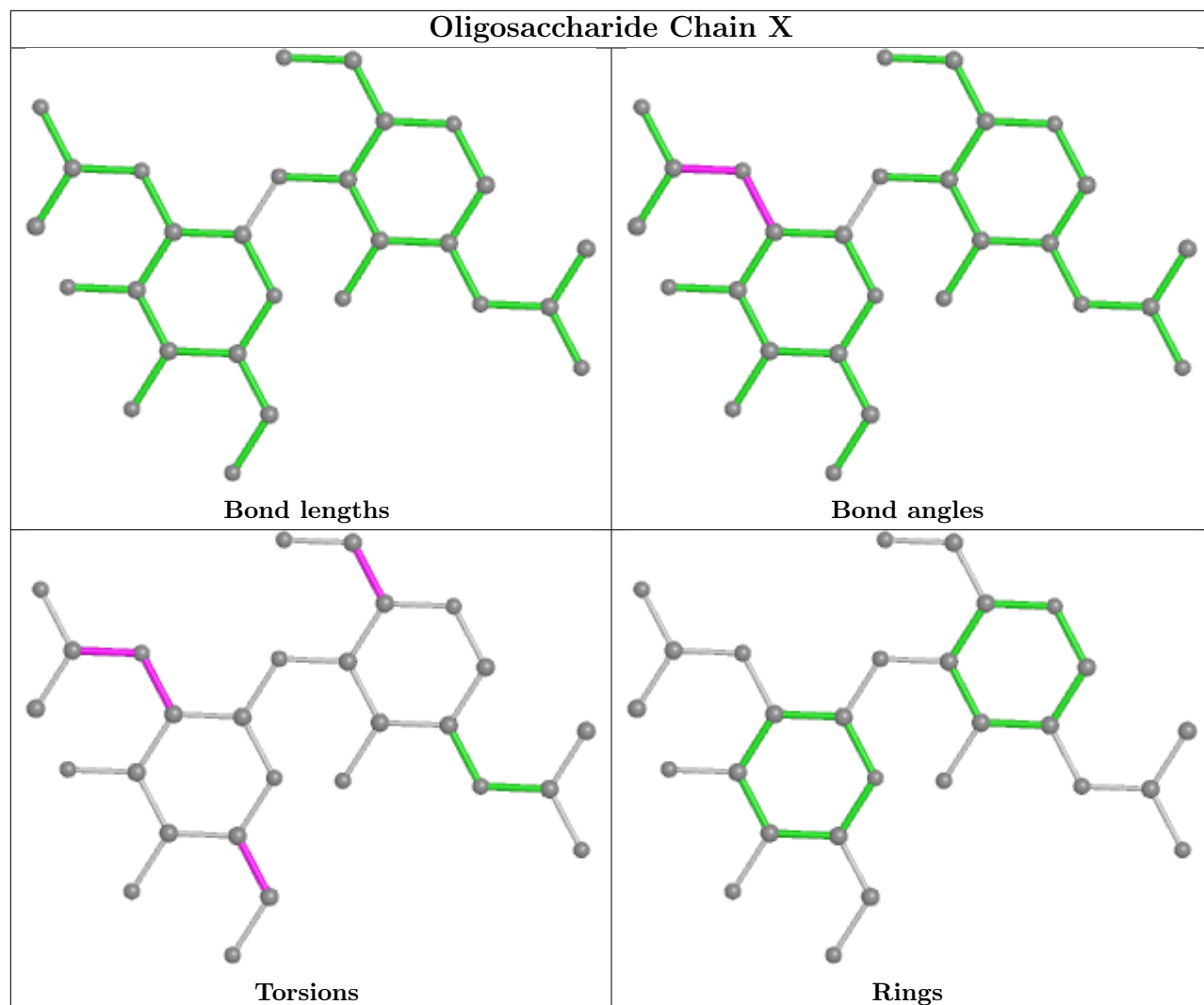


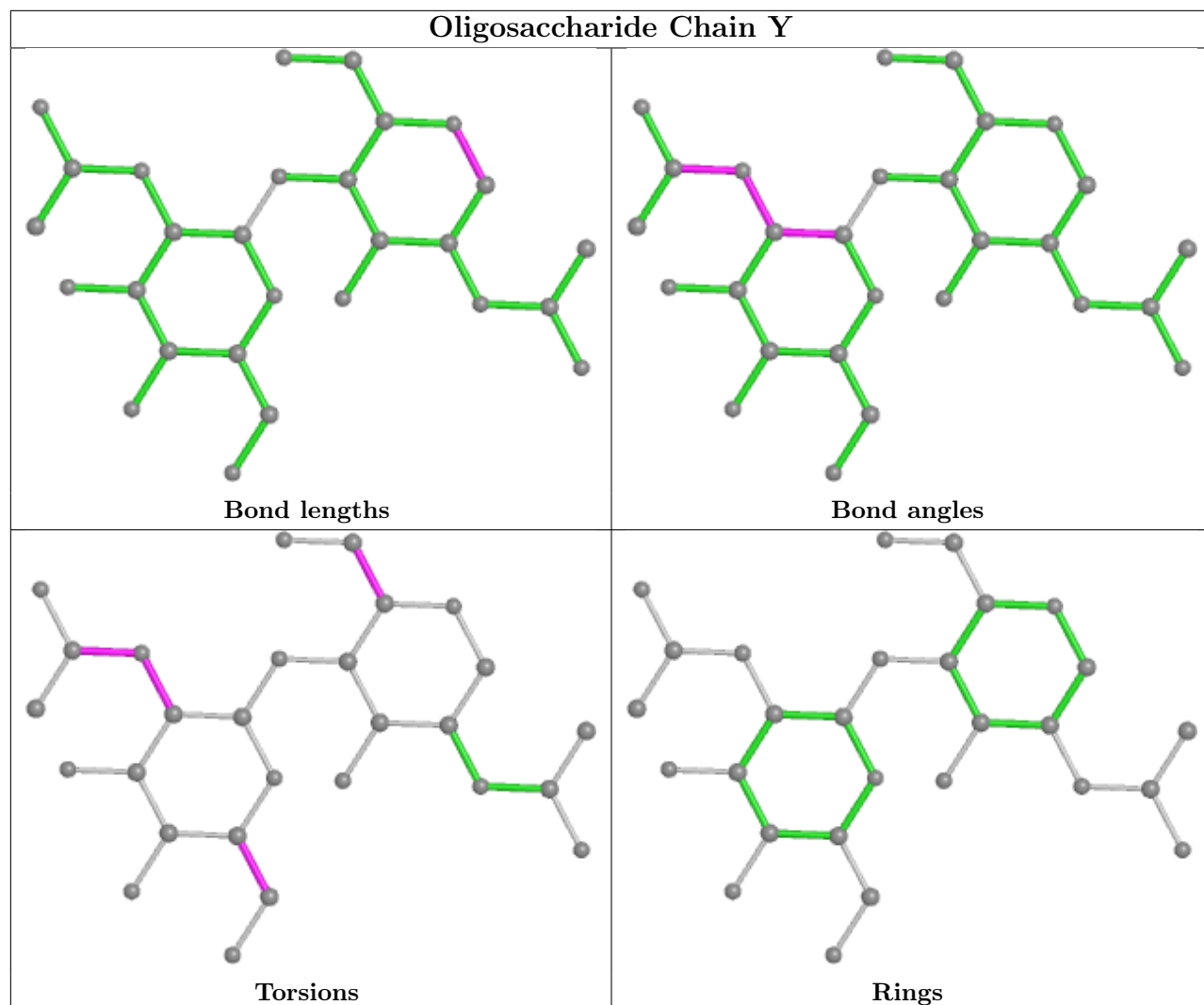


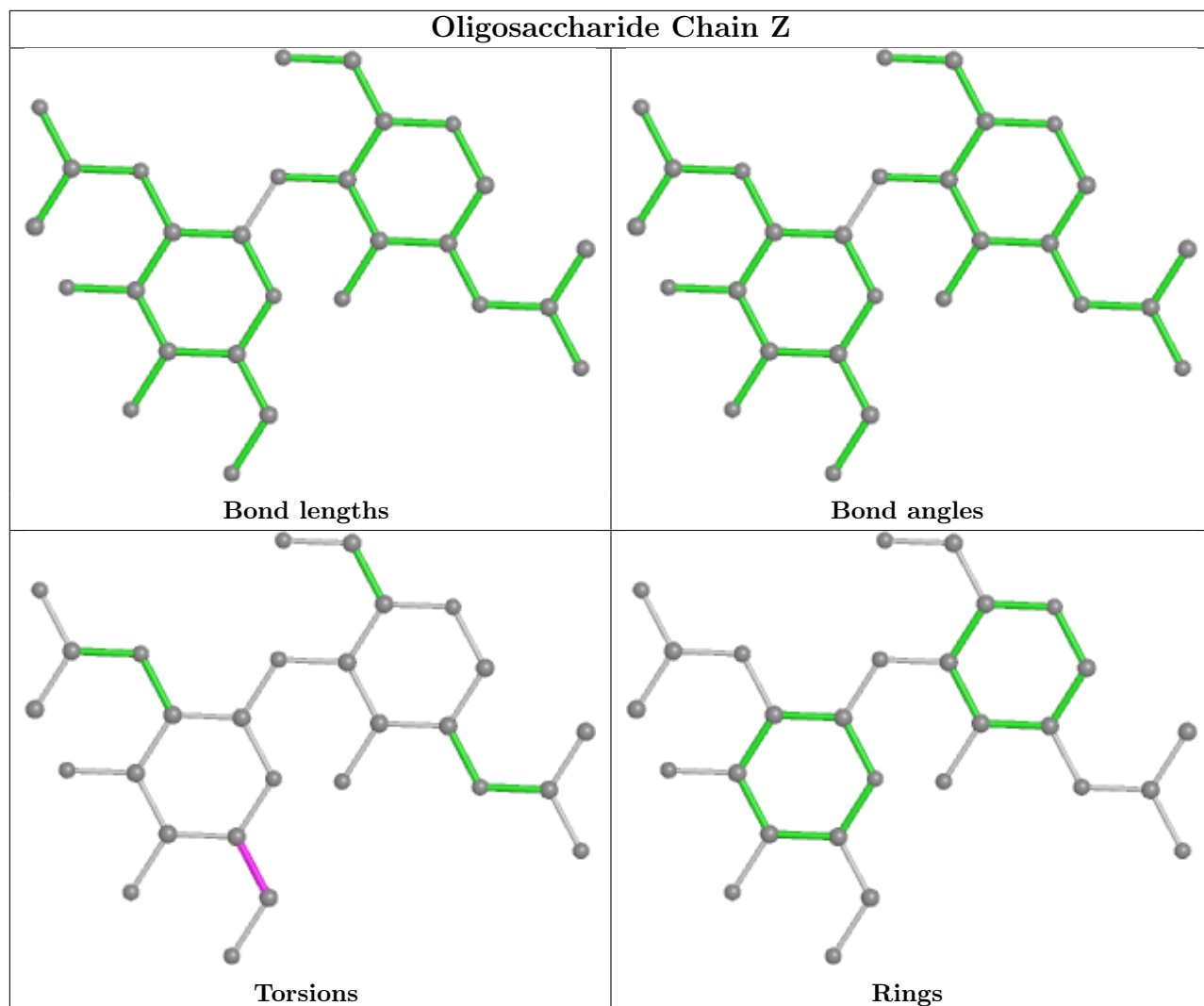


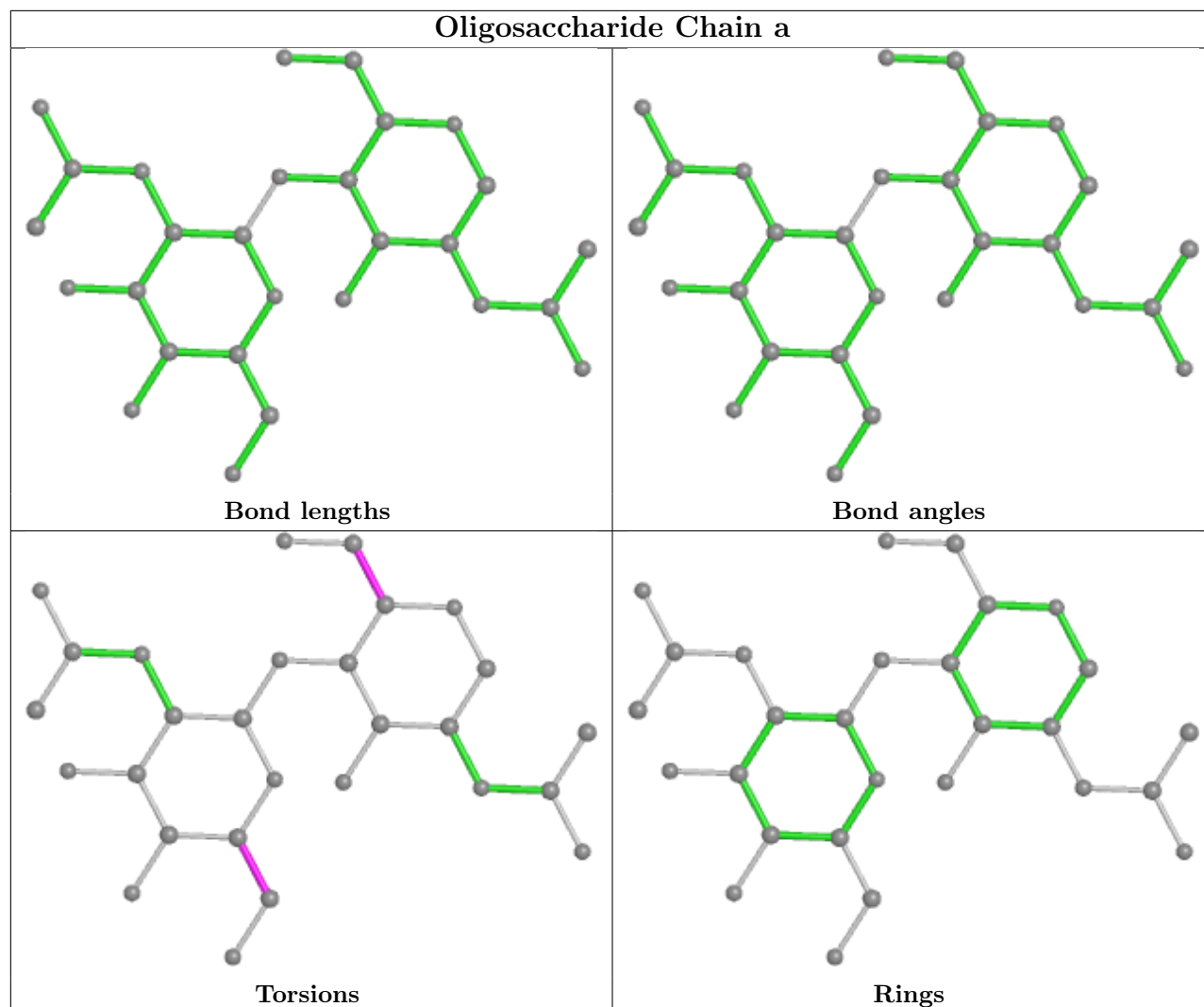


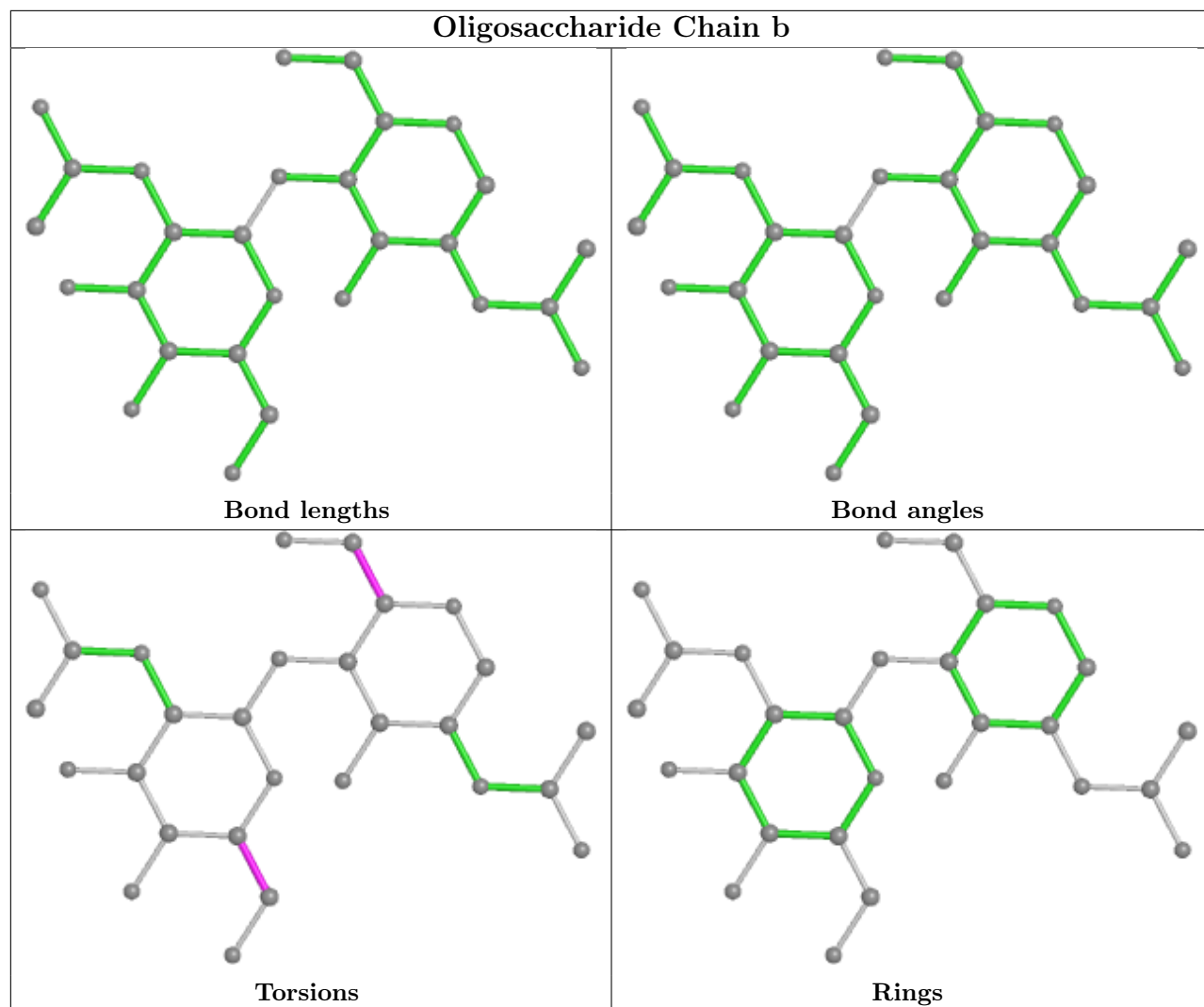




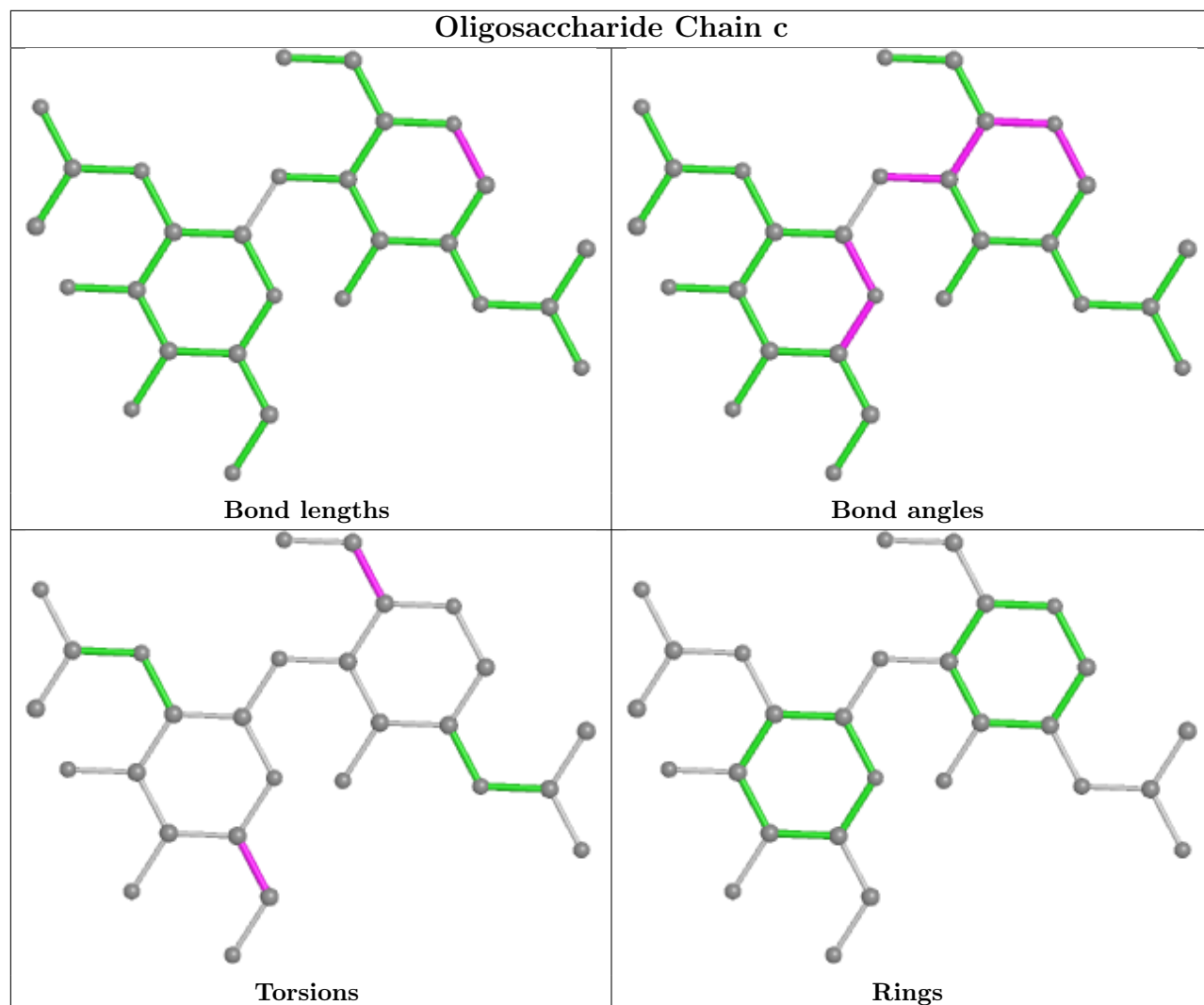


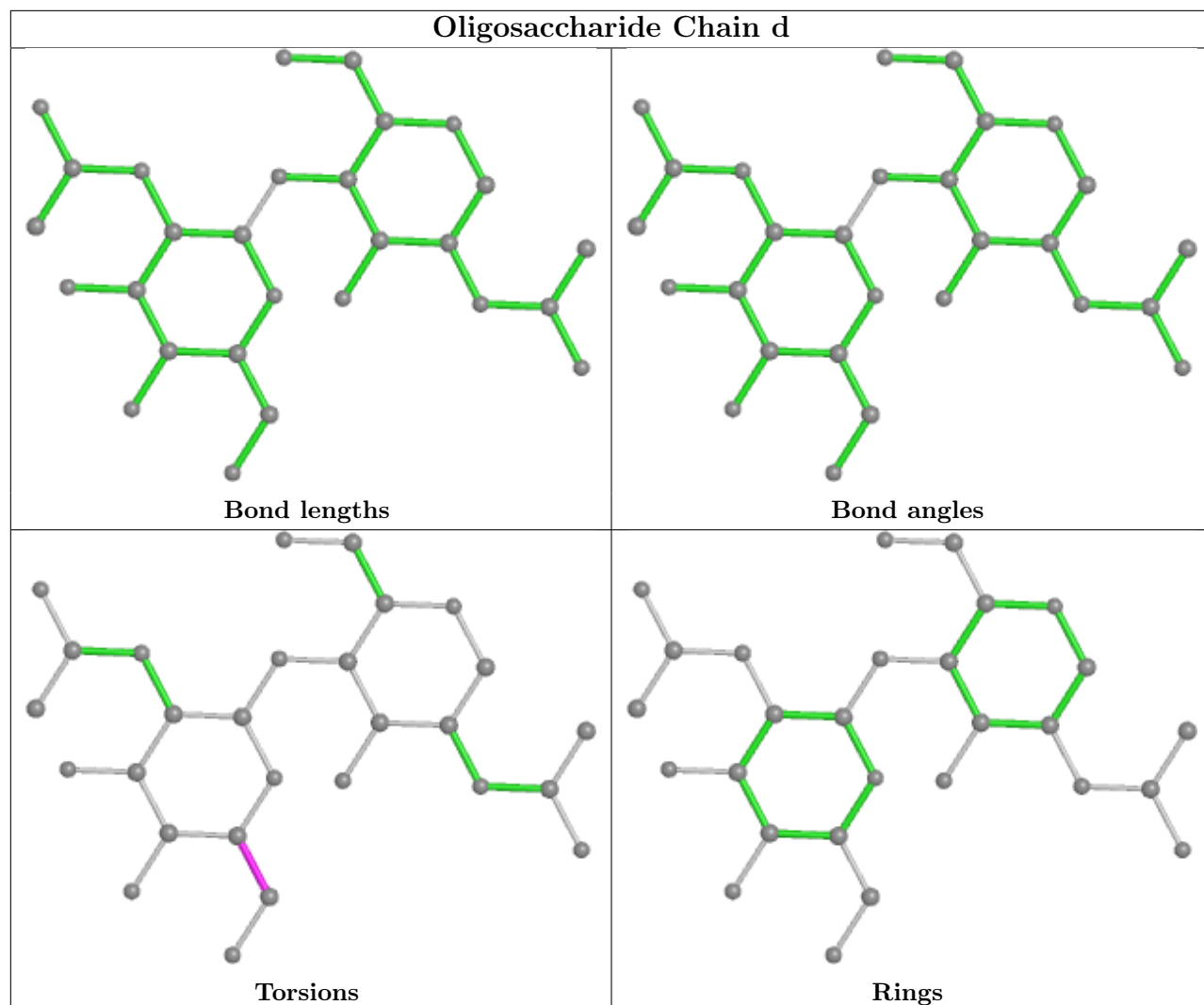


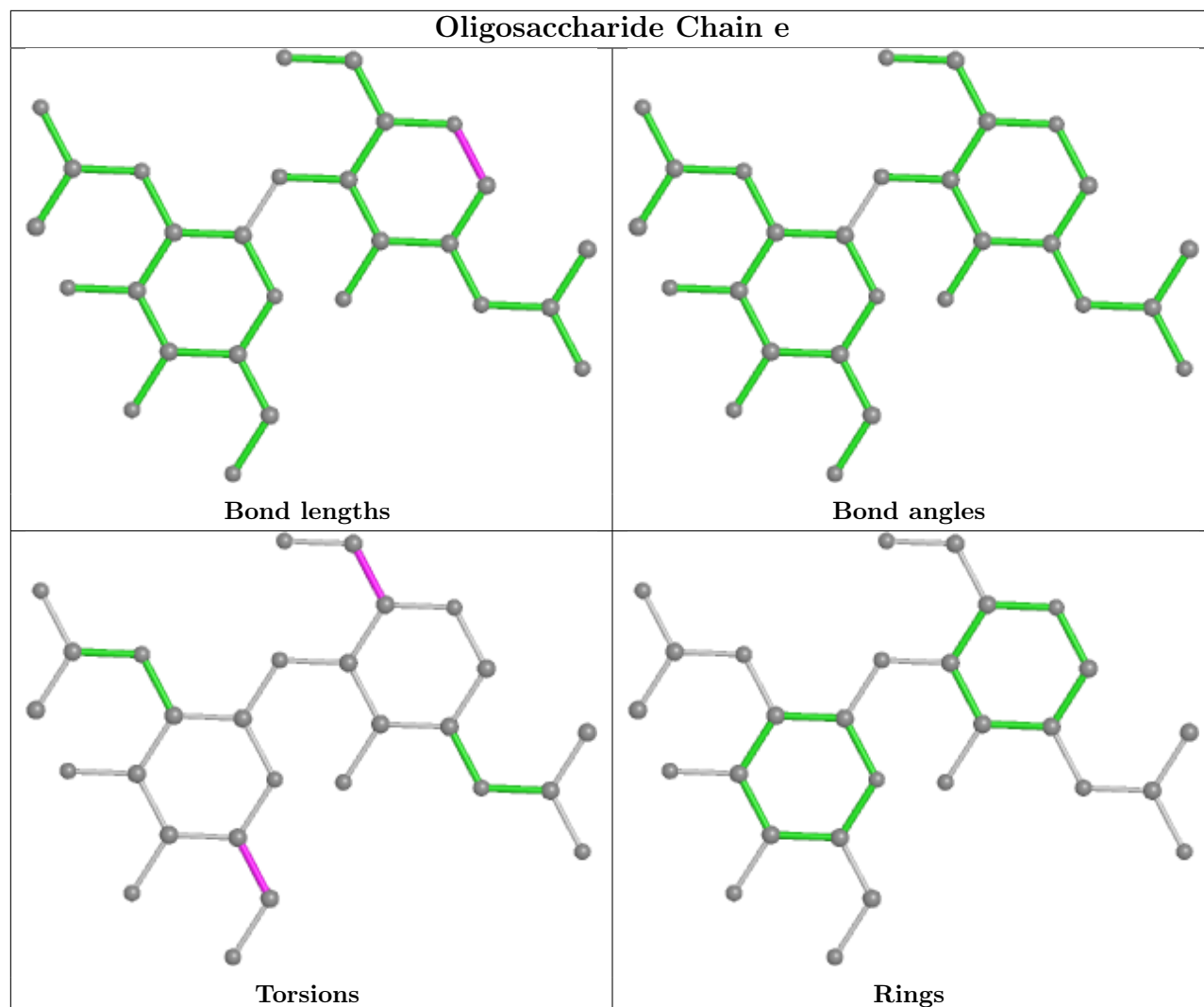


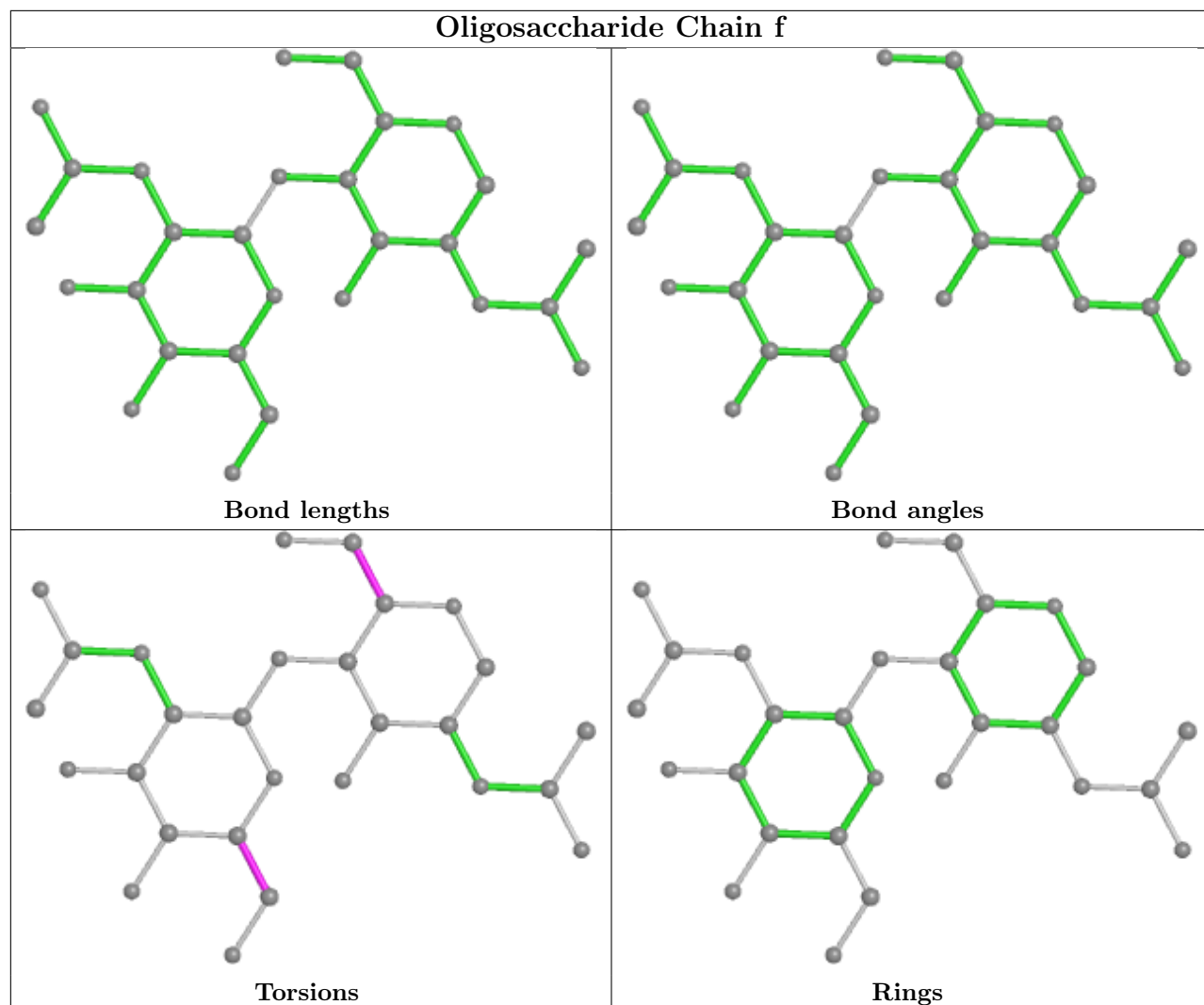


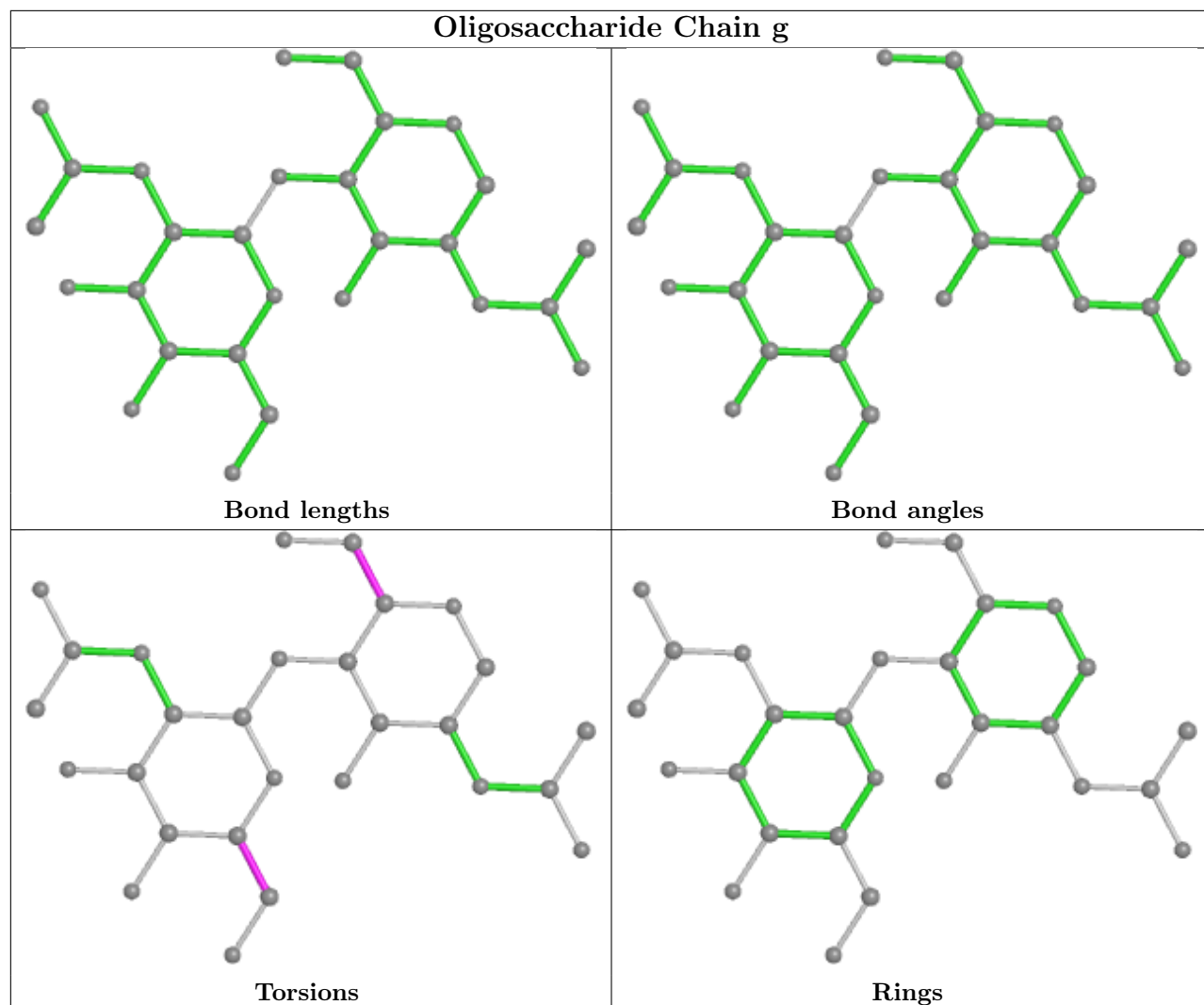


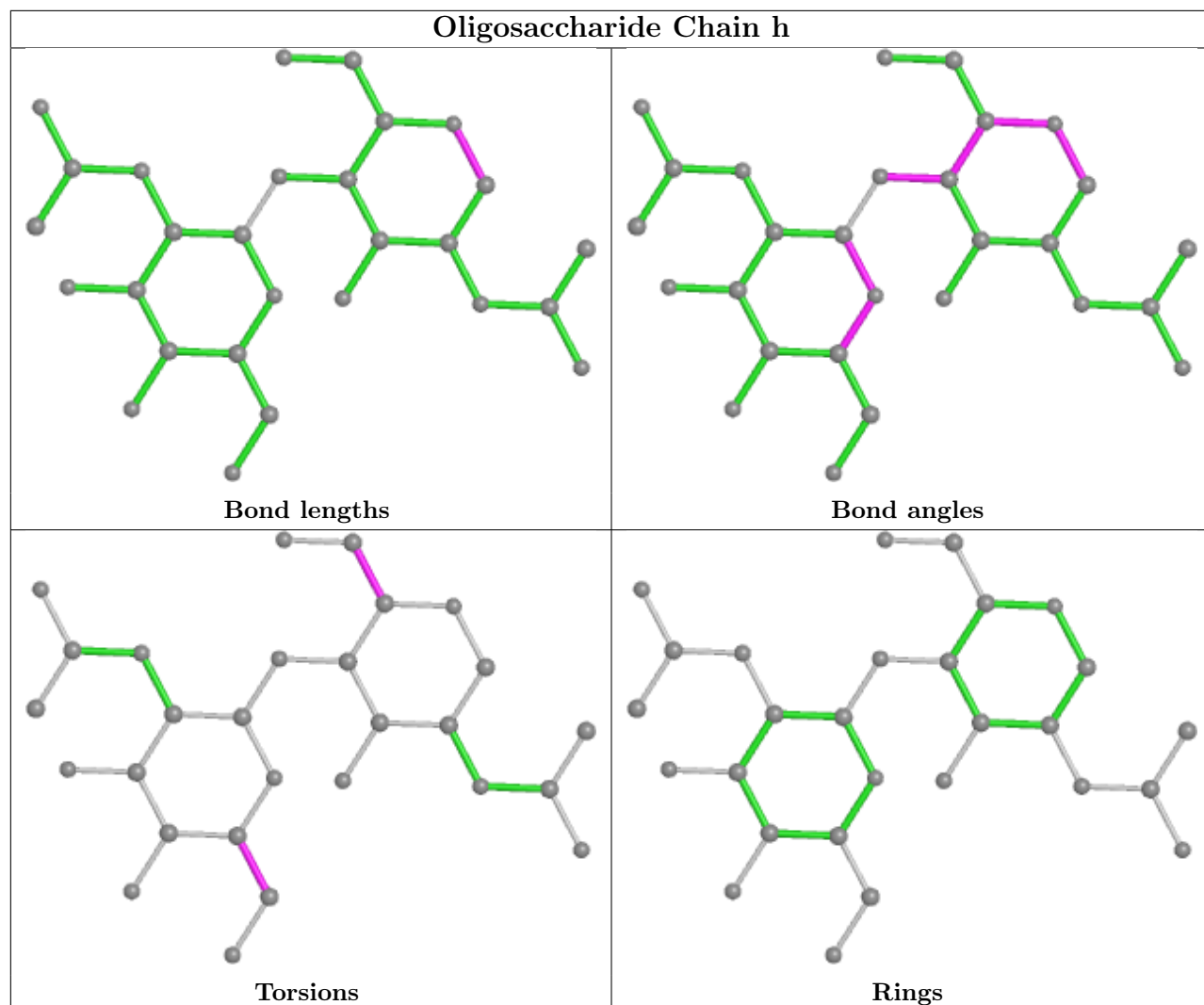


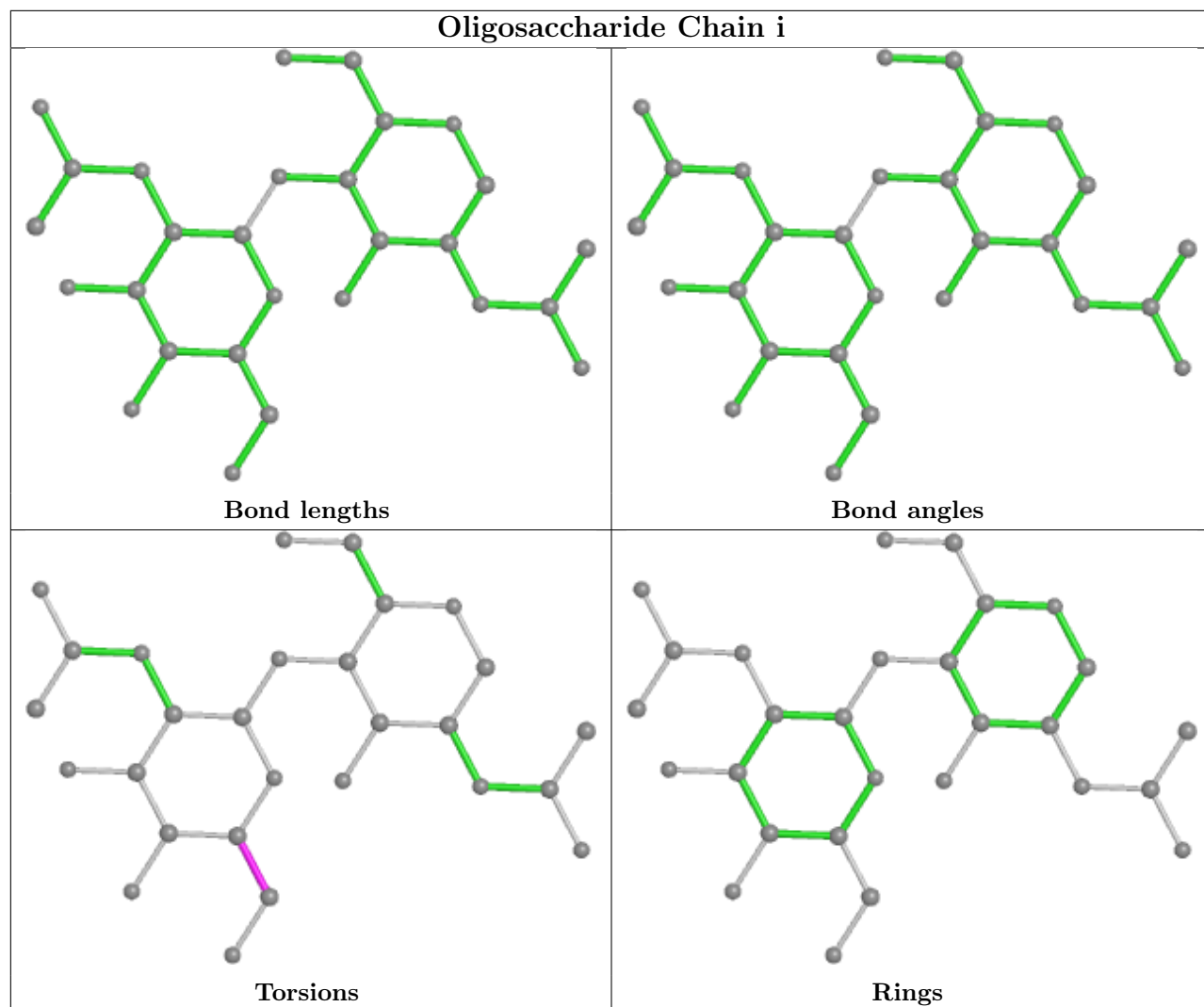


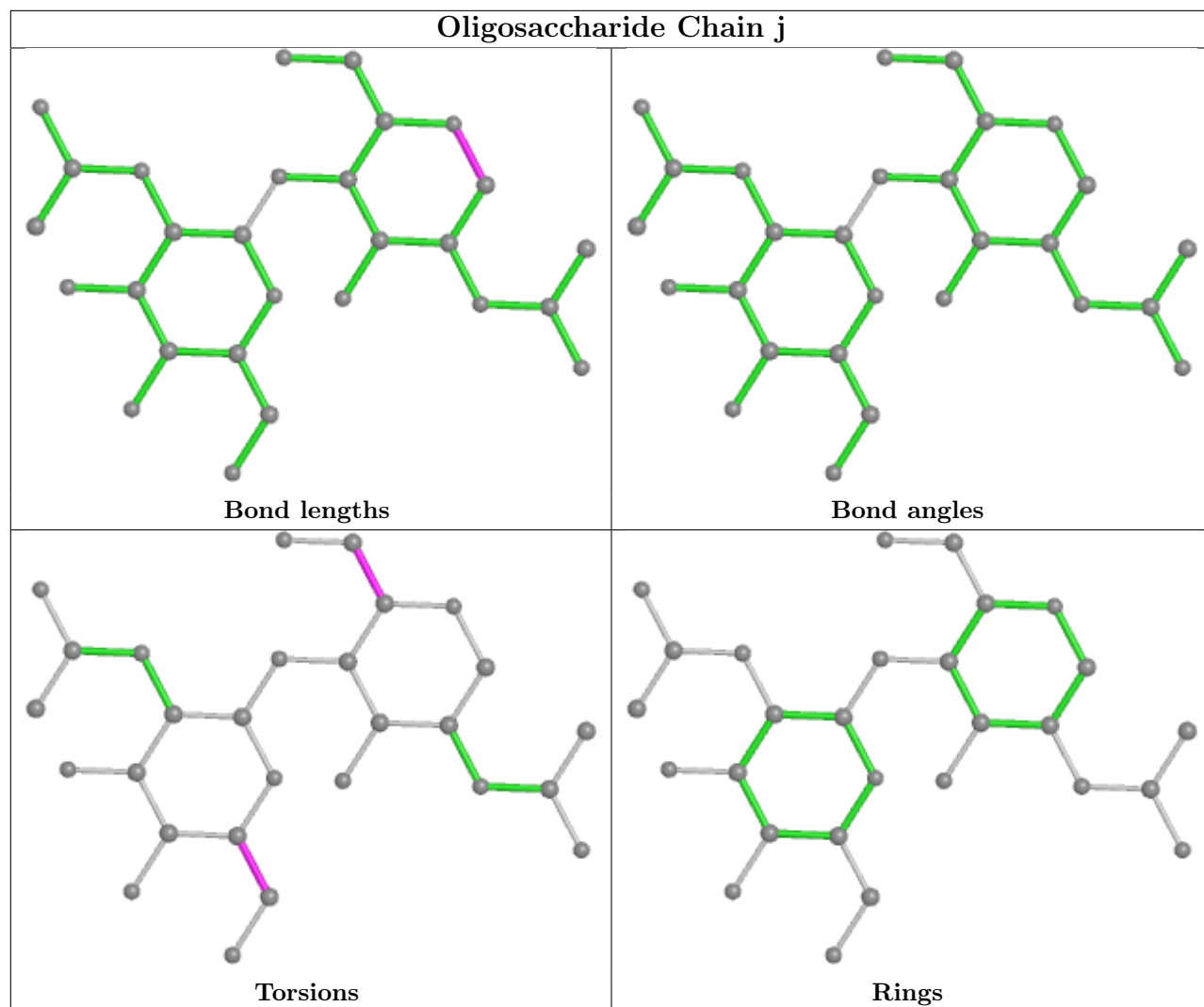




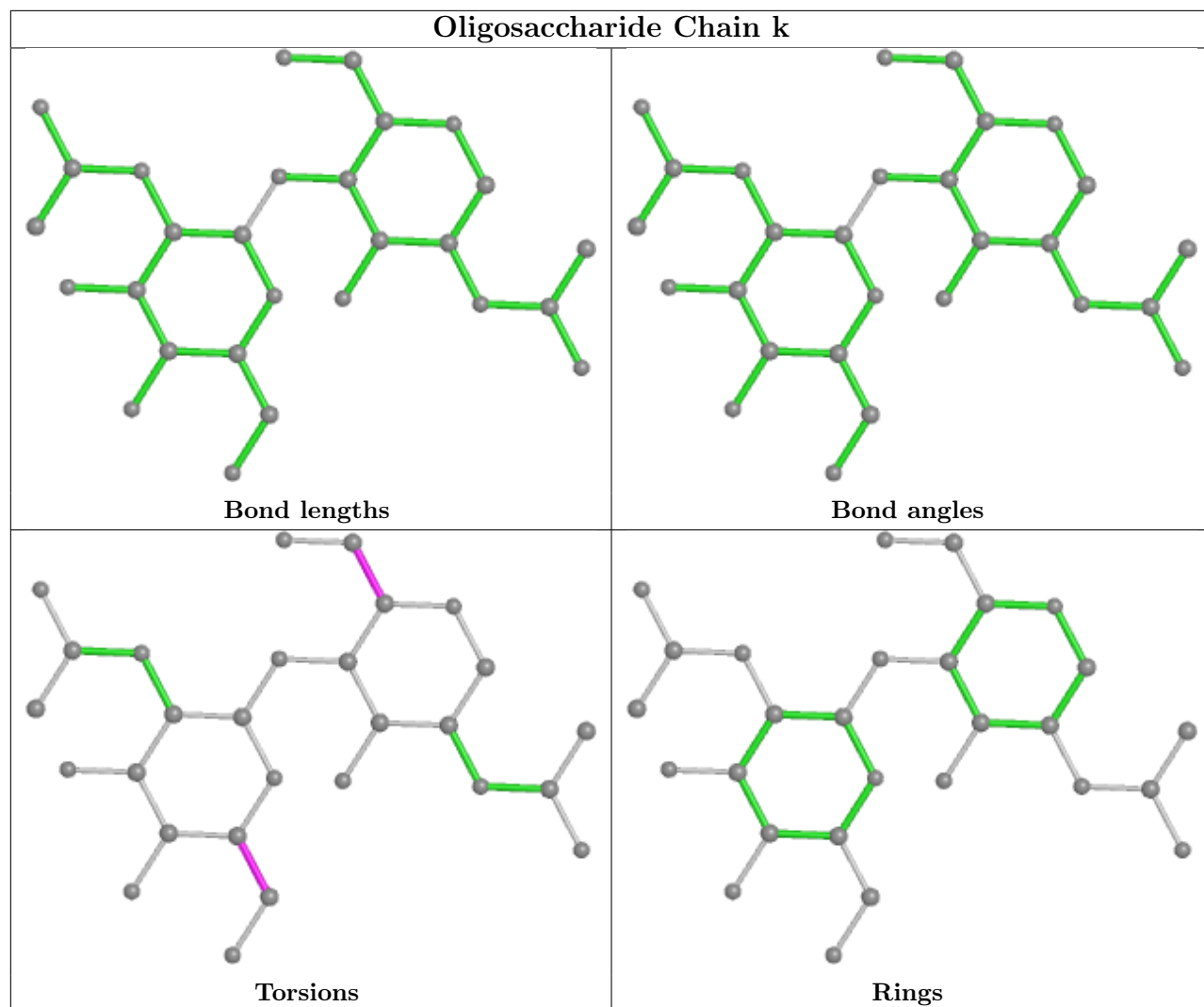


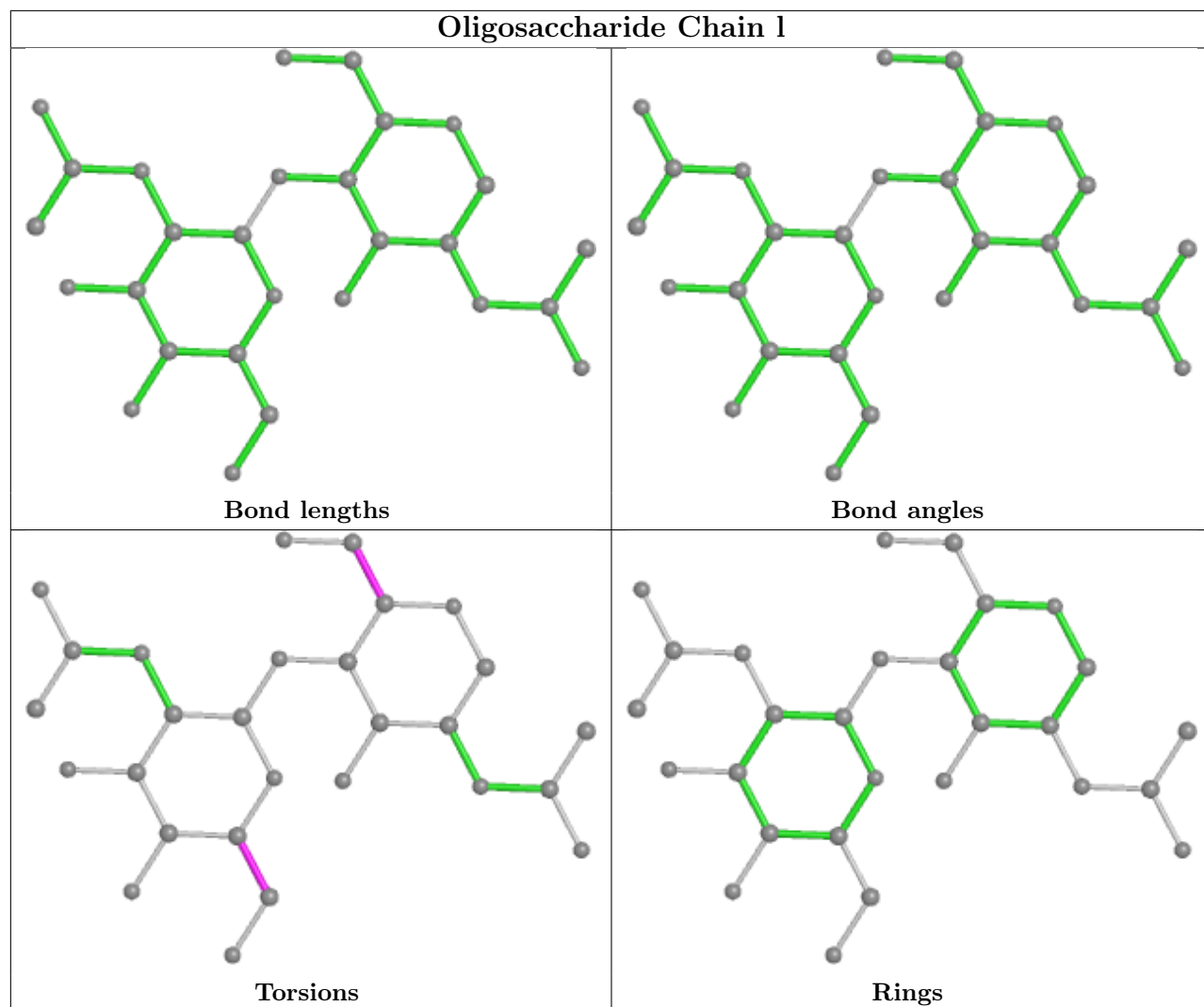


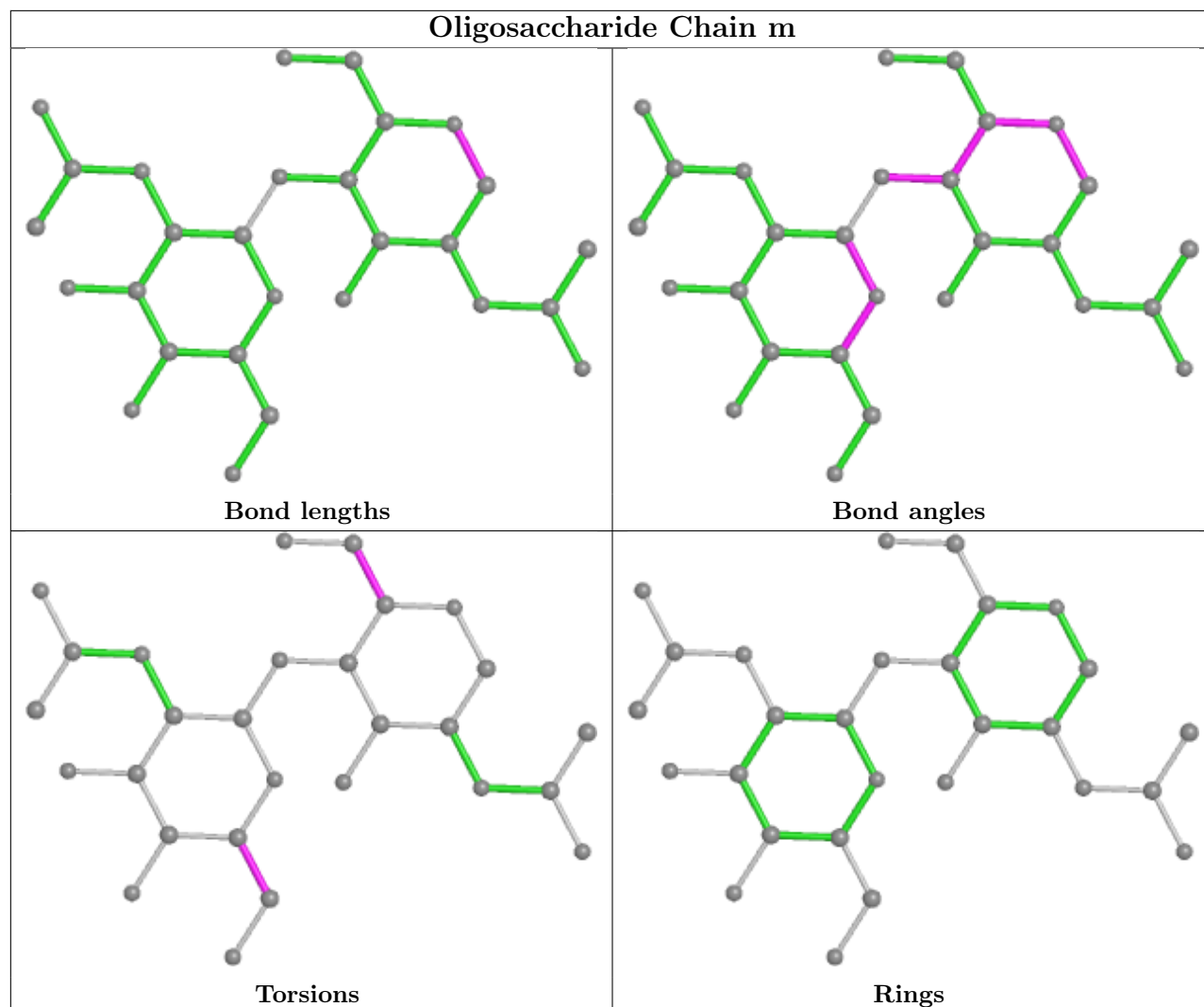


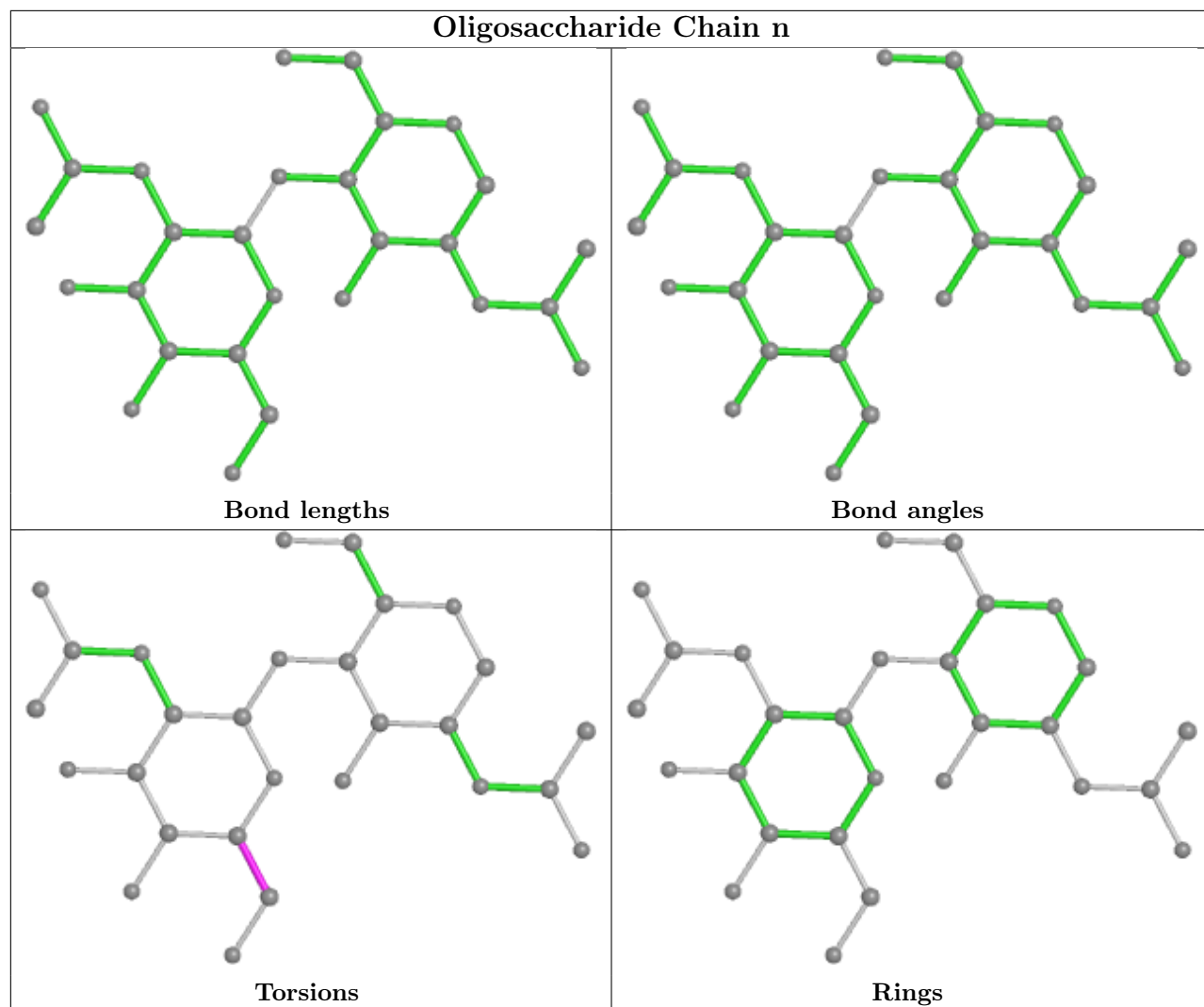


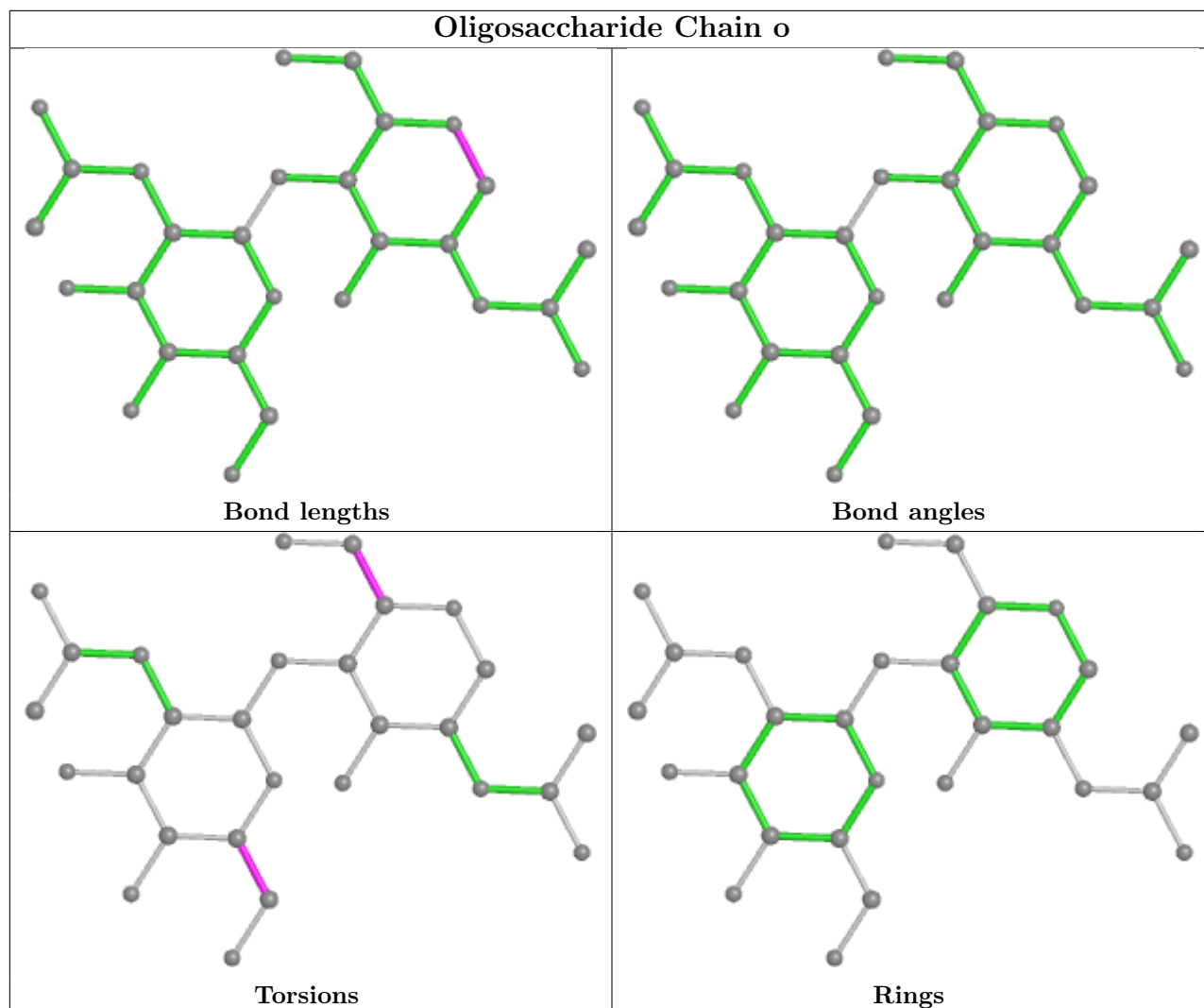












## 5.6 Ligand geometry [i](#)

34 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	$\# Z  > 2$
4	NAG	A	1405	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
4	NAG	B	1412	4	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	C	1408	1	14,14,15	0.29	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	901	2	14,14,15	0.49	0	17,19,21	0.48	0
4	NAG	C	1410	1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	B	1407	4	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	B	1411	1,4	14,14,15	0.40	0	17,19,21	1.15	1 (5%)
4	NAG	C	1404	1	14,14,15	0.46	0	17,19,21	0.54	0
4	NAG	C	1406	1,4	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	E	901	2	14,14,15	0.49	0	17,19,21	0.48	0
4	NAG	B	1403	1	14,14,15	0.19	0	17,19,21	0.39	0
4	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.62	0
4	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	B	1401	1	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	C	1407	4	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
4	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	B	1406	1,4	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
4	NAG	C	1409	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1403	1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	F	901	2	14,14,15	0.49	0	17,19,21	0.47	0
4	NAG	B	1409	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	A	1409	1	14,14,15	0.51	0	17,19,21	0.36	0
4	NAG	C	1401	1	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	C	1405	1	14,14,15	0.56	0	17,19,21	1.25	1 (5%)
4	NAG	A	1404	1	14,14,15	0.45	0	17,19,21	0.54	0
4	NAG	B	1404	1	14,14,15	0.46	0	17,19,21	0.55	0
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	A	1401	1	14,14,15	0.32	0	17,19,21	0.34	0
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	B	1408	1	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	NAG	B	1410	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	B	1405	1	14,14,15	0.56	0	17,19,21	1.24	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1412	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	F	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	4.27	128.98	122.90
4	A	1405	NAG	C2-N2-C7	4.25	128.96	122.90
4	B	1405	NAG	C2-N2-C7	4.22	128.91	122.90
4	B	1408	NAG	C1-O5-C5	2.41	115.46	112.19
4	C	1406	NAG	C8-C7-N2	2.38	120.13	116.10

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6

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.



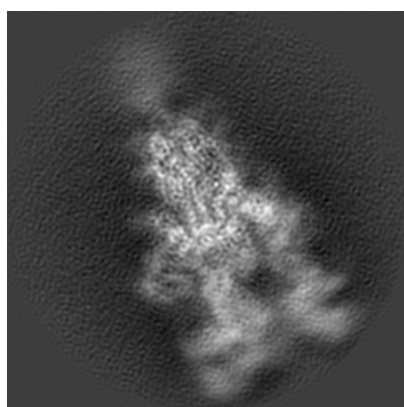
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30460. These allow visual inspection of the internal detail of the map and identification of artifacts.

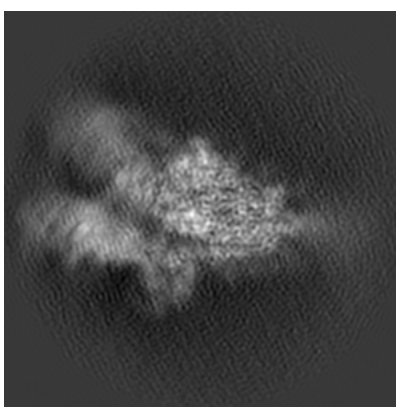
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

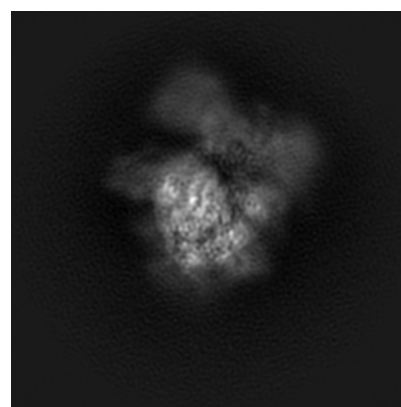
#### 6.1.1 Primary map



X



Y

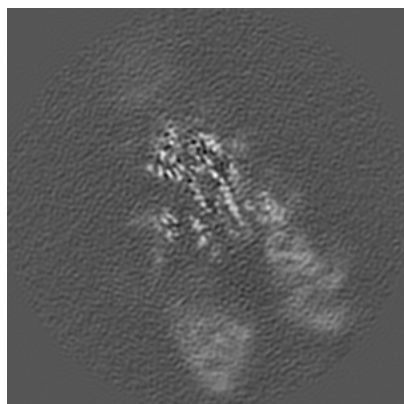


Z

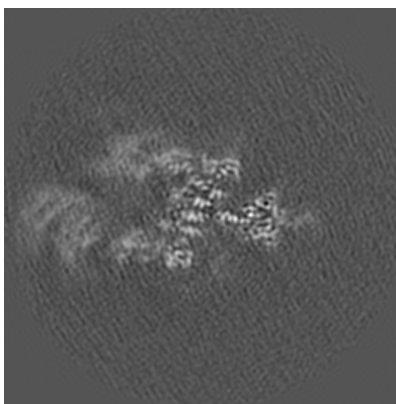
The images above show the map projected in three orthogonal directions.

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

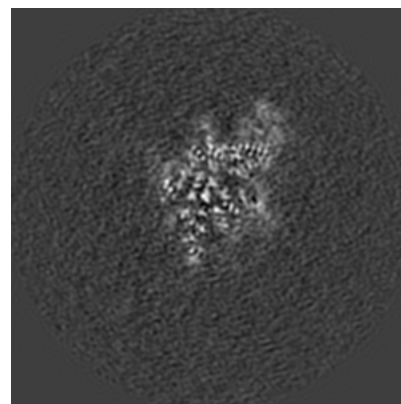
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

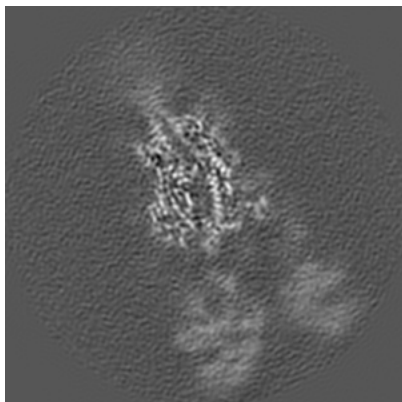


Z Index: 144

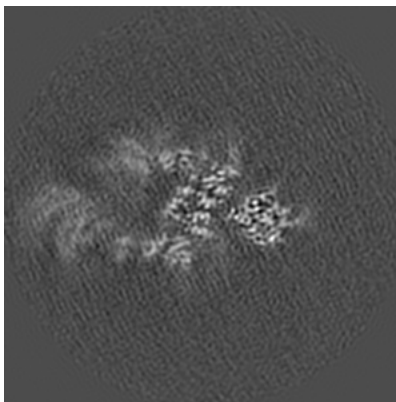
The images above show central slices of the map in three orthogonal directions.

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

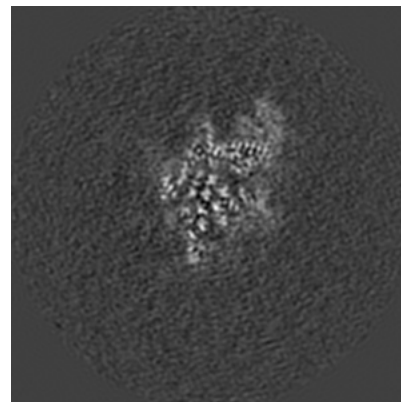
### 6.3.1 Primary map



X Index: 130



Y Index: 141



Z Index: 143

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

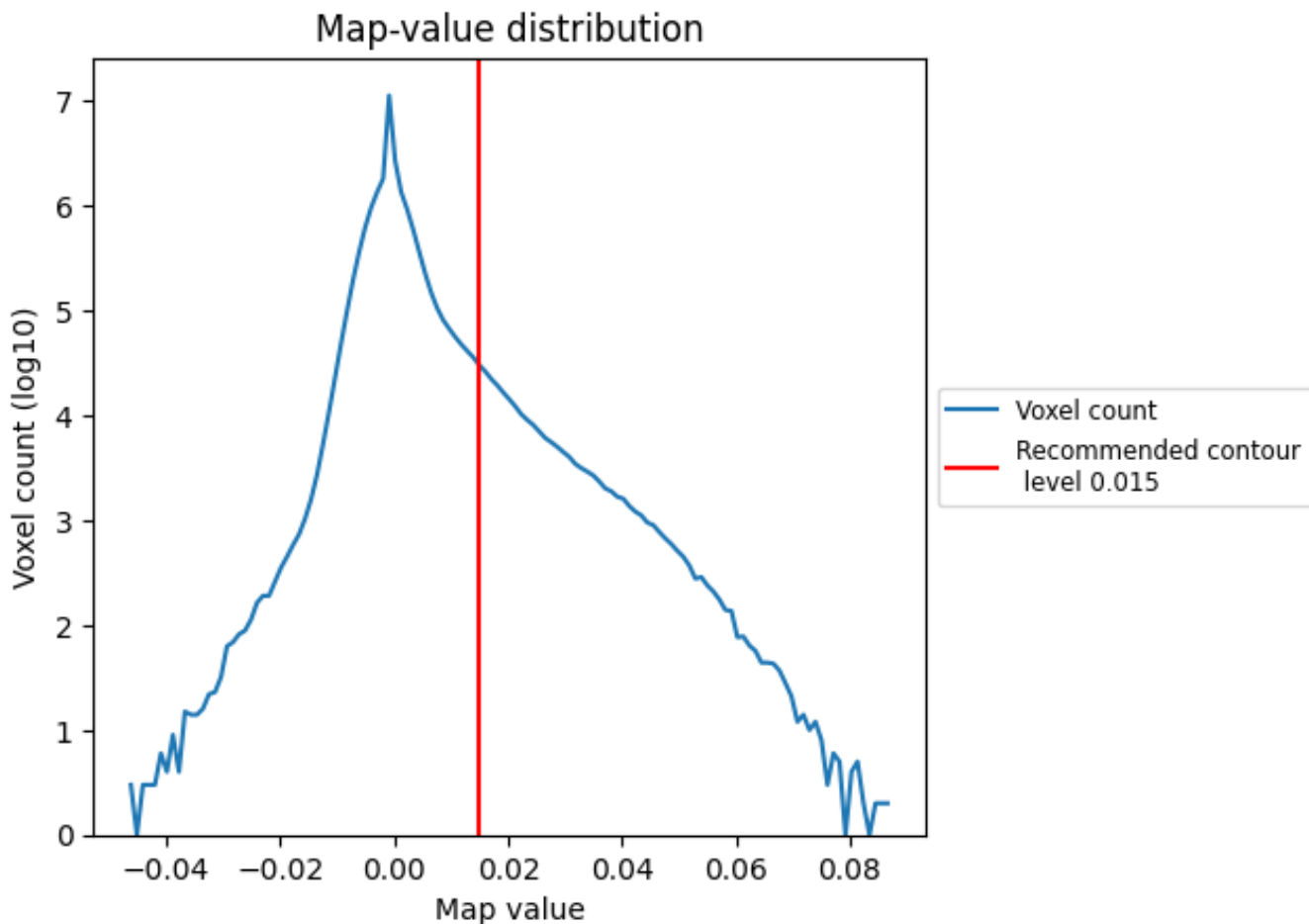
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

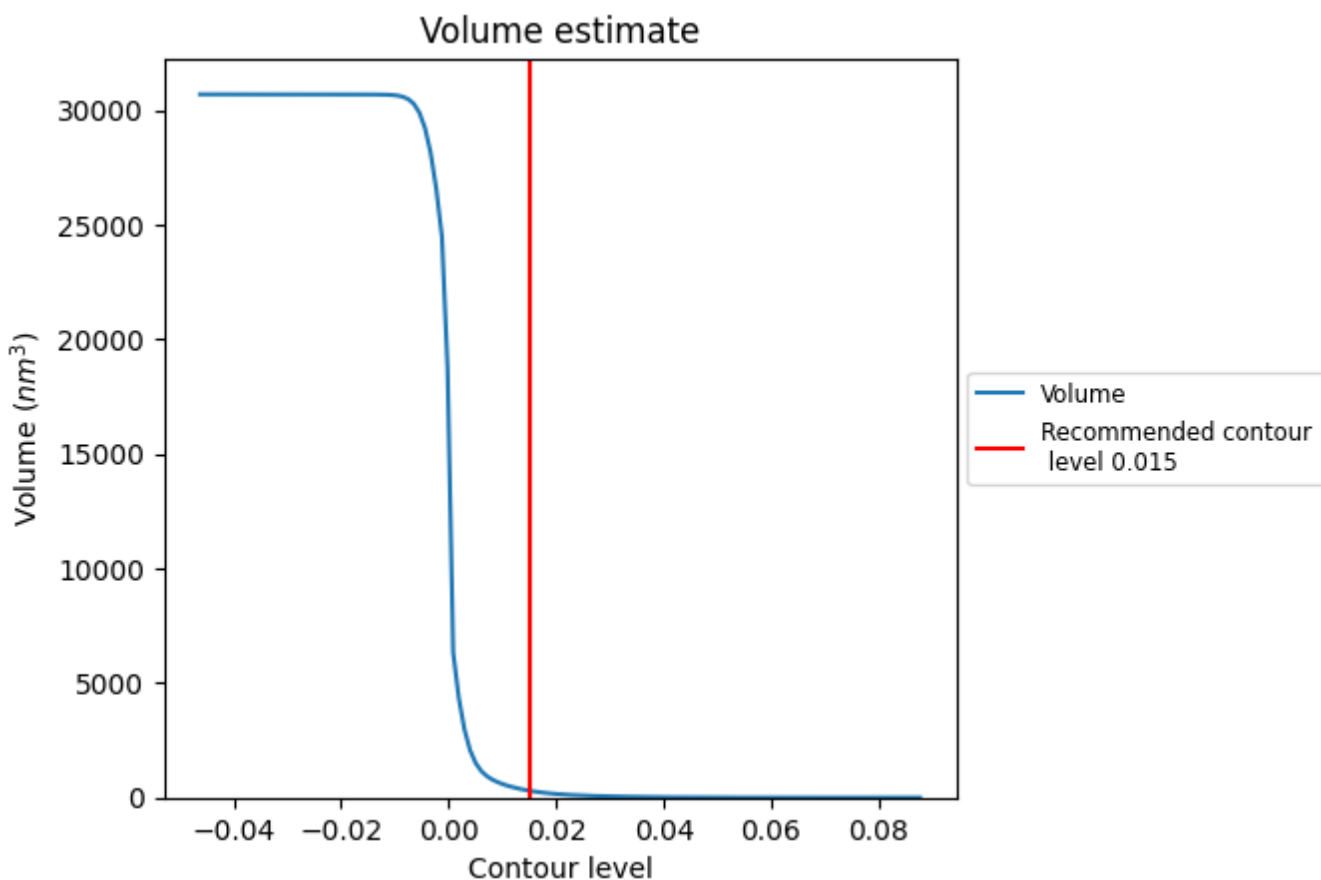
This section contains the results of statistical analysis of the map.

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



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

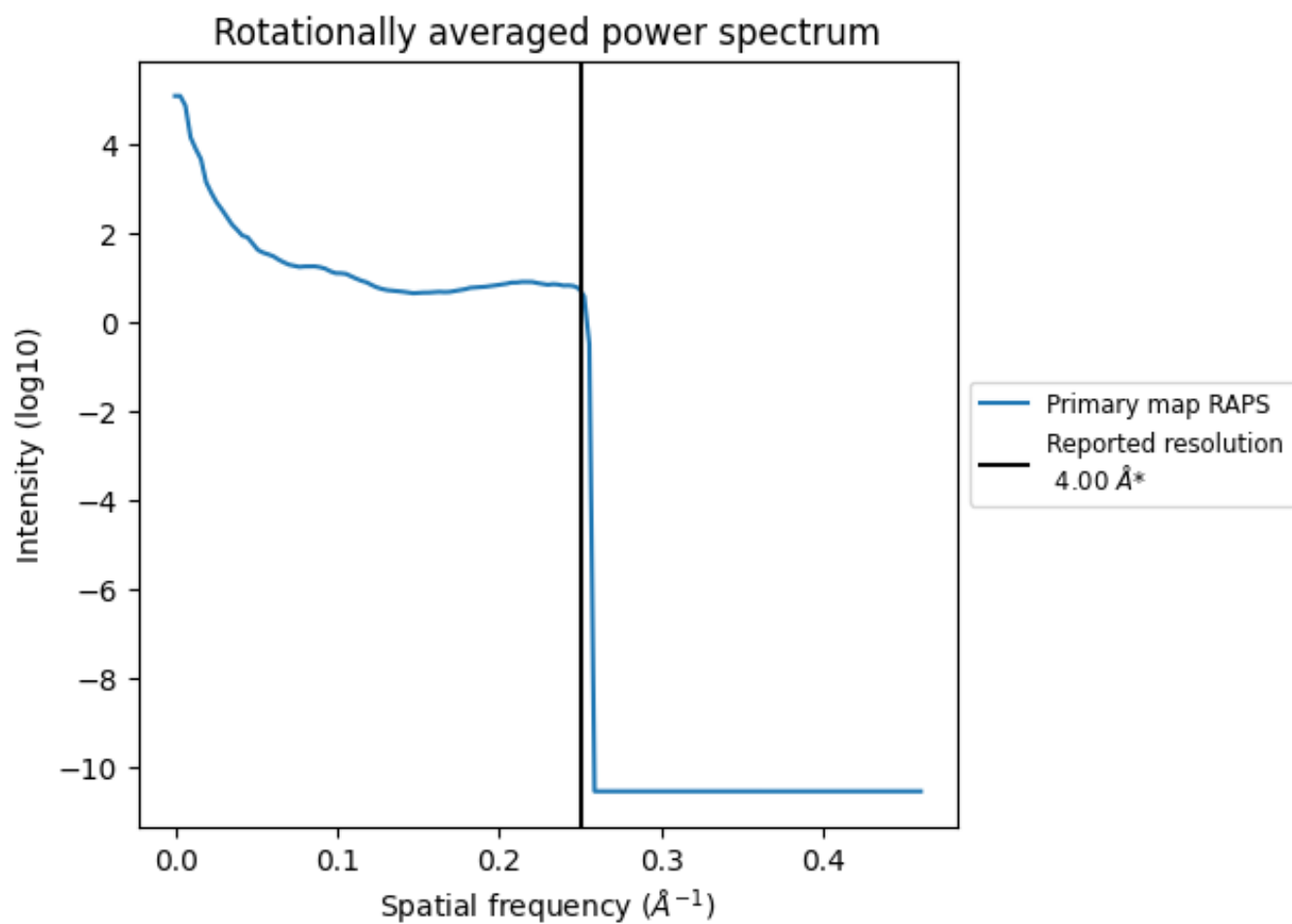
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299  $\text{nm}^3$ ; this corresponds to an approximate mass of 270 kDa.

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

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



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

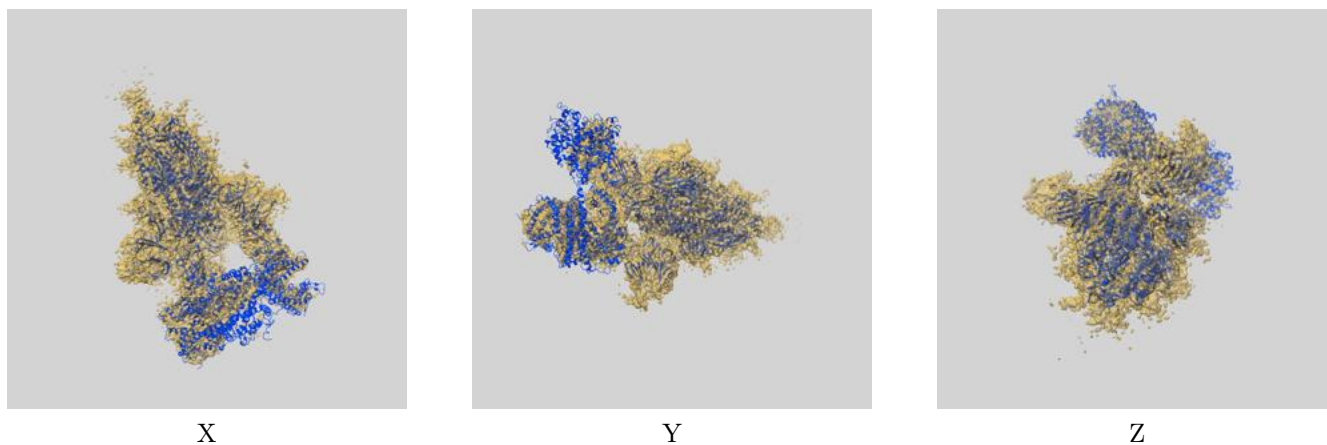
## 8 Fourier-Shell correlation

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-30460 and PDB model 7CT5. Per-residue inclusion information can be found in section 3 on page 15.

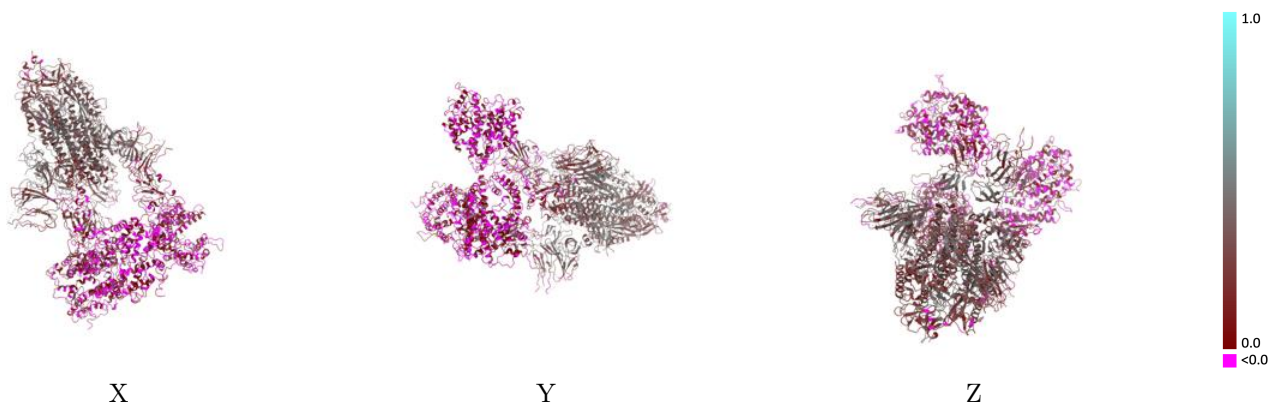
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

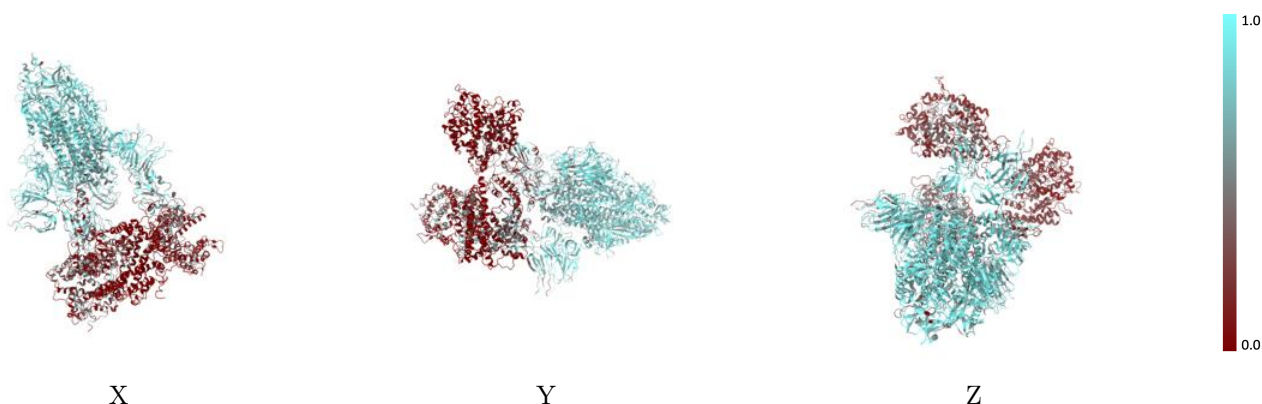


## 9.2 Q-score mapped to coordinate model [i](#)



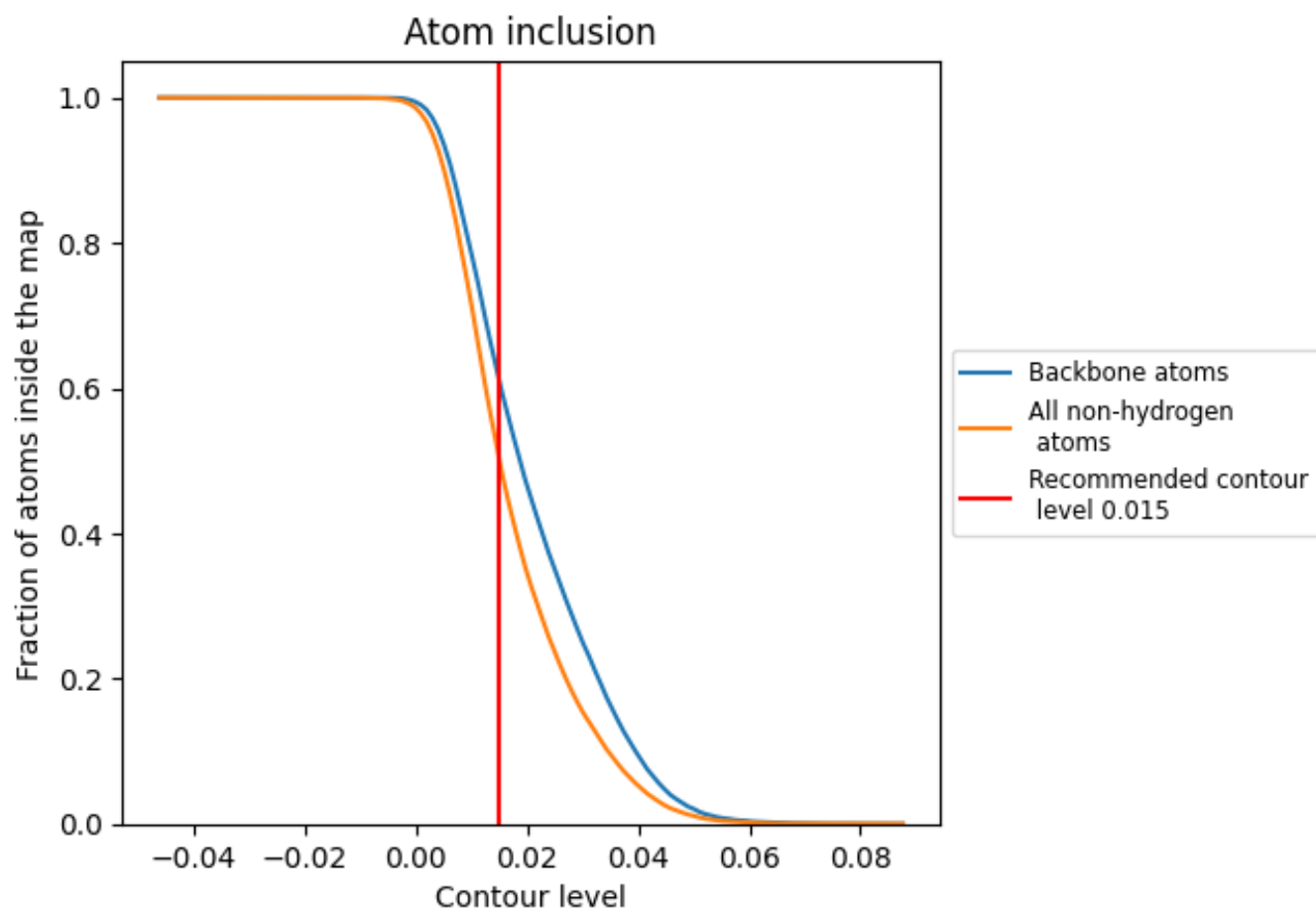
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 50% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5012	 0.1860
A	 0.6999	 0.2650
B	 0.7001	 0.2710
C	 0.7354	 0.2970
D	 0.1485	 0.0320
E	 0.0487	 0.0180
F	 0.2966	 0.0630
G	 0.7143	 0.3250
H	 0.3571	 0.1000
I	 0.7143	 0.3640
J	 0.7143	 0.3390
K	 0.5357	 0.2820
L	 0.7500	 0.2860
M	 0.5714	 0.2910
N	 0.0714	 0.0170
O	 0.4643	 0.2090
P	 0.6071	 0.2600
Q	 0.6786	 0.2600
R	 0.7143	 0.2600
S	 0.7500	 0.3610
T	 0.4643	 0.3000
U	 0.4643	 0.2050
V	 0.6786	 0.3760
W	 0.6429	 0.2440
X	 0.2857	 0.0940
Y	 0.8214	 0.2980
Z	 0.7143	 0.3070
a	 0.0000	 -0.0170
b	 0.0000	 -0.0750
c	 0.0000	 0.0180
d	 0.0000	 0.1300
e	 0.0000	 0.1150
f	 0.0000	 -0.0890
g	 0.0000	 -0.0210
h	 0.0000	 0.1310



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Chain	Atom inclusion	Q-score
i	 0.0000	 -0.0670
j	 0.0000	 0.0730
k	 0.0000	 -0.0600
l	 0.1429	 -0.0620
m	 0.0714	 0.0520
n	 0.0000	 0.1620
o	 0.1071	 0.1620