



## wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 05:53 AM EST

PDB ID : 7RSO  
EMDB ID : EMD-24676  
Title : AMC016 SOSIP.v4.2 in complex with PGV04 Fab  
Authors : Bader, D.L.V.; Cottrell, C.A.; Ward, A.B.  
Deposited on : 2021-08-11  
Resolution : 4.10 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:

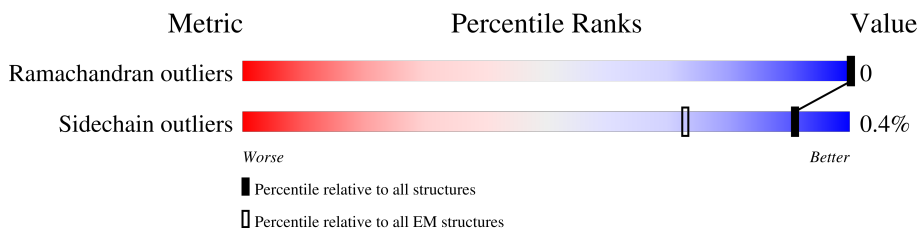
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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





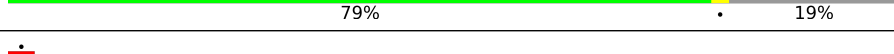




The reported resolution of this entry is 4.10 Å.

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.





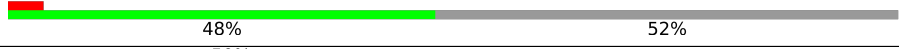
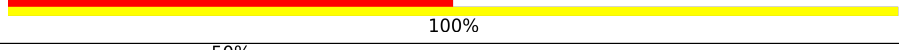
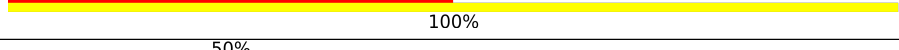

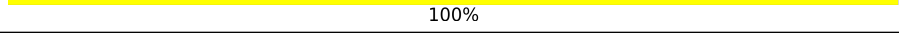
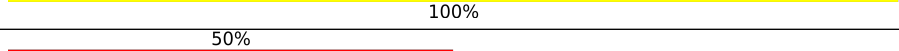
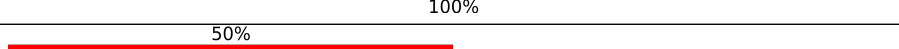
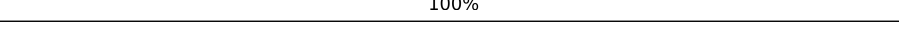
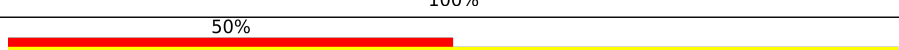
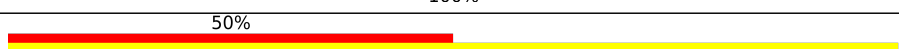
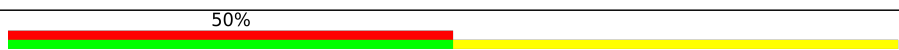
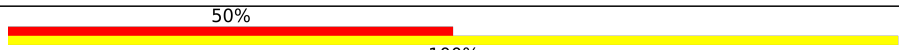
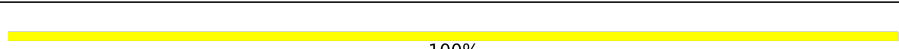


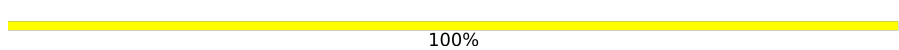
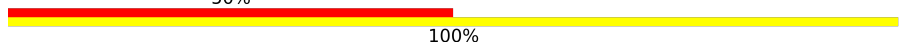


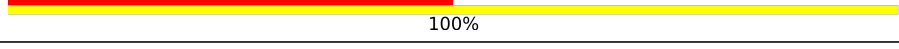
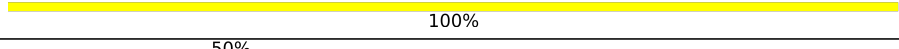
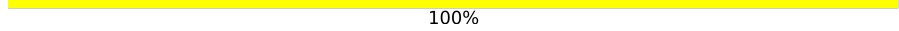

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	486	 87%      • 10%
1	C	486	 87%      • 10%
1	D	486	 87%      • 10%
2	B	154	 79%      • 19%
2	E	154	 79%      • 19%
2	F	154	 79%      • 19%
3	G	229	 52%      • 46%
3	H	229	 52%      • 46%
3	I	229	 52%      • 46%

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Mol	Chain	Length	Quality of chain
4	J	208	 48% 52%
4	K	208	 48% 52%
4	L	208	 48% 52%
5	M	2	 50% 100%
5	N	2	 50% 100%
5	R	2	 50% 50%
5	S	2	 50% 100%
5	T	2	 100%
5	U	2	 50% 100%
5	V	2	 50% 100%
5	X	2	 100%
5	Y	2	 50% 100%
5	Z	2	 50% 100%
5	d	2	 50% 50%
5	e	2	 50% 100%
5	f	2	 100%
5	g	2	 50% 100%
5	h	2	 50% 100%
5	j	2	 100%
5	k	2	 50% 100%
5	l	2	 50% 100%
5	p	2	 50% 50%
5	q	2	 50% 100%
5	r	2	 100%
5	s	2	 50% 100%

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Mol	Chain	Length	Quality of chain
5	t	2	50% 100%
5	v	2	100%
6	O	3	67% 100%
6	W	3	67% 100%
6	a	3	67% 100%
6	i	3	67% 100%
6	m	3	67% 100%
6	u	3	67% 100%
7	P	6	17% 17% 83%
7	b	6	17% 17% 83%
7	n	6	17% 17% 83%
8	Q	5	100%
8	c	5	100%
8	o	5	100%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20568 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 AMC016 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	437	Total	C	N	O	S	0	0
			3453	2175	602	650	26		
1	C	437	Total	C	N	O	S	0	0
			3453	2175	602	650	26		
1	D	437	Total	C	N	O	S	0	0
			3453	2175	602	650	26		

- Molecule 2 is a protein called AMC016 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	124	Total	C	N	O	S	0	0
			989	628	167	187	7		
2	E	124	Total	C	N	O	S	0	0
			989	628	167	187	7		
2	F	124	Total	C	N	O	S	0	0
			989	628	167	187	7		

- Molecule 3 is a protein called PGV04 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	124	Total	C	N	O	S	0	0
			985	627	177	178	3		
3	G	124	Total	C	N	O	S	0	0
			985	627	177	178	3		
3	I	124	Total	C	N	O	S	0	0
			985	627	177	178	3		

- Molecule 4 is a protein called PGV04 kappa chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	100	Total	C	N	O	S	0	0
			784	500	131	149	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
4	K	100	Total	C	N	O	S	0	0
			784	500	131	149	4		

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

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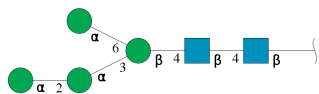
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	j	2	28	16	2	10	0	0
5	k	2	28	16	2	10	0	0
5	l	2	28	16	2	10	0	0
5	p	2	28	16	2	10	0	0
5	q	2	28	16	2	10	0	0
5	r	2	28	16	2	10	0	0
5	s	2	28	16	2	10	0	0
5	t	2	28	16	2	10	0	0
5	v	2	28	16	2	10	0	0

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



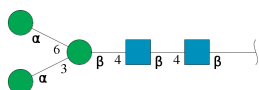
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	O	3	39	22	2	15	0	0
6	W	3	39	22	2	15	0	0
6	a	3	39	22	2	15	0	0
6	i	3	39	22	2	15	0	0
6	m	3	39	22	2	15	0	0
6	u	3	39	22	2	15	0	0

- 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
			Total	C	N	O		
7	P	6	72	40	2	30	0	0
7	b	6	72	40	2	30	0	0
7	n	6	72	40	2	30	0	0

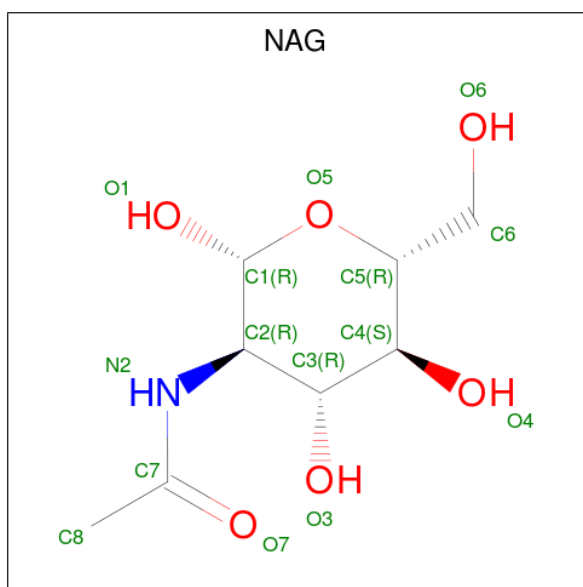
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	A	1	168	96	12	60	0
9	B	1	42	24	3	15	0
9	B	1	42	24	3	15	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	42	24	3	15	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	C	1	168	96	12	60	0
9	E	1	42	24	3	15	0
9	E	1	42	24	3	15	0
9	E	1	42	24	3	15	0
9	D	1	168	96	12	60	0
9	D	1	168	96	12	60	0
9	D	1	168	96	12	60	0
9	D	1	168	96	12	60	0
9	D	1	168	96	12	60	0

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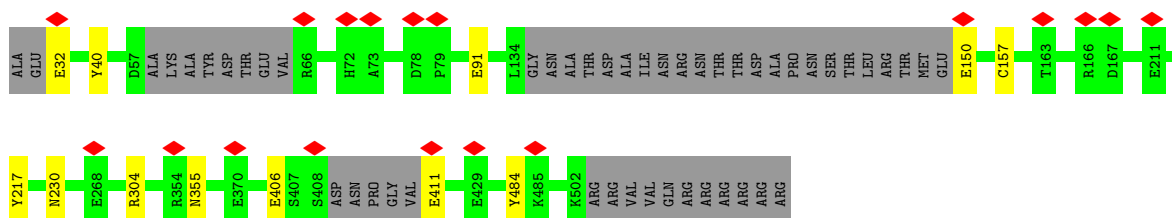
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	D	1	Total 168	96	12	60	0
9	F	1	Total 42	24	3	15	0
9	F	1	Total 42	24	3	15	0
9	F	1	Total 42	24	3	15	0

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


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

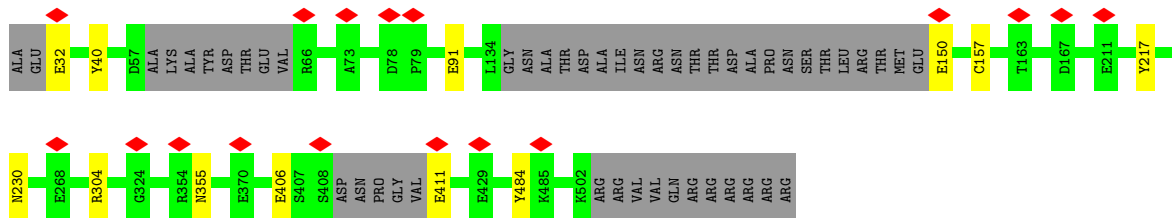
- Molecule 1: AMC016 gp120

Chain A:  87% 10%




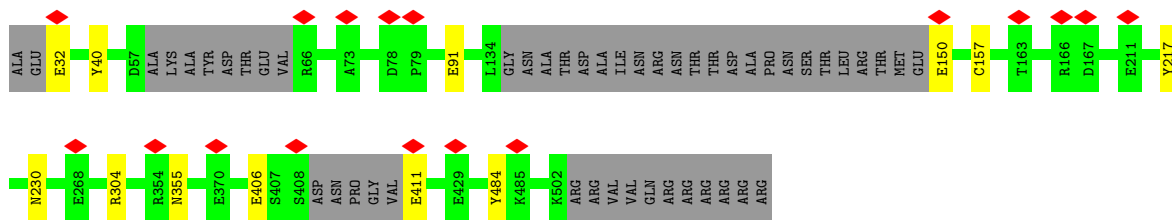
- Molecule 1: AMC016 gp120

Chain C:  87% 10%




- Molecule 1: AMC016 gp120

Chain D:  87% 10%



- Molecule 2: AMC016 gp41

Chain B:  79% 19%







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



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



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



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



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




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





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

Chain X:  100%



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

Chain Y:  50%  
100%



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

Chain Z:  50%  
100%



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

Chain d:  50%  
50% 50%




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

Chain e:  50%  
100%



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

Chain f:  100%



MAG1  
MAG2

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

MAG1  
MAG2

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

MAG1  
MAG2

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

MAG1  
MAG2

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

MAG1  
MAG2

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

MAG1  
MAG2

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





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



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



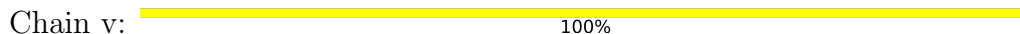
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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



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



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



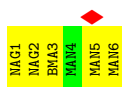
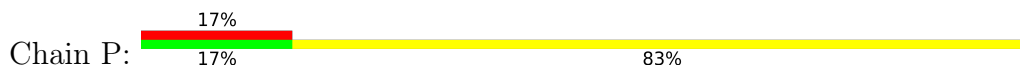
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



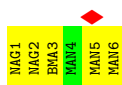
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



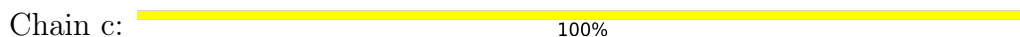
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



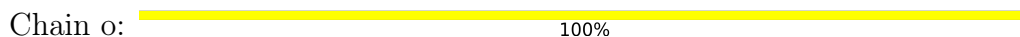
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	77068	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.708	Depositor
Minimum map value	-1.449	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	1.05	9/3527 (0.3%)	0.90	4/4790 (0.1%)
1	C	1.05	9/3527 (0.3%)	0.90	4/4790 (0.1%)
1	D	1.05	9/3527 (0.3%)	0.90	4/4790 (0.1%)
2	B	1.13	3/1006 (0.3%)	0.78	0/1362
2	E	1.13	3/1006 (0.3%)	0.78	0/1362
2	F	1.13	3/1006 (0.3%)	0.78	0/1362
3	G	1.18	6/1011 (0.6%)	0.95	1/1371 (0.1%)
3	H	1.18	6/1011 (0.6%)	0.95	1/1371 (0.1%)
3	I	1.18	6/1011 (0.6%)	0.95	1/1371 (0.1%)
4	J	1.06	0/804	0.93	1/1087 (0.1%)
4	K	1.06	0/804	0.93	1/1087 (0.1%)
4	L	1.06	0/804	0.93	1/1087 (0.1%)
All	All	1.09	54/19044 (0.3%)	0.89	18/25830 (0.1%)

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	100(E)	TYR	CB-CG	-10.93	1.35	1.51
3	I	100(E)	TYR	CB-CG	-10.93	1.35	1.51
3	H	100(E)	TYR	CB-CG	-10.92	1.35	1.51
1	C	484	TYR	CB-CG	-9.04	1.38	1.51
1	D	484	TYR	CB-CG	-9.03	1.38	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	C	484	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	D	484	TYR	CB-CG-CD1	-7.69	116.38	121.00
1	A	217	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	D	217	TYR	CB-CG-CD2	-7.02	116.79	121.00

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	429/486 (88%)	422 (98%)	7 (2%)	0	100	100
1	C	429/486 (88%)	422 (98%)	7 (2%)	0	100	100
1	D	429/486 (88%)	422 (98%)	7 (2%)	0	100	100
2	B	120/154 (78%)	119 (99%)	1 (1%)	0	100	100
2	E	120/154 (78%)	119 (99%)	1 (1%)	0	100	100
2	F	120/154 (78%)	119 (99%)	1 (1%)	0	100	100
3	G	122/229 (53%)	122 (100%)	0	0	100	100
3	H	122/229 (53%)	122 (100%)	0	0	100	100
3	I	122/229 (53%)	122 (100%)	0	0	100	100
4	J	98/208 (47%)	95 (97%)	3 (3%)	0	100	100
4	K	98/208 (47%)	95 (97%)	3 (3%)	0	100	100
4	L	98/208 (47%)	95 (97%)	3 (3%)	0	100	100
All	All	2307/3231 (71%)	2274 (99%)	33 (1%)	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	393/434 (91%)	391 (100%)	2 (0%)	88	93
1	C	393/434 (91%)	391 (100%)	2 (0%)	88	93
1	D	393/434 (91%)	391 (100%)	2 (0%)	88	93
2	B	107/130 (82%)	107 (100%)	0	100	100
2	E	107/130 (82%)	107 (100%)	0	100	100
2	F	107/130 (82%)	107 (100%)	0	100	100
3	G	103/194 (53%)	102 (99%)	1 (1%)	76	85
3	H	103/194 (53%)	102 (99%)	1 (1%)	76	85
3	I	103/194 (53%)	102 (99%)	1 (1%)	76	85
4	J	85/182 (47%)	85 (100%)	0	100	100
4	K	85/182 (47%)	85 (100%)	0	100	100
4	L	85/182 (47%)	85 (100%)	0	100	100
All	All	2064/2820 (73%)	2055 (100%)	9 (0%)	91	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	71	ARG
3	I	71	ARG
1	C	230	ASN
1	C	355	ASN
1	D	230	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

99 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	M	1	1,5	14,14,15	2.14	6 (42%)	17,19,21	1.08	2 (11%)
5	NAG	M	2	5	14,14,15	2.01	6 (42%)	17,19,21	0.94	1 (5%)
5	NAG	N	1	1,5	14,14,15	2.35	6 (42%)	17,19,21	1.02	1 (5%)
5	NAG	N	2	5	14,14,15	2.04	7 (50%)	17,19,21	0.92	1 (5%)
6	NAG	O	1	1,6	14,14,15	2.06	5 (35%)	17,19,21	1.18	1 (5%)
6	NAG	O	2	6	14,14,15	2.09	6 (42%)	17,19,21	0.90	1 (5%)
6	BMA	O	3	6	11,11,12	2.02	5 (45%)	15,15,17	0.72	0
7	NAG	P	1	1,7	14,14,15	2.04	6 (42%)	17,19,21	1.11	1 (5%)
7	NAG	P	2	7	14,14,15	1.97	6 (42%)	17,19,21	0.96	1 (5%)
7	BMA	P	3	7	11,11,12	1.47	3 (27%)	15,15,17	0.62	0
7	MAN	P	4	7	11,11,12	0.80	0	15,15,17	0.90	0
7	MAN	P	5	7	11,11,12	2.02	6 (54%)	15,15,17	0.71	0
7	MAN	P	6	7	11,11,12	1.96	5 (45%)	15,15,17	0.72	0
8	NAG	Q	1	1,8	14,14,15	2.09	6 (42%)	17,19,21	1.08	2 (11%)
8	NAG	Q	2	8	14,14,15	2.02	6 (42%)	17,19,21	1.04	2 (11%)
8	BMA	Q	3	8	11,11,12	1.51	3 (27%)	15,15,17	0.62	0
8	MAN	Q	4	8	11,11,12	1.95	6 (54%)	15,15,17	0.77	0
8	MAN	Q	5	8	11,11,12	1.95	5 (45%)	15,15,17	0.73	0
5	NAG	R	1	1,5	14,14,15	0.56	0	17,19,21	1.20	1 (5%)
5	NAG	R	2	5	14,14,15	0.32	0	17,19,21	0.67	0
5	NAG	S	1	1,5	14,14,15	2.10	6 (42%)	17,19,21	1.11	1 (5%)
5	NAG	S	2	5	14,14,15	2.08	7 (50%)	17,19,21	1.03	1 (5%)
5	NAG	T	1	1,5	14,14,15	2.07	5 (35%)	17,19,21	0.99	0
5	NAG	T	2	5	14,14,15	2.01	7 (50%)	17,19,21	0.94	2 (11%)
5	NAG	U	1	1,5	14,14,15	2.22	6 (42%)	17,19,21	1.01	1 (5%)
5	NAG	U	2	5	14,14,15	2.03	7 (50%)	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	V	1	1,5	14,14,15	2.25	5 (35%)	17,19,21	1.11	3 (17%)
5	NAG	V	2	5	14,14,15	2.00	6 (42%)	17,19,21	0.92	1 (5%)
6	NAG	W	1	1,6	14,14,15	2.22	6 (42%)	17,19,21	1.08	1 (5%)
6	NAG	W	2	6	14,14,15	2.15	5 (35%)	17,19,21	0.86	1 (5%)
6	BMA	W	3	6	11,11,12	2.05	6 (54%)	15,15,17	0.74	0
5	NAG	X	1	1,5	14,14,15	2.16	6 (42%)	17,19,21	1.03	1 (5%)
5	NAG	X	2	5	14,14,15	1.92	6 (42%)	17,19,21	6.46	2 (11%)
5	NAG	Y	1	1,5	14,14,15	2.14	6 (42%)	17,19,21	1.08	2 (11%)
5	NAG	Y	2	5	14,14,15	2.01	6 (42%)	17,19,21	0.94	1 (5%)
5	NAG	Z	1	1,5	14,14,15	2.36	6 (42%)	17,19,21	1.02	1 (5%)
5	NAG	Z	2	5	14,14,15	2.04	7 (50%)	17,19,21	0.92	1 (5%)
6	NAG	a	1	1,6	14,14,15	2.05	5 (35%)	17,19,21	1.18	1 (5%)
6	NAG	a	2	6	14,14,15	2.09	6 (42%)	17,19,21	0.90	1 (5%)
6	BMA	a	3	6	11,11,12	2.02	5 (45%)	15,15,17	0.71	0
7	NAG	b	1	1,7	14,14,15	2.04	6 (42%)	17,19,21	1.11	1 (5%)
7	NAG	b	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.96	1 (5%)
7	BMA	b	3	7	11,11,12	1.47	3 (27%)	15,15,17	0.62	0
7	MAN	b	4	7	11,11,12	0.80	0	15,15,17	0.90	0
7	MAN	b	5	7	11,11,12	2.01	6 (54%)	15,15,17	0.71	0
7	MAN	b	6	7	11,11,12	1.96	5 (45%)	15,15,17	0.72	0
8	NAG	c	1	1,8	14,14,15	2.09	6 (42%)	17,19,21	1.08	2 (11%)
8	NAG	c	2	8	14,14,15	2.03	6 (42%)	17,19,21	1.05	2 (11%)
8	BMA	c	3	8	11,11,12	1.51	3 (27%)	15,15,17	0.62	0
8	MAN	c	4	8	11,11,12	1.95	6 (54%)	15,15,17	0.77	0
8	MAN	c	5	8	11,11,12	1.94	5 (45%)	15,15,17	0.73	0
5	NAG	d	1	1,5	14,14,15	0.56	0	17,19,21	1.20	1 (5%)
5	NAG	d	2	5	14,14,15	0.32	0	17,19,21	0.67	0
5	NAG	e	1	1,5	14,14,15	2.10	6 (42%)	17,19,21	1.11	1 (5%)
5	NAG	e	2	5	14,14,15	2.07	7 (50%)	17,19,21	1.03	1 (5%)
5	NAG	f	1	1,5	14,14,15	2.07	5 (35%)	17,19,21	0.99	0
5	NAG	f	2	5	14,14,15	2.00	6 (42%)	17,19,21	0.94	2 (11%)
5	NAG	g	1	1,5	14,14,15	2.21	6 (42%)	17,19,21	1.00	1 (5%)
5	NAG	g	2	5	14,14,15	2.03	7 (50%)	17,19,21	0.86	1 (5%)
5	NAG	h	1	1,5	14,14,15	2.25	5 (35%)	17,19,21	1.11	2 (11%)
5	NAG	h	2	5	14,14,15	1.99	6 (42%)	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	i	1	1,6	14,14,15	2.21	6 (42%)	17,19,21	1.08	1 (5%)
6	NAG	i	2	6	14,14,15	2.15	5 (35%)	17,19,21	0.86	1 (5%)
6	BMA	i	3	6	11,11,12	2.06	6 (54%)	15,15,17	0.74	0
5	NAG	j	1	1,5	14,14,15	2.15	6 (42%)	17,19,21	1.03	1 (5%)
5	NAG	j	2	5	14,14,15	1.92	6 (42%)	17,19,21	6.46	2 (11%)
5	NAG	k	1	1,5	14,14,15	2.13	6 (42%)	17,19,21	1.07	2 (11%)
5	NAG	k	2	5	14,14,15	2.01	7 (50%)	17,19,21	0.93	1 (5%)
5	NAG	l	1	1,5	14,14,15	2.35	6 (42%)	17,19,21	1.02	1 (5%)
5	NAG	l	2	5	14,14,15	2.04	7 (50%)	17,19,21	0.92	1 (5%)
6	NAG	m	1	1,6	14,14,15	2.06	5 (35%)	17,19,21	1.18	1 (5%)
6	NAG	m	2	6	14,14,15	2.10	6 (42%)	17,19,21	0.90	1 (5%)
6	BMA	m	3	6	11,11,12	2.02	5 (45%)	15,15,17	0.72	0
7	NAG	n	1	1,7	14,14,15	2.04	6 (42%)	17,19,21	1.11	1 (5%)
7	NAG	n	2	7	14,14,15	1.97	6 (42%)	17,19,21	0.96	1 (5%)
7	BMA	n	3	7	11,11,12	1.47	3 (27%)	15,15,17	0.62	0
7	MAN	n	4	7	11,11,12	0.79	0	15,15,17	0.90	0
7	MAN	n	5	7	11,11,12	2.01	6 (54%)	15,15,17	0.71	0
7	MAN	n	6	7	11,11,12	1.96	6 (54%)	15,15,17	0.72	0
8	NAG	o	1	1,8	14,14,15	2.08	6 (42%)	17,19,21	1.08	2 (11%)
8	NAG	o	2	8	14,14,15	2.02	6 (42%)	17,19,21	1.04	1 (5%)
8	BMA	o	3	8	11,11,12	1.51	3 (27%)	15,15,17	0.63	0
8	MAN	o	4	8	11,11,12	1.95	6 (54%)	15,15,17	0.77	0
8	MAN	o	5	8	11,11,12	1.94	6 (54%)	15,15,17	0.73	0
5	NAG	p	1	1,5	14,14,15	0.56	0	17,19,21	1.21	1 (5%)
5	NAG	p	2	5	14,14,15	0.32	0	17,19,21	0.67	0
5	NAG	q	1	1,5	14,14,15	2.09	6 (42%)	17,19,21	1.11	1 (5%)
5	NAG	q	2	5	14,14,15	2.08	7 (50%)	17,19,21	1.03	1 (5%)
5	NAG	r	1	1,5	14,14,15	2.07	5 (35%)	17,19,21	0.99	0
5	NAG	r	2	5	14,14,15	2.00	7 (50%)	17,19,21	0.94	2 (11%)
5	NAG	s	1	1,5	14,14,15	2.21	6 (42%)	17,19,21	1.00	1 (5%)
5	NAG	s	2	5	14,14,15	2.03	7 (50%)	17,19,21	0.85	1 (5%)
5	NAG	t	1	1,5	14,14,15	2.25	5 (35%)	17,19,21	1.11	2 (11%)
5	NAG	t	2	5	14,14,15	2.00	6 (42%)	17,19,21	0.92	1 (5%)
6	NAG	u	1	1,6	14,14,15	2.21	6 (42%)	17,19,21	1.08	1 (5%)
6	NAG	u	2	6	14,14,15	2.15	7 (50%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	u	3	6	11,11,12	2.05	6 (54%)	15,15,17	0.74	0
5	NAG	v	1	1,5	14,14,15	2.16	6 (42%)	17,19,21	1.03	1 (5%)
5	NAG	v	2	5	14,14,15	1.92	6 (42%)	17,19,21	6.46	2 (11%)

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	M	1	1,5	-	0/6/23/26	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
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	0/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	1/2/19/22	0/1/1/1
7	MAN	P	5	7	-	2/2/19/22	0/1/1/1
7	MAN	P	6	7	-	1/2/19/22	0/1/1/1
8	NAG	Q	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	1/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	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	-	0/6/23/26	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	-	1/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	BMA	W	3	6	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	m	3	6	-	0/2/19/22	0/1/1/1
7	NAG	n	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
7	BMA	n	3	7	-	0/2/19/22	0/1/1/1
7	MAN	n	4	7	-	1/2/19/22	0/1/1/1
7	MAN	n	5	7	-	2/2/19/22	0/1/1/1
7	MAN	n	6	7	-	1/2/19/22	0/1/1/1
8	NAG	o	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
8	BMA	o	3	8	-	0/2/19/22	0/1/1/1
8	MAN	o	4	8	-	1/2/19/22	0/1/1/1
8	MAN	o	5	8	-	1/2/19/22	0/1/1/1
5	NAG	p	1	1,5	-	4/6/23/26	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	-	0/6/23/26	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
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	-	1/6/23/26	0/1/1/1
6	NAG	u	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	u	2	6	-	0/6/23/26	0/1/1/1
6	BMA	u	3	6	-	1/2/19/22	0/1/1/1
5	NAG	v	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	v	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	1	NAG	C1-C2	5.84	1.61	1.52
5	N	1	NAG	C1-C2	5.83	1.61	1.52
5	l	1	NAG	C1-C2	5.80	1.61	1.52
5	V	1	NAG	C1-C2	5.63	1.60	1.52
5	t	1	NAG	C1-C2	5.62	1.60	1.52

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	v	2	NAG	C2-N2-C7	26.31	160.37	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	j	2	NAG	C2-N2-C7	26.31	160.37	122.90
5	X	2	NAG	C2-N2-C7	26.30	160.36	122.90
5	p	1	NAG	C2-N2-C7	-3.15	118.42	122.90
5	d	1	NAG	C2-N2-C7	-3.14	118.44	122.90

There are no chirality outliers.

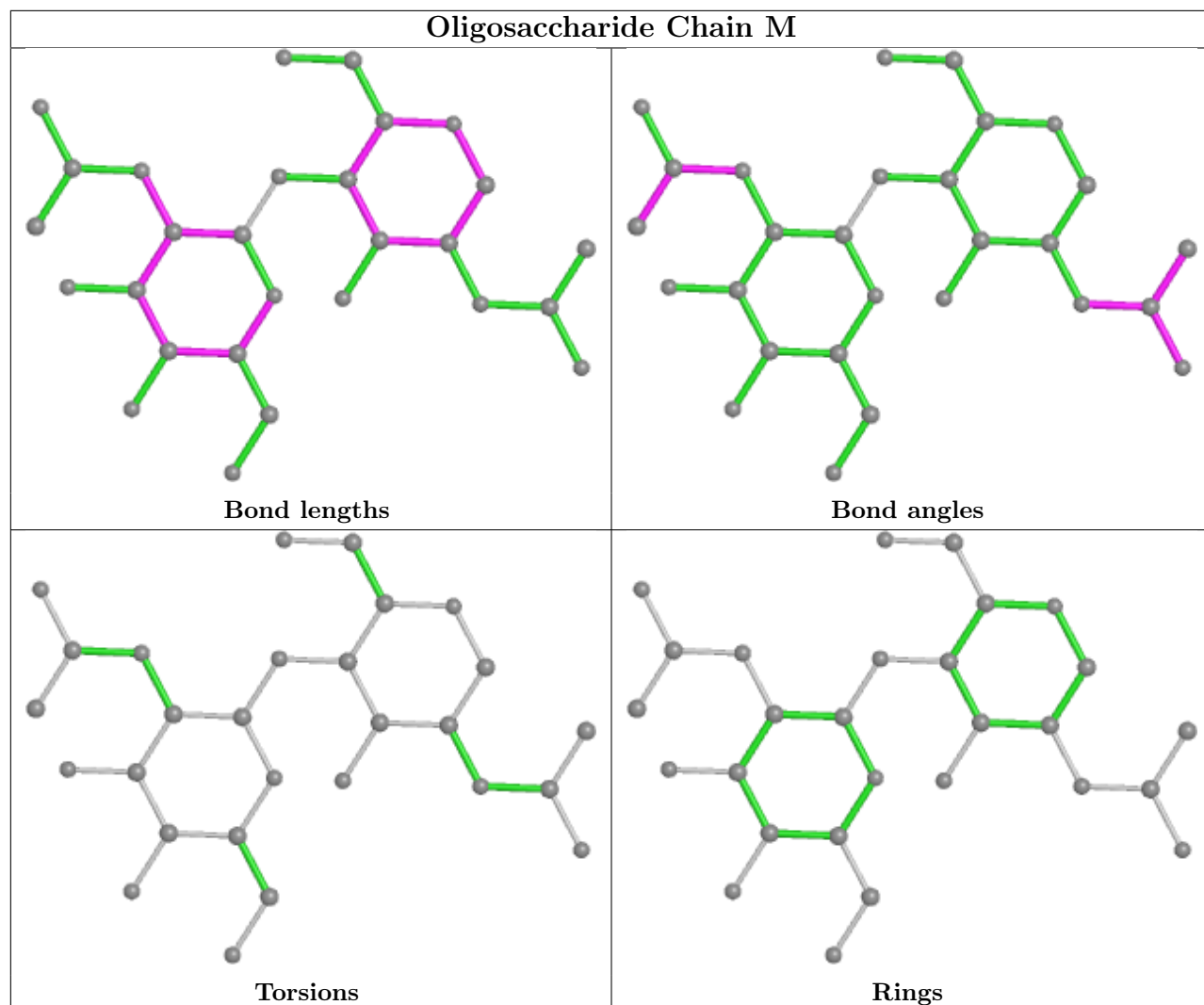
5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	b	4	MAN	O5-C5-C6-O6
7	P	4	MAN	O5-C5-C6-O6
7	n	4	MAN	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6

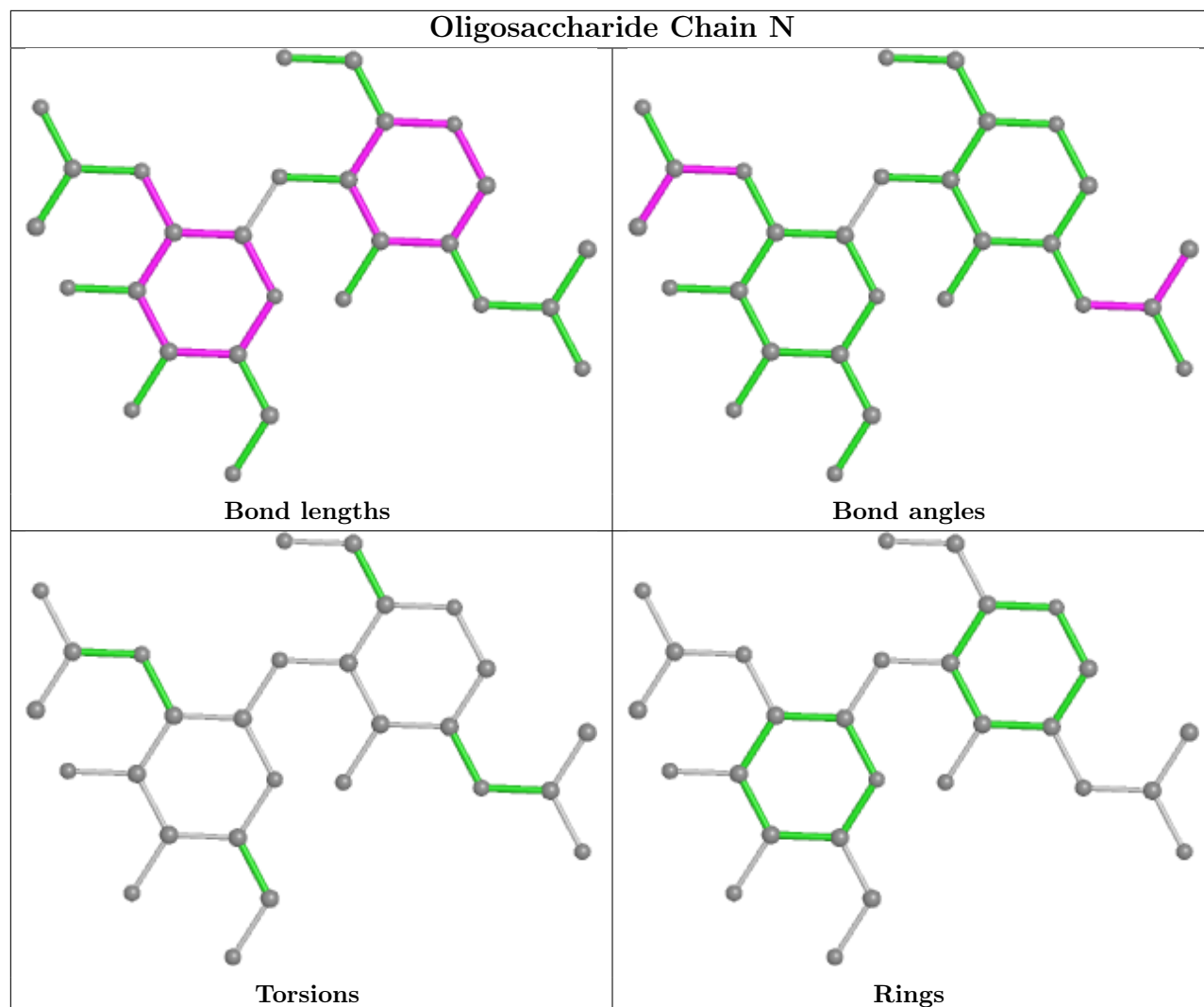
There are no ring outliers.

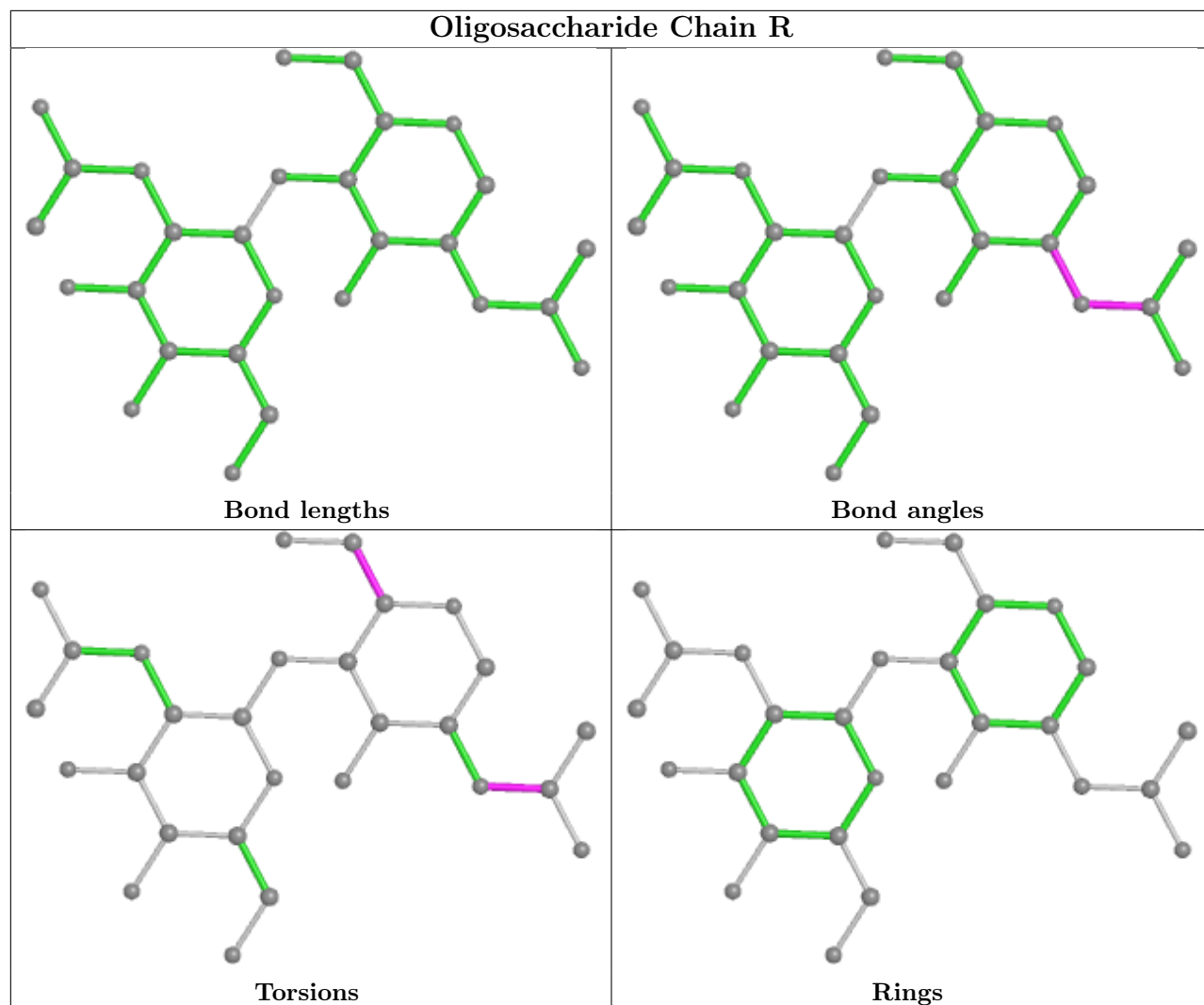
No monomer is involved in short contacts.

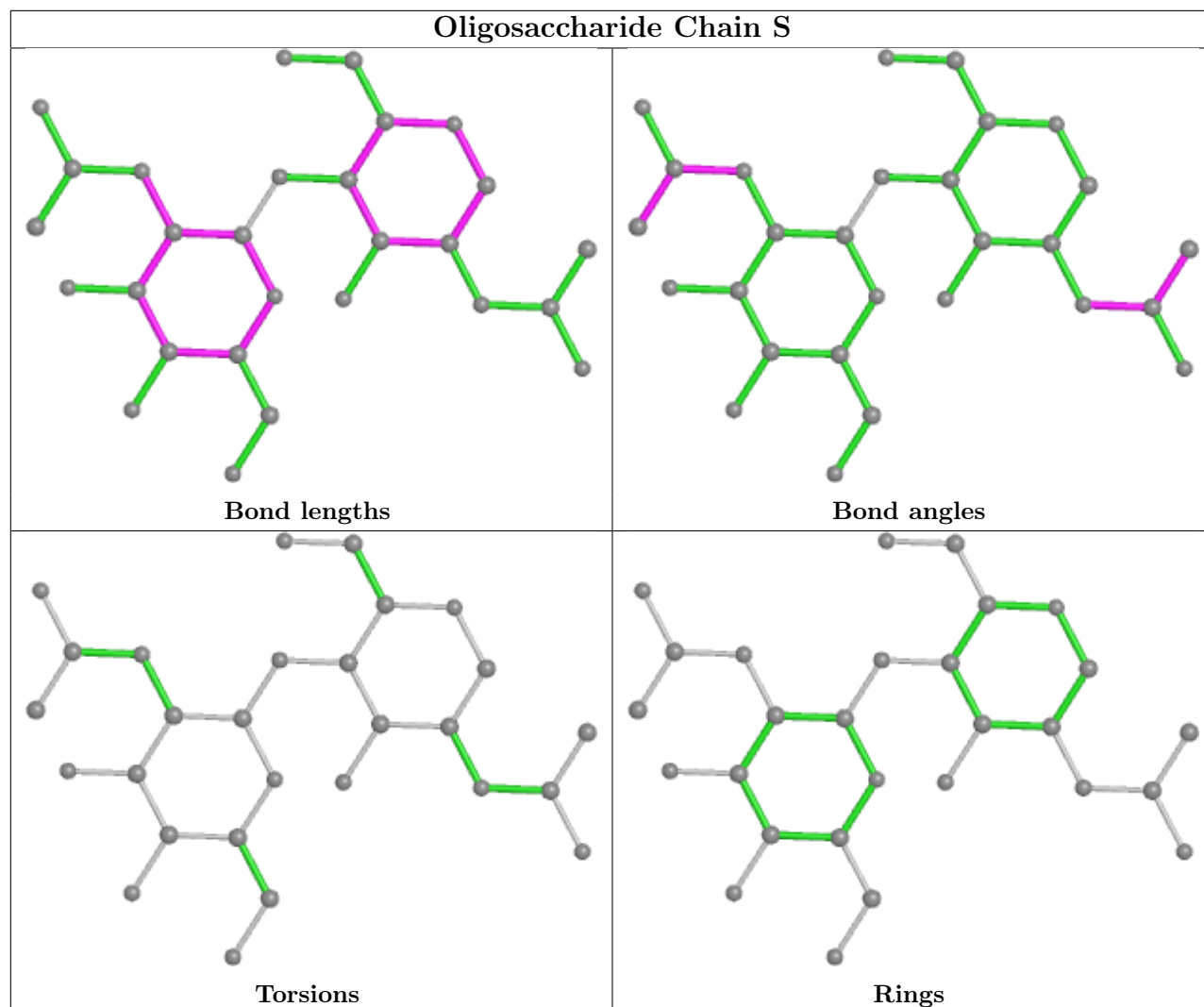
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

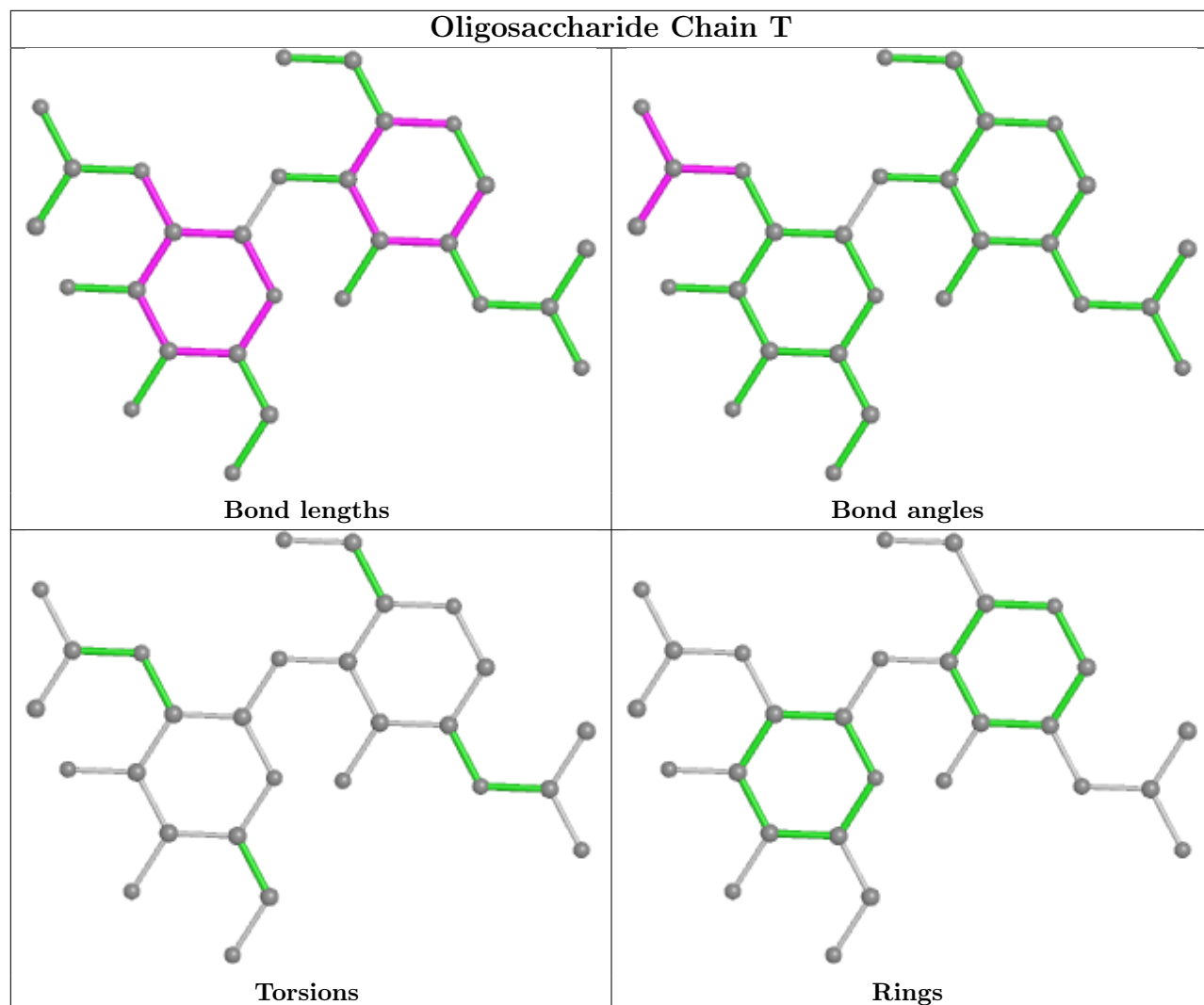


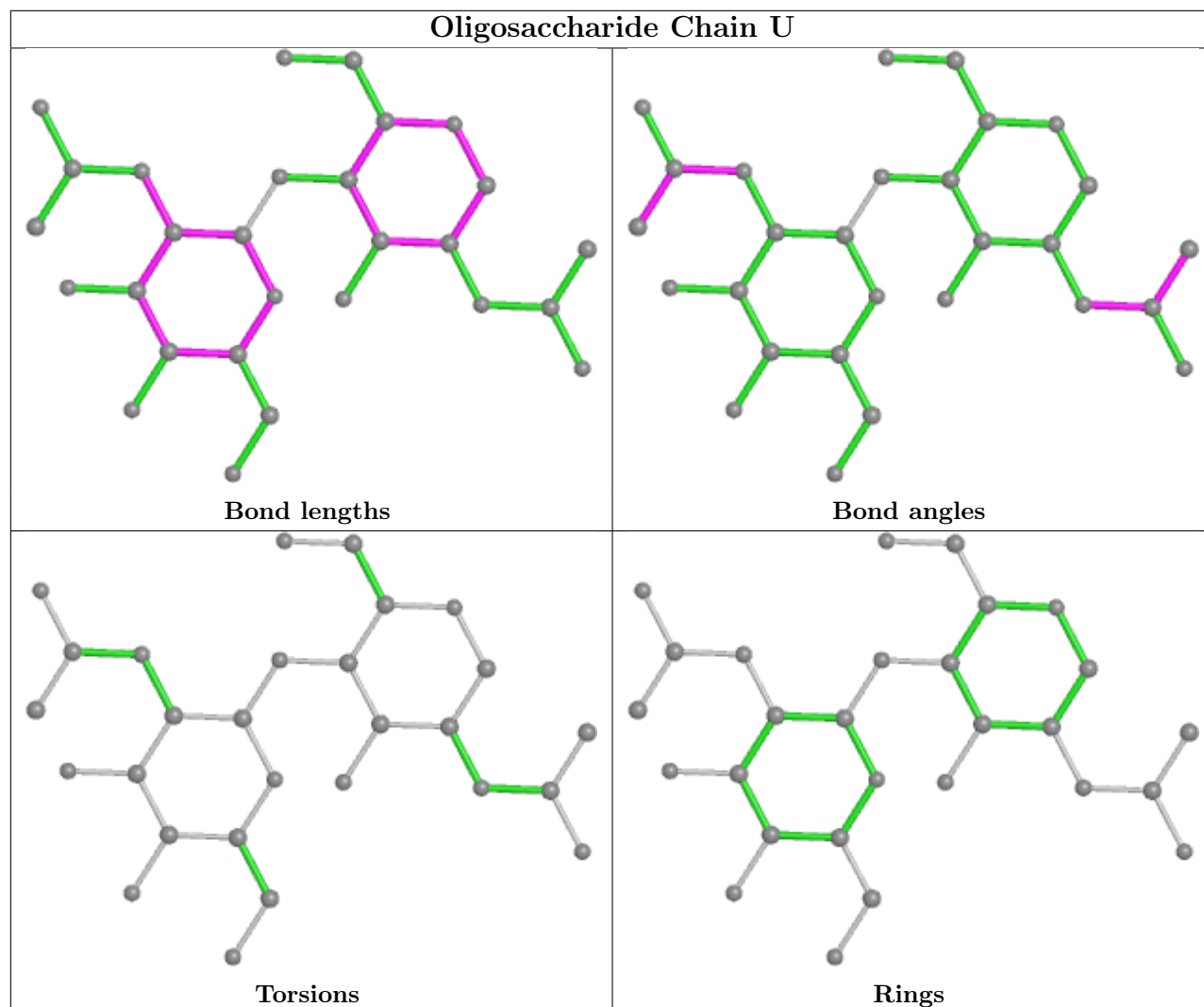


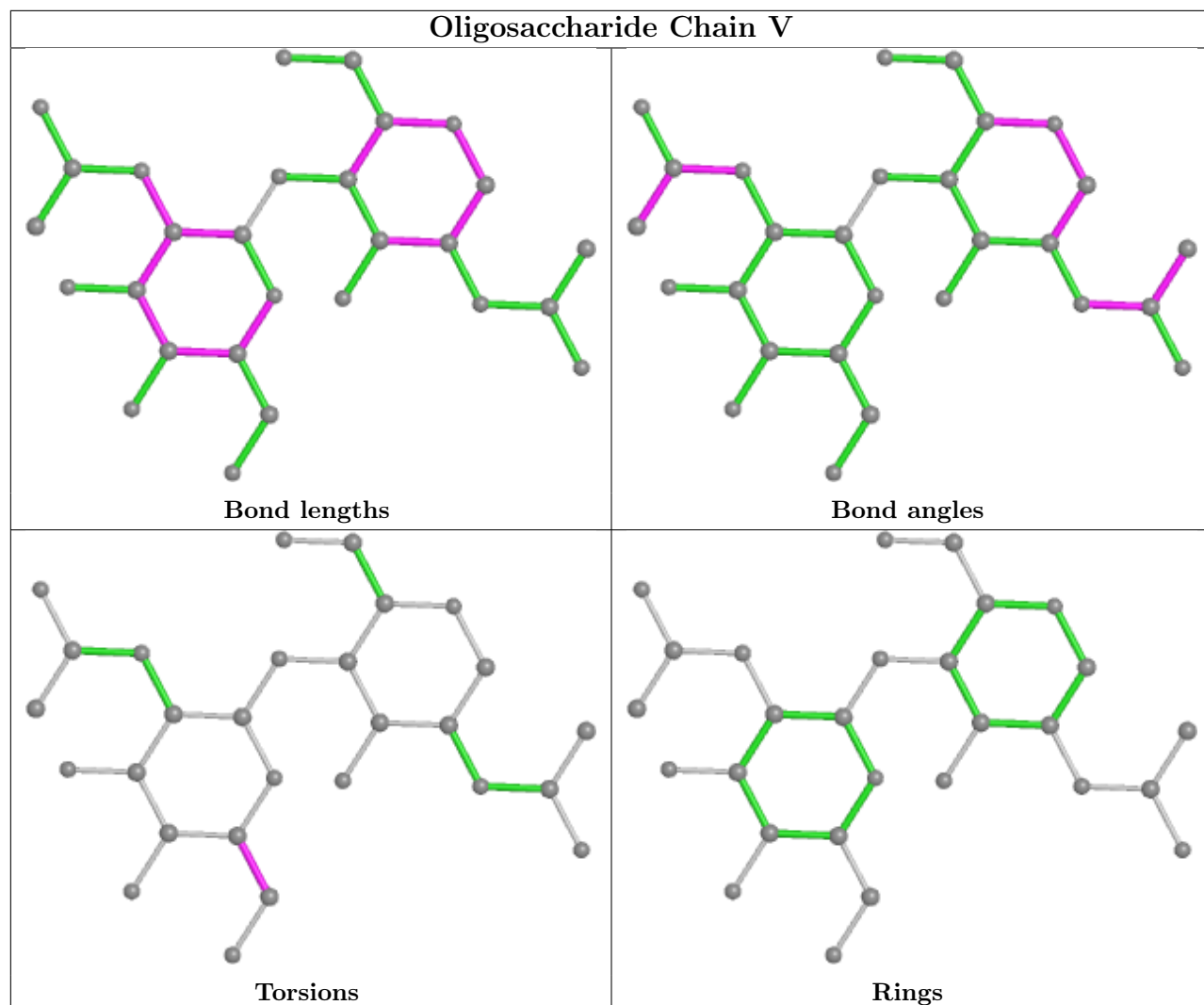


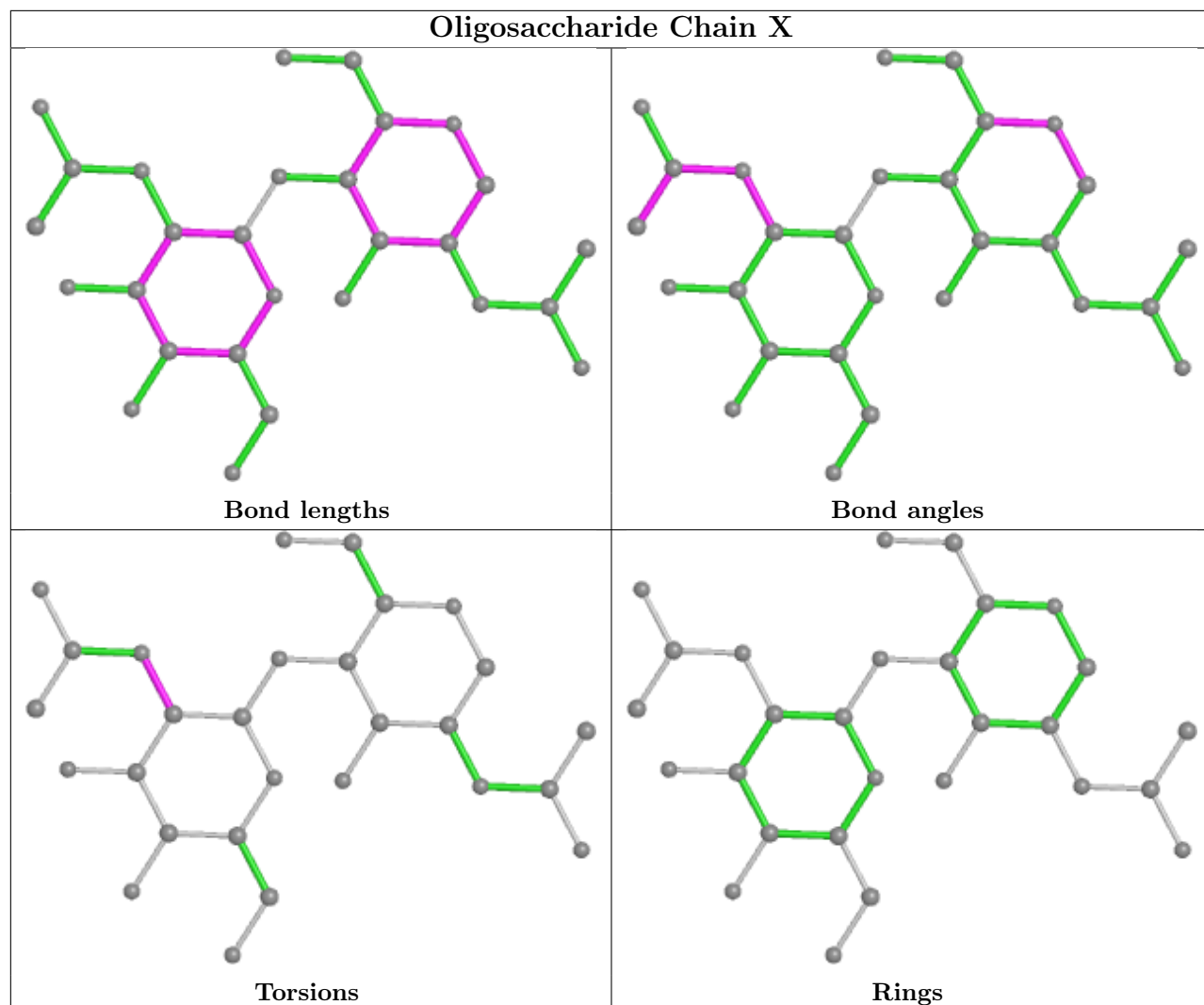


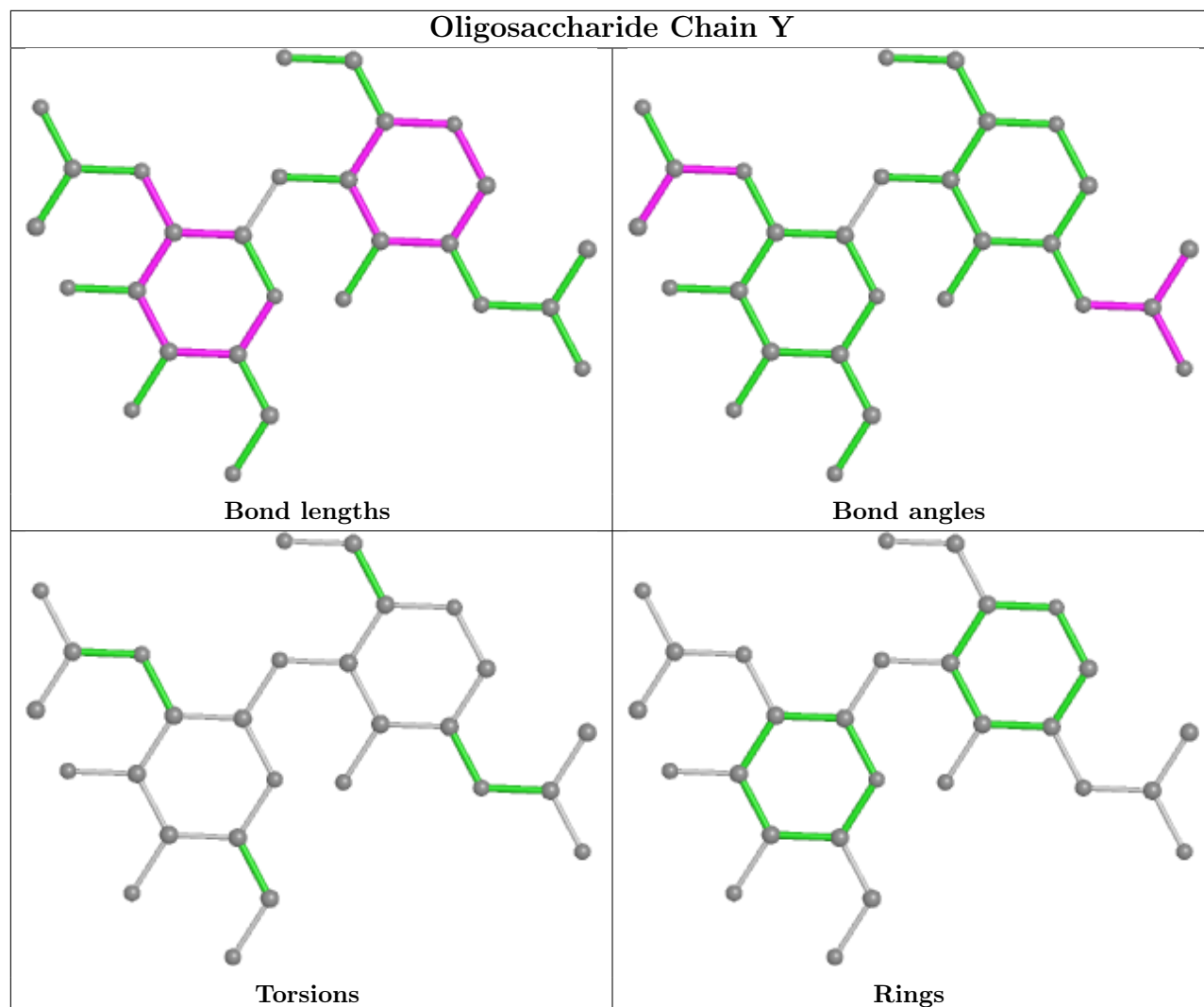




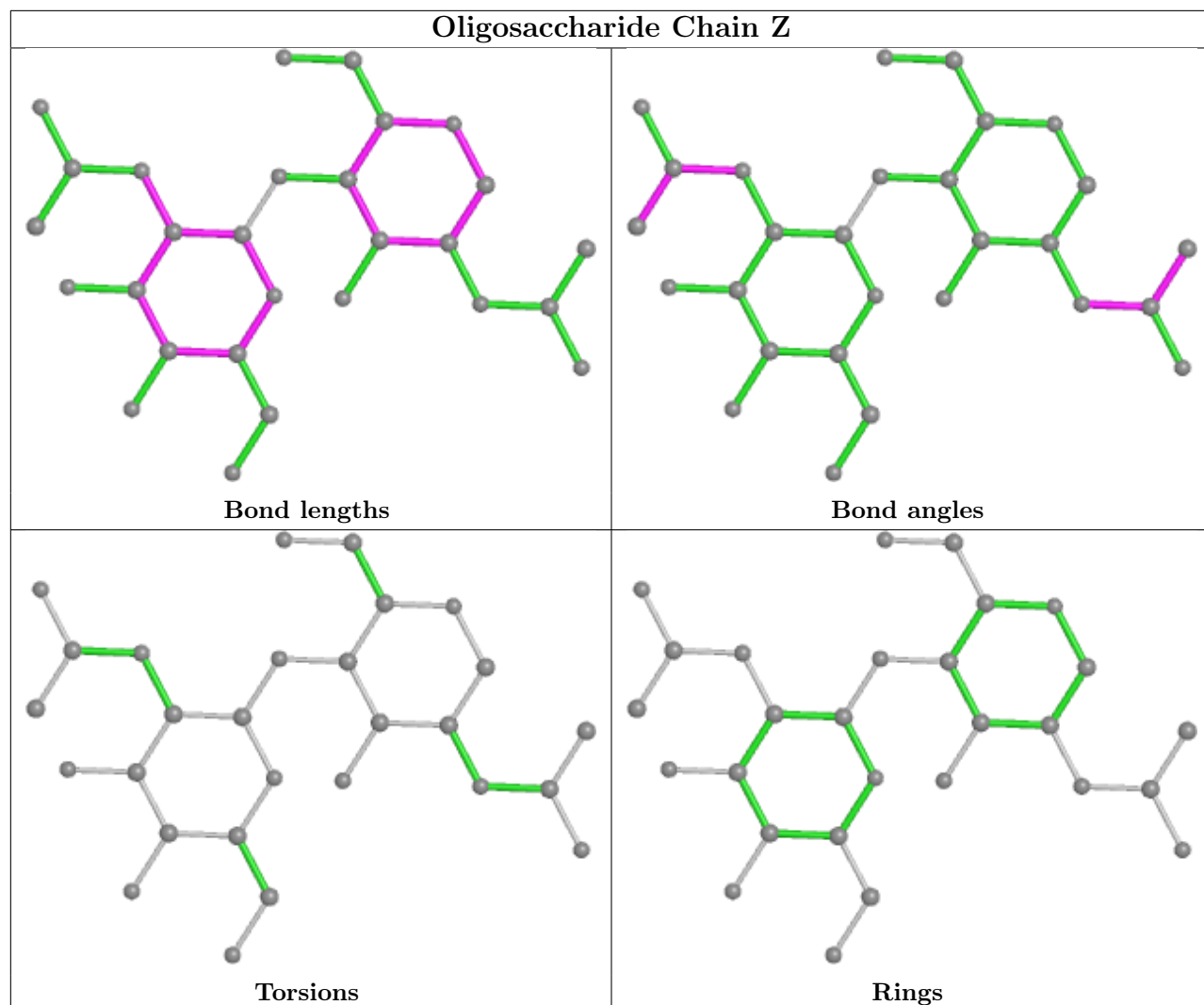


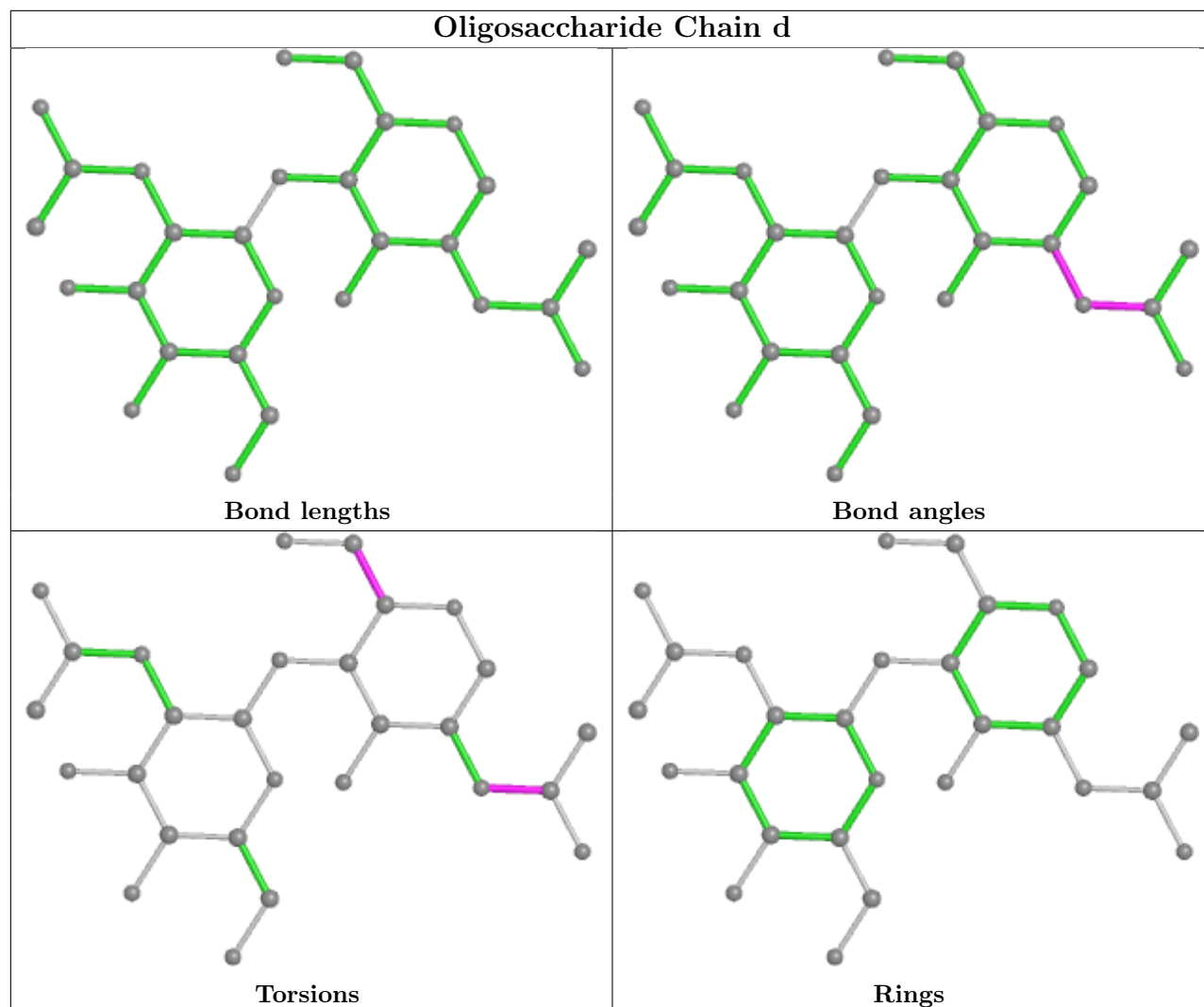


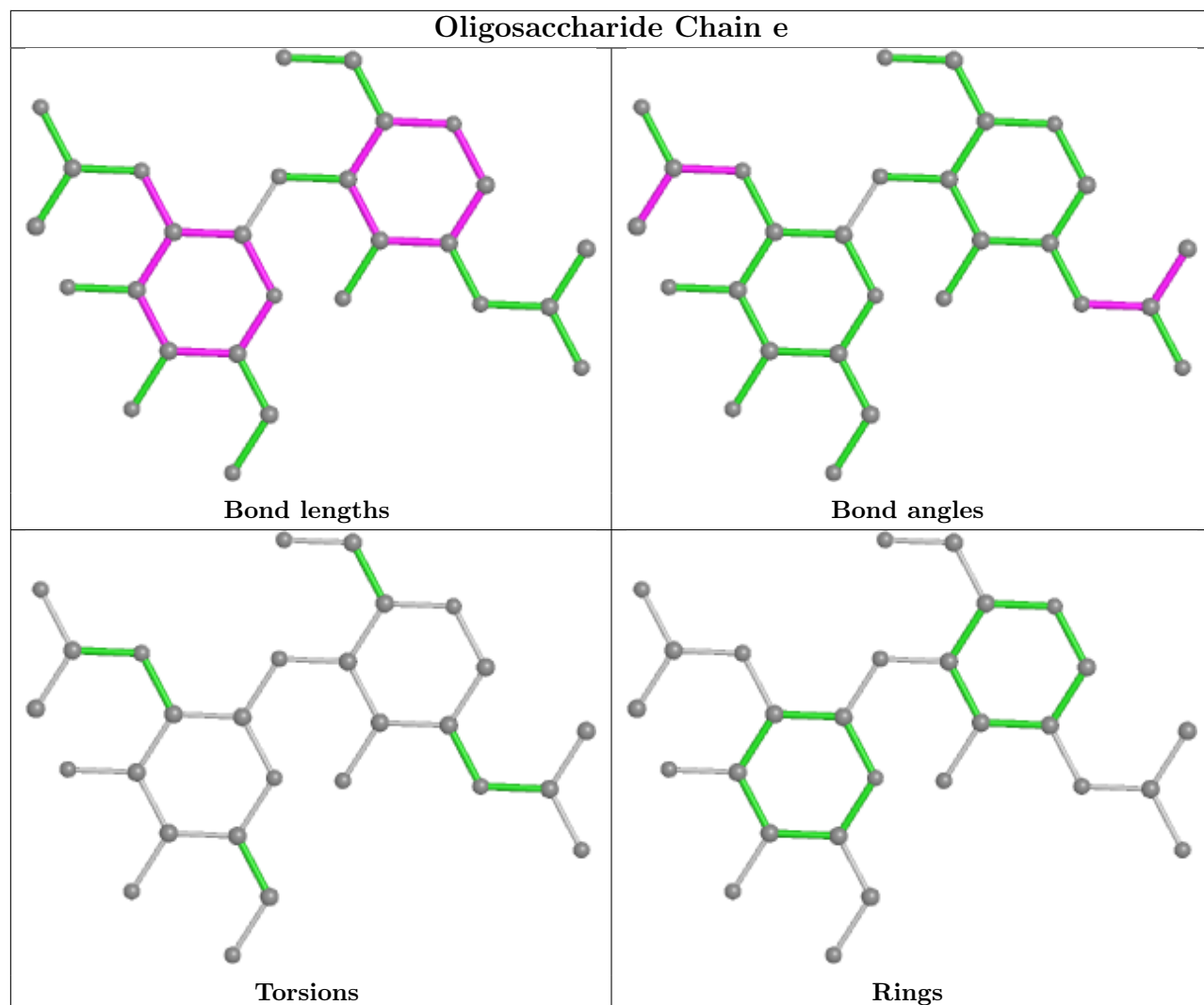


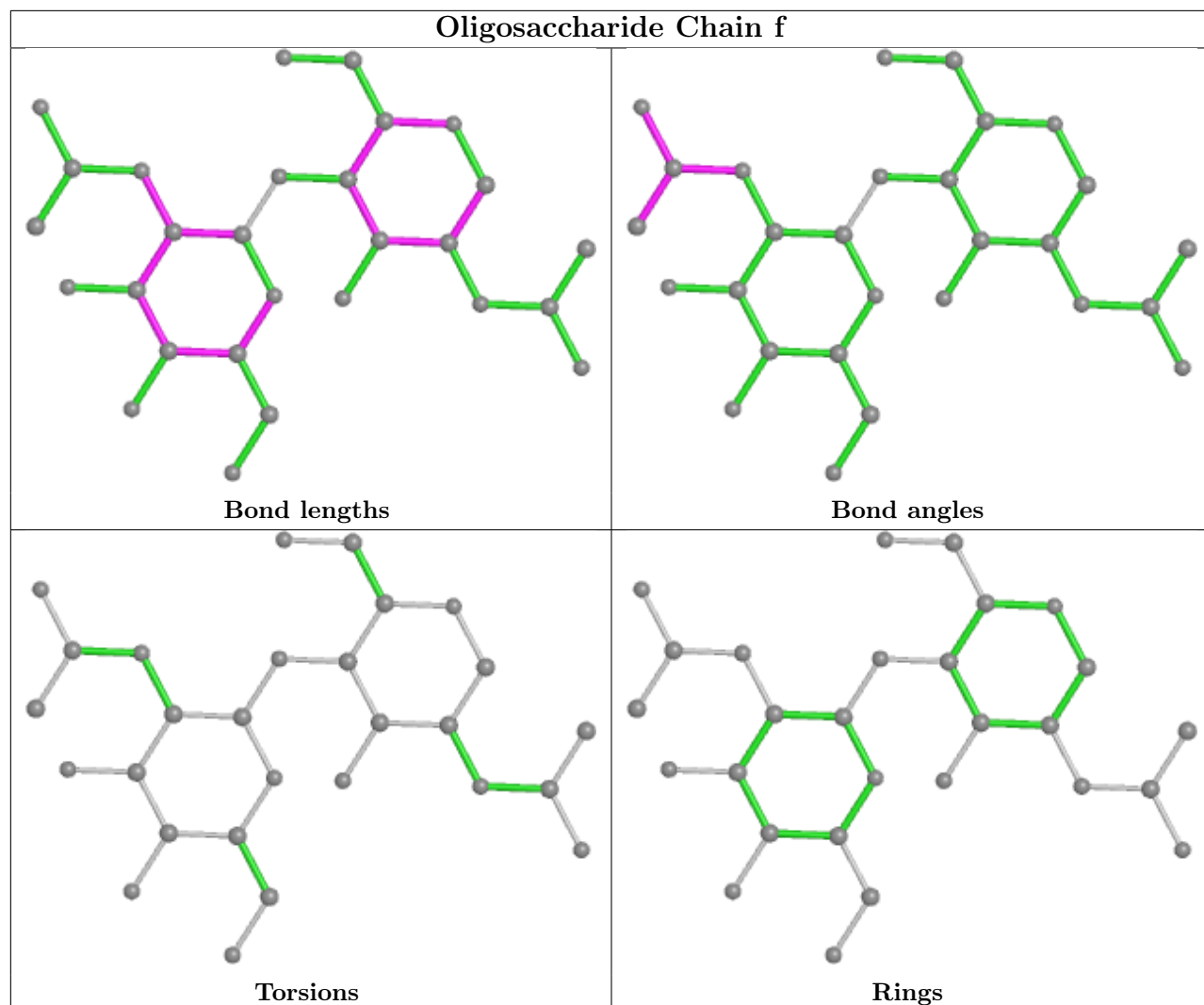


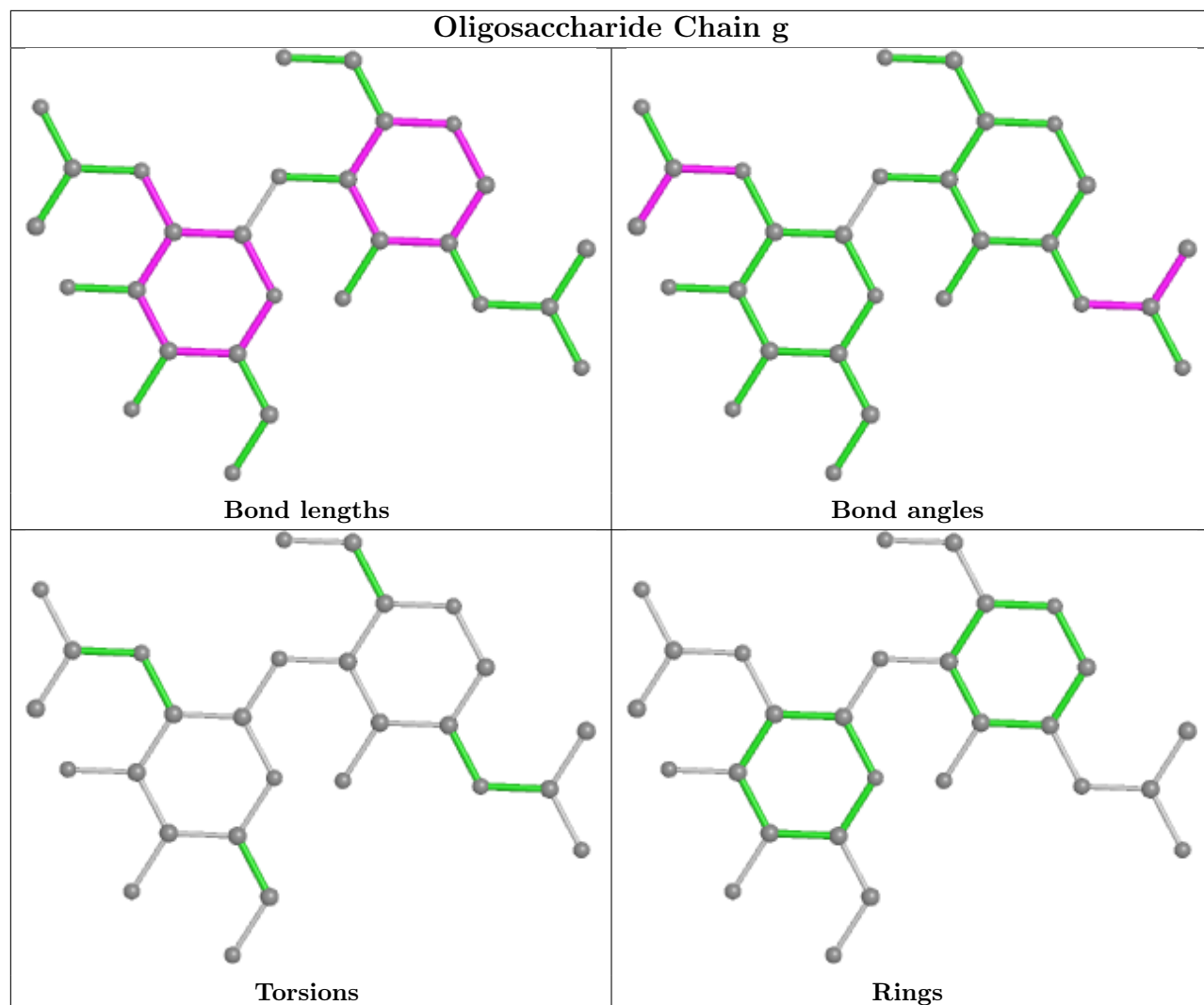


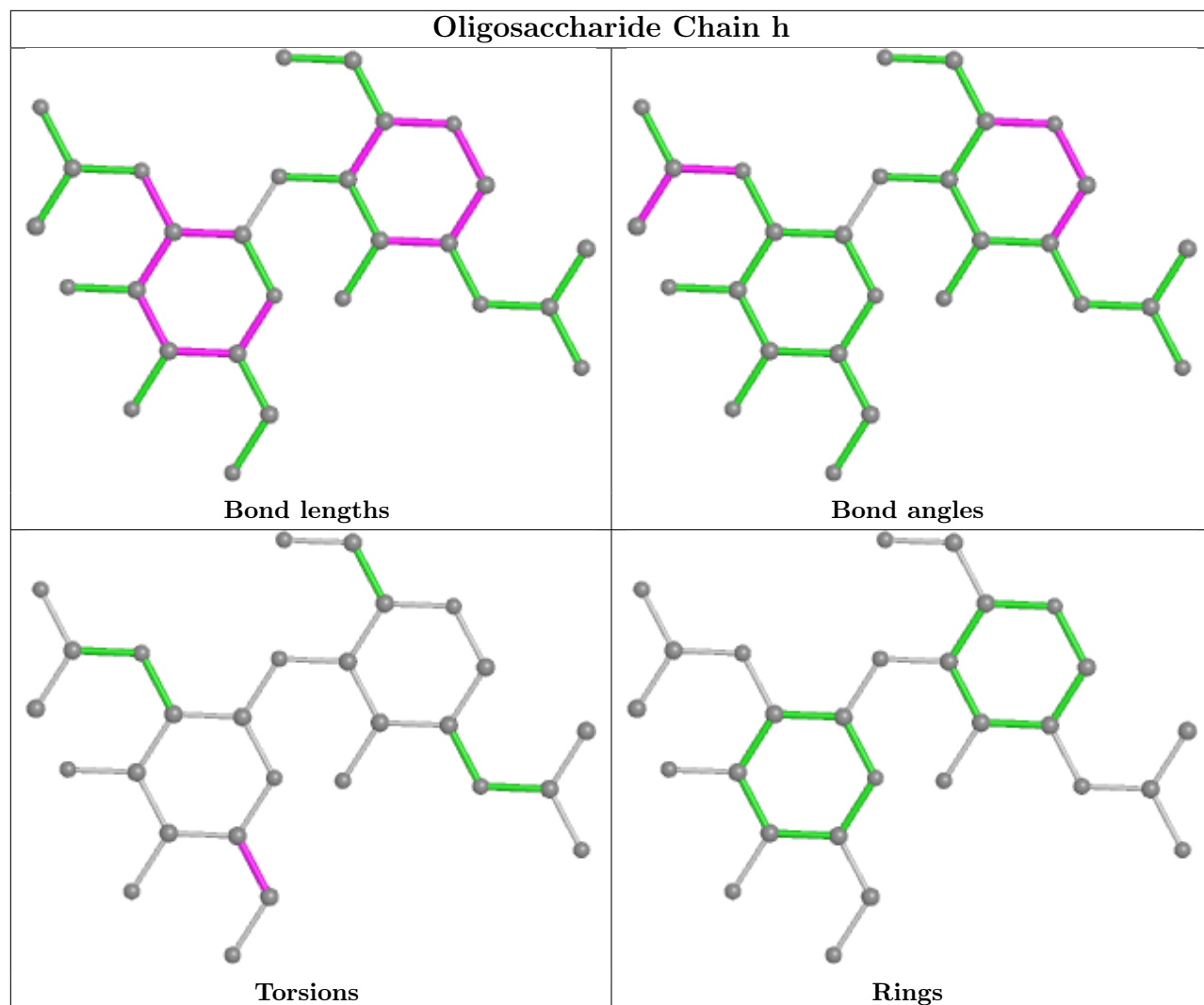


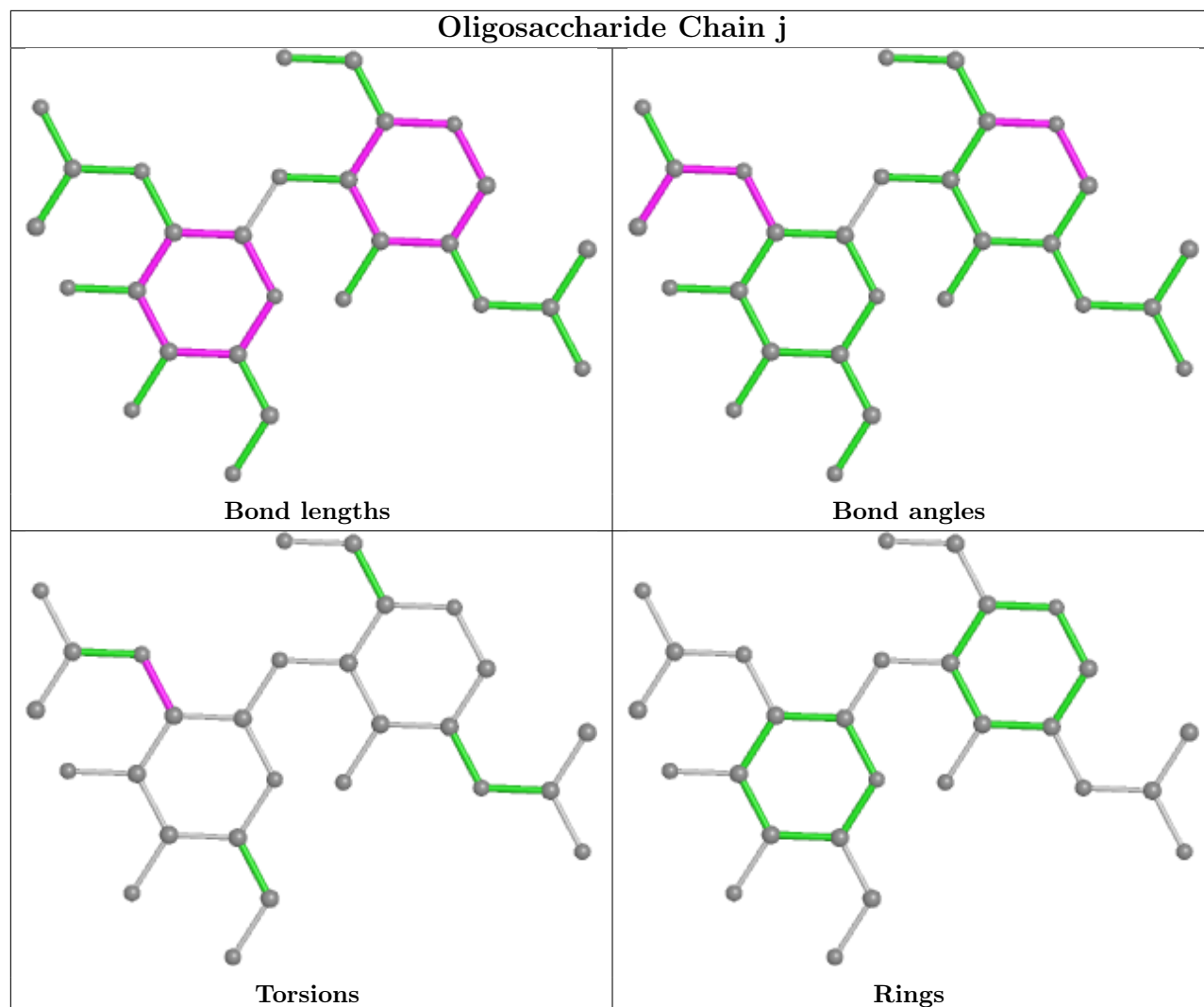


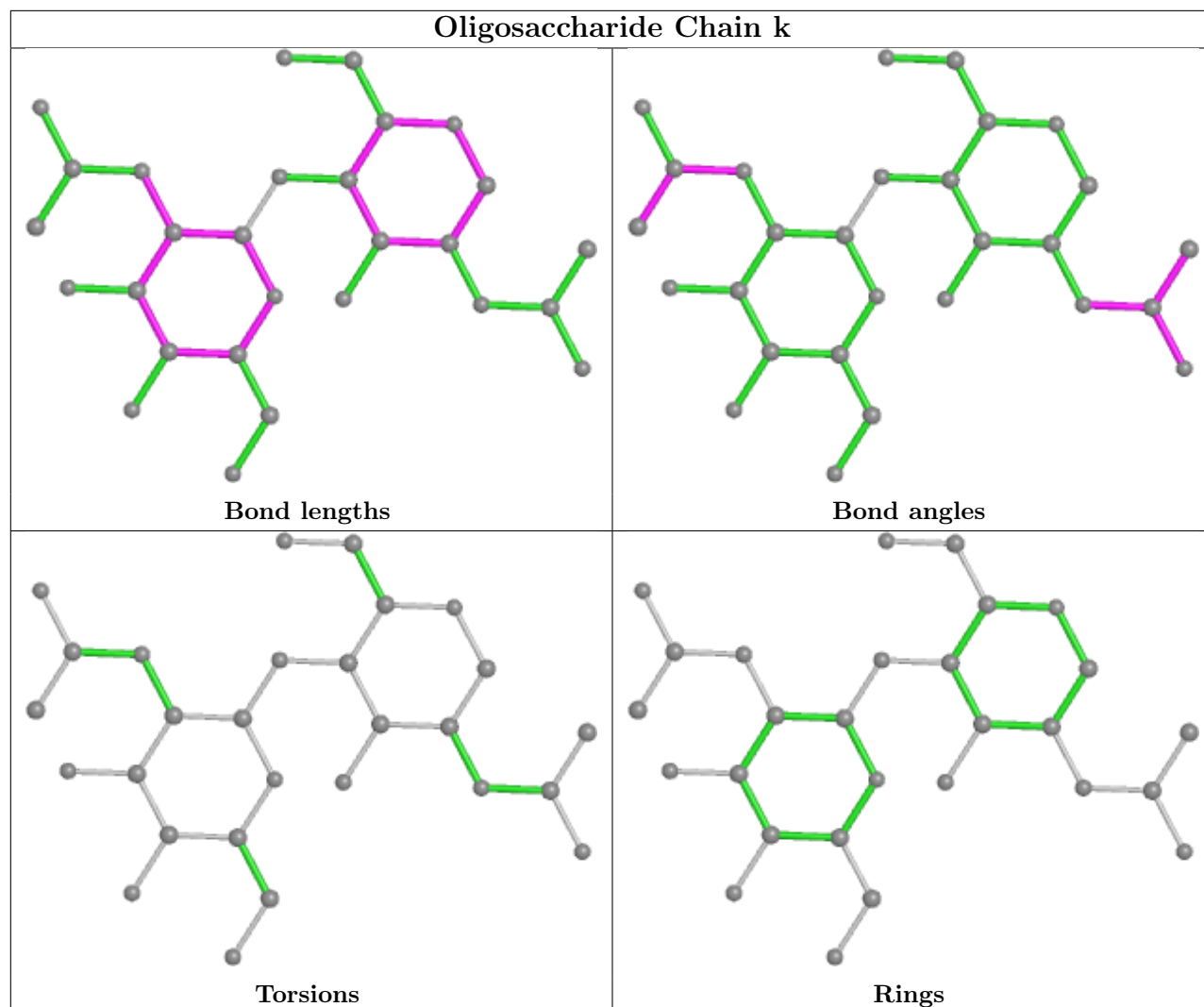




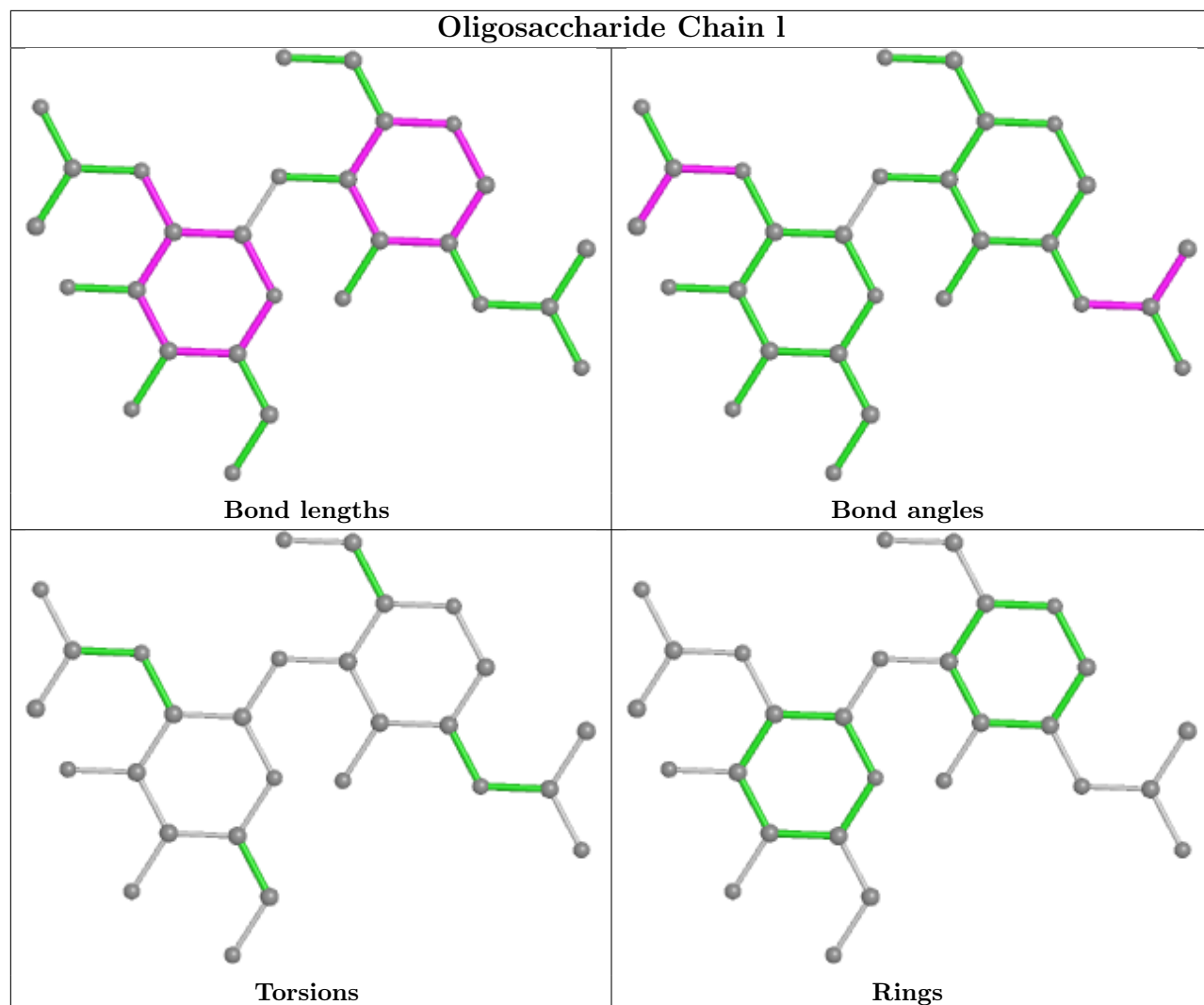


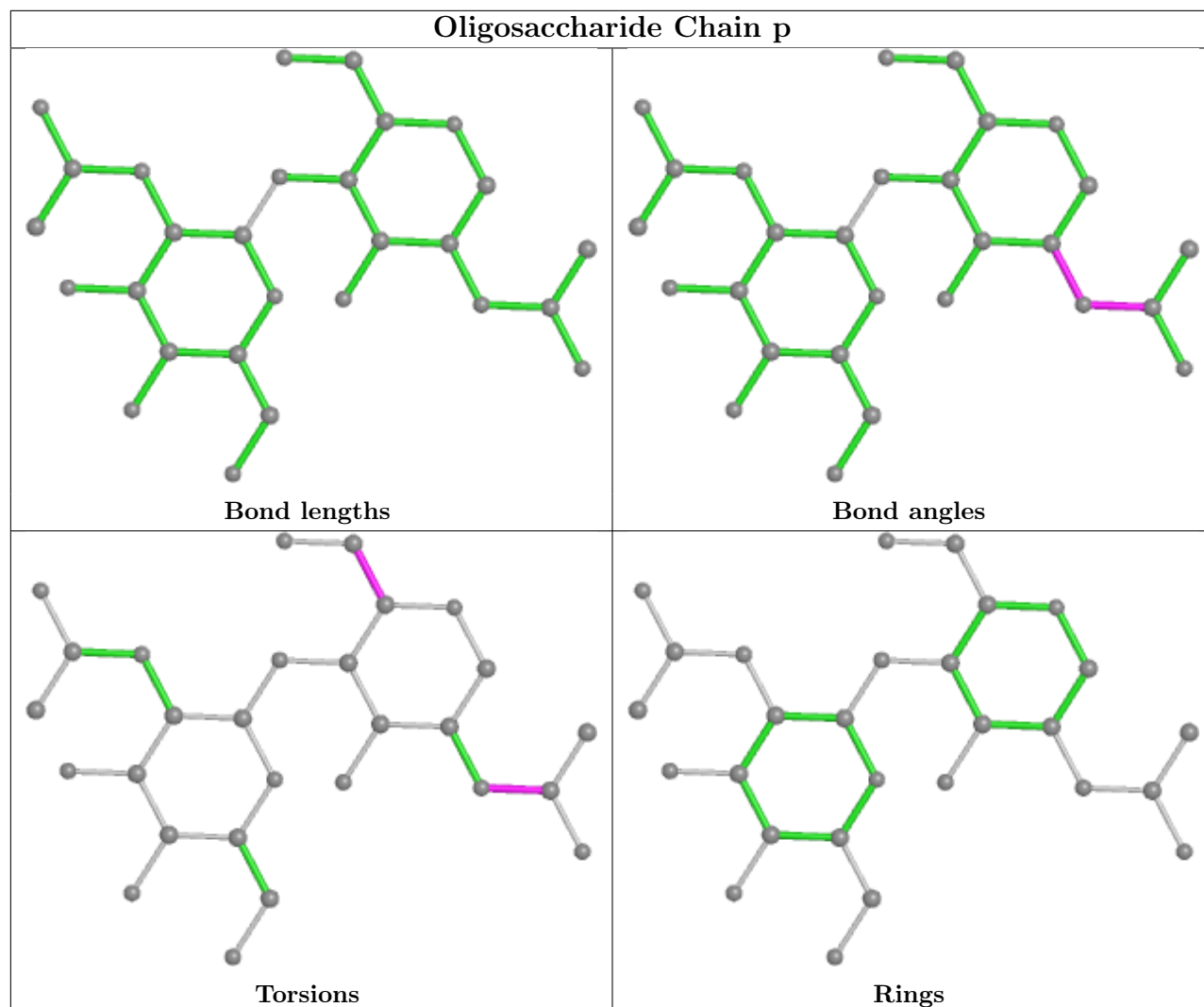


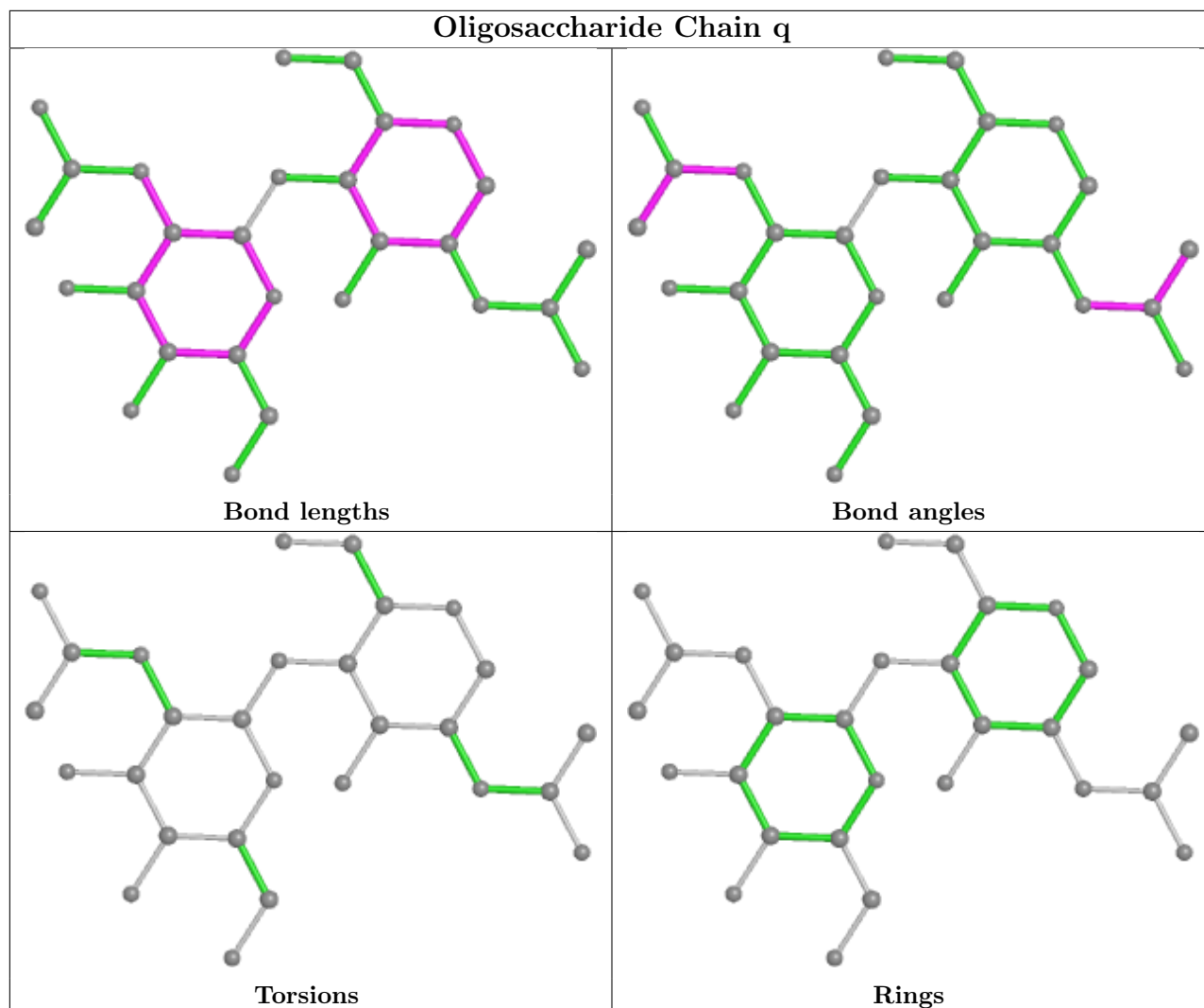


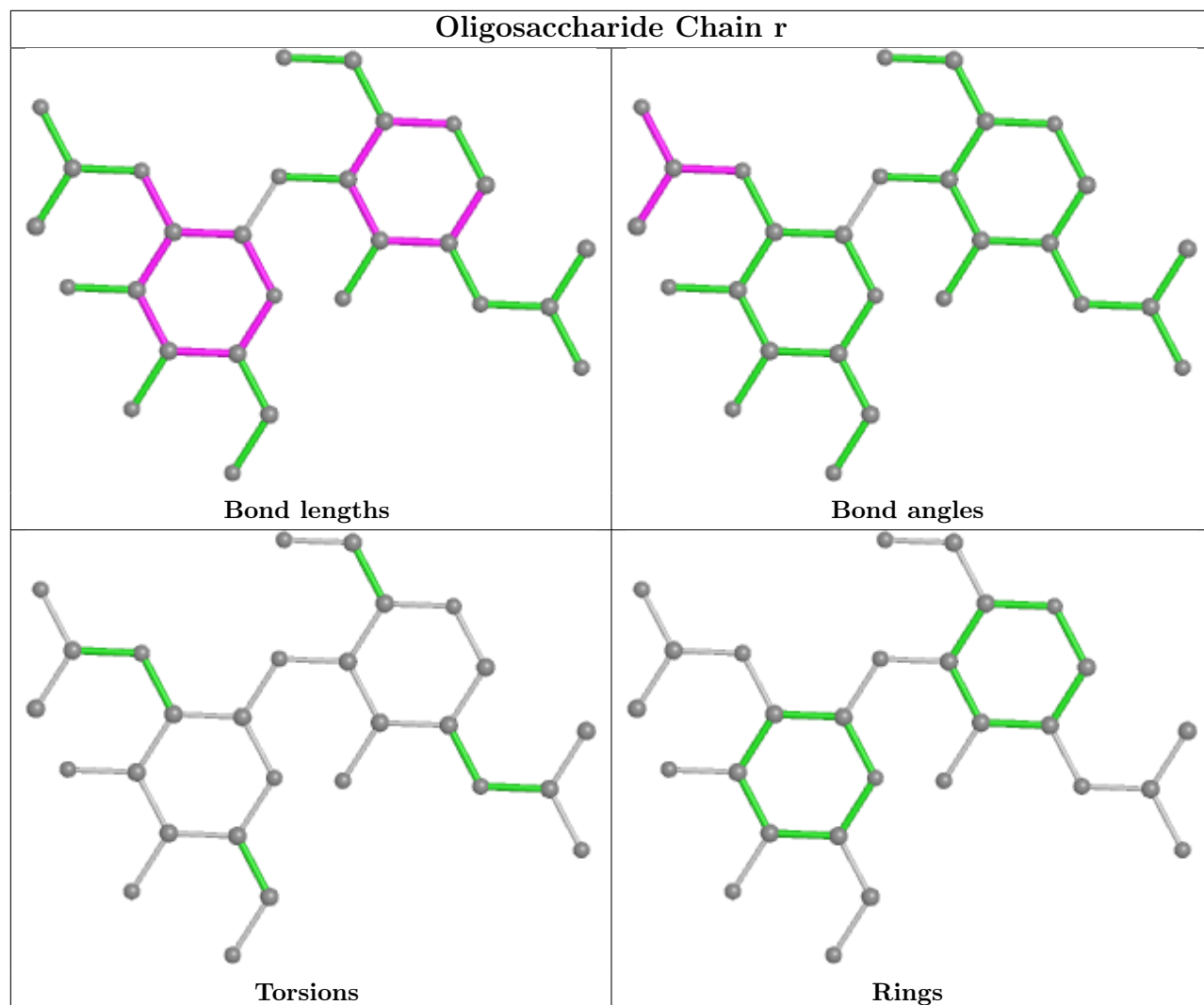


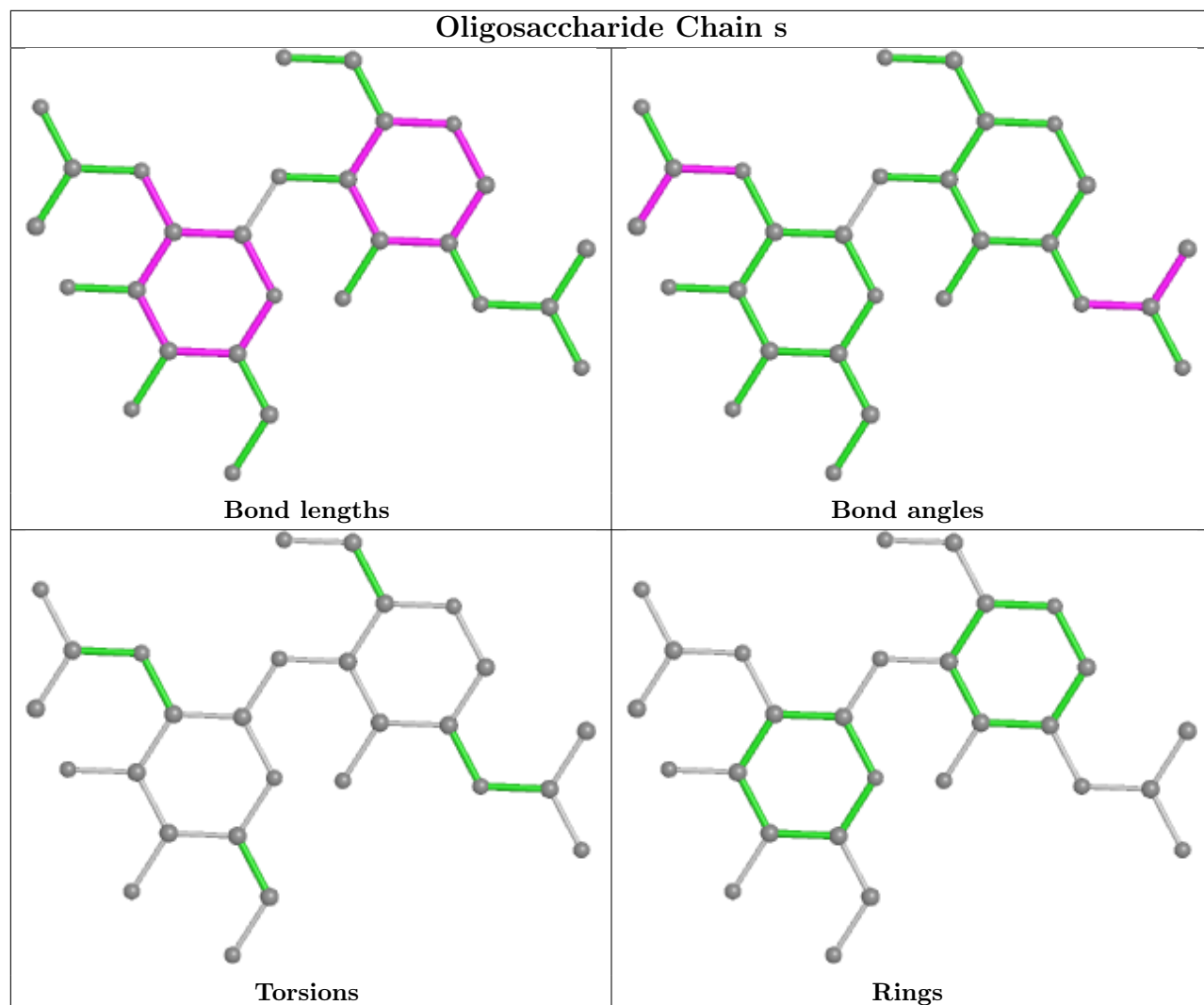


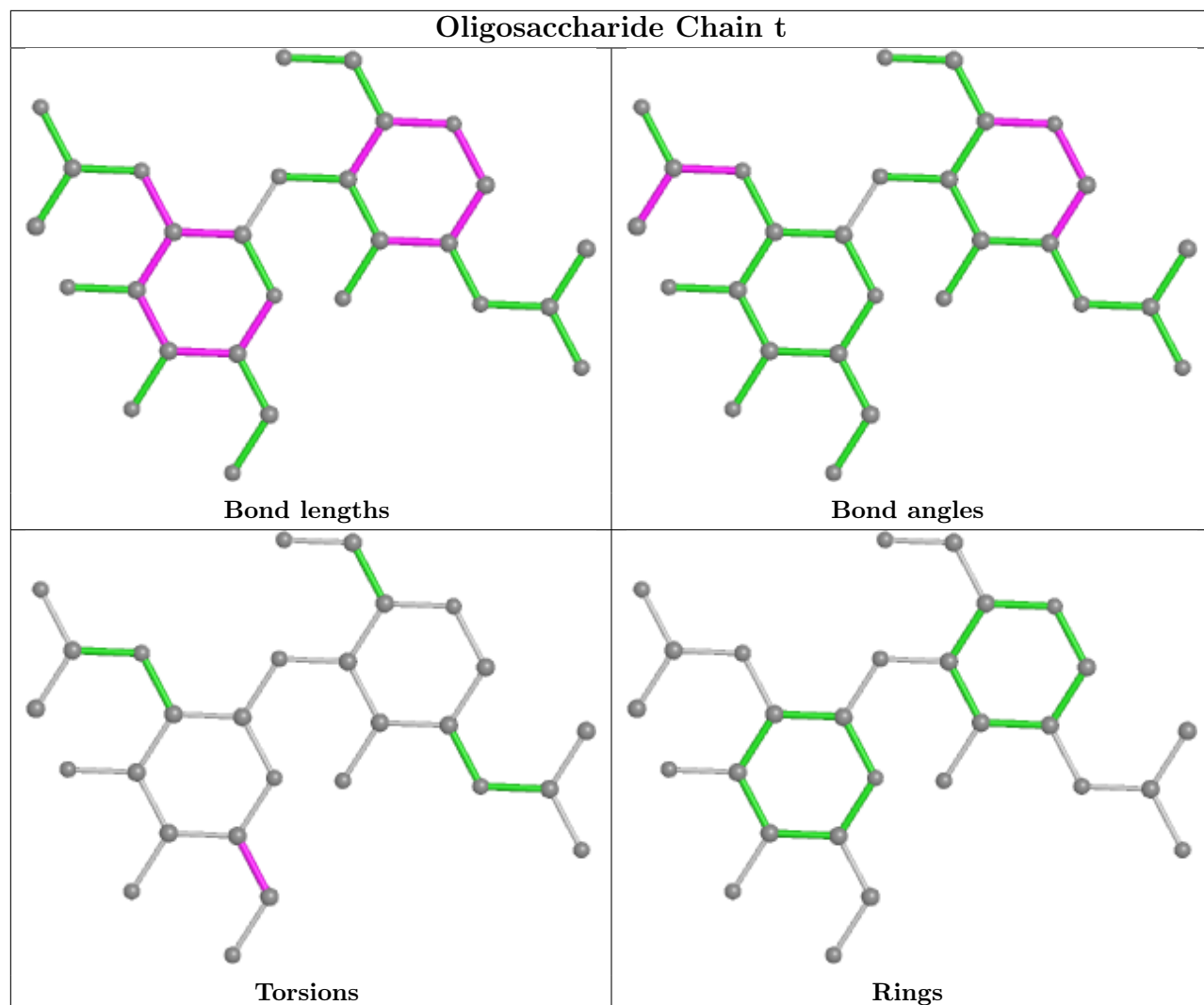


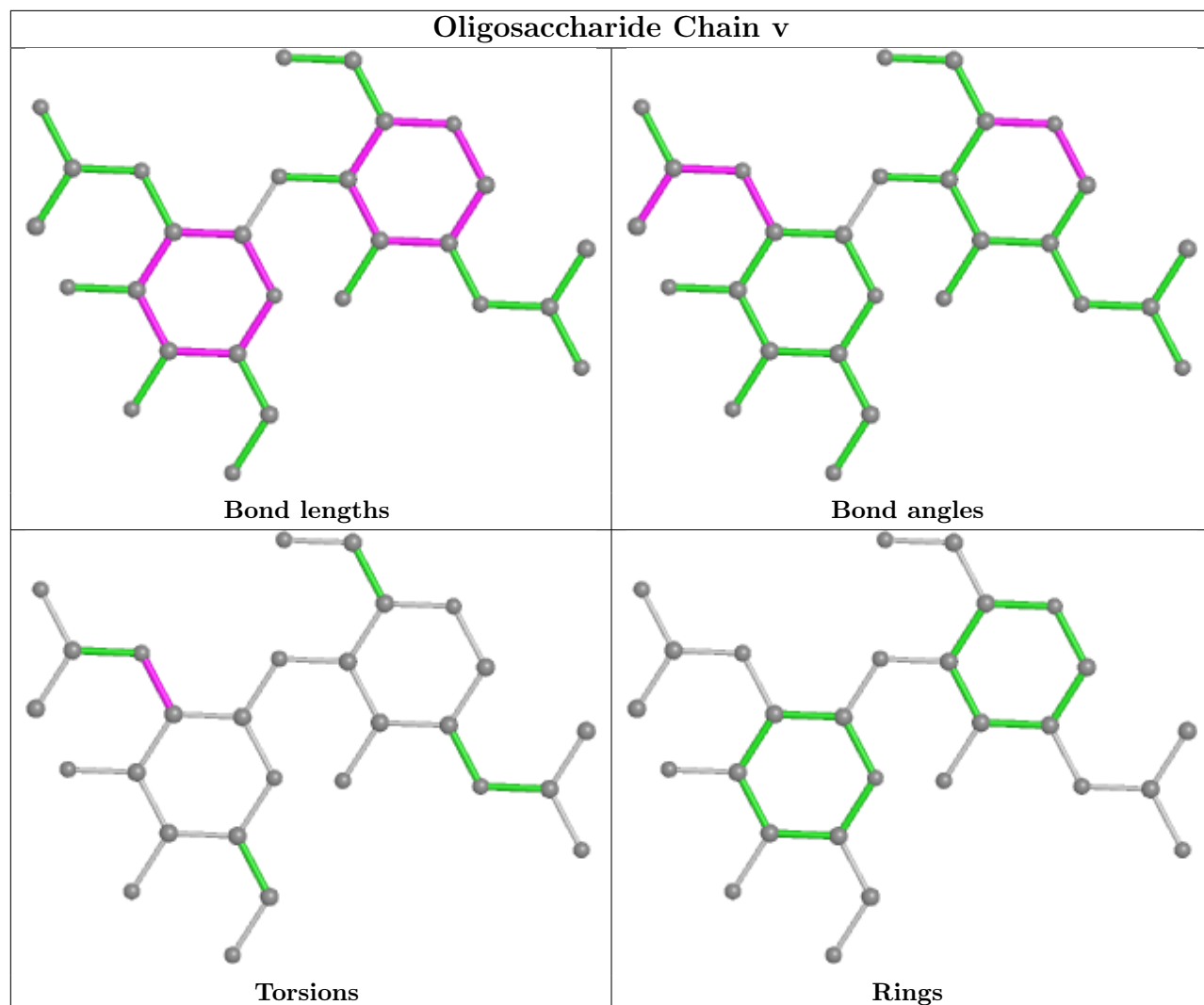


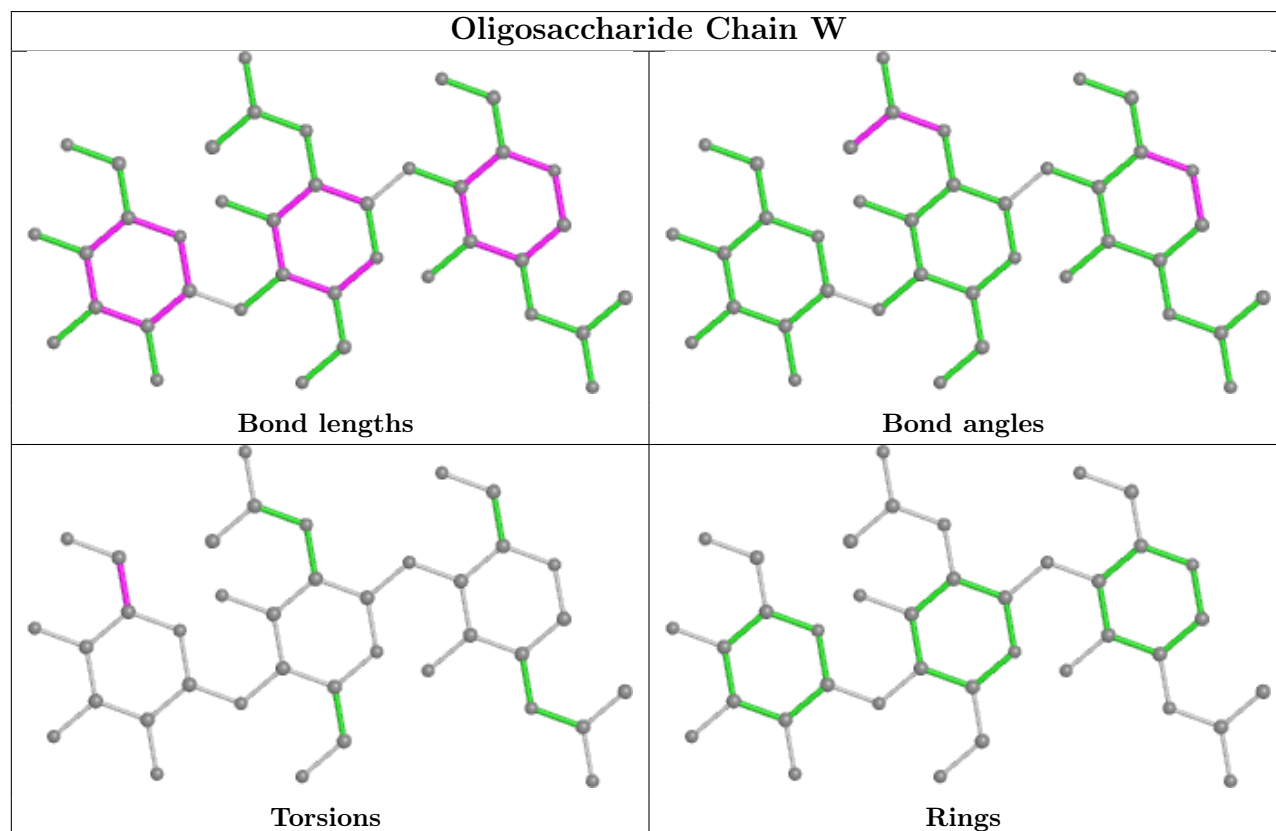
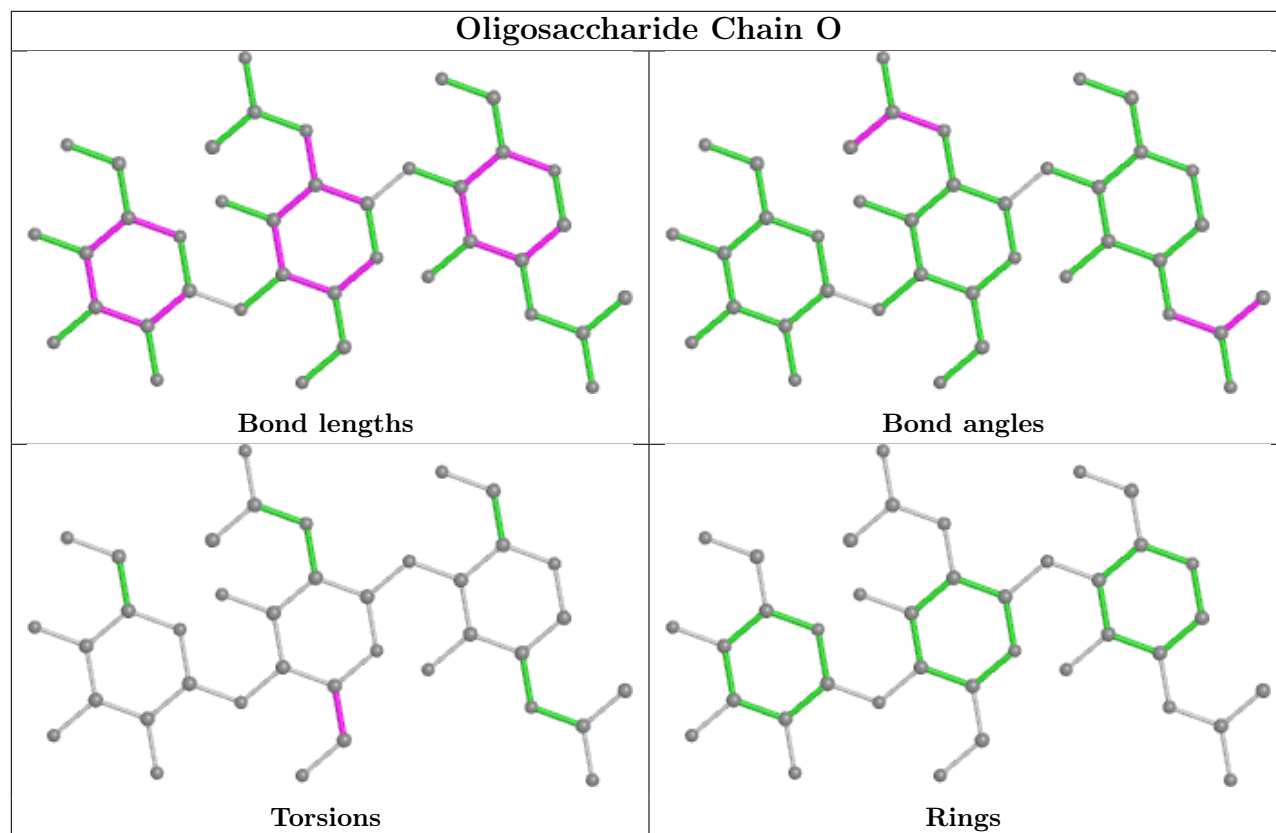




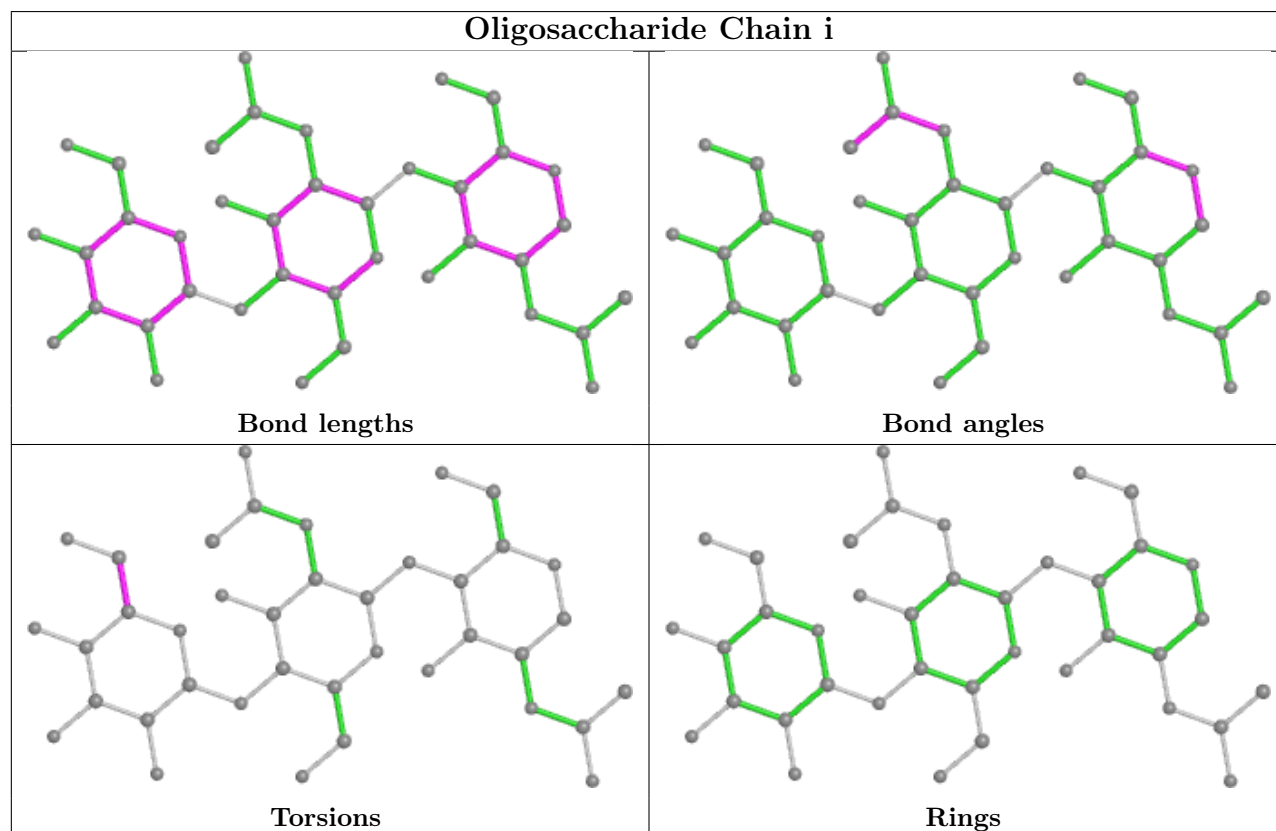
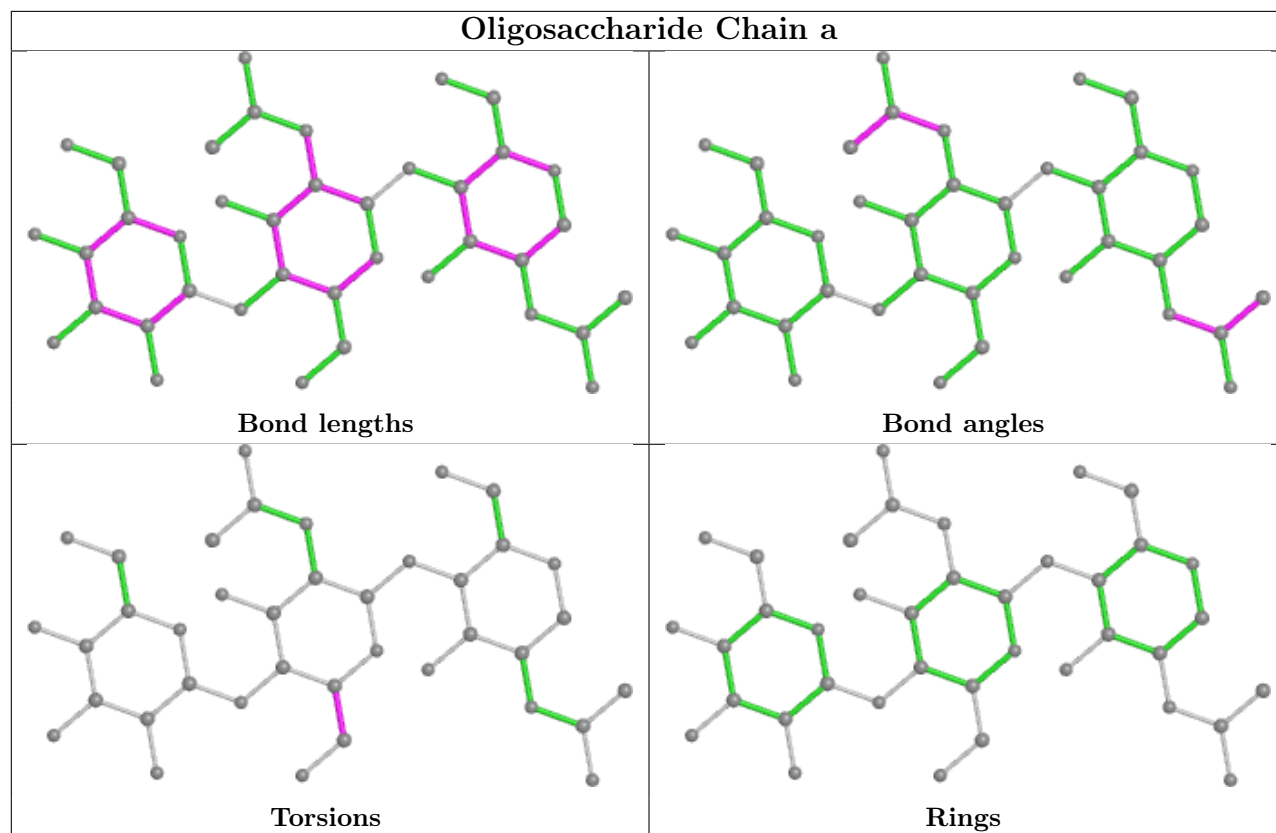


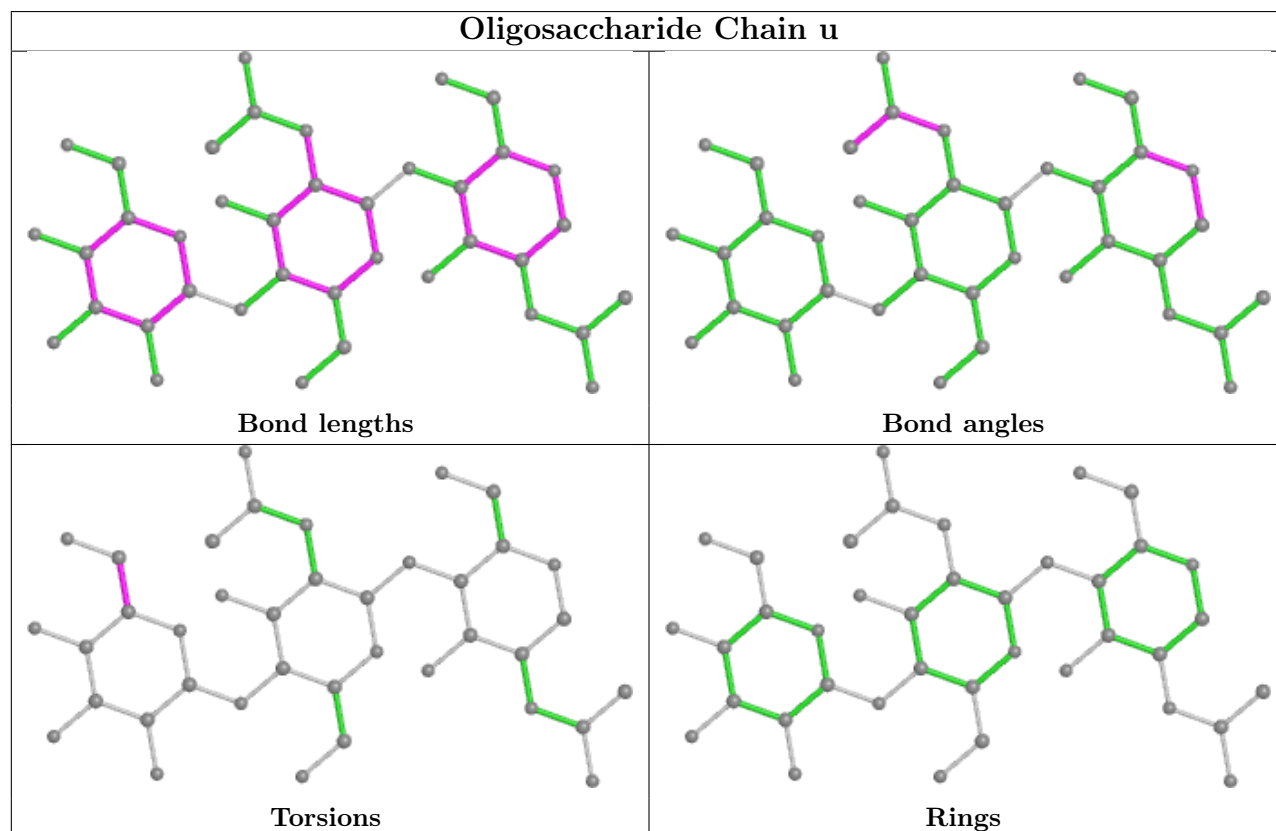
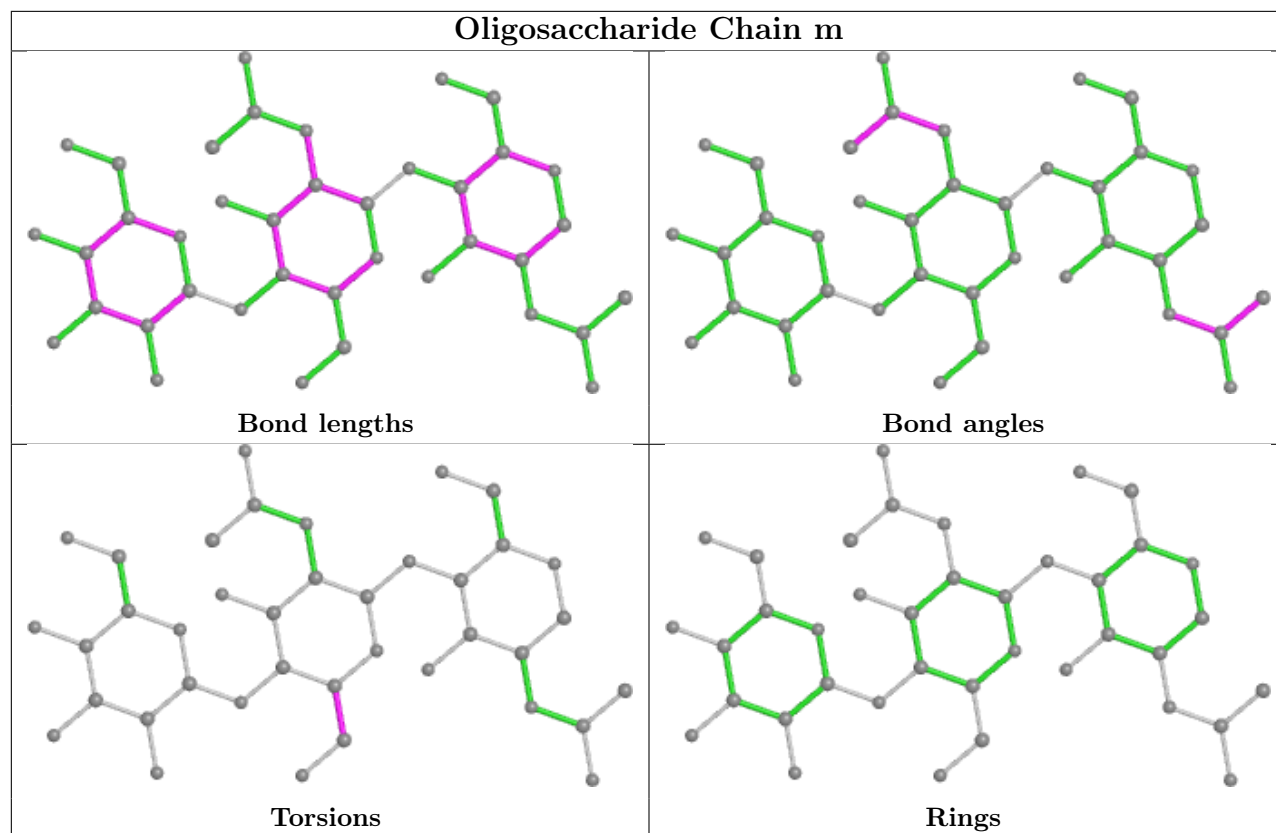


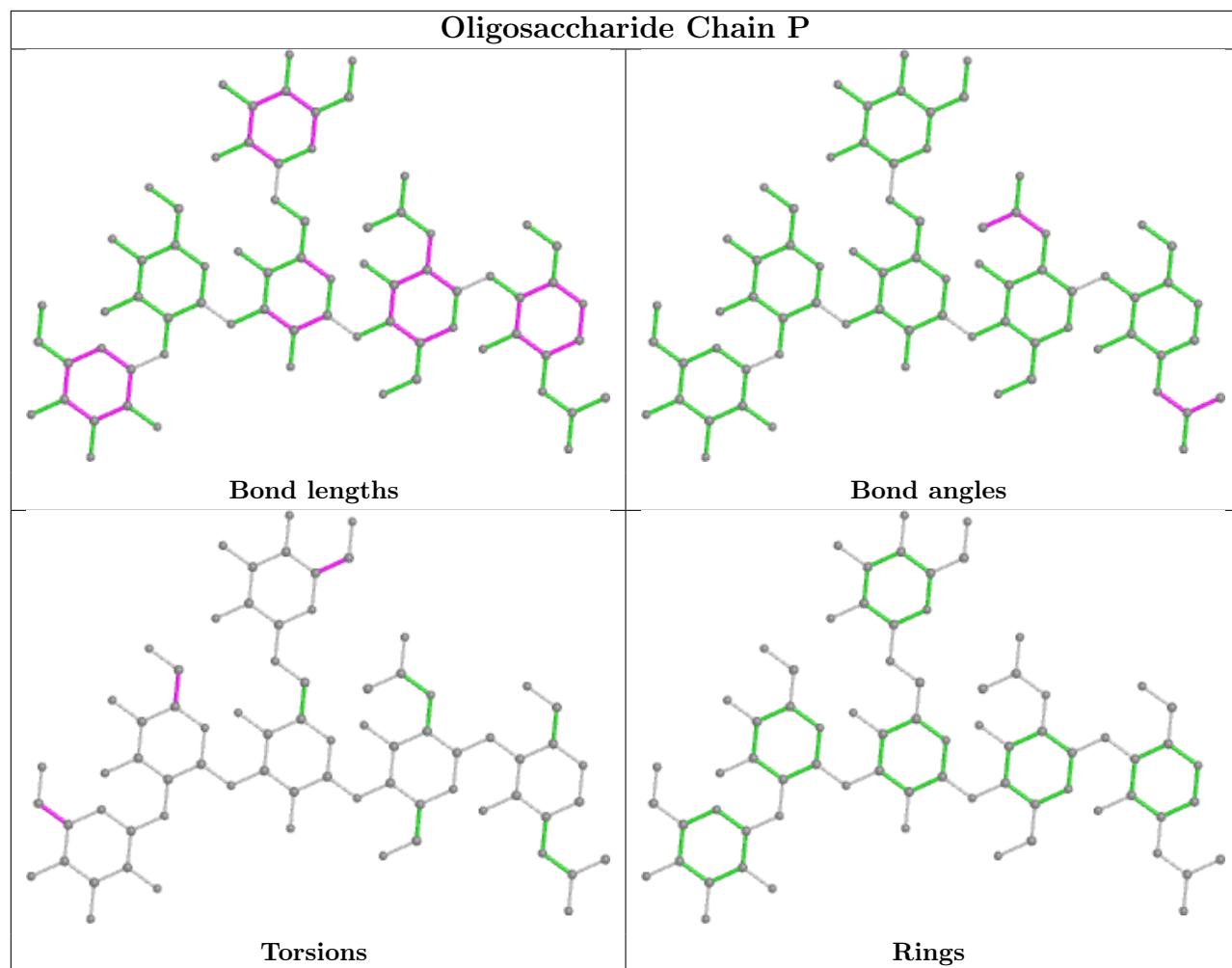


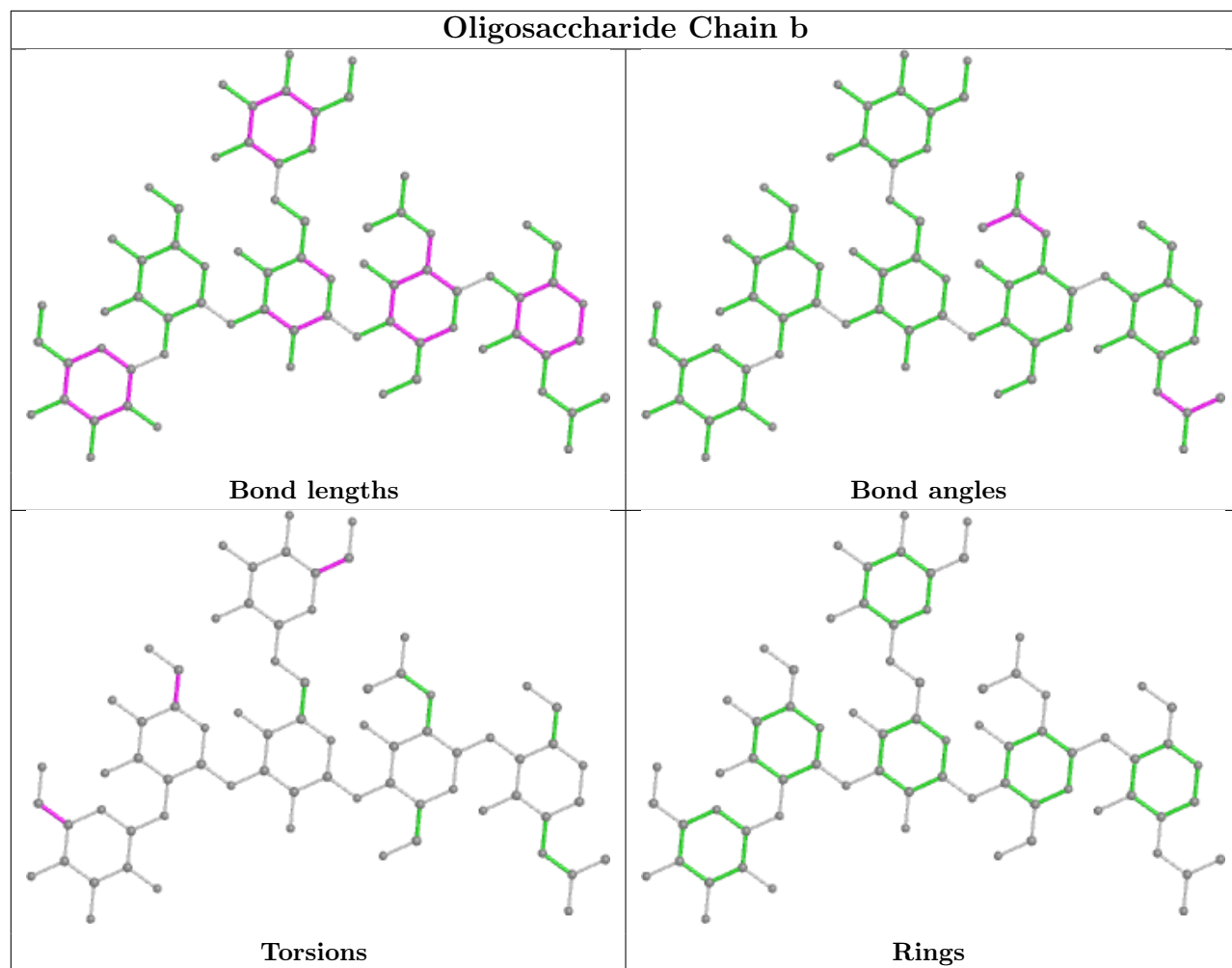


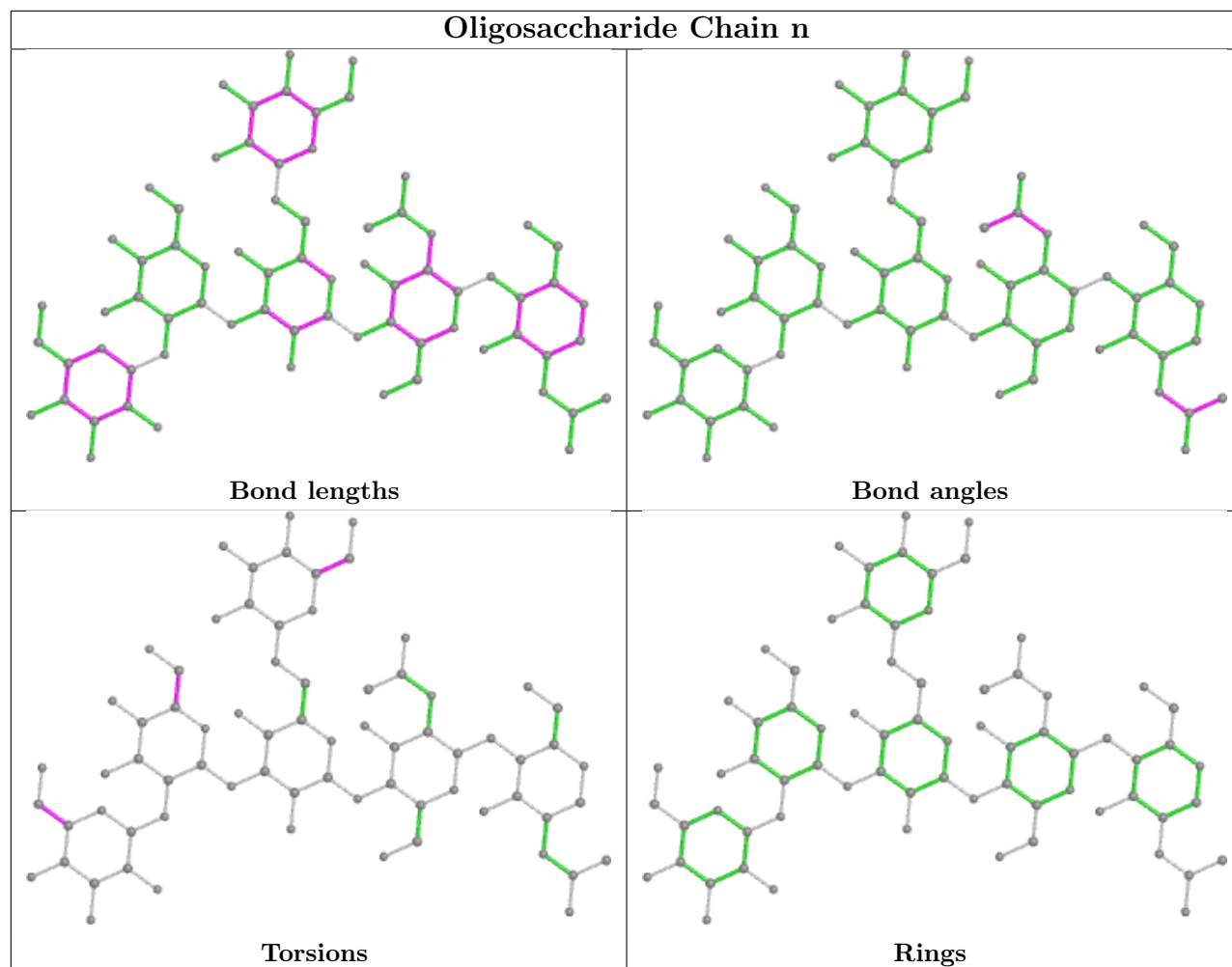


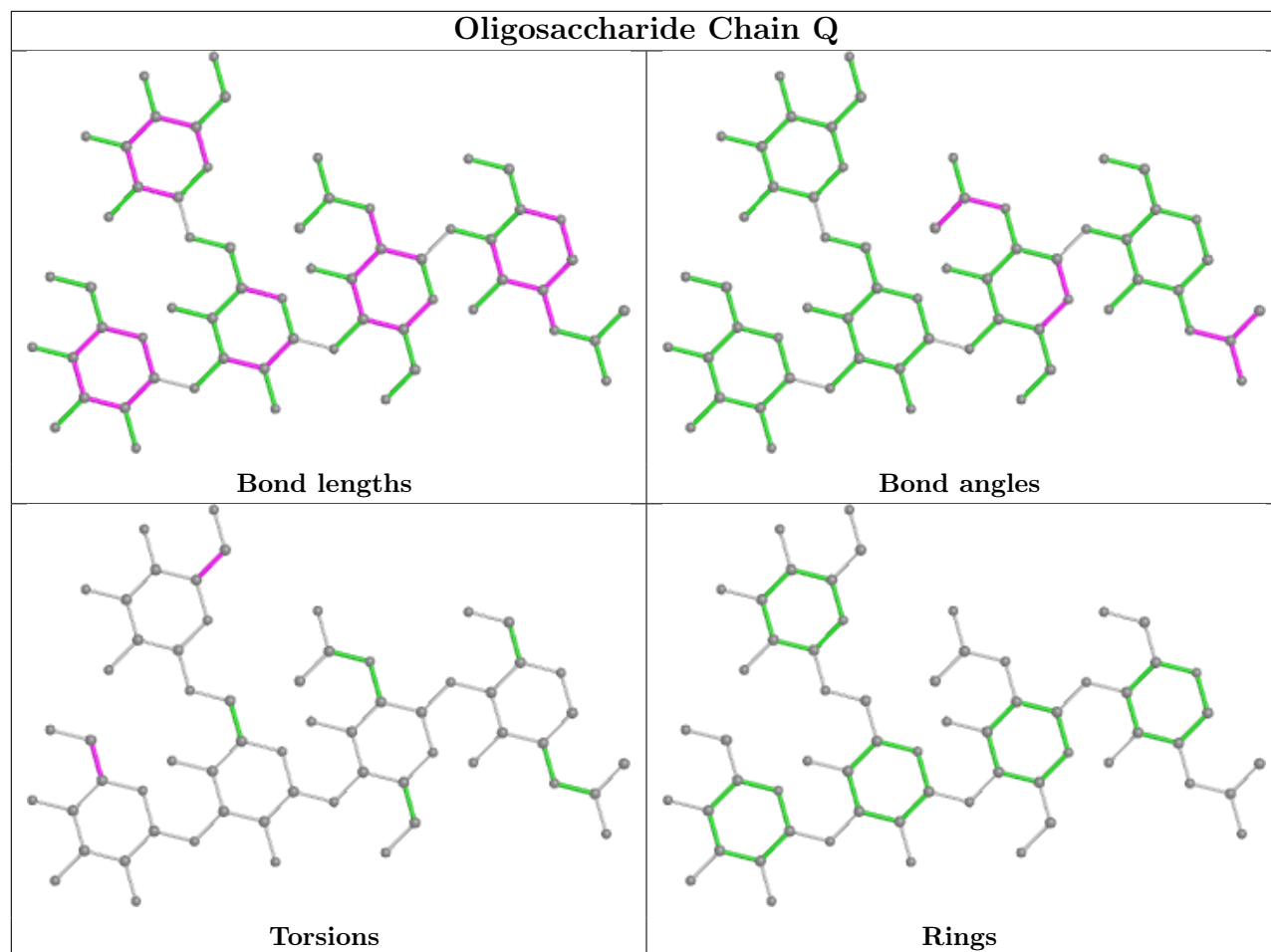


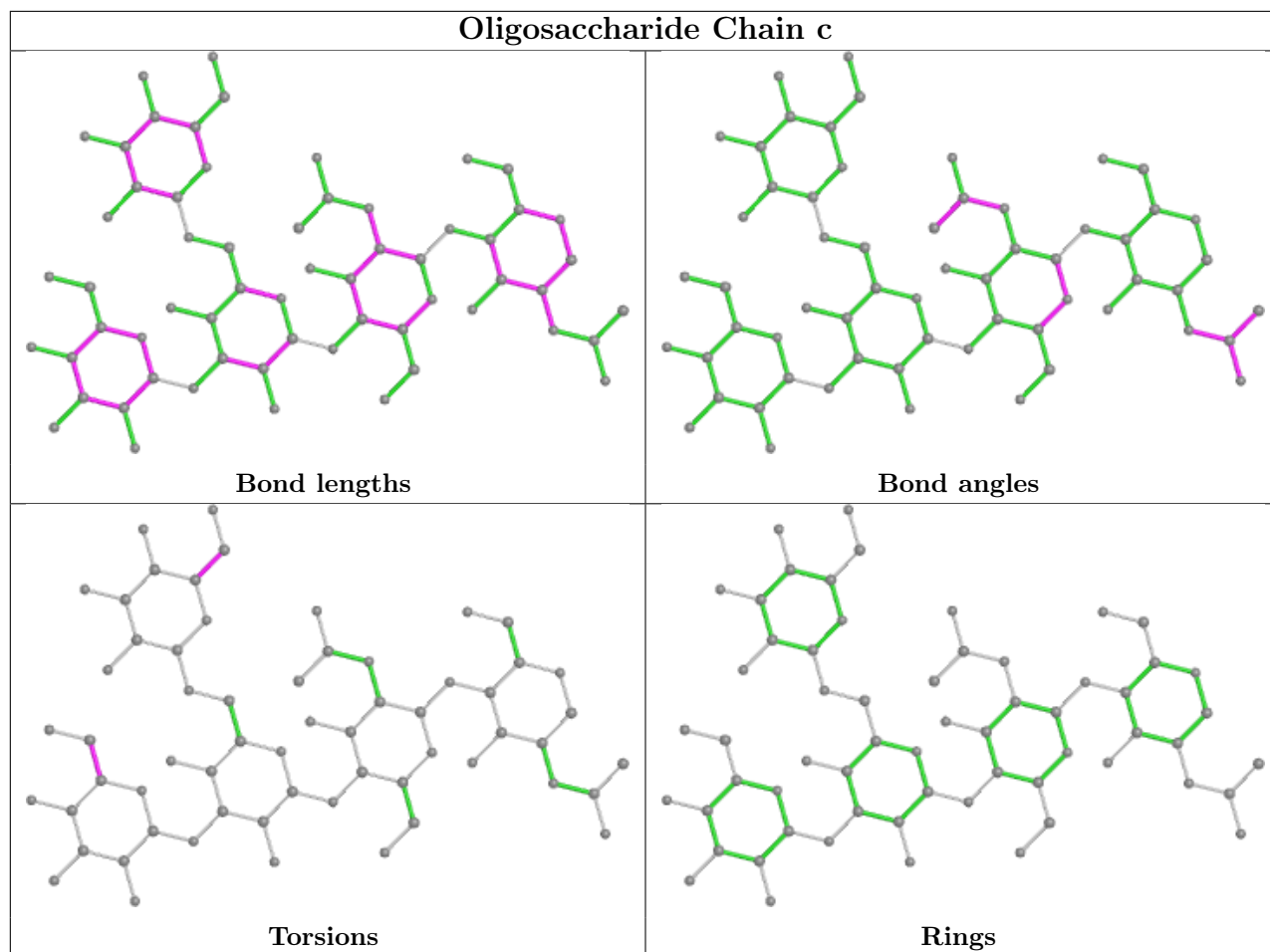


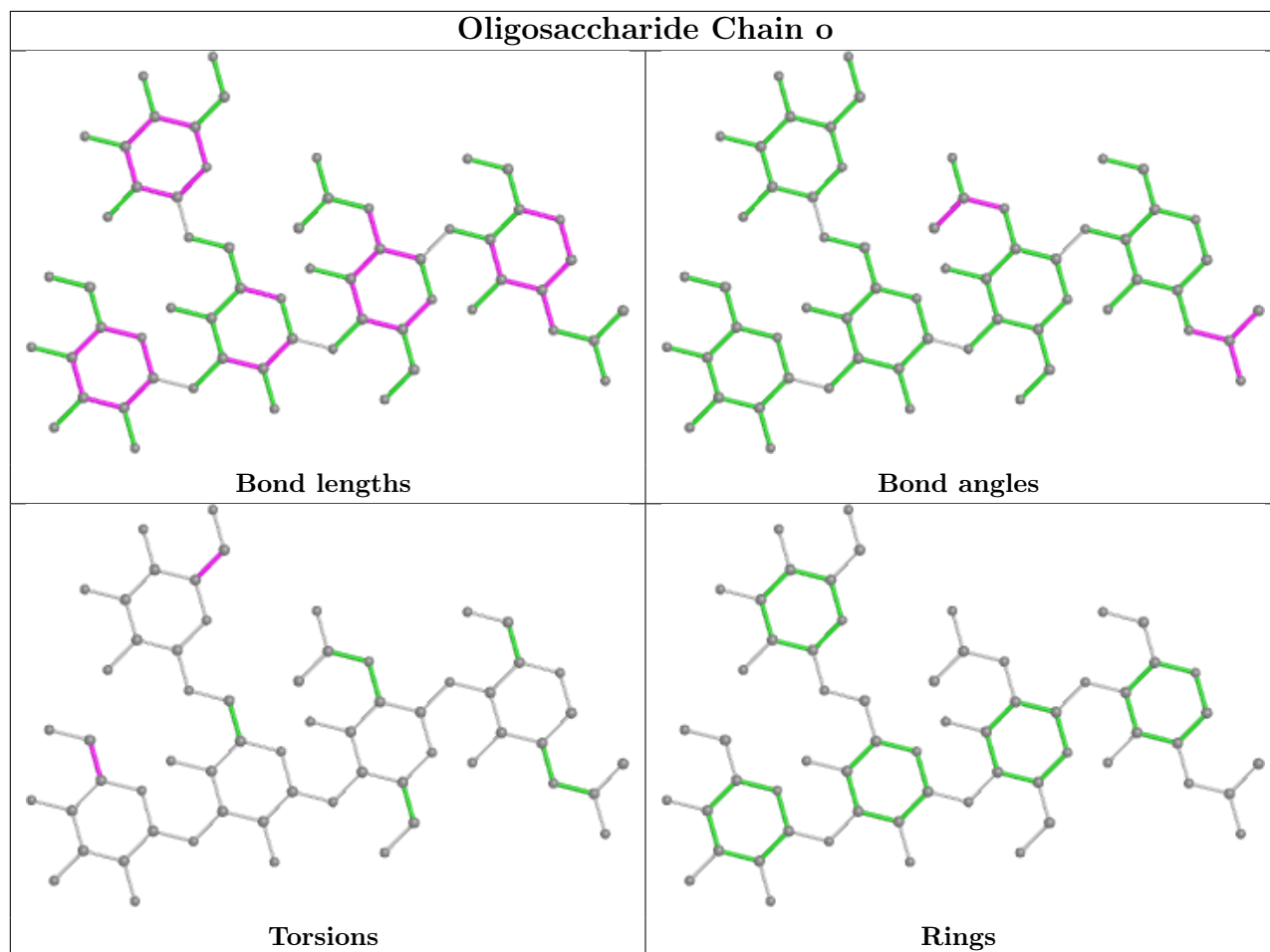












## 5.6 Ligand geometry [i](#)

45 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$
9	NAG	D	606	1	14,14,15	2.05	7 (50%)	17,19,21	1.09	1 (5%)
9	NAG	A	610	1	14,14,15	2.18	6 (42%)	17,19,21	1.03	2 (11%)
9	NAG	A	611	1	14,14,15	2.04	6 (42%)	17,19,21	1.00	1 (5%)
9	NAG	C	605	1	14,14,15	2.17	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	A	612	1	14,14,15	2.22	6 (42%)	17,19,21	0.95	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	C	607	1	14,14,15	2.13	5 (35%)	17,19,21	0.94	0
9	NAG	D	612	1	14,14,15	2.21	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	F	701	2	14,14,15	2.28	6 (42%)	17,19,21	1.06	1 (5%)
9	NAG	A	603	1	14,14,15	2.17	6 (42%)	17,19,21	2.08	2 (11%)
9	NAG	D	602	1	14,14,15	2.12	7 (50%)	17,19,21	1.07	2 (11%)
9	NAG	D	611	1	14,14,15	2.04	6 (42%)	17,19,21	1.00	1 (5%)
9	NAG	D	605	1	14,14,15	2.17	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	B	703	2	14,14,15	2.20	5 (35%)	17,19,21	0.94	0
9	NAG	C	601	1	14,14,15	2.11	6 (42%)	17,19,21	1.02	1 (5%)
9	NAG	D	609	1	14,14,15	1.89	6 (42%)	17,19,21	6.60	3 (17%)
9	NAG	C	606	1	14,14,15	2.04	7 (50%)	17,19,21	1.09	1 (5%)
9	NAG	A	602	1	14,14,15	2.12	7 (50%)	17,19,21	1.07	1 (5%)
9	NAG	B	702	2	14,14,15	2.20	6 (42%)	17,19,21	1.05	2 (11%)
9	NAG	C	602	1	14,14,15	2.12	7 (50%)	17,19,21	1.07	1 (5%)
9	NAG	D	601	1	14,14,15	2.11	6 (42%)	17,19,21	1.02	1 (5%)
9	NAG	C	611	1	14,14,15	2.03	6 (42%)	17,19,21	1.00	1 (5%)
9	NAG	C	608	1	14,14,15	2.25	6 (42%)	17,19,21	1.11	1 (5%)
9	NAG	B	701	2	14,14,15	2.27	6 (42%)	17,19,21	1.06	1 (5%)
9	NAG	F	703	2	14,14,15	2.20	5 (35%)	17,19,21	0.94	0
9	NAG	C	604	1	14,14,15	2.23	5 (35%)	17,19,21	0.97	0
9	NAG	C	612	1	14,14,15	2.22	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	A	606	1	14,14,15	2.04	7 (50%)	17,19,21	1.08	1 (5%)
9	NAG	E	703	2	14,14,15	2.20	5 (35%)	17,19,21	0.94	0
9	NAG	E	702	2	14,14,15	2.20	7 (50%)	17,19,21	1.05	2 (11%)
9	NAG	A	604	1	14,14,15	2.22	5 (35%)	17,19,21	0.97	0
9	NAG	F	702	2	14,14,15	2.20	6 (42%)	17,19,21	1.06	2 (11%)
9	NAG	D	610	1	14,14,15	2.17	7 (50%)	17,19,21	1.03	1 (5%)
9	NAG	A	605	1	14,14,15	2.17	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	D	608	1	14,14,15	2.25	6 (42%)	17,19,21	1.11	1 (5%)
9	NAG	A	607	1	14,14,15	2.13	5 (35%)	17,19,21	0.94	0
9	NAG	D	603	1	14,14,15	2.17	6 (42%)	17,19,21	2.08	2 (11%)
9	NAG	E	701	2	14,14,15	2.28	6 (42%)	17,19,21	1.06	1 (5%)
9	NAG	C	610	1	14,14,15	2.17	6 (42%)	17,19,21	1.02	2 (11%)
9	NAG	A	601	1	14,14,15	2.12	6 (42%)	17,19,21	1.01	1 (5%)
9	NAG	A	608	1	14,14,15	2.25	6 (42%)	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	609	1	14,14,15	1.88	6 (42%)	17,19,21	6.59	3 (17%)
9	NAG	D	607	1	14,14,15	2.13	5 (35%)	17,19,21	0.94	0
9	NAG	C	609	1	14,14,15	1.88	6 (42%)	17,19,21	6.60	3 (17%)
9	NAG	C	603	1	14,14,15	2.17	6 (42%)	17,19,21	2.08	2 (11%)
9	NAG	D	604	1	14,14,15	2.23	5 (35%)	17,19,21	0.97	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
9	NAG	D	606	1	-	1/6/23/26	0/1/1/1
9	NAG	A	610	1	-	0/6/23/26	0/1/1/1
9	NAG	A	611	1	-	0/6/23/26	0/1/1/1
9	NAG	C	605	1	-	0/6/23/26	0/1/1/1
9	NAG	A	612	1	-	0/6/23/26	0/1/1/1
9	NAG	C	607	1	-	1/6/23/26	0/1/1/1
9	NAG	D	612	1	-	0/6/23/26	0/1/1/1
9	NAG	F	701	2	-	0/6/23/26	0/1/1/1
9	NAG	A	603	1	-	3/6/23/26	0/1/1/1
9	NAG	D	602	1	-	1/6/23/26	0/1/1/1
9	NAG	D	611	1	-	0/6/23/26	0/1/1/1
9	NAG	D	605	1	-	0/6/23/26	0/1/1/1
9	NAG	B	703	2	-	0/6/23/26	0/1/1/1
9	NAG	C	601	1	-	0/6/23/26	0/1/1/1
9	NAG	D	609	1	-	0/6/23/26	0/1/1/1
9	NAG	C	606	1	-	1/6/23/26	0/1/1/1
9	NAG	A	602	1	-	1/6/23/26	0/1/1/1
9	NAG	B	702	2	-	0/6/23/26	0/1/1/1
9	NAG	C	602	1	-	1/6/23/26	0/1/1/1
9	NAG	D	601	1	-	0/6/23/26	0/1/1/1
9	NAG	C	611	1	-	0/6/23/26	0/1/1/1
9	NAG	C	608	1	-	2/6/23/26	0/1/1/1
9	NAG	B	701	2	-	0/6/23/26	0/1/1/1
9	NAG	F	703	2	-	0/6/23/26	0/1/1/1
9	NAG	C	604	1	-	0/6/23/26	0/1/1/1
9	NAG	C	612	1	-	0/6/23/26	0/1/1/1
9	NAG	A	606	1	-	1/6/23/26	0/1/1/1
9	NAG	E	703	2	-	0/6/23/26	0/1/1/1
9	NAG	E	702	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	604	1	-	0/6/23/26	0/1/1/1
9	NAG	F	702	2	-	0/6/23/26	0/1/1/1
9	NAG	D	610	1	-	0/6/23/26	0/1/1/1
9	NAG	A	605	1	-	0/6/23/26	0/1/1/1
9	NAG	D	608	1	-	2/6/23/26	0/1/1/1
9	NAG	A	607	1	-	1/6/23/26	0/1/1/1
9	NAG	D	603	1	-	3/6/23/26	0/1/1/1
9	NAG	E	701	2	-	0/6/23/26	0/1/1/1
9	NAG	C	610	1	-	0/6/23/26	0/1/1/1
9	NAG	A	601	1	-	0/6/23/26	0/1/1/1
9	NAG	A	608	1	-	2/6/23/26	0/1/1/1
9	NAG	A	609	1	-	0/6/23/26	0/1/1/1
9	NAG	D	607	1	-	1/6/23/26	0/1/1/1
9	NAG	C	609	1	-	0/6/23/26	0/1/1/1
9	NAG	C	603	1	-	3/6/23/26	0/1/1/1
9	NAG	D	604	1	-	0/6/23/26	0/1/1/1

The worst 5 of 269 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	701	NAG	C1-C2	6.03	1.61	1.52
9	E	701	NAG	C1-C2	5.99	1.61	1.52
9	B	701	NAG	C1-C2	5.98	1.61	1.52
9	D	604	NAG	C1-C2	5.72	1.60	1.52
9	C	604	NAG	C1-C2	5.71	1.60	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	609	NAG	C2-N2-C7	26.73	160.97	122.90
9	D	609	NAG	C2-N2-C7	26.72	160.96	122.90
9	A	609	NAG	C2-N2-C7	26.72	160.95	122.90
9	A	603	NAG	C8-C7-N2	6.59	127.26	116.10
9	D	603	NAG	C8-C7-N2	6.59	127.25	116.10

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	603	NAG	C8-C7-N2-C2
9	A	603	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	C	603	NAG	C8-C7-N2-C2
9	C	603	NAG	O7-C7-N2-C2
9	D	603	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

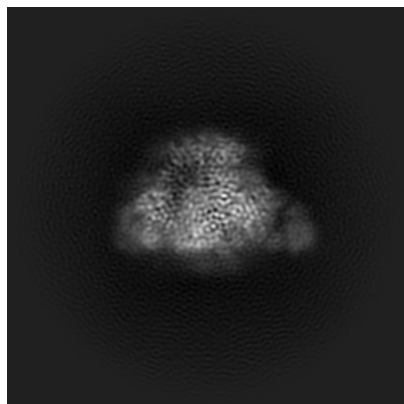
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24676. These allow visual inspection of the internal detail of the map and identification of artifacts.

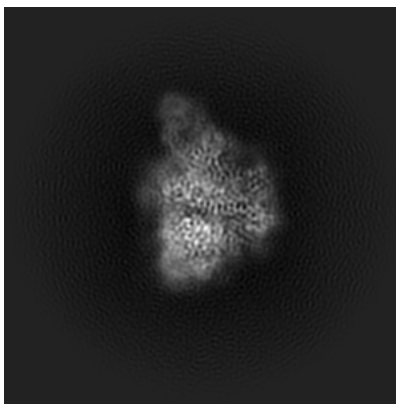
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

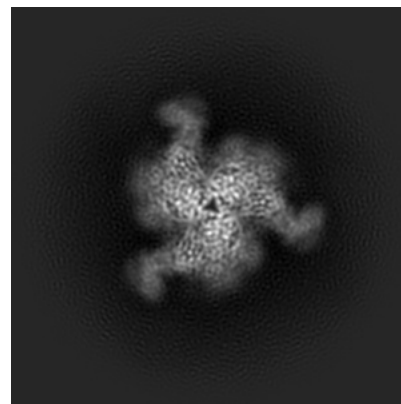
#### 6.1.1 Primary map



X

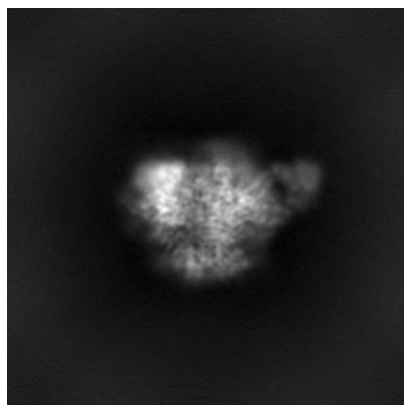


Y

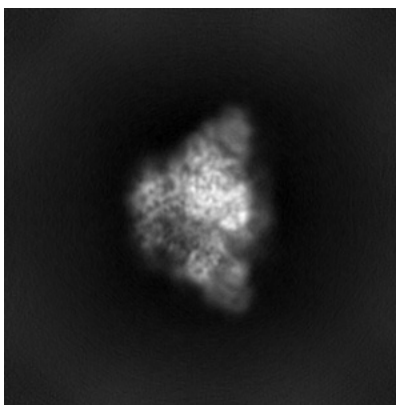


Z

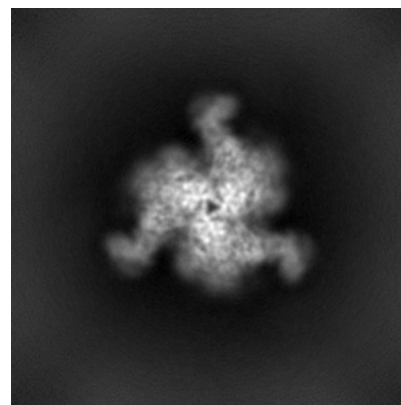
#### 6.1.2 Raw map



X



Y

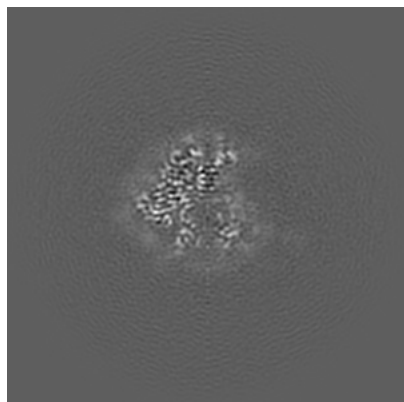


Z

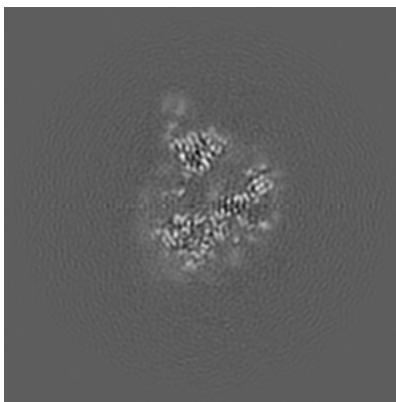
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

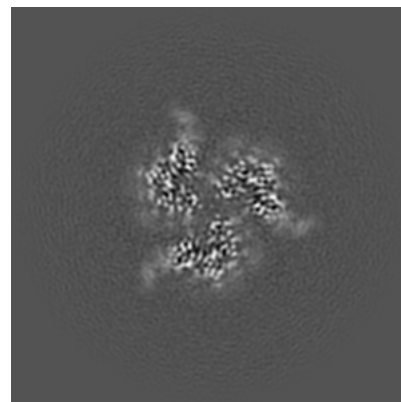
### 6.2.1 Primary map



X Index: 128

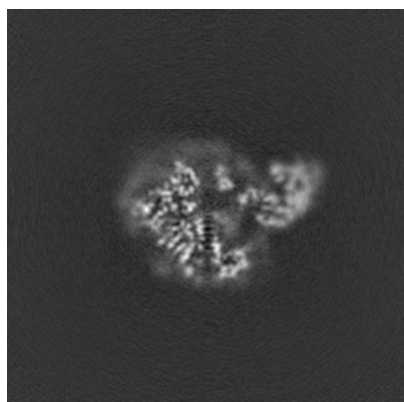


Y Index: 128

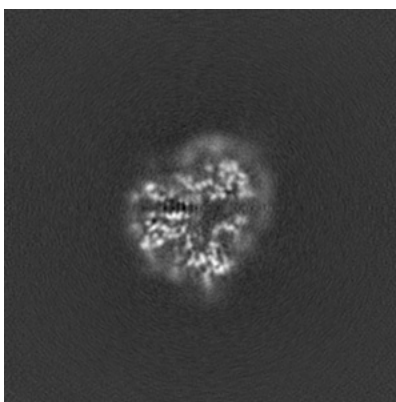


Z Index: 128

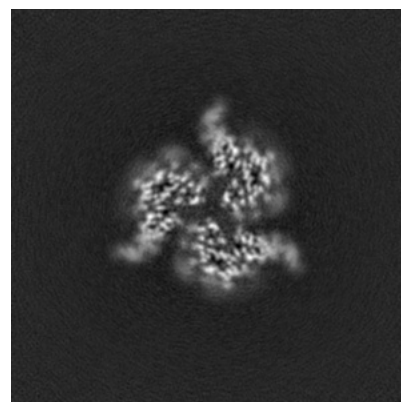
### 6.2.2 Raw map



X Index: 128



Y Index: 128

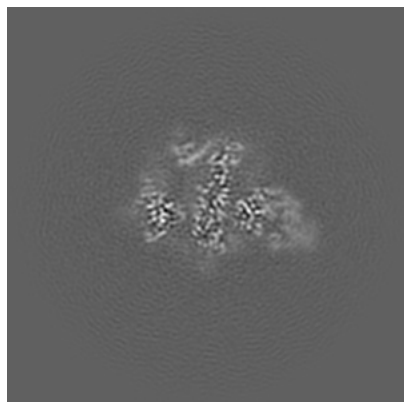


Z Index: 128

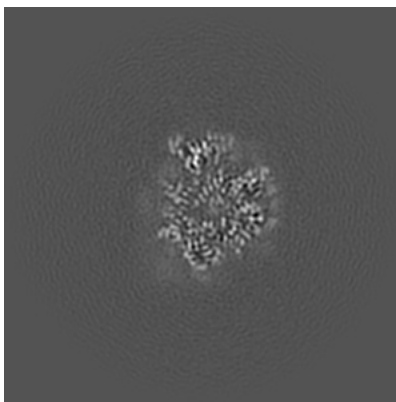
The images above show central slices of the map in three orthogonal directions.

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

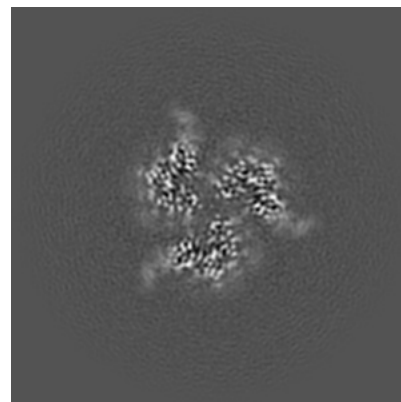
### 6.3.1 Primary map



X Index: 114

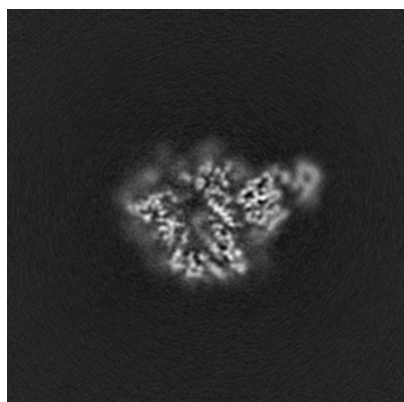


Y Index: 134

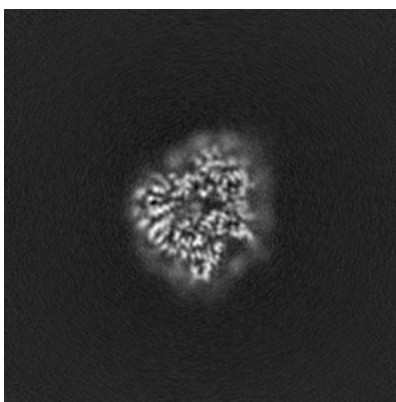


Z Index: 128

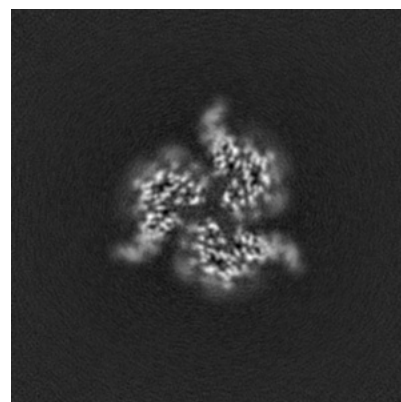
### 6.3.2 Raw map



X Index: 138



Y Index: 135

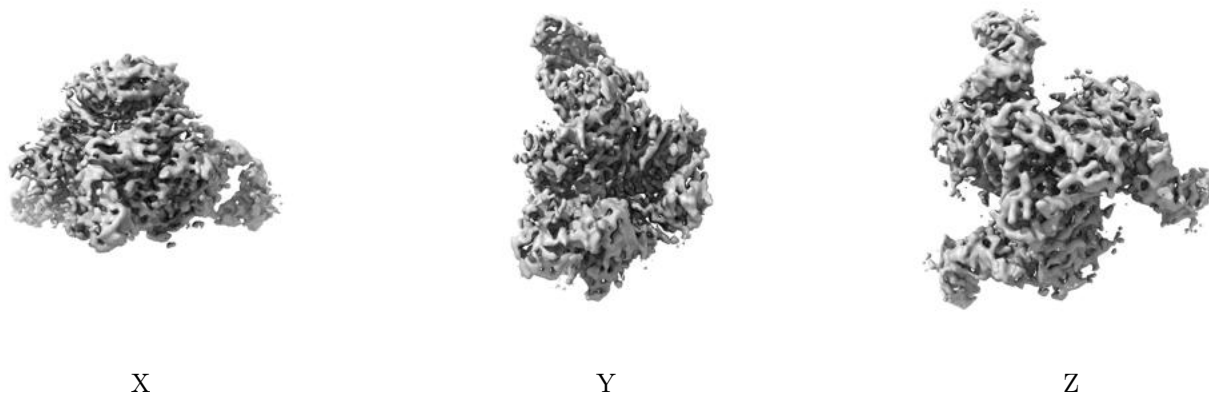


Z Index: 128

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



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

## 6.5 Mask visualisation [i](#)

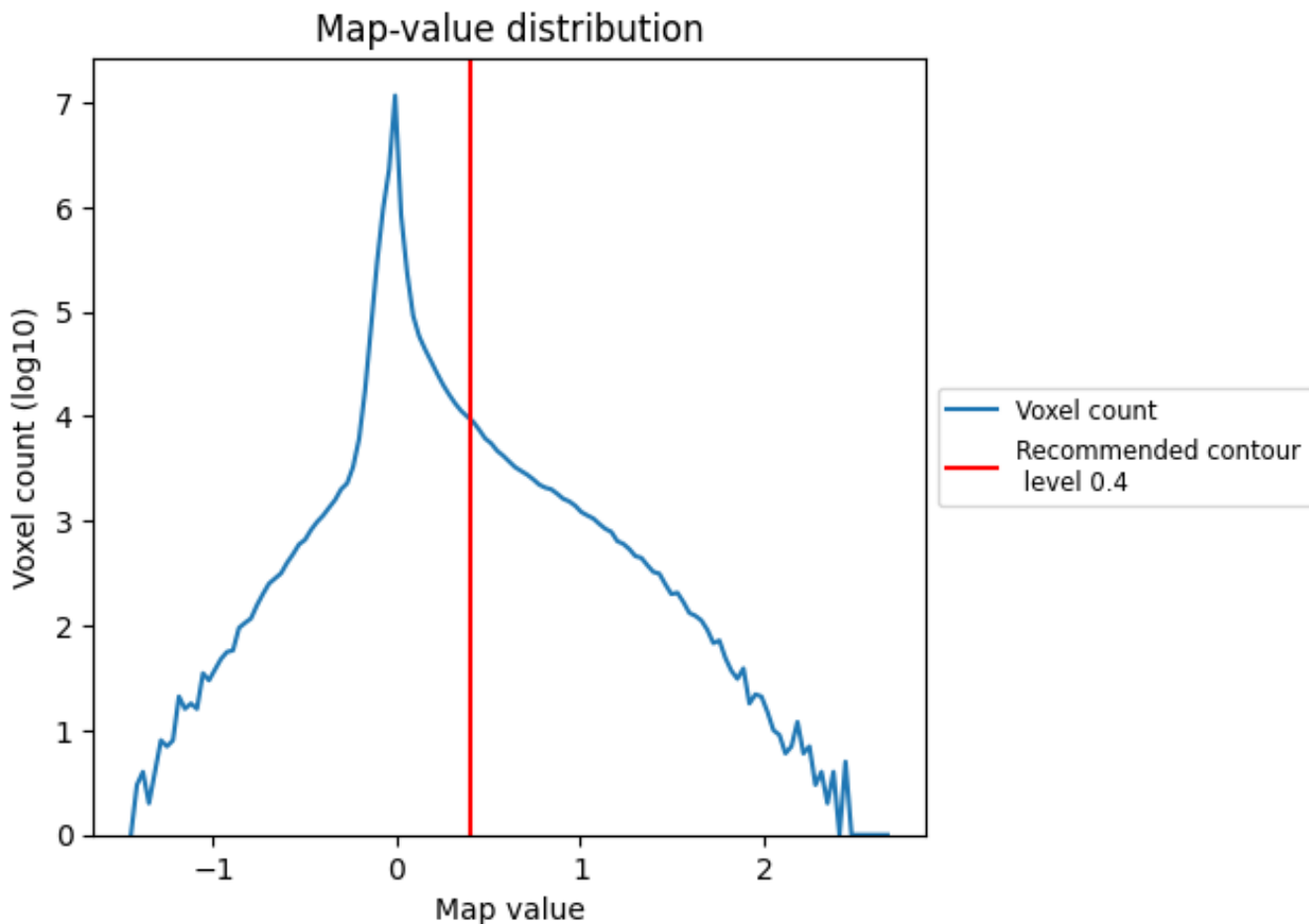
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

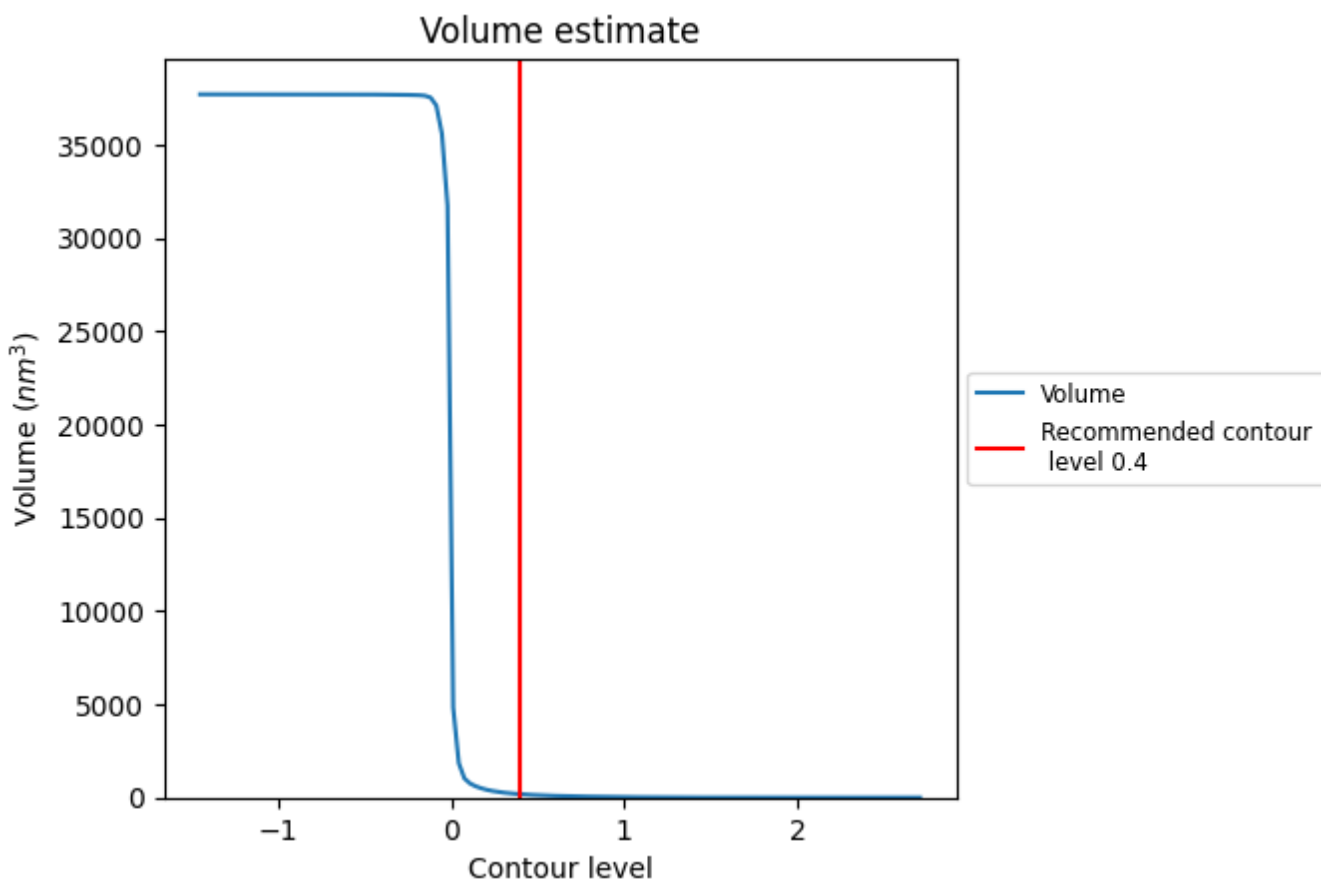
This section contains the results of statistical analysis of the map.

### 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.

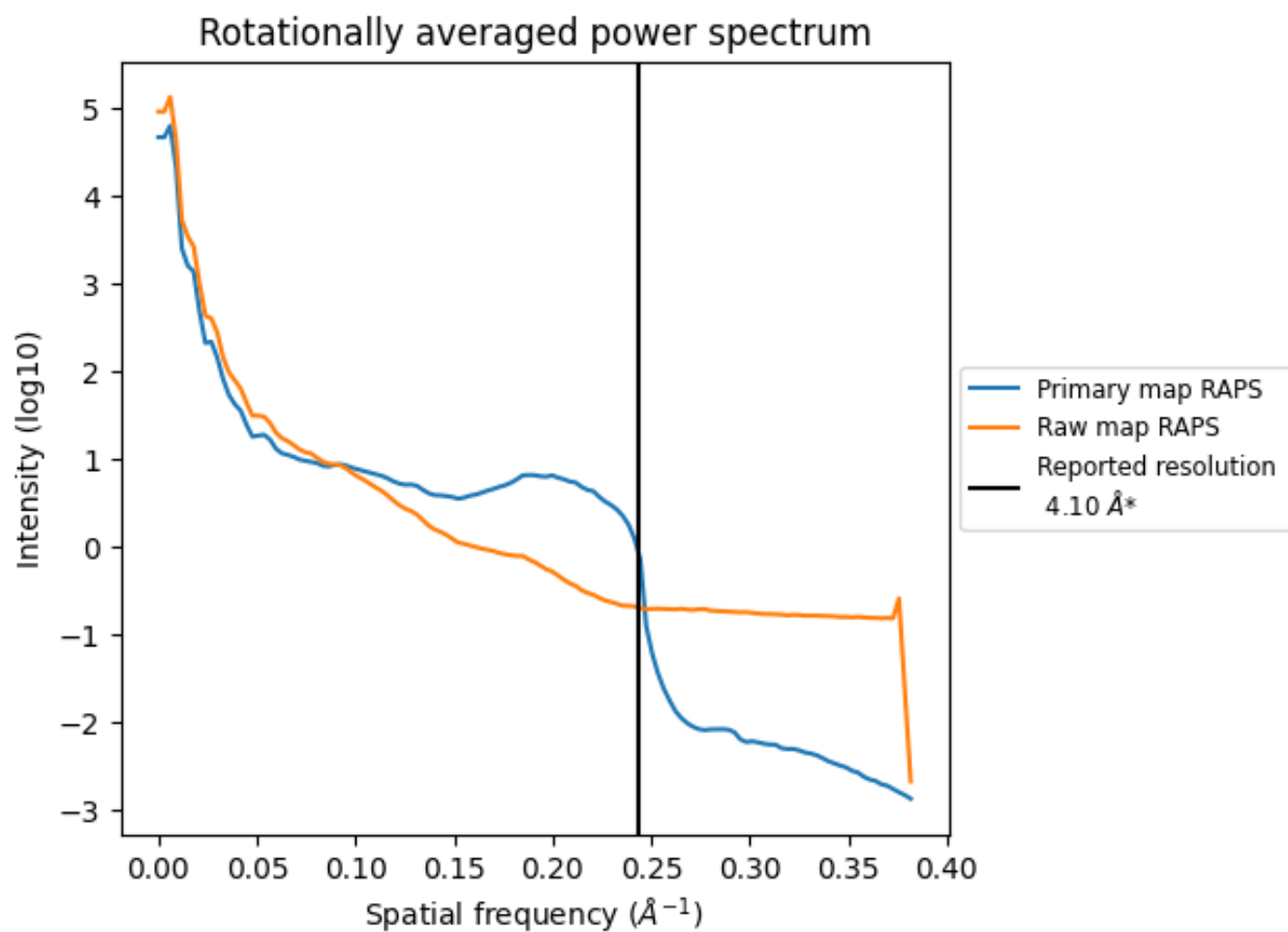
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 182 nm<sup>3</sup>; this corresponds to an approximate mass of 165 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

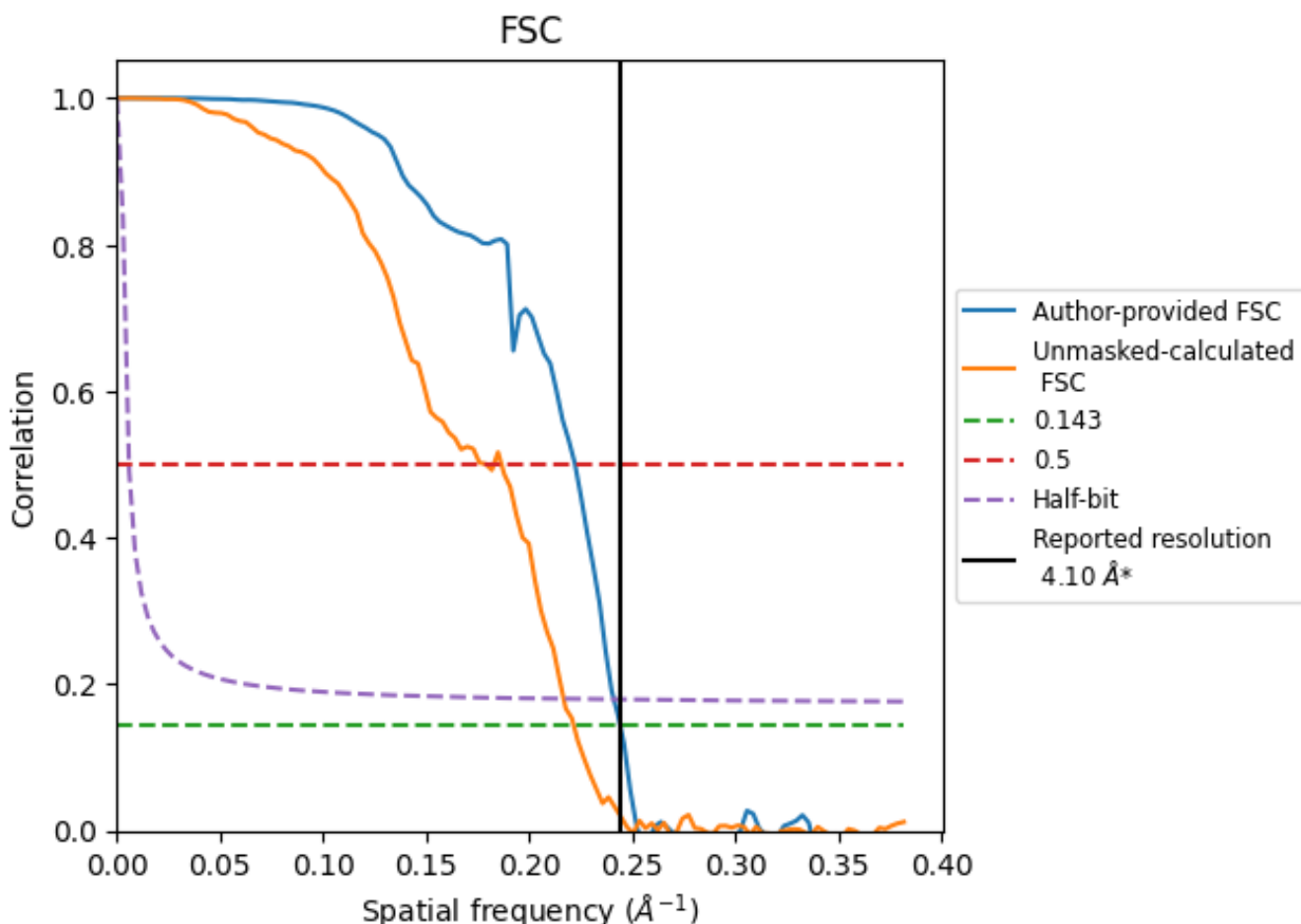


\*Reported resolution corresponds to spatial frequency of  $0.244 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

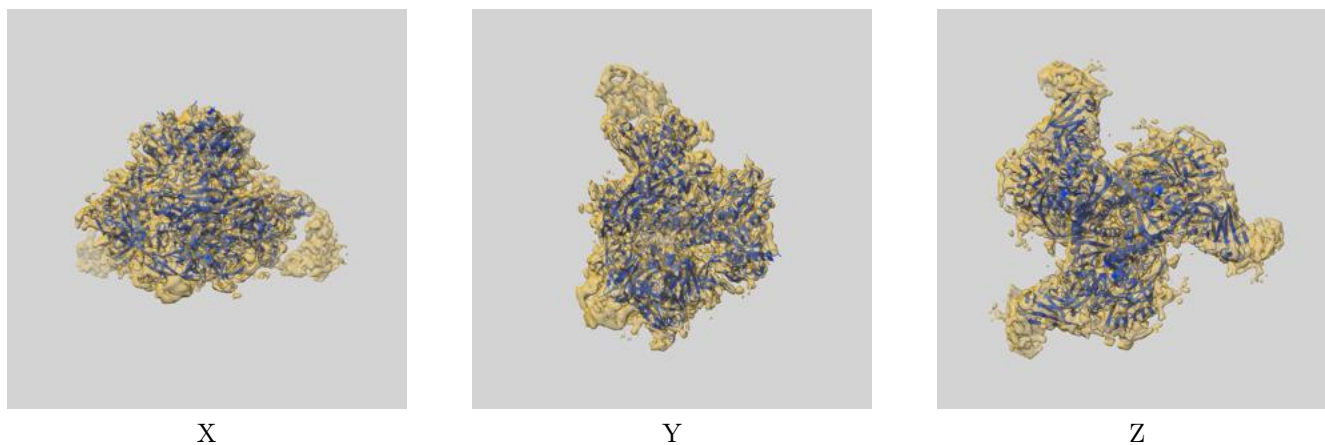
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	4.50	4.15
Unmasked-calculated*	4.51	5.58	4.61

\*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 4.51 differs from the reported value 4.1 by more than 10 %

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

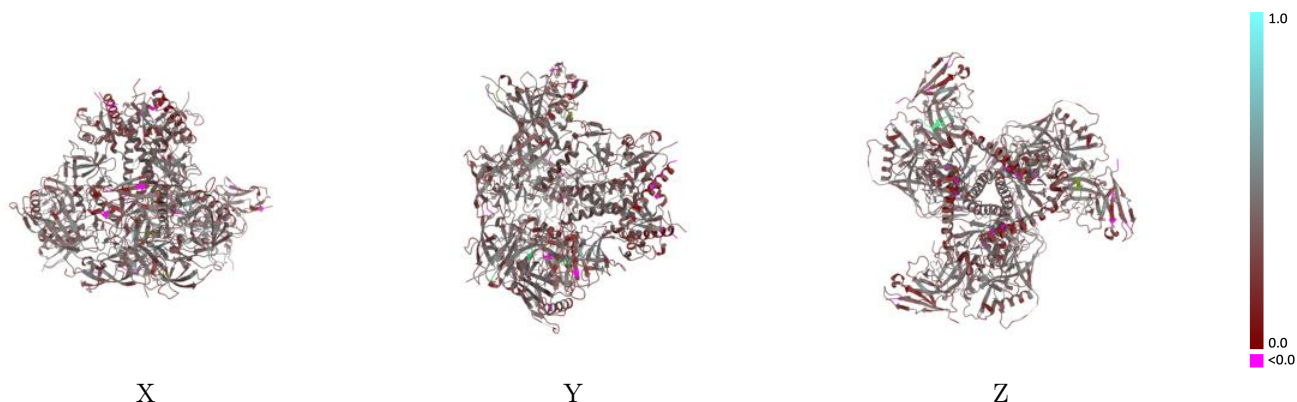
This section contains information regarding the fit between EMDB map EMD-24676 and PDB model 7RSO. Per-residue inclusion information can be found in section 3 on page 12.

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



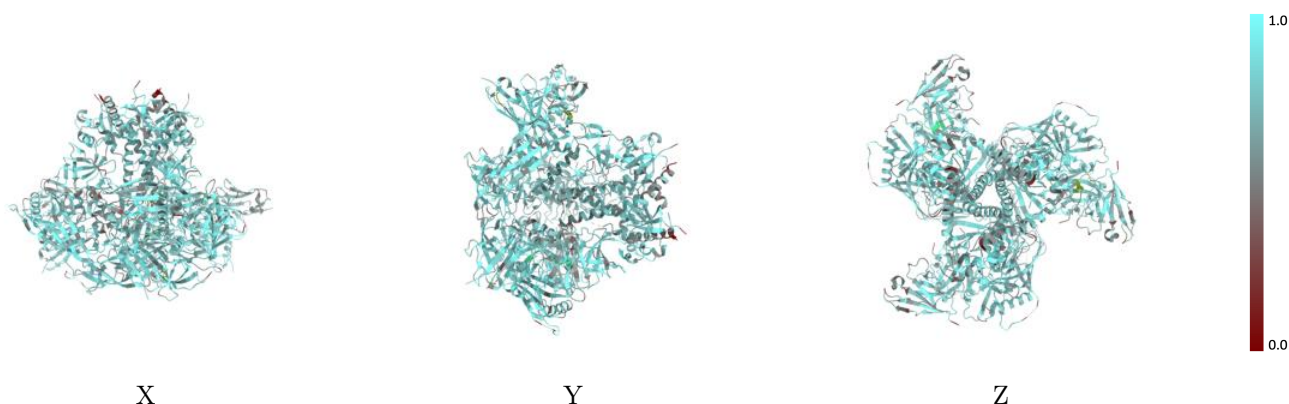
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



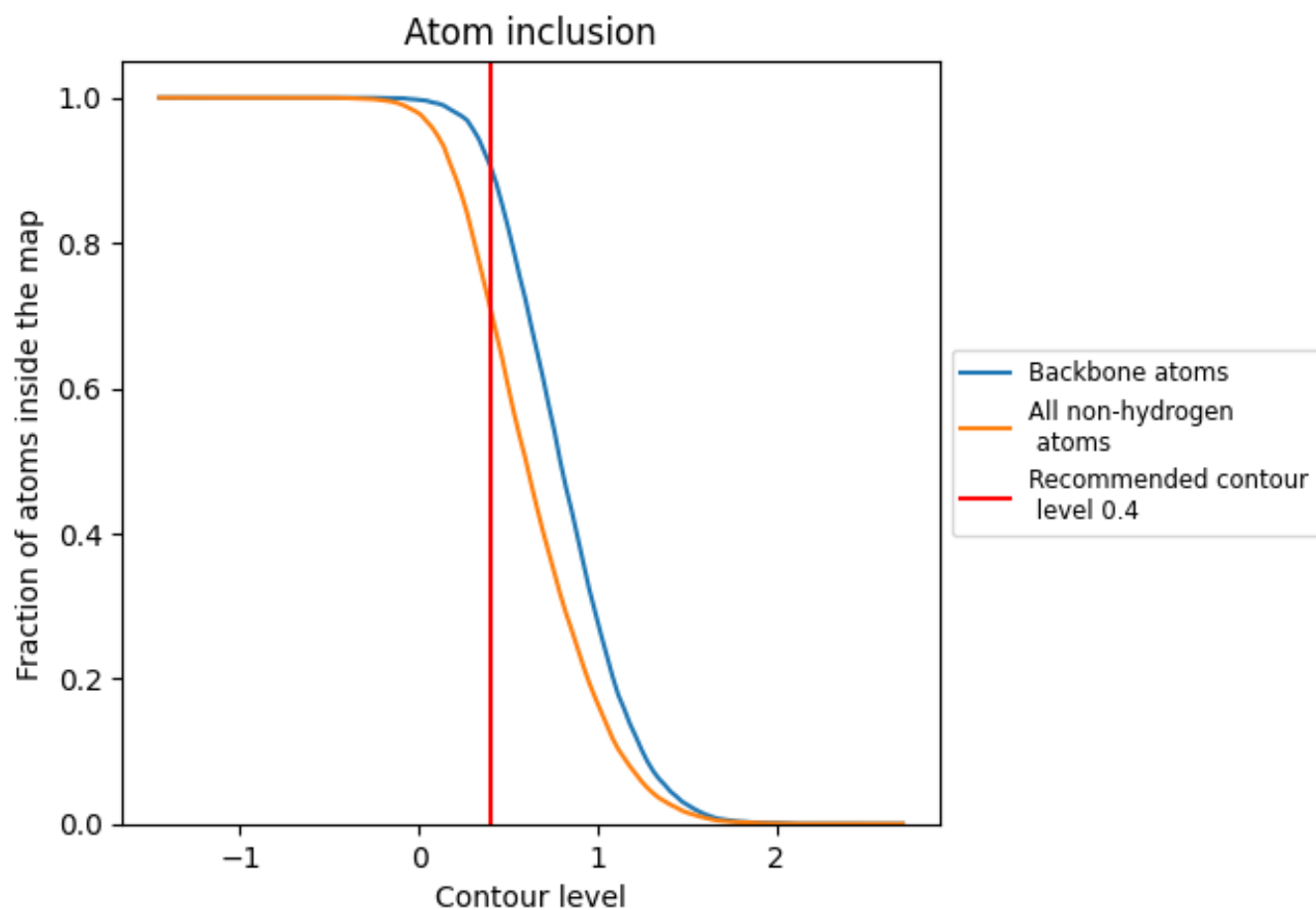
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 91% of all backbone atoms, 71% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.3490
A	 0.7328	 0.3690
B	 0.6916	 0.3030
C	 0.7365	 0.3690
D	 0.7339	 0.3690
E	 0.6887	 0.3030
F	 0.6877	 0.3080
G	 0.7594	 0.3720
H	 0.7626	 0.3750
I	 0.7615	 0.3730
J	 0.6693	 0.3020
K	 0.6654	 0.3040
L	 0.6732	 0.3030
M	 0.4643	 0.3030
N	 0.5357	 0.3790
O	 0.4359	 0.3290
P	 0.6250	 0.3550
Q	 0.7049	 0.3230
R	 0.4286	 0.4490
S	 0.4286	 0.2610
T	 0.6786	 0.3440
U	 0.4286	 0.3020
V	 0.3571	 0.1210
W	 0.4359	 0.2540
X	 0.6429	 0.3390
Y	 0.4643	 0.2870
Z	 0.5357	 0.3760
a	 0.4359	 0.3150
b	 0.6111	 0.3550
c	 0.7049	 0.3240
d	 0.4643	 0.4460
e	 0.3929	 0.2410
f	 0.6786	 0.3330
g	 0.4286	 0.2970
h	 0.3571	 0.1230



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Chain	Atom inclusion	Q-score
i	 0.4359	 0.2600
j	 0.6786	 0.3500
k	 0.4643	 0.2970
l	 0.5357	 0.3700
m	 0.4359	 0.3320
n	 0.6111	 0.3640
o	 0.6885	 0.3330
p	 0.3929	 0.4520
q	 0.4286	 0.2390
r	 0.6786	 0.3370
s	 0.4286	 0.2970
t	 0.3571	 0.1050
u	 0.4359	 0.2620
v	 0.6786	 0.3390