



wwPDB EM Validation Summary Report ⓘ

Apr 28, 2024 – 12:19 AM JST

PDB ID : 8JTM
EMDB ID : EMD-36649
Title : CNE55.664 trimer in complex with broadly neutralizing HIV antibody PGT145
Authors : Chatterjee, A.; Chen, C.; Lee, K.; Mangala Prasad, V.
Deposited on : 2023-06-22
Resolution : 5.14 Å(reported)
Based on initial model : 5V8L

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

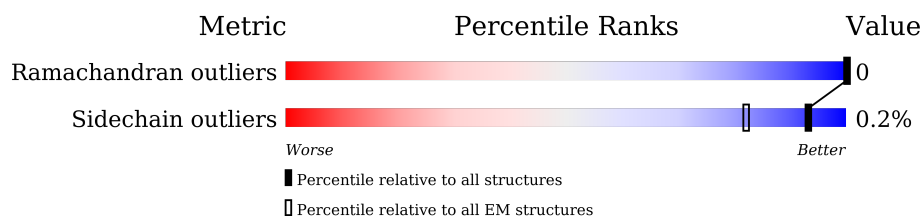
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

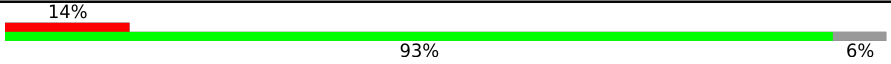
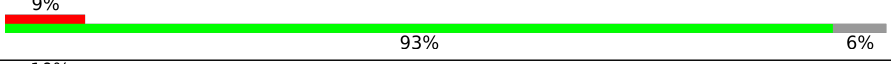
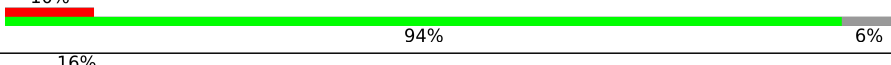



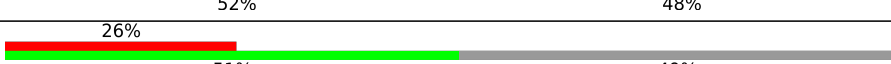
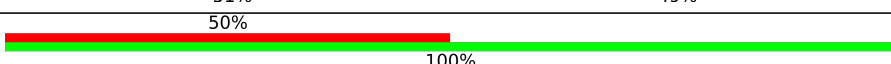

The reported resolution of this entry is 5.14 Å.

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






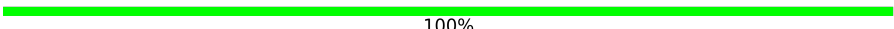


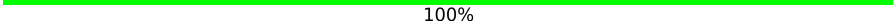

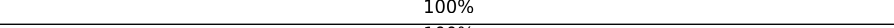
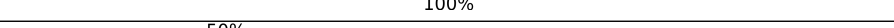
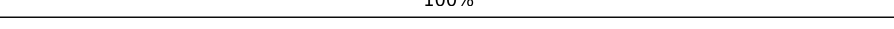
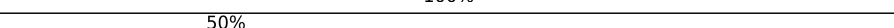
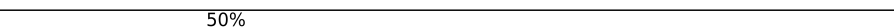












Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	481	
1	C	481	
1	D	481	
2	B	153	
2	E	153	
2	F	153	
3	J	267	
4	N	219	
5	0	2	

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Mol	Chain	Length	Quality of chain
5	1	2	100% 
5	O	2	50% 
5	P	2	100% 
5	Q	2	100% 
5	R	2	100% 
5	V	2	100% 
5	W	2	50% 
5	Z	2	50% 
5	a	2	100% 
5	b	2	100% 
5	c	2	50% 
5	e	2	100% 
5	h	2	50% 
5	i	2	50% 
5	j	2	50% 
5	m	2	50% 
5	n	2	100% 
5	o	2	50% 
5	p	2	50% 
5	r	2	100% 
5	u	2	50% 
5	v	2	50% 
5	w	2	100% 
5	z	2	100% 
6	S	3	33% 

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Mol	Chain	Length	Quality of chain
6	X	3	<div>100%</div> <div>100%</div>
6	d	3	<div>33%</div> <div>100%</div>
6	l	3	<div>67%</div> <div>33%</div>
6	y	3	<div>33%</div> <div>100%</div>
7	T	6	<div>17%</div> <div>50%</div> <div>50%</div>
8	Y	5	<div>60%</div> <div>60%</div> <div>40%</div>
8	k	5	<div>80%</div> <div>60%</div> <div>40%</div>
8	x	5	<div>60%</div> <div>40%</div> <div>60%</div>
9	f	7	<div>14%</div> <div>43%</div> <div>57%</div>
9	s	7	<div>43%</div> <div>57%</div>
10	q	8	<div>25%</div> <div>50%</div> <div>50%</div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17275 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 gp120 protein of HIV envelope trimer.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3545	2227	625	665	28		
1	C	451	Total	C	N	O	S	0	0
			3553	2231	627	667	28		
1	D	452	Total	C	N	O	S	0	0
			3562	2236	628	670	28		

- Molecule 2 is a protein called gp41 protein of HIV envelope trimer.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1004	635	173	190	6		
2	E	124	Total	C	N	O	S	0	0
			987	623	170	188	6		
2	F	123	Total	C	N	O	S	0	0
			981	620	169	186	6		

- Molecule 3 is a protein called PGT145 antibody fragment, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	140	Total	C	N	O	S	0	0
			1094	685	191	213	5		

- Molecule 4 is a protein called PGT145 antibody fragment, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	112	Total	C	N	O	S	0	0
			859	542	153	160	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	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	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	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		
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	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	r	2	Total	C	N	O	0	0
			28	16	2	10		

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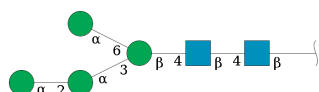
Mol	Chain	Residues	Atoms				AltConf	Trace
5	u	2	Total	C	N	O	0	0
			28	16	2	10		
5	v	2	Total	C	N	O	0	0
			28	16	2	10		
5	w	2	Total	C	N	O	0	0
			28	16	2	10		
5	z	2	Total	C	N	O	0	0
			28	16	2	10		
5	0	2	Total	C	N	O	0	0
			28	16	2	10		
5	1	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



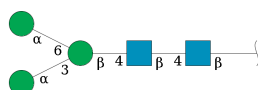
Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		
6	d	3	Total	C	N	O	0	0
			39	22	2	15		
6	l	3	Total	C	N	O	0	0
			39	22	2	15		
6	y	3	Total	C	N	O	0	0
			39	22	2	15		

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



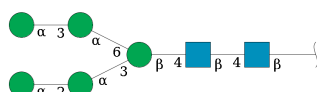
Mol	Chain	Residues	Atoms				AltConf	Trace
7	T	6	Total	C	N	O	0	0
			72	40	2	30		

- 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.



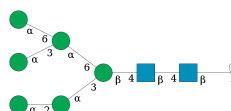
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	5	Total	C	N	O	0	0
			61	34	2	25		
8	k	5	Total	C	N	O	0	0
			61	34	2	25		
8	x	5	Total	C	N	O	0	0
			61	34	2	25		

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



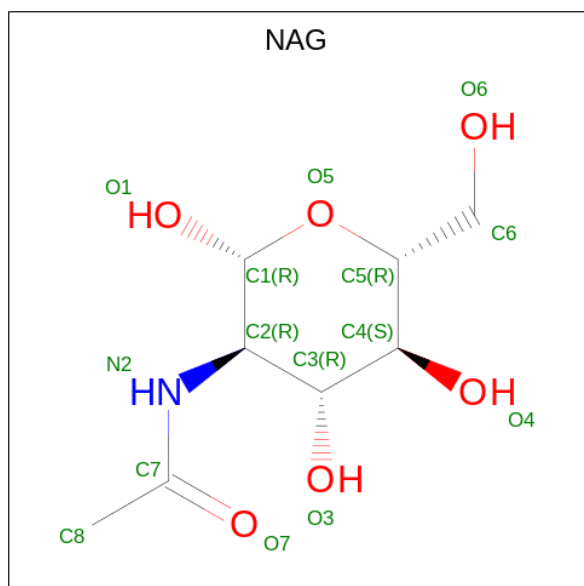
Mol	Chain	Residues	Atoms				AltConf	Trace
9	f	7	Total	C	N	O	0	0
			83	46	2	35		
9	s	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



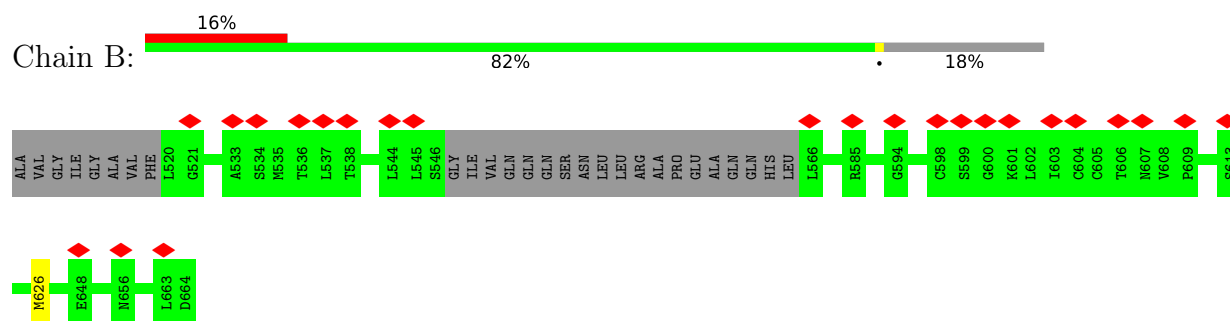
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	C	1	Total	C	N	O	0
			14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

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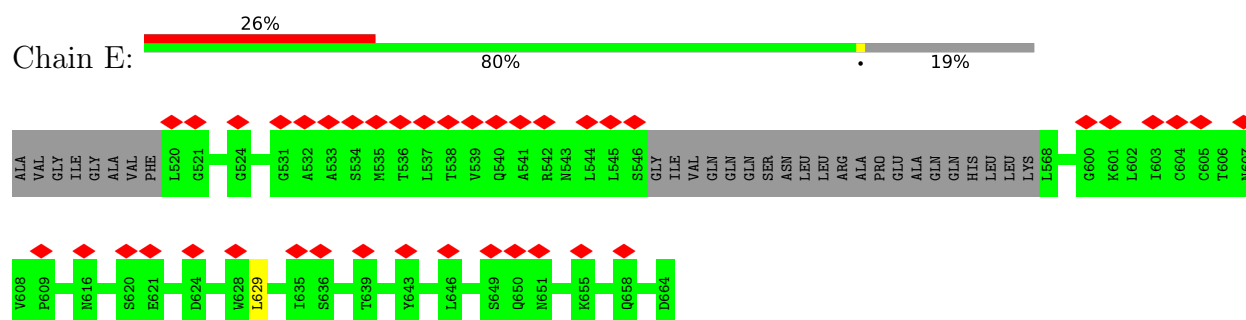
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Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	E	1	Total 14	C 8	N 1	O 5	0
11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

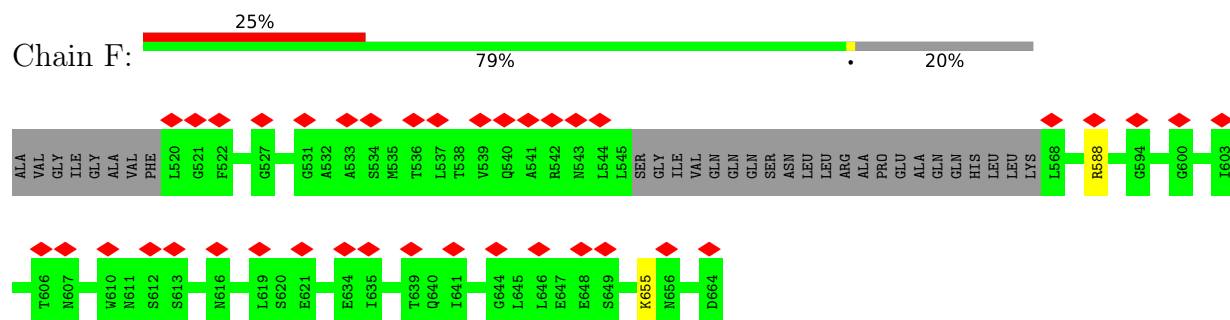
- Molecule 2: gp41 protein of HIV envelope trimer



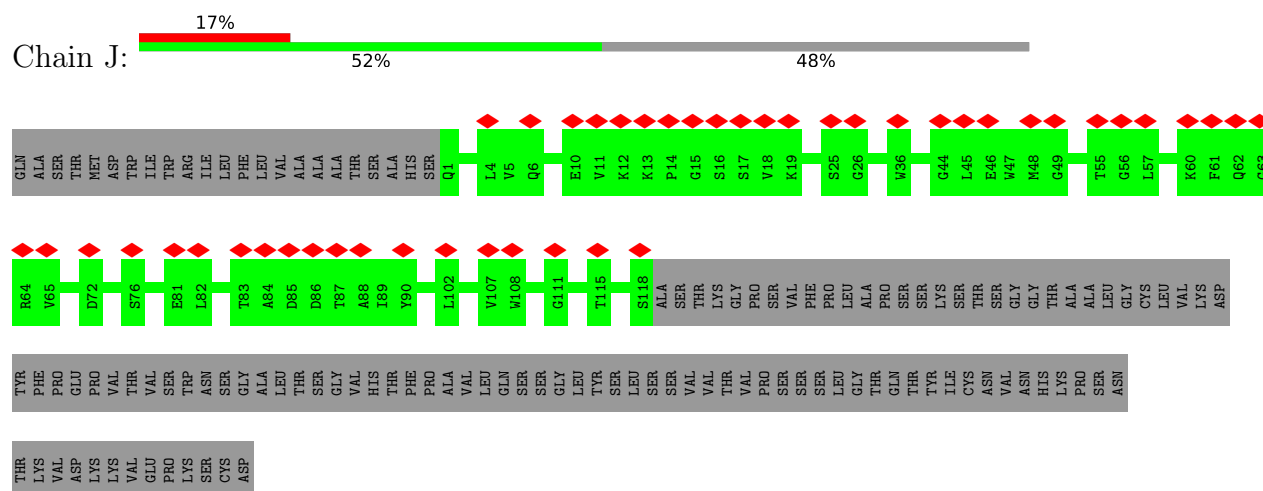
- Molecule 2: gp41 protein of HIV envelope trimer



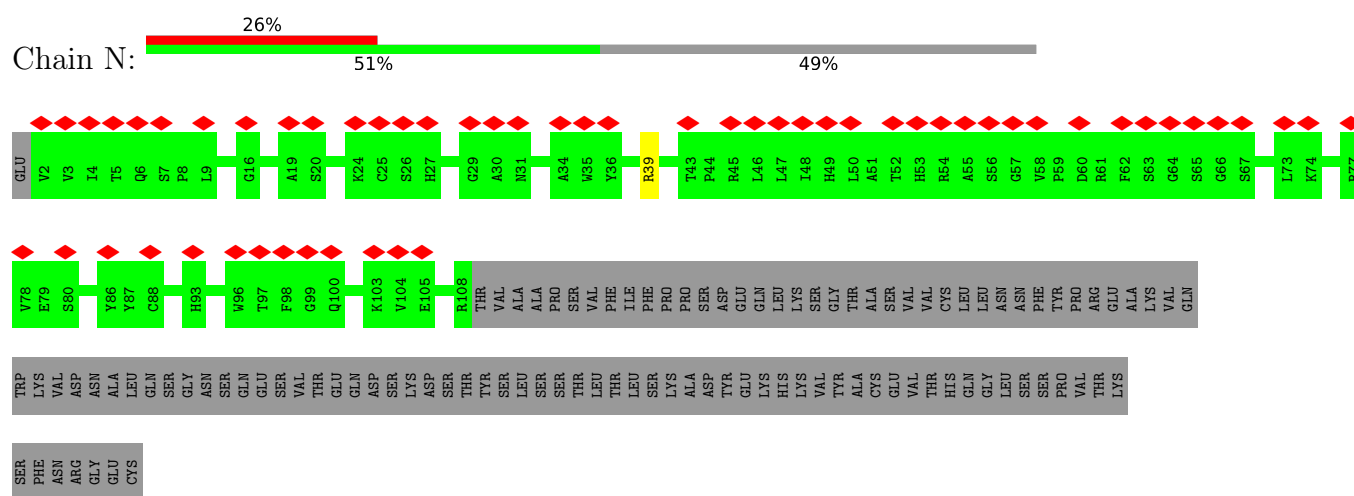
- Molecule 2: gp41 protein of HIV envelope trimer



- Molecule 3: PGT145 antibody fragment, heavy chain



- Molecule 4: PGT145 antibody fragment, light chain



- 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



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- 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 e:  100%



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

Chain h:  50%
 100%



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

Chain i:  50%
 100%



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

Chain j:  50%
 100%



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

Chain m:  50%
 50%



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

Chain n:  100%



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



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



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

Chain z:  100%



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

Chain 0:  50%
100%



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

Chain 1:  100%
100%



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

Chain S:  33%
100%



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

Chain X:  100%
100%



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

Chain d:  33%
100%



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

Chain l:  67% 33%



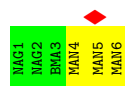
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  33% 100%



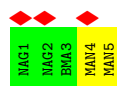
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  17% 50% 50%




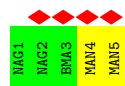
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  60% 60% 40%



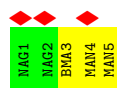
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  80% 60% 40%



- 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

Chain x:  60% 40% 60%



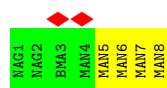
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	527385	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 ($e^-/\text{\AA}^2$)	43.89	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	40.303	Depositor
Minimum map value	-20.685	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.46	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	0.28	0/3619	0.58	0/4914
1	C	0.28	0/3627	0.55	0/4925
1	D	0.29	0/3636	0.58	0/4937
2	B	0.29	0/1021	0.59	0/1384
2	E	0.30	0/1004	0.62	1/1362 (0.1%)
2	F	0.34	0/998	0.62	1/1354 (0.1%)
3	J	0.25	0/1121	0.53	0/1519
4	N	0.24	0/882	0.55	0/1199
All	All	0.29	0/15908	0.57	2/21594 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	629	LEU	CA-CB-CG	7.12	131.68	115.30
2	F	655	LYS	CD-CE-NZ	-6.77	96.12	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ASN	Peptide
1	A	338	TRP	Peptide
1	C	217	TYR	Peptide

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	444/481 (92%)	426 (96%)	18 (4%)	0	100	100
1	C	445/481 (92%)	429 (96%)	16 (4%)	0	100	100
1	D	446/481 (93%)	431 (97%)	15 (3%)	0	100	100
2	B	122/153 (80%)	118 (97%)	4 (3%)	0	100	100
2	E	120/153 (78%)	116 (97%)	4 (3%)	0	100	100
2	F	119/153 (78%)	115 (97%)	4 (3%)	0	100	100
3	J	138/267 (52%)	137 (99%)	1 (1%)	0	100	100
4	N	110/219 (50%)	108 (98%)	2 (2%)	0	100	100
All	All	1944/2388 (81%)	1880 (97%)	64 (3%)	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	402/428 (94%)	402 (100%)	0	100	100
1	C	403/428 (94%)	402 (100%)	1 (0%)	93	96
1	D	404/428 (94%)	404 (100%)	0	100	100
2	B	109/129 (84%)	108 (99%)	1 (1%)	78	87
2	E	107/129 (83%)	107 (100%)	0	100	100
2	F	106/129 (82%)	105 (99%)	1 (1%)	78	87
3	J	115/223 (52%)	115 (100%)	0	100	100
4	N	95/191 (50%)	94 (99%)	1 (1%)	73	85
All	All	1741/2085 (84%)	1737 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	626	MET
1	C	207	LYS
2	F	588	ARG
4	N	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	GLN
1	D	302	ASN
3	J	98	HIS
1	D	114	GLN
1	D	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

108 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	0	1	2,5	14,14,15	0.21	0	17,19,21	0.55	0
5	NAG	0	2	5	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	1	1	2,5	14,14,15	0.33	0	17,19,21	0.47	0
5	NAG	1	2	5	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	O	1	1,5	14,14,15	0.24	0	17,19,21	0.65	1 (5%)
5	NAG	O	2	5	14,14,15	0.42	0	17,19,21	1.29	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	P	2	5	14,14,15	0.28	0	17,19,21	0.50	0
5	NAG	Q	1	1,5	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	Q	2	5	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	R	1	1,5	14,14,15	0.62	0	17,19,21	0.72	0
5	NAG	R	2	5	14,14,15	0.27	0	17,19,21	0.43	0
6	NAG	S	1	1,6	14,14,15	0.24	0	17,19,21	0.54	0
6	NAG	S	2	6	14,14,15	0.19	0	17,19,21	0.49	0
6	BMA	S	3	6	11,11,12	0.57	0	15,15,17	0.82	0
7	NAG	T	1	1,7	14,14,15	0.28	0	17,19,21	0.57	0
7	NAG	T	2	7	14,14,15	0.22	0	17,19,21	0.49	0
7	BMA	T	3	7	11,11,12	0.72	0	15,15,17	0.99	0
7	MAN	T	4	7	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
7	MAN	T	5	7	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
7	MAN	T	6	7	11,11,12	0.73	1 (9%)	15,15,17	1.05	2 (13%)
5	NAG	V	1	1,5	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	W	1	1,5	14,14,15	0.60	0	17,19,21	0.76	0
5	NAG	W	2	5	14,14,15	0.30	0	17,19,21	0.58	0
6	NAG	X	1	1,6	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	X	2	6	14,14,15	0.20	0	17,19,21	0.47	0
6	BMA	X	3	6	11,11,12	0.65	0	15,15,17	1.00	0
8	NAG	Y	1	1,8	14,14,15	0.26	0	17,19,21	0.52	0
8	NAG	Y	2	8	14,14,15	0.24	0	17,19,21	0.38	0
8	BMA	Y	3	8	11,11,12	0.59	0	15,15,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	Y	4	8	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
8	MAN	Y	5	8	11,11,12	0.68	0	15,15,17	0.91	1 (6%)
5	NAG	Z	1	1,5	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
5	NAG	Z	2	5	14,14,15	0.35	0	17,19,21	0.38	0
5	NAG	a	1	1,5	14,14,15	0.32	0	17,19,21	0.65	0
5	NAG	a	2	5	14,14,15	0.26	0	17,19,21	0.35	0
5	NAG	b	1	1,5	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	b	2	5	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	c	1	1,5	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	c	2	5	14,14,15	0.28	0	17,19,21	0.49	0
6	NAG	d	1	1,6	14,14,15	0.23	0	17,19,21	0.48	0
6	NAG	d	2	6	14,14,15	0.25	0	17,19,21	0.47	0
6	BMA	d	3	6	11,11,12	0.60	0	15,15,17	0.93	0
5	NAG	e	1	1,5	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	e	2	5	14,14,15	0.32	0	17,19,21	0.51	0
9	NAG	f	1	1,9	14,14,15	0.36	0	17,19,21	0.45	0
9	NAG	f	2	9	14,14,15	0.22	0	17,19,21	0.40	0
9	BMA	f	3	9	11,11,12	0.55	0	15,15,17	0.89	0
9	MAN	f	4	9	11,11,12	0.62	0	15,15,17	1.21	2 (13%)
9	MAN	f	5	9	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
9	MAN	f	6	9	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
9	MAN	f	7	9	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
5	NAG	h	1	1,5	14,14,15	0.36	0	17,19,21	0.39	0
5	NAG	h	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	i	1	1,5	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	i	2	5	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	j	1	1,5	14,14,15	0.36	0	17,19,21	0.50	0
5	NAG	j	2	5	14,14,15	0.31	0	17,19,21	0.52	0
8	NAG	k	1	1,8	14,14,15	0.56	0	17,19,21	0.54	0
8	NAG	k	2	8	14,14,15	0.30	0	17,19,21	0.42	0
8	BMA	k	3	8	11,11,12	0.62	0	15,15,17	0.87	0
8	MAN	k	4	8	11,11,12	0.60	0	15,15,17	1.09	2 (13%)
8	MAN	k	5	8	11,11,12	0.73	0	15,15,17	0.87	1 (6%)
6	NAG	l	1	1,6	14,14,15	0.64	1 (7%)	17,19,21	0.75	1 (5%)
6	NAG	l	2	6	14,14,15	0.24	0	17,19,21	0.57	0
6	BMA	l	3	6	11,11,12	0.63	0	15,15,17	0.97	0
5	NAG	m	1	1,5	14,14,15	0.67	1 (7%)	17,19,21	0.53	0
5	NAG	m	2	5	14,14,15	0.21	0	17,19,21	0.47	0
5	NAG	n	1	1,5	14,14,15	0.34	0	17,19,21	0.48	0
5	NAG	n	2	5	14,14,15	0.26	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	o	1	1,5	14,14,15	0.30	0	17,19,21	0.60	0
5	NAG	o	2	5	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
5	NAG	p	1	1,5	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	p	2	5	14,14,15	0.24	0	17,19,21	0.43	0
10	NAG	q	1	1,10	14,14,15	0.18	0	17,19,21	0.46	0
10	NAG	q	2	10	14,14,15	0.21	0	17,19,21	0.44	0
10	BMA	q	3	10	11,11,12	0.53	0	15,15,17	0.74	0
10	MAN	q	4	10	11,11,12	0.78	0	15,15,17	0.89	0
10	MAN	q	5	10	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
10	MAN	q	6	10	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
10	MAN	q	7	10	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
10	MAN	q	8	10	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
5	NAG	r	1	1,5	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	r	2	5	14,14,15	0.35	0	17,19,21	0.56	0
9	NAG	s	1	1,9	14,14,15	0.19	0	17,19,21	0.42	0
9	NAG	s	2	9	14,14,15	0.20	0	17,19,21	0.44	0
9	BMA	s	3	9	11,11,12	0.76	0	15,15,17	0.85	0
9	MAN	s	4	9	11,11,12	0.69	0	15,15,17	1.26	2 (13%)
9	MAN	s	5	9	11,11,12	0.68	0	15,15,17	0.95	2 (13%)
9	MAN	s	6	9	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
9	MAN	s	7	9	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
5	NAG	u	1	1,5	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	u	2	5	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	v	1	1,5	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
5	NAG	v	2	5	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	w	1	1,5	14,14,15	0.42	0	17,19,21	0.48	0
5	NAG	w	2	5	14,14,15	0.28	0	17,19,21	0.52	0
8	NAG	x	1	1,8	14,14,15	0.23	0	17,19,21	0.38	0
8	NAG	x	2	8	14,14,15	0.26	0	17,19,21	0.48	0
8	BMA	x	3	8	11,11,12	0.63	0	15,15,17	0.95	1 (6%)
8	MAN	x	4	8	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
8	MAN	x	5	8	11,11,12	0.64	0	15,15,17	0.98	2 (13%)
6	NAG	y	1	1,6	14,14,15	0.42	0	17,19,21	0.72	0
6	NAG	y	2	6	14,14,15	0.21	0	17,19,21	0.55	0
6	BMA	y	3	6	11,11,12	0.58	0	15,15,17	0.89	0
5	NAG	z	1	1,5	14,14,15	0.39	0	17,19,21	0.51	0
5	NAG	z	2	5	14,14,15	0.27	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
5	NAG	e	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
9	NAG	f	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
9	BMA	f	3	9	-	0/2/19/22	0/1/1/1
9	MAN	f	4	9	-	0/2/19/22	0/1/1/1
9	MAN	f	5	9	-	0/2/19/22	0/1/1/1
9	MAN	f	6	9	-	0/2/19/22	0/1/1/1
9	MAN	f	7	9	-	0/2/19/22	0/1/1/1
5	NAG	h	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	0/6/23/26	0/1/1/1
5	NAG	i	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	0/6/23/26	0/1/1/1
5	NAG	j	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1
8	NAG	k	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	BMA	k	3	8	-	2/2/19/22	0/1/1/1
8	MAN	k	4	8	-	0/2/19/22	0/1/1/1
8	MAN	k	5	8	-	0/2/19/22	0/1/1/1
6	NAG	l	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1
6	BMA	l	3	6	-	1/2/19/22	0/1/1/1
5	NAG	m	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	2/6/23/26	0/1/1/1
5	NAG	n	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	n	2	5	-	0/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	5/6/23/26	0/1/1/1
5	NAG	p	1	1,5	-	2/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	v	1	NAG	O5-C1	-2.49	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	1	NAG	O5-C1	-2.41	1.39	1.43
6	l	1	NAG	O5-C1	2.09	1.47	1.43
7	T	6	MAN	C1-C2	2.02	1.56	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2	NAG	C2-N2-C7	4.34	129.08	122.90
5	o	2	NAG	C2-N2-C7	4.28	129.00	122.90
9	f	4	MAN	C1-O5-C5	3.34	116.71	112.19
9	s	4	MAN	C1-O5-C5	3.30	116.67	112.19
9	s	4	MAN	O2-C2-C3	-3.04	104.06	110.14

There are no chirality outliers.

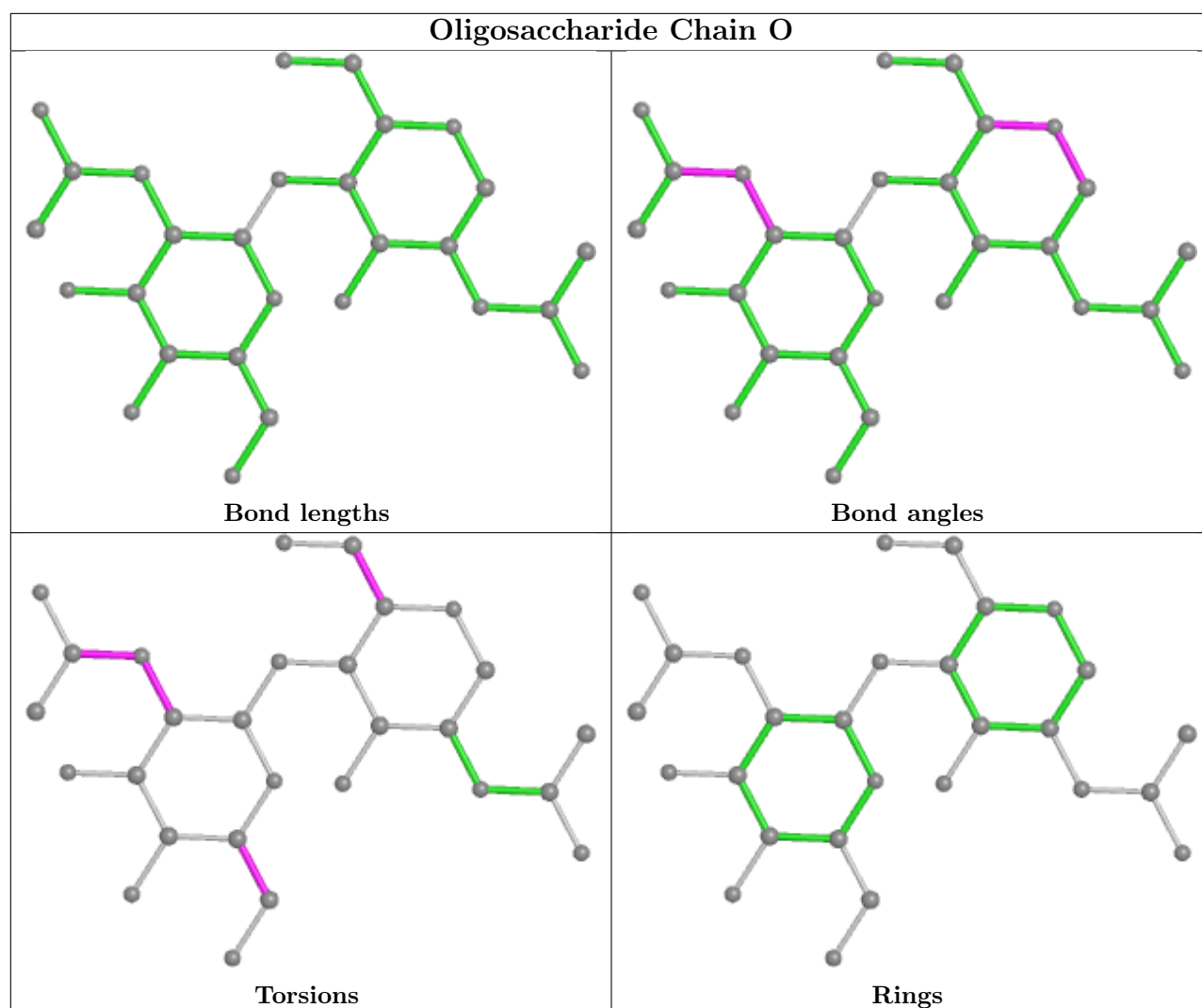
5 of 124 torsion outliers are listed below:

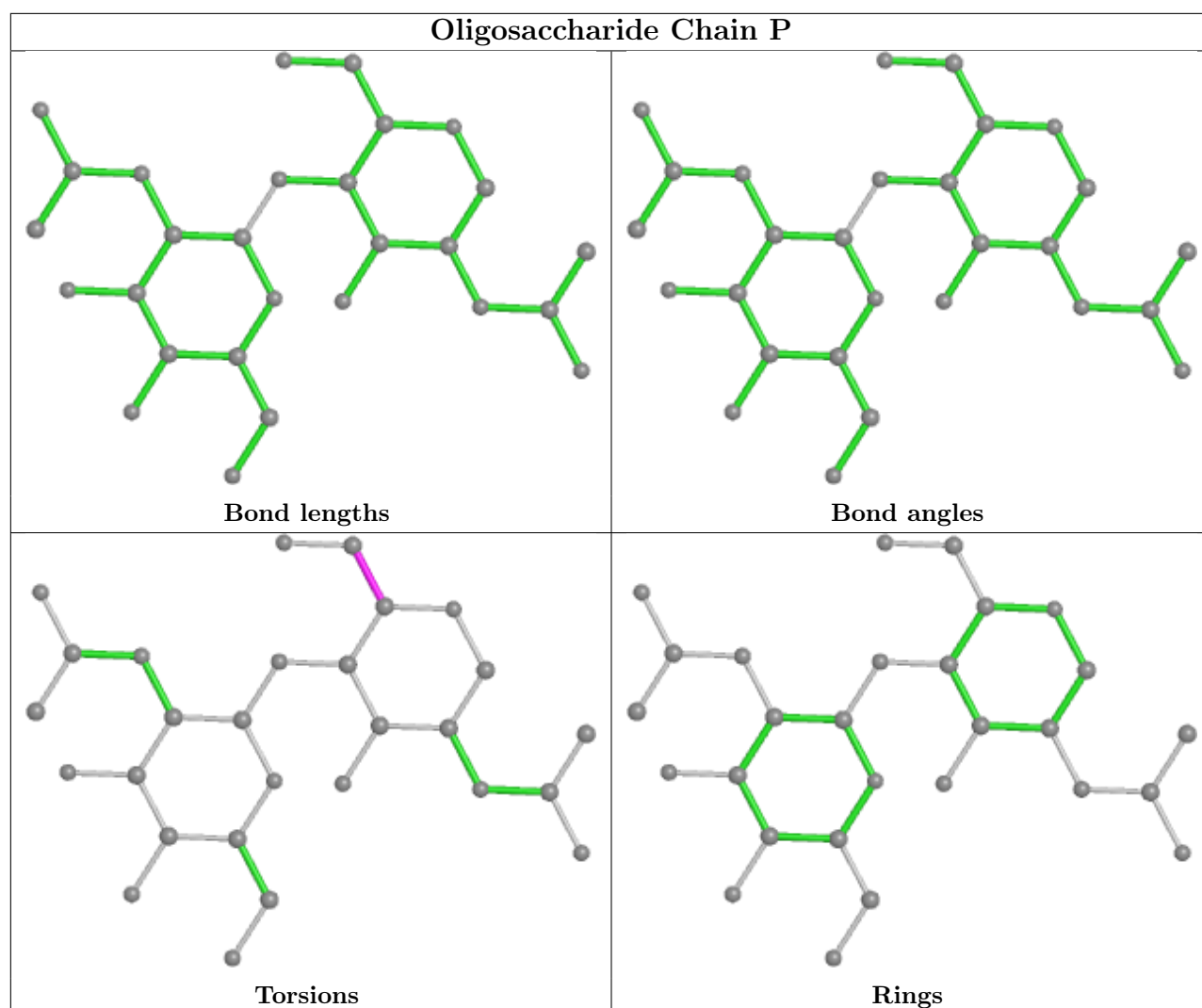
Mol	Chain	Res	Type	Atoms
5	c	1	NAG	O5-C5-C6-O6
5	h	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	u	1	NAG	O5-C5-C6-O6

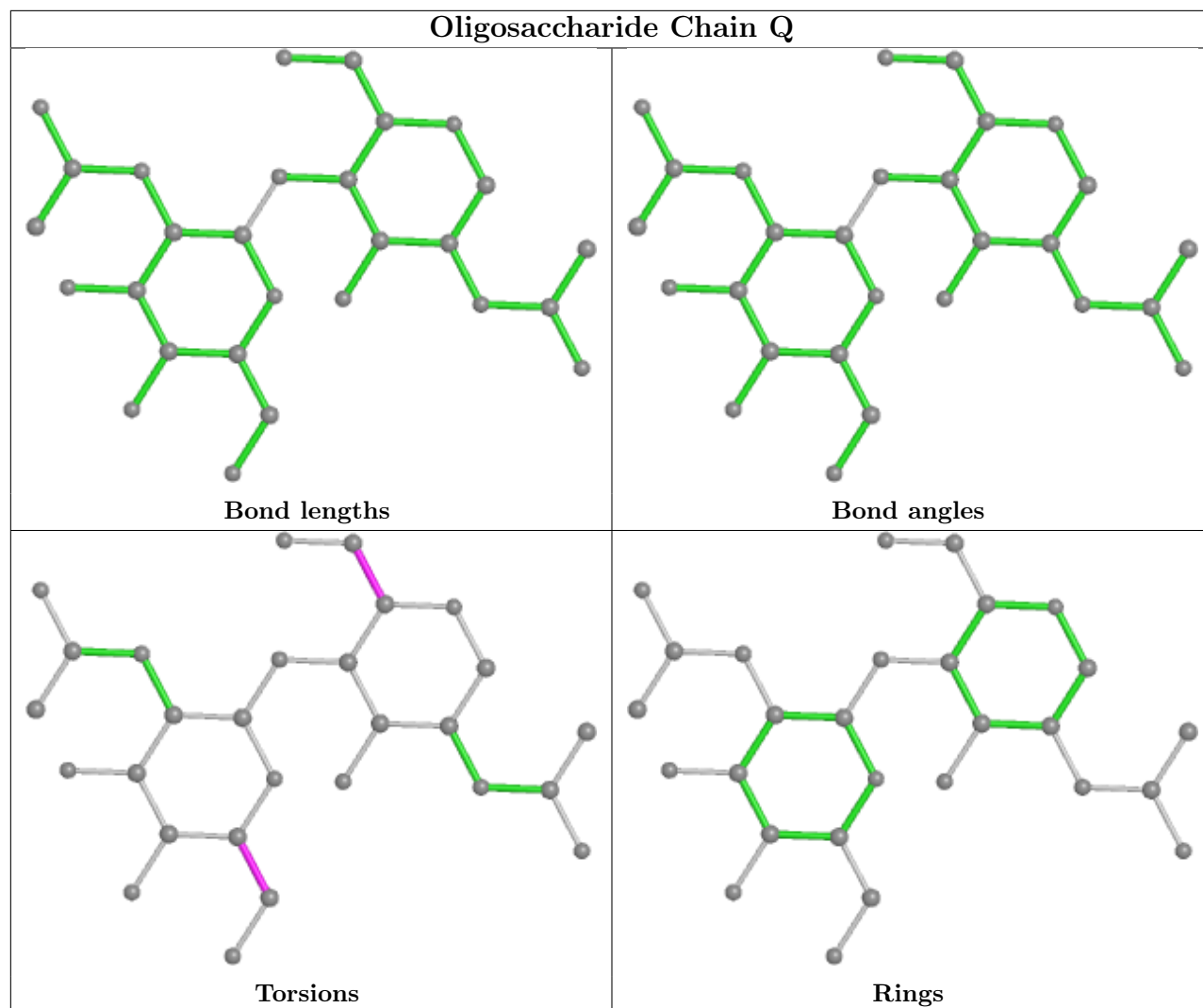
There are no ring outliers.

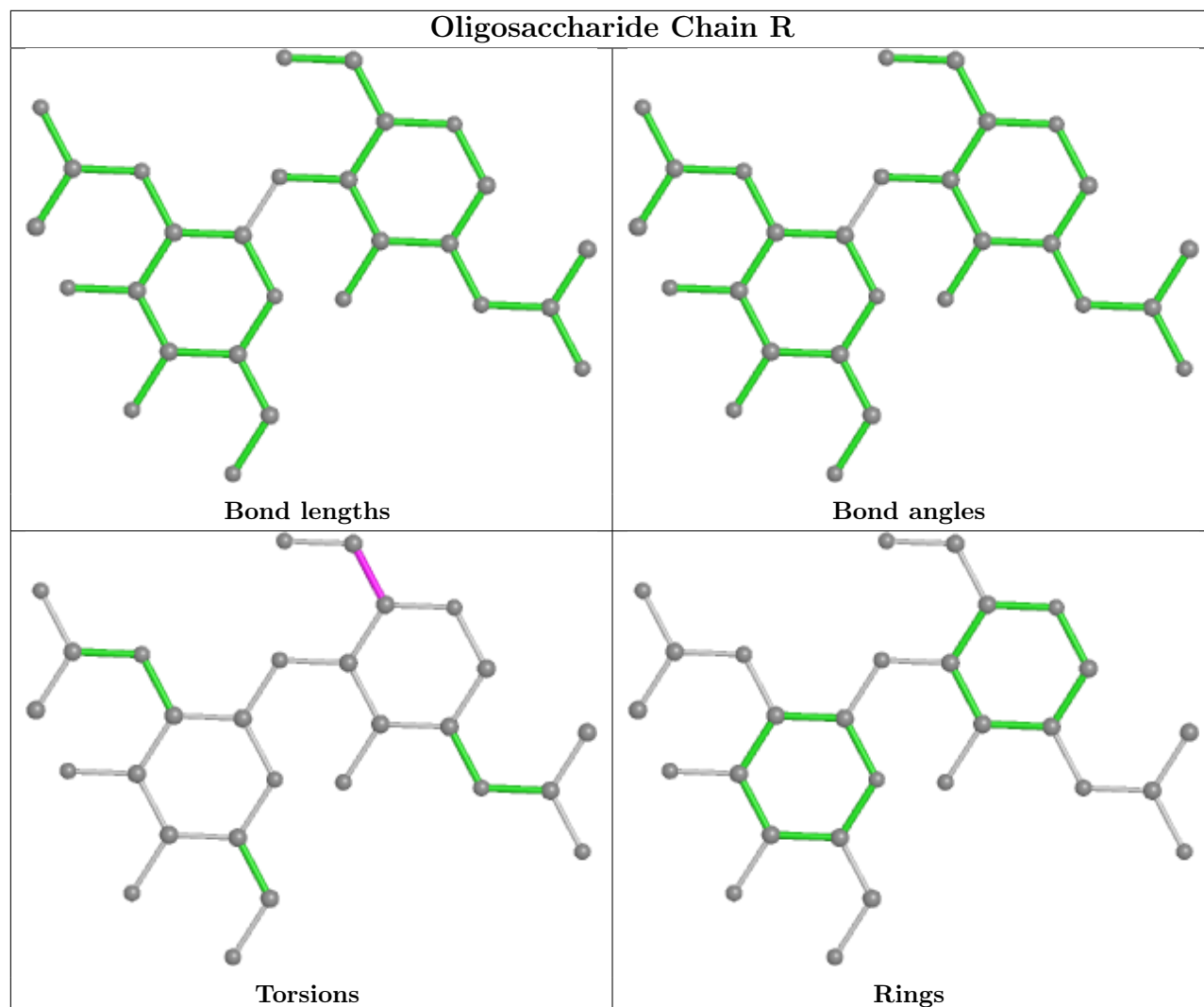
No monomer is involved in short contacts.

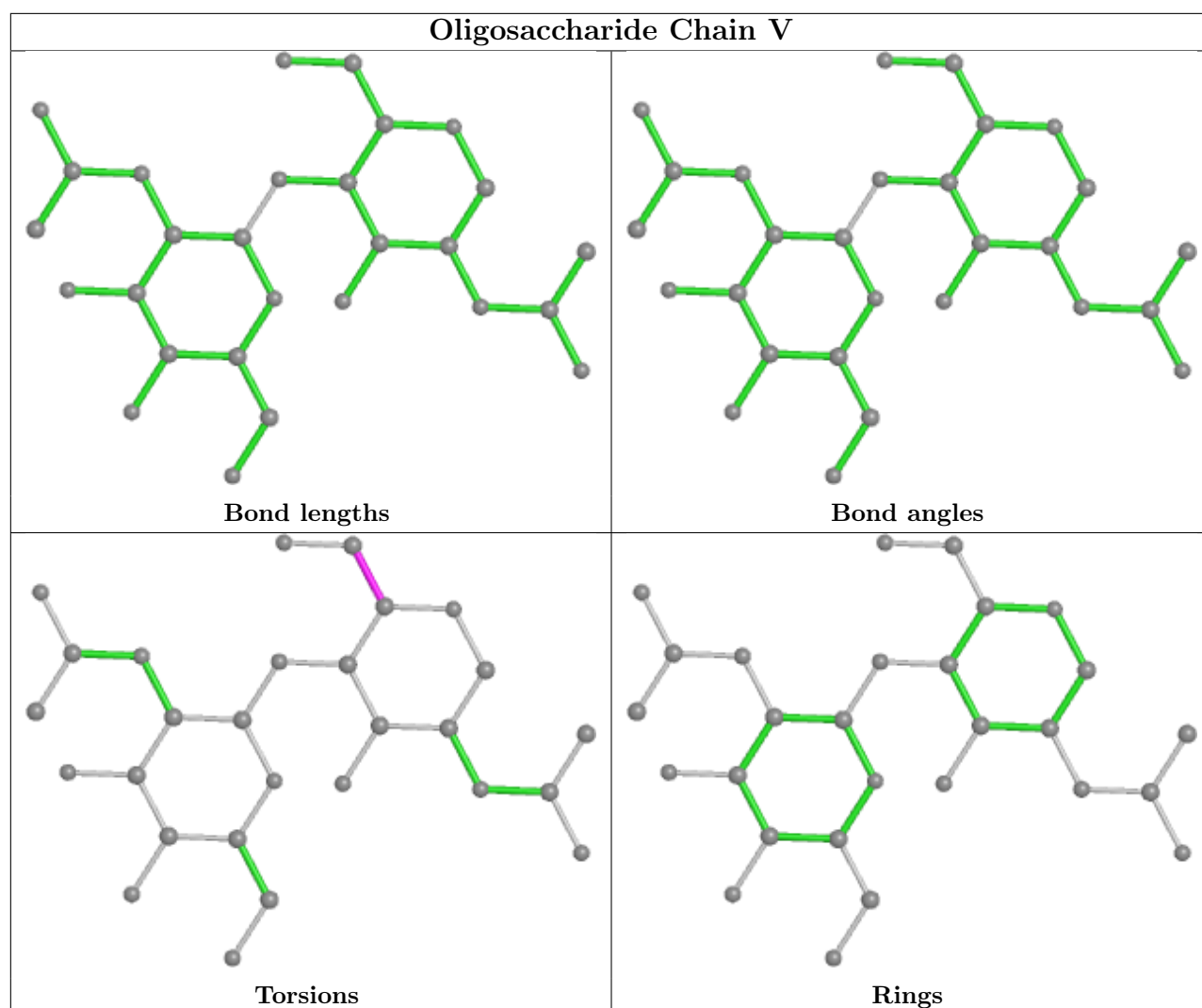
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

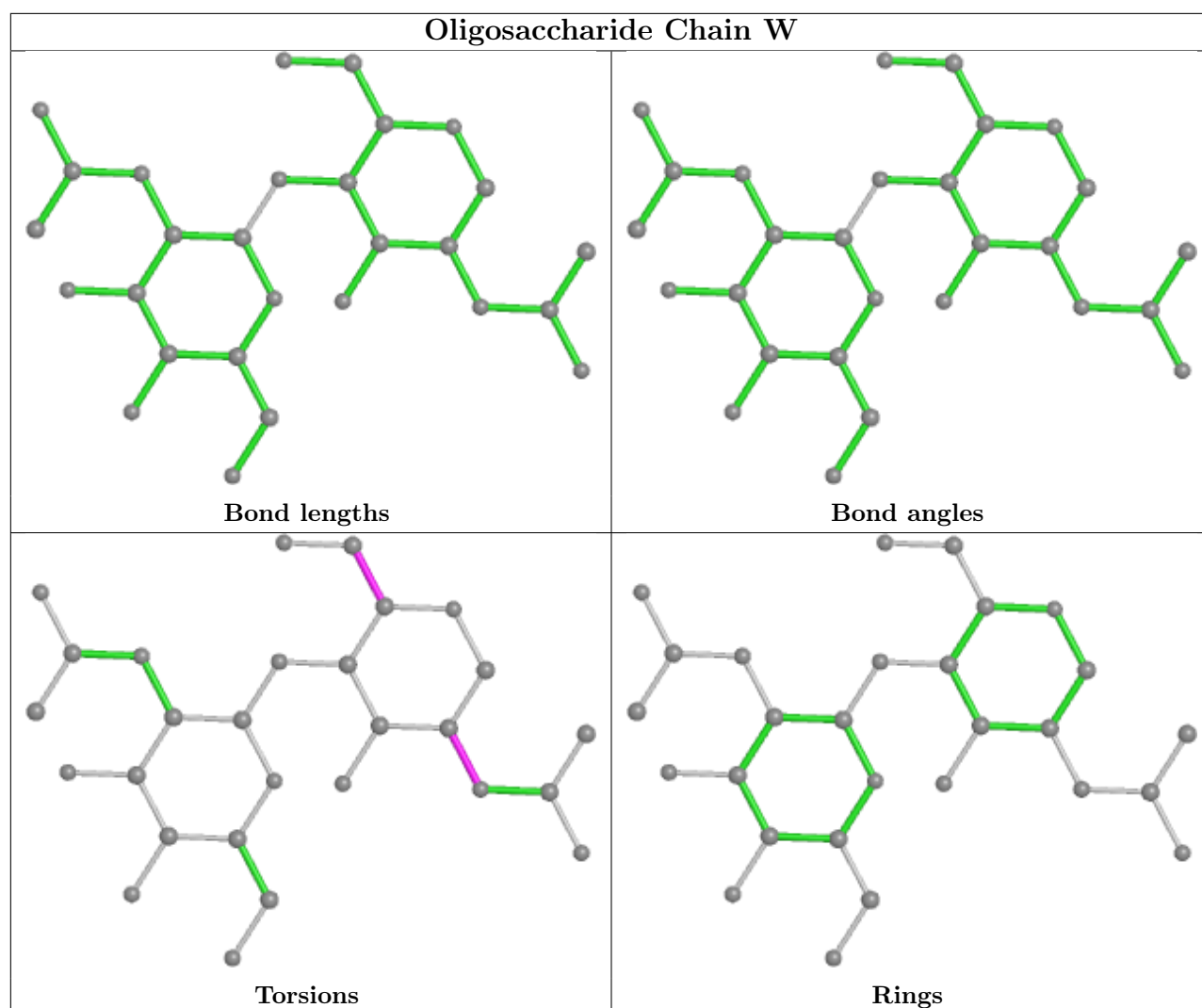


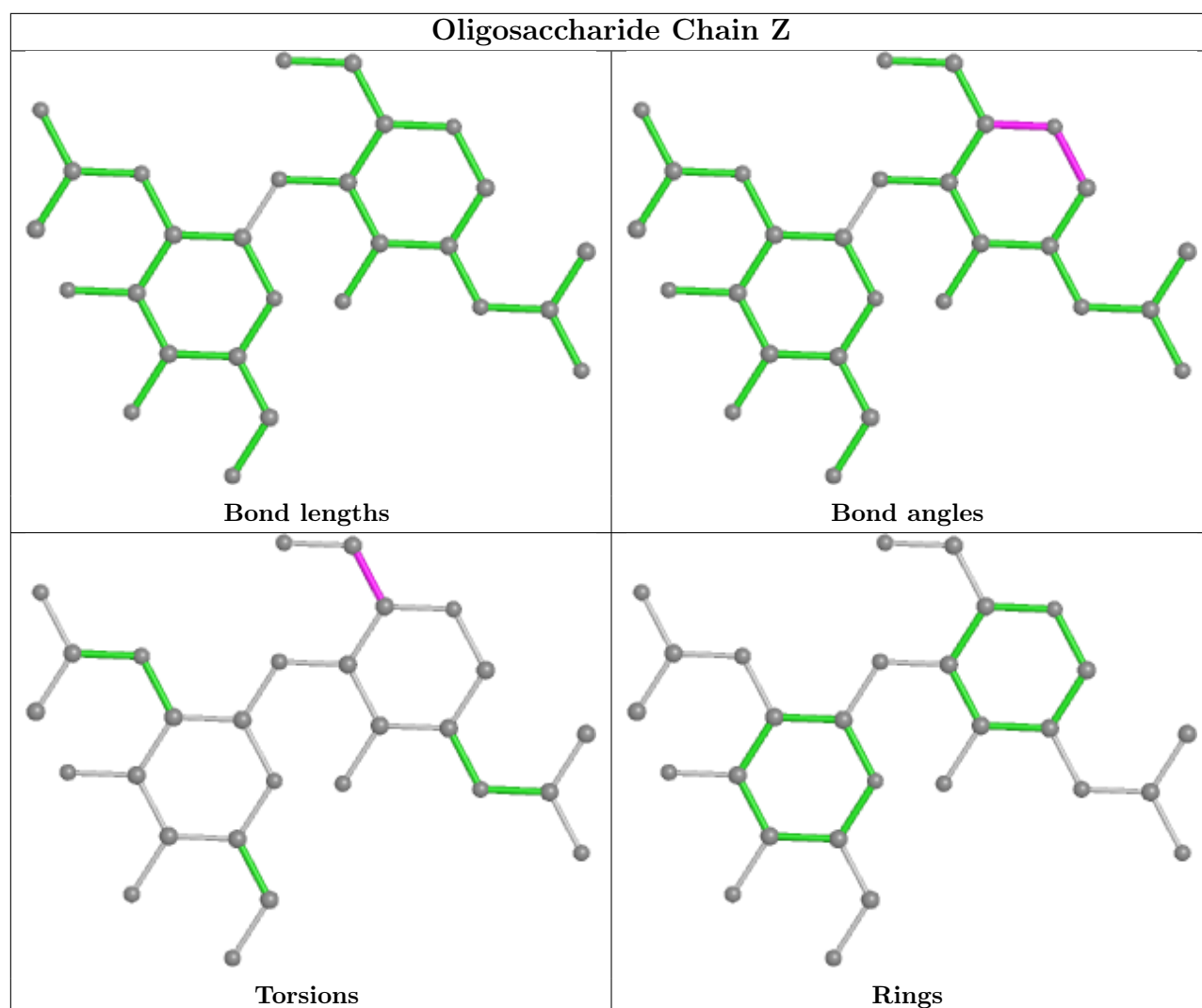


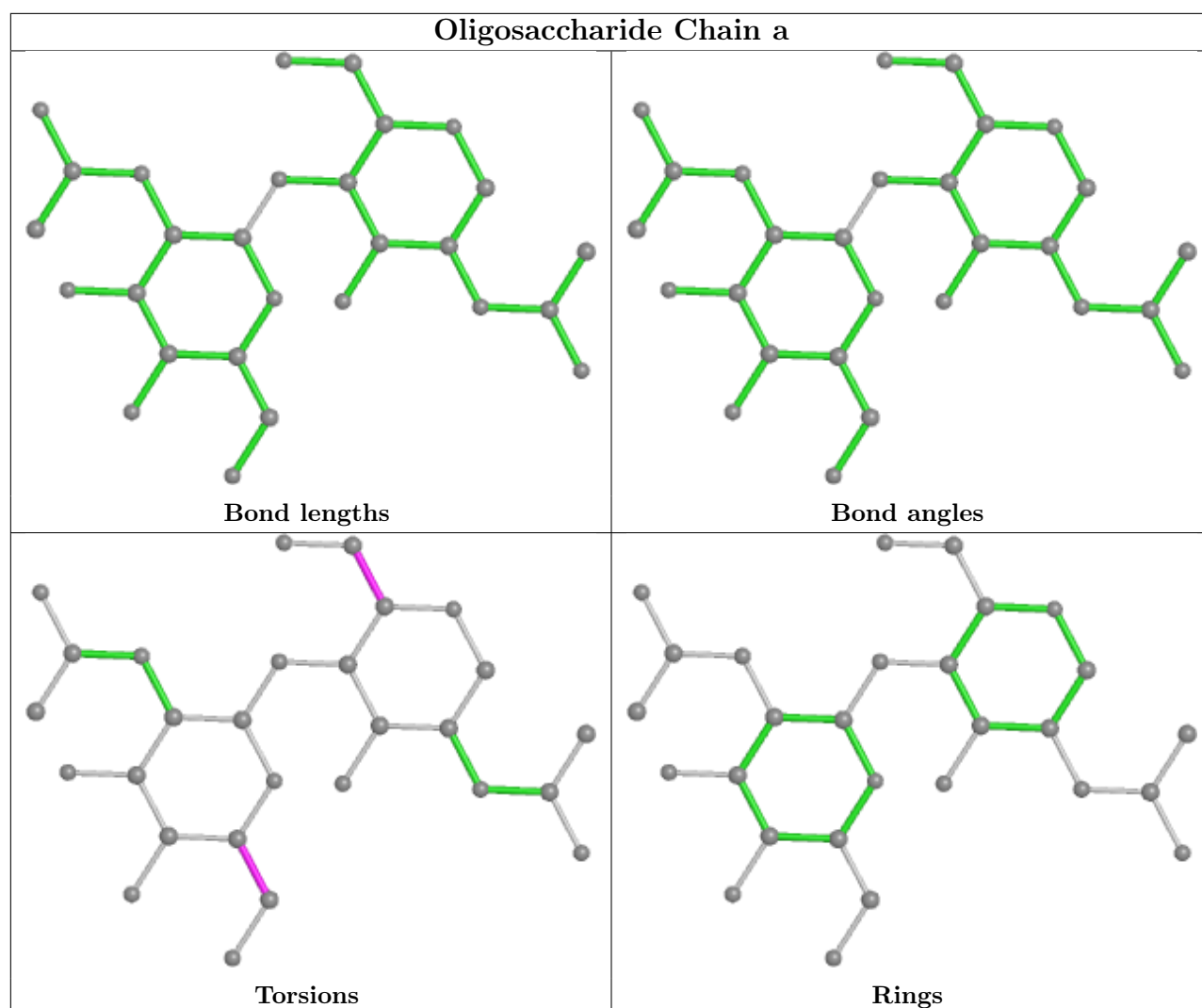


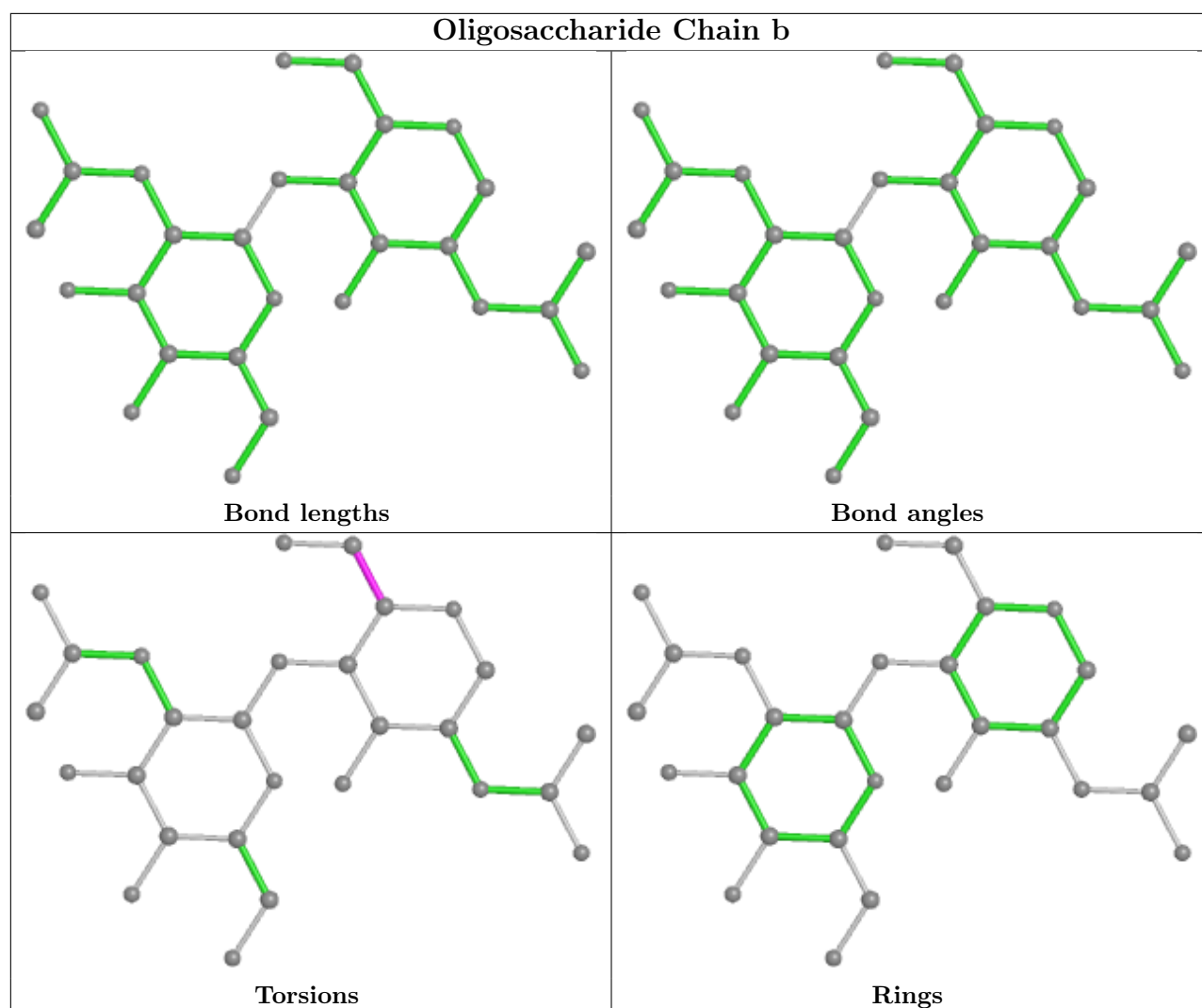


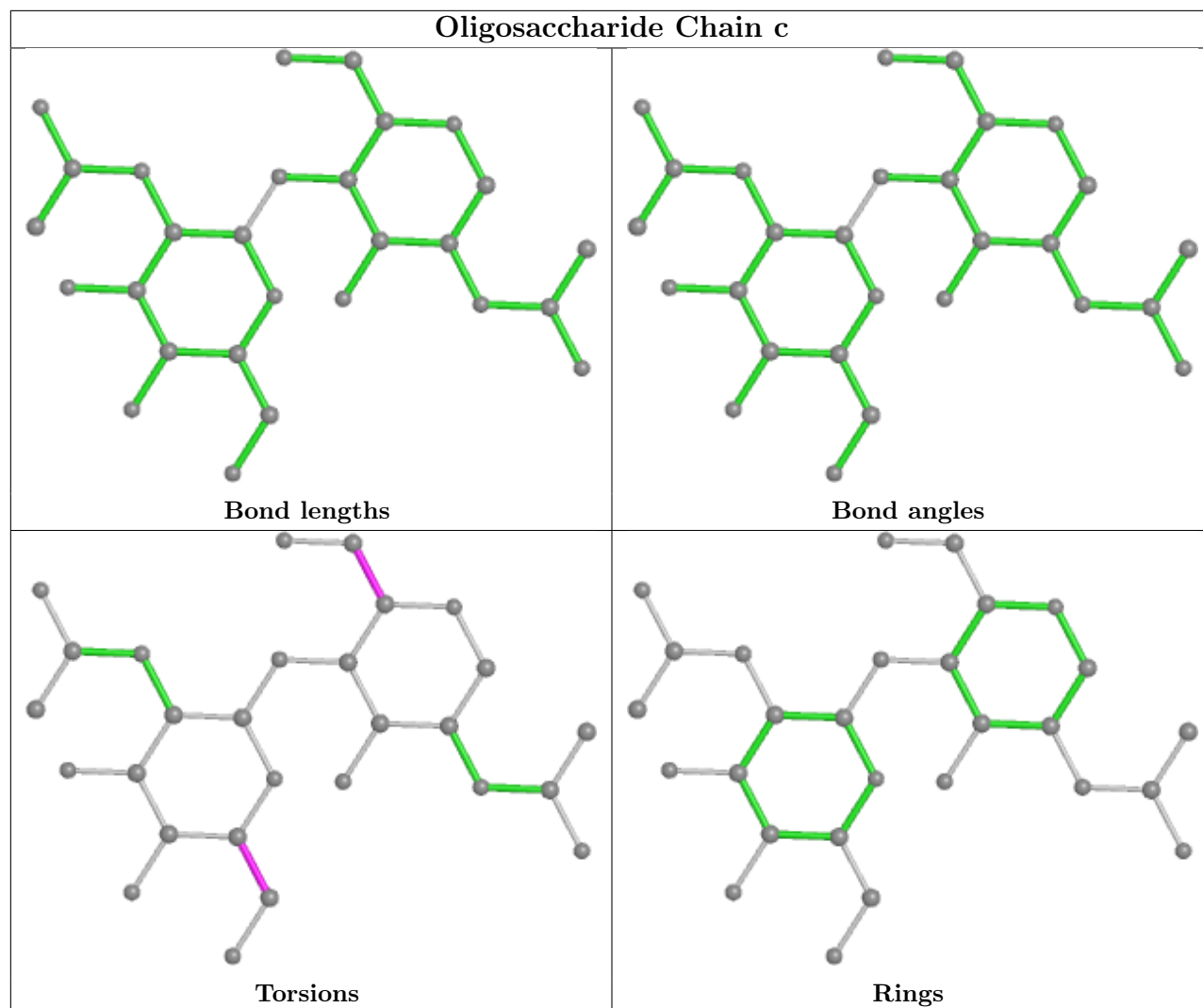


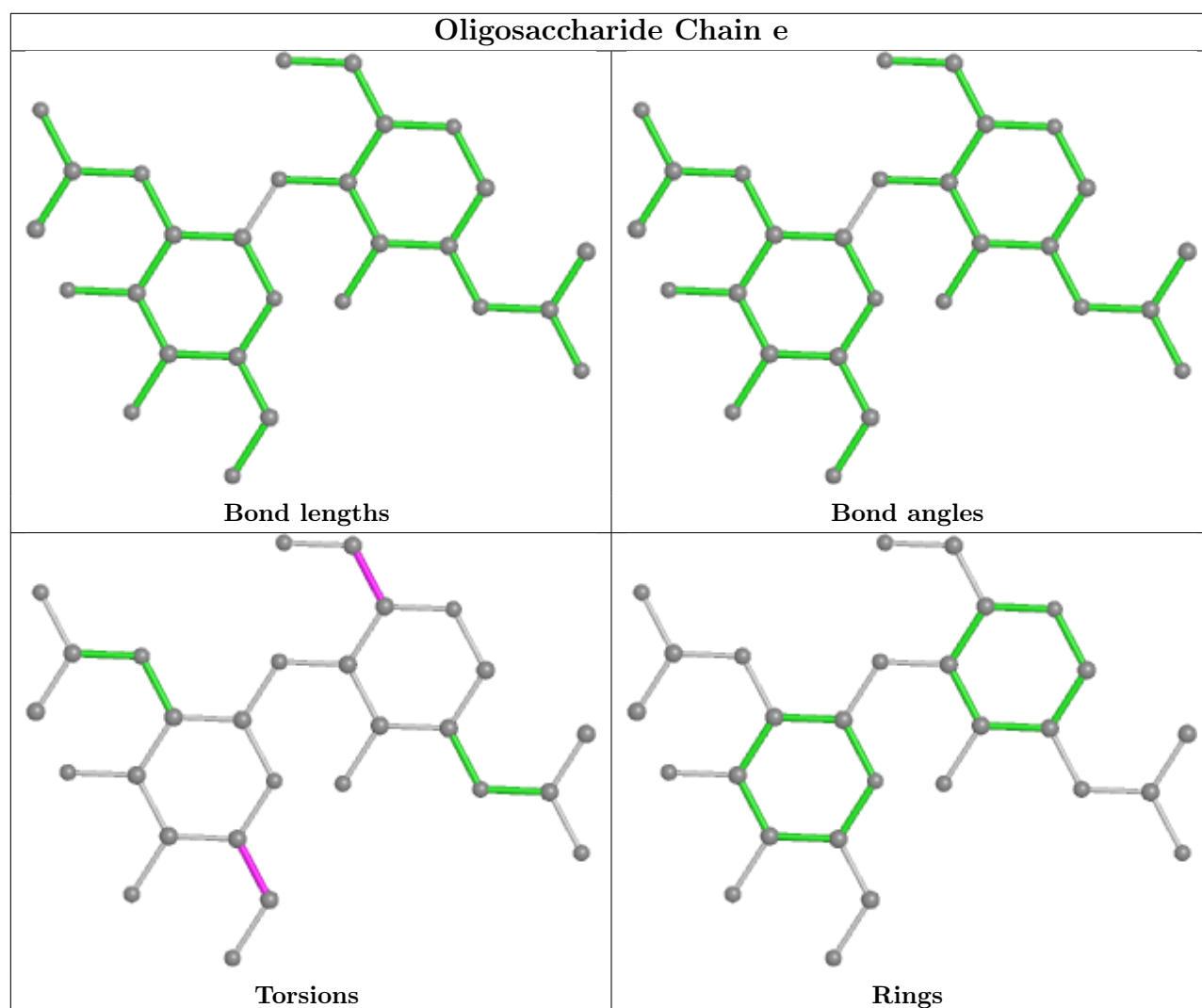


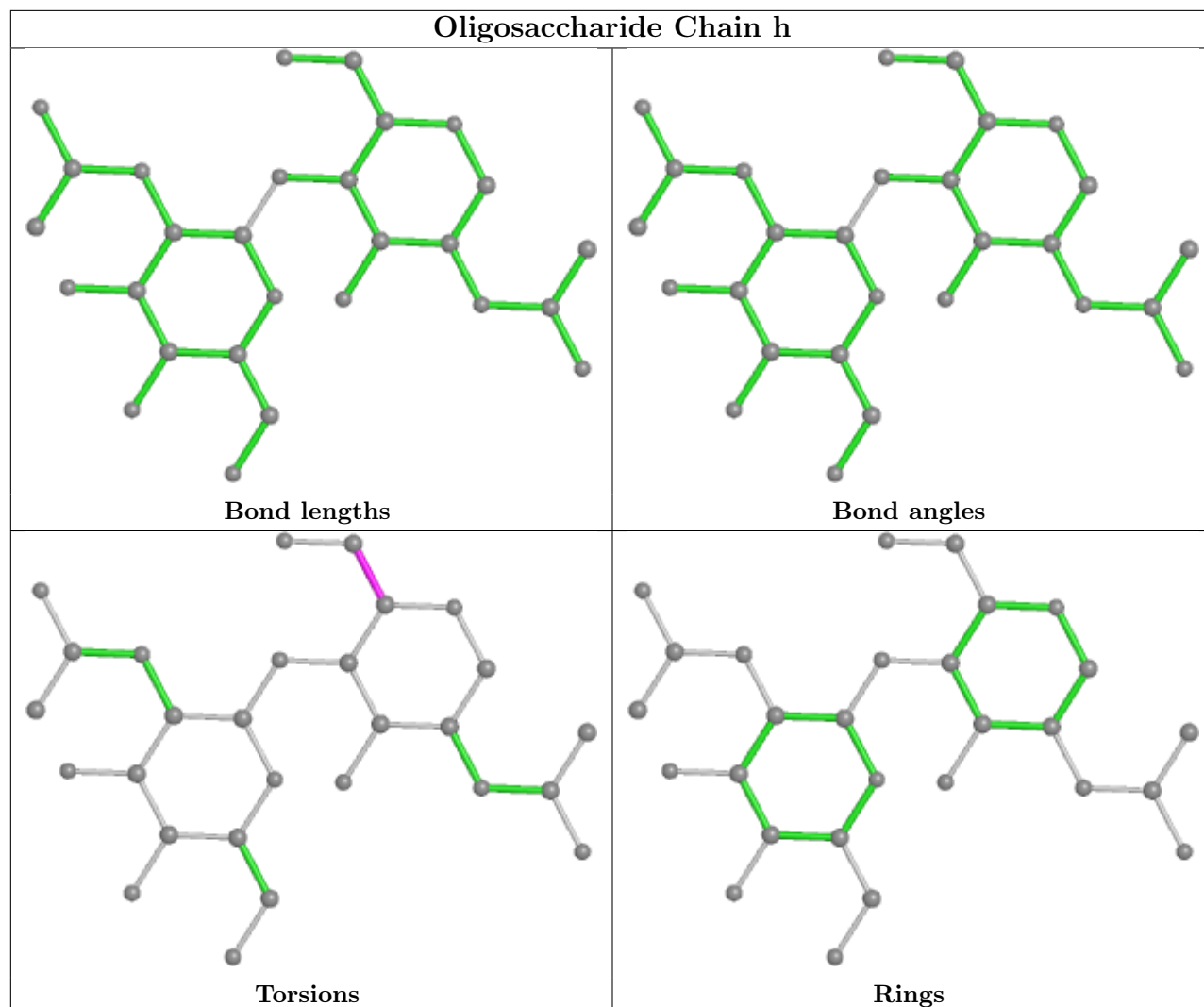


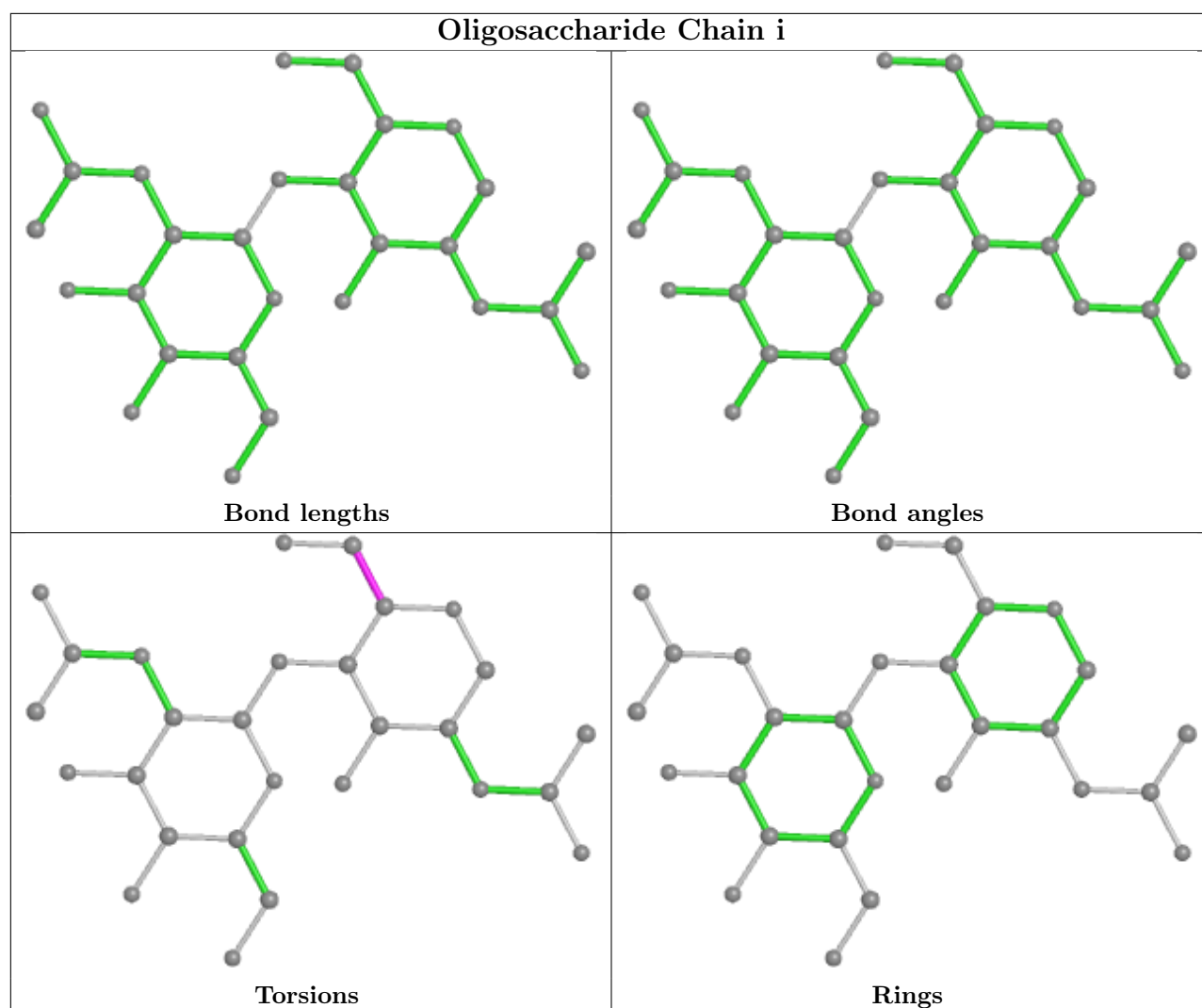


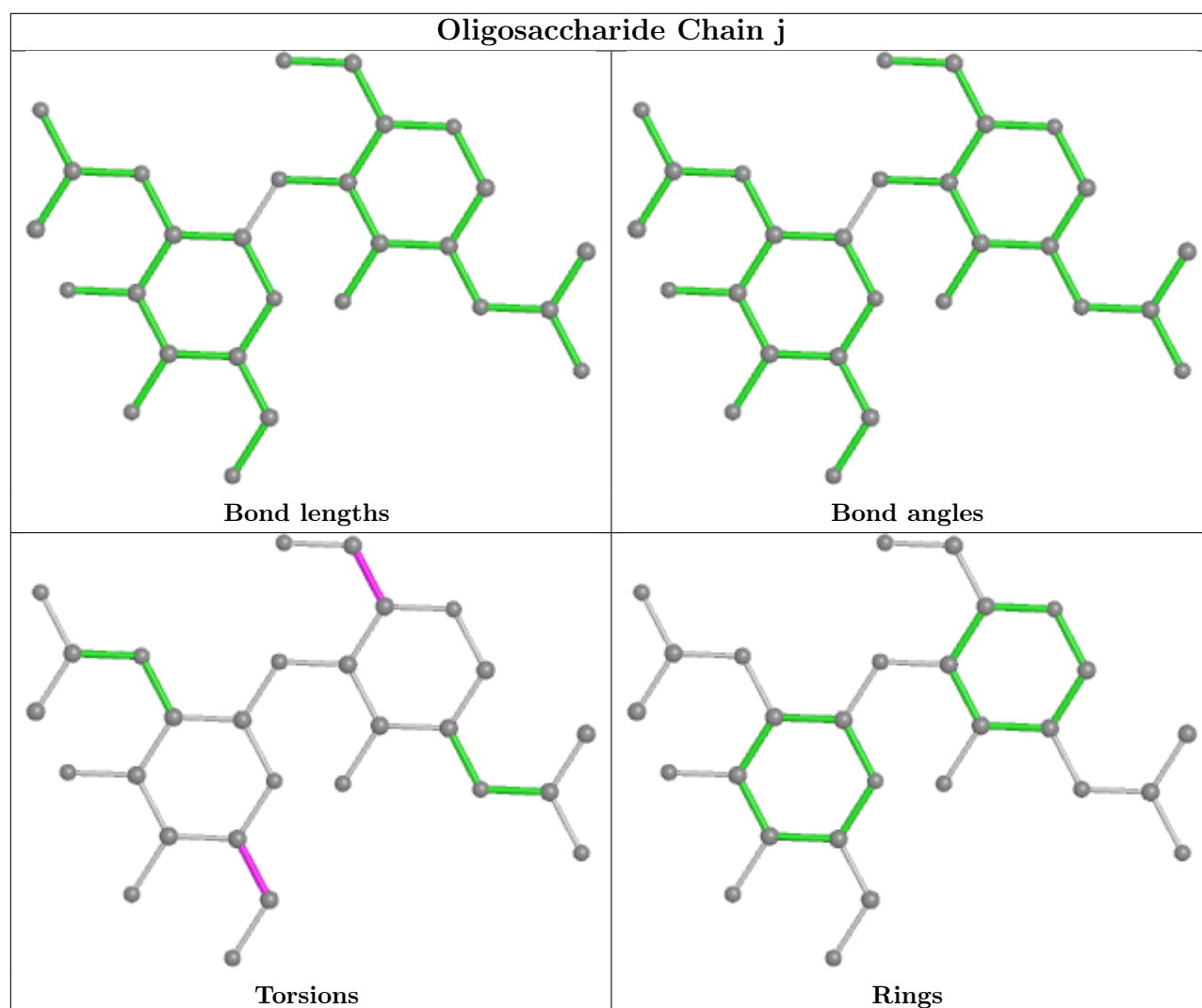


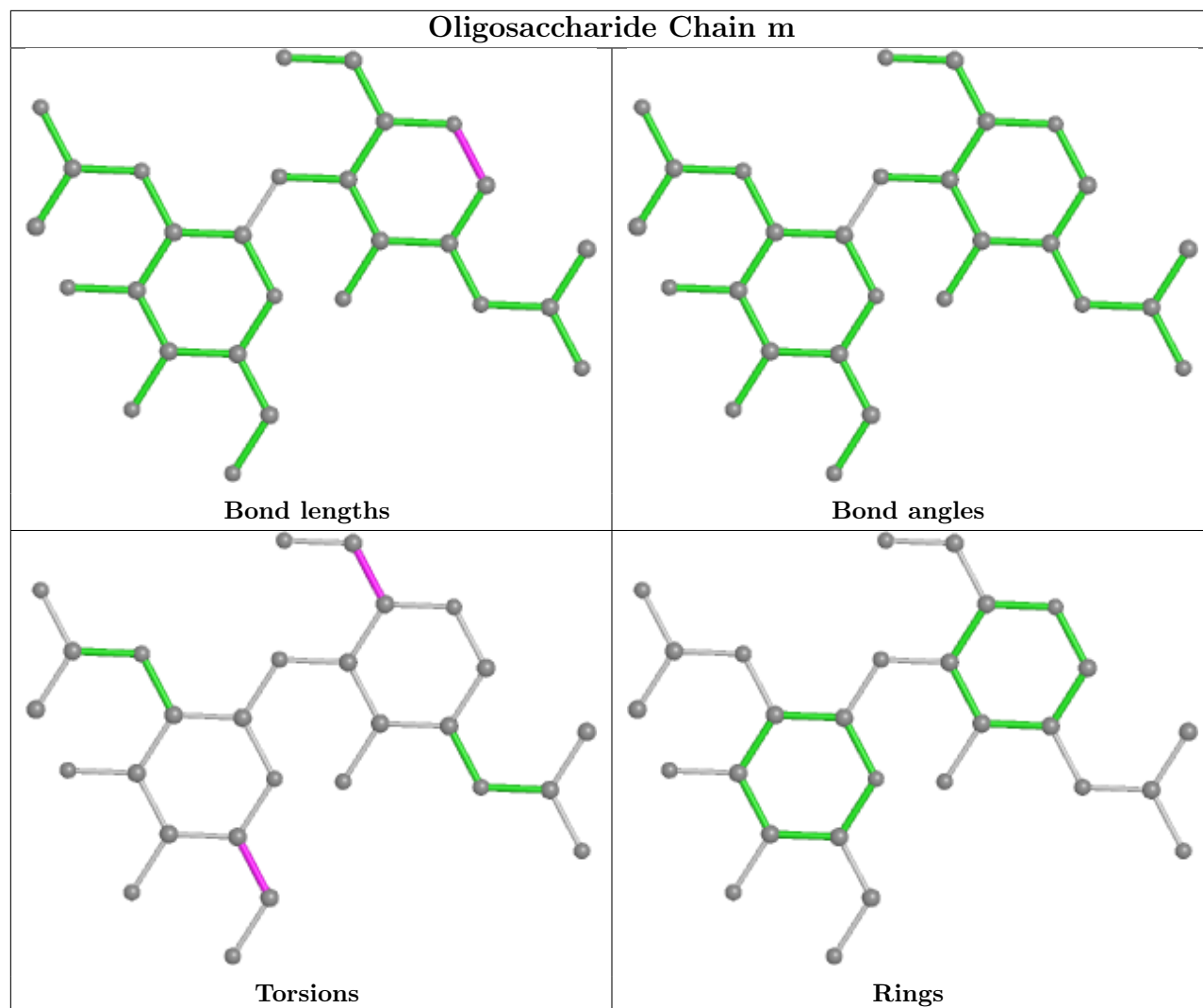


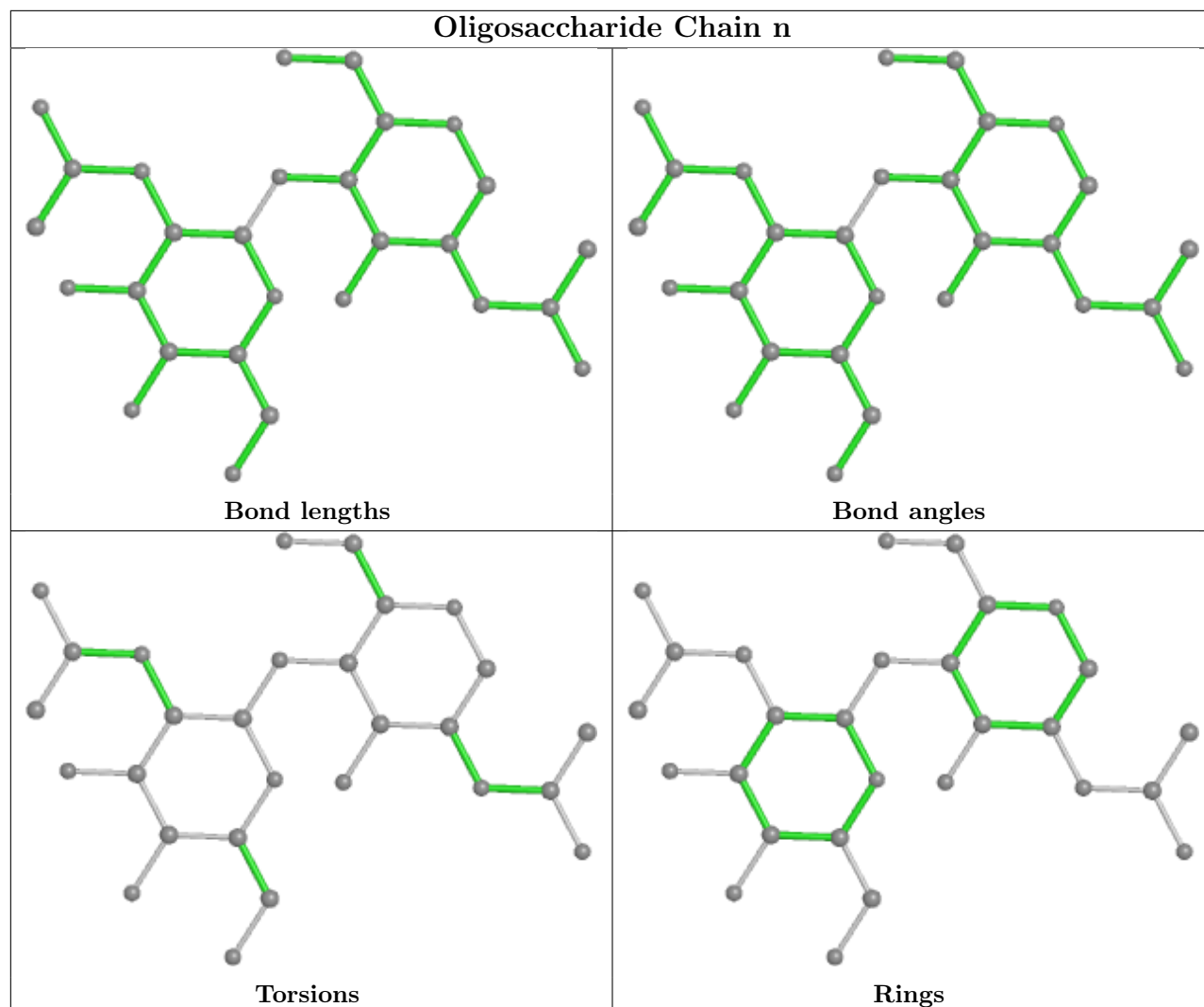


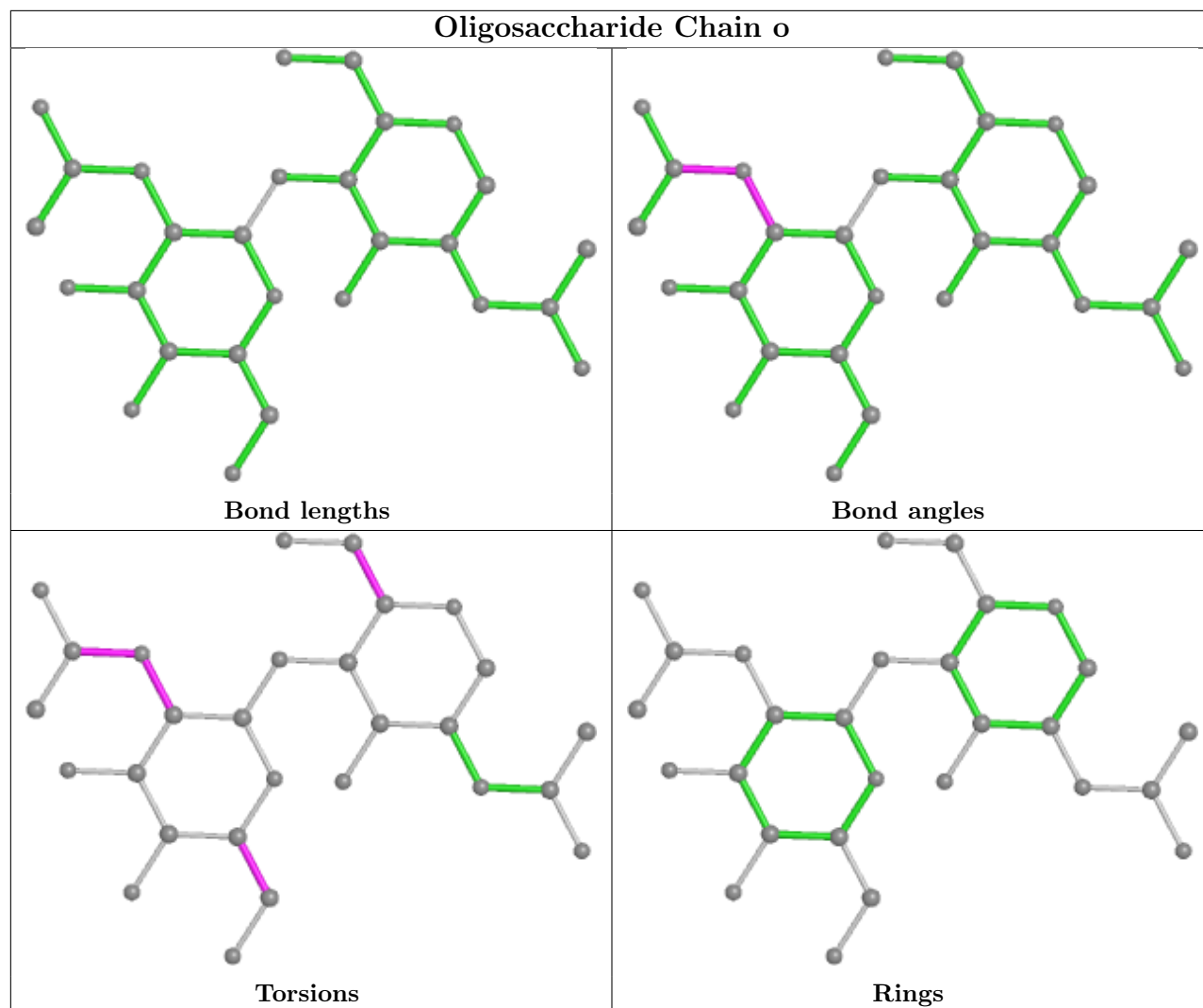


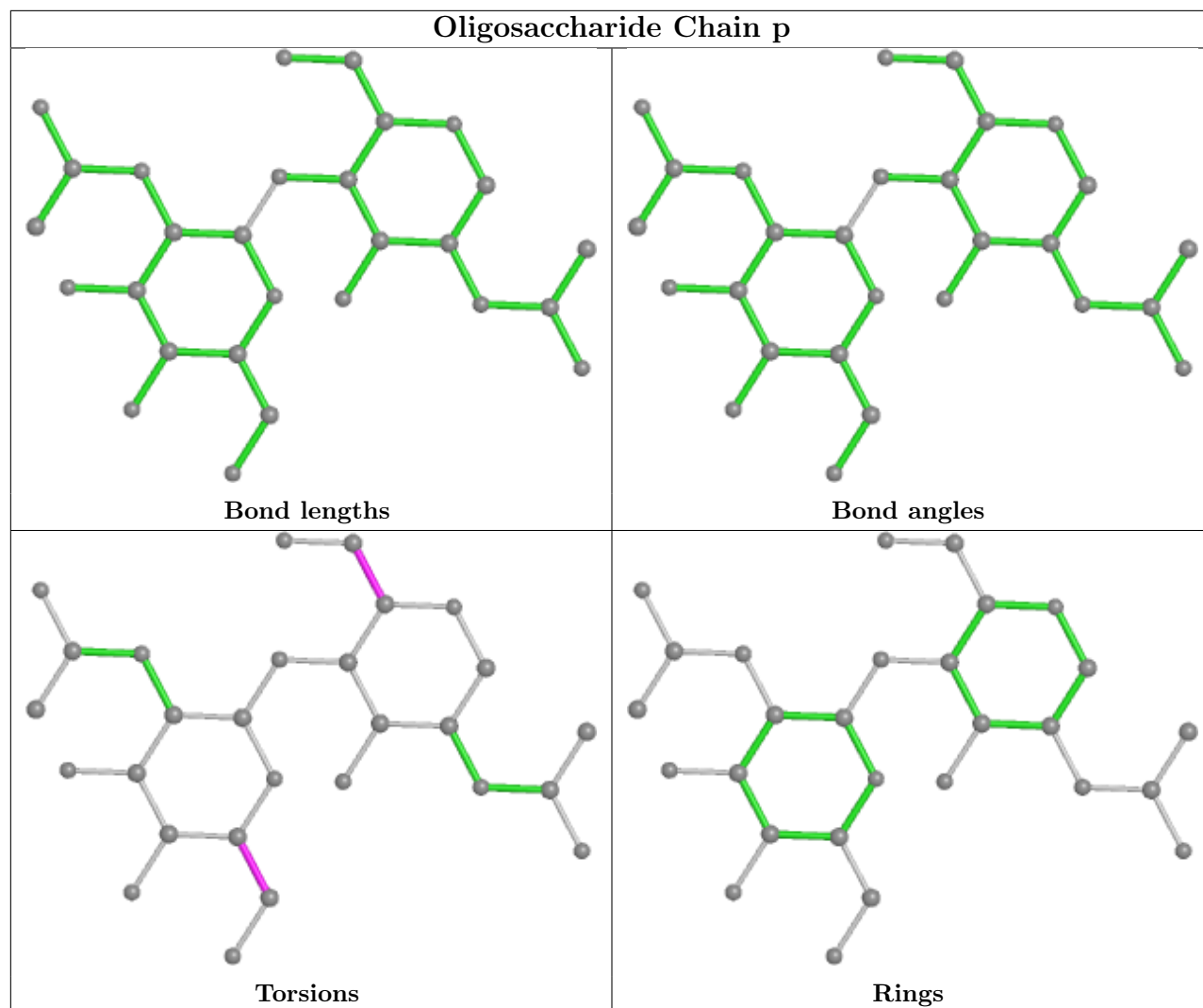


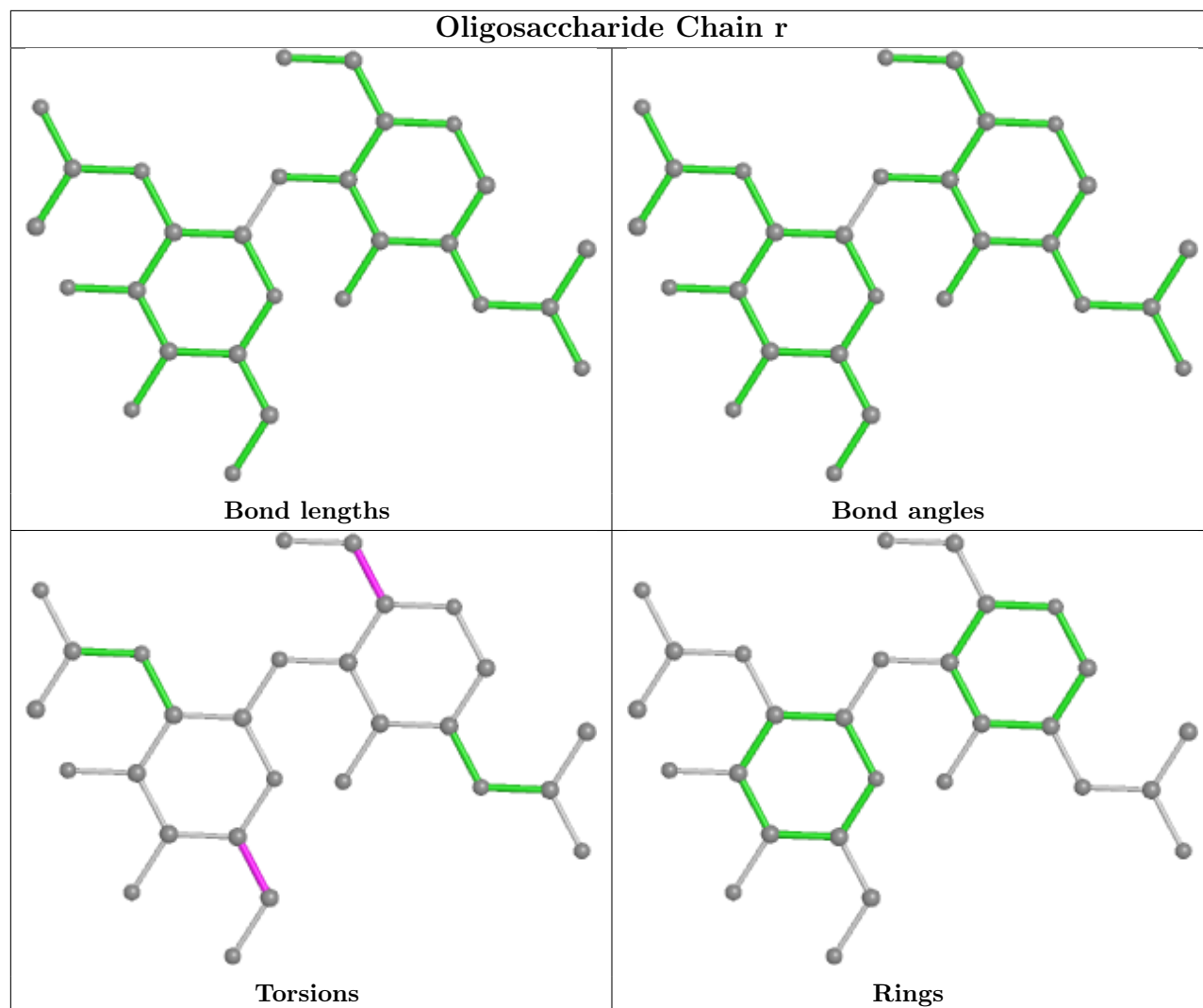


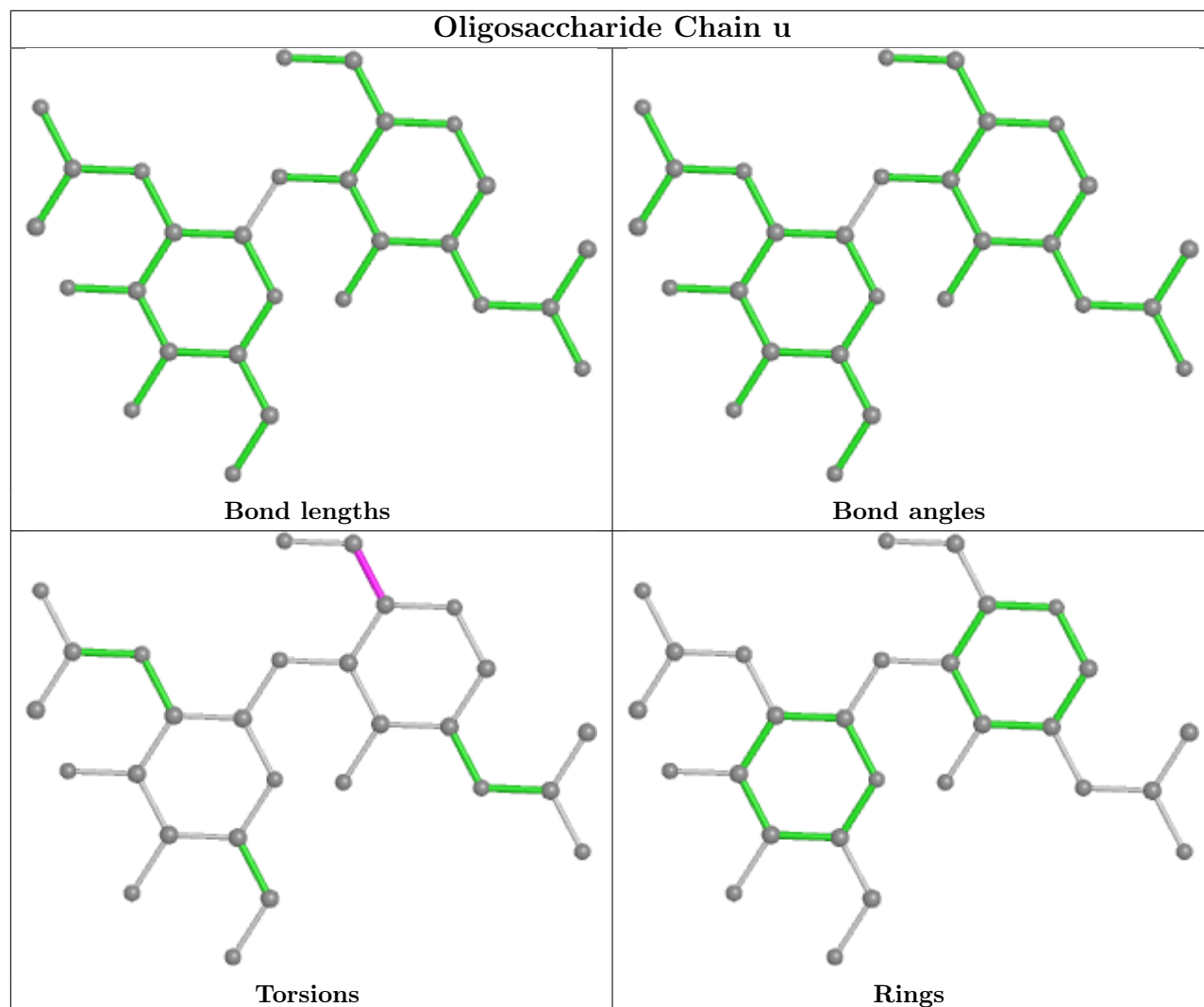


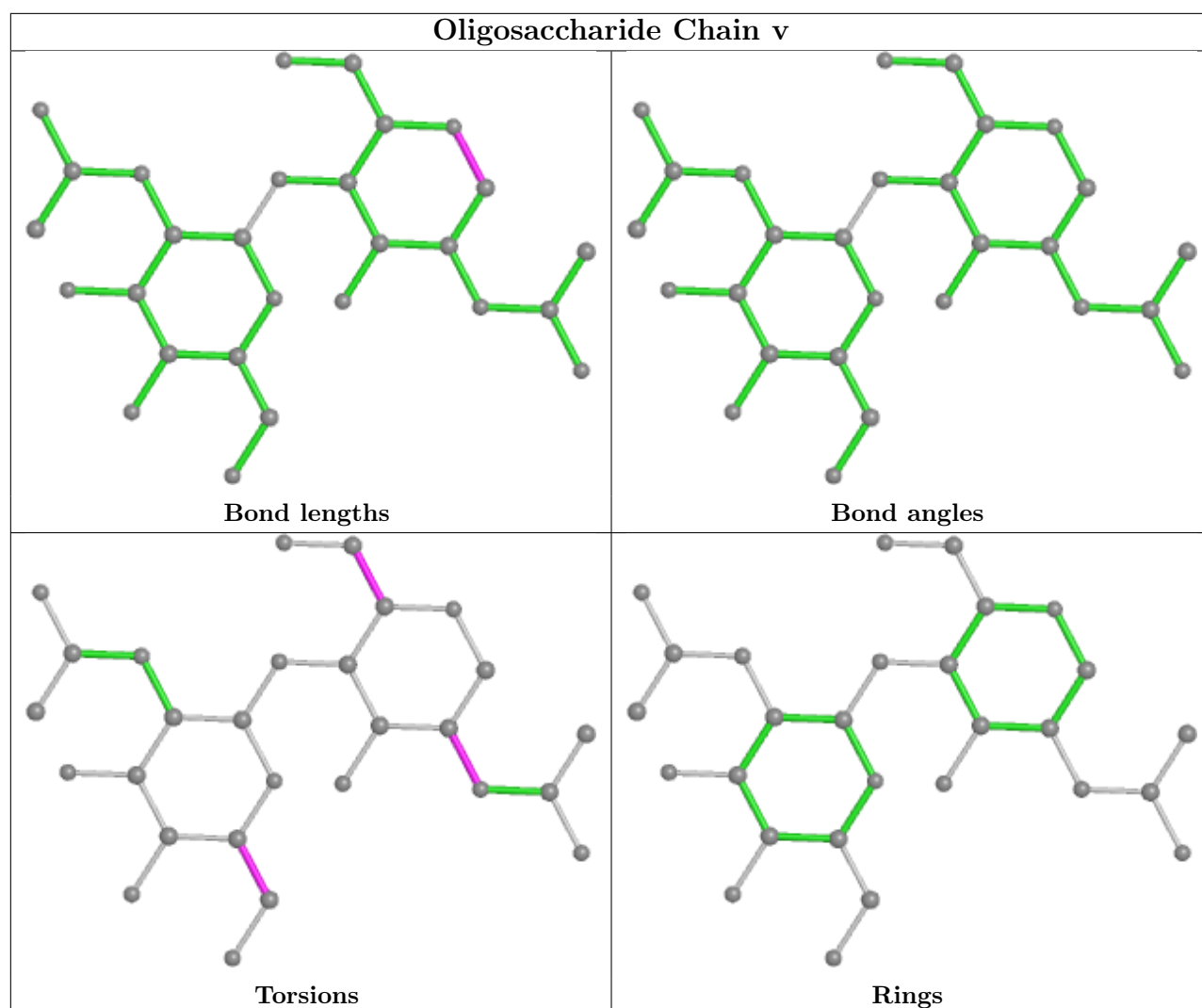


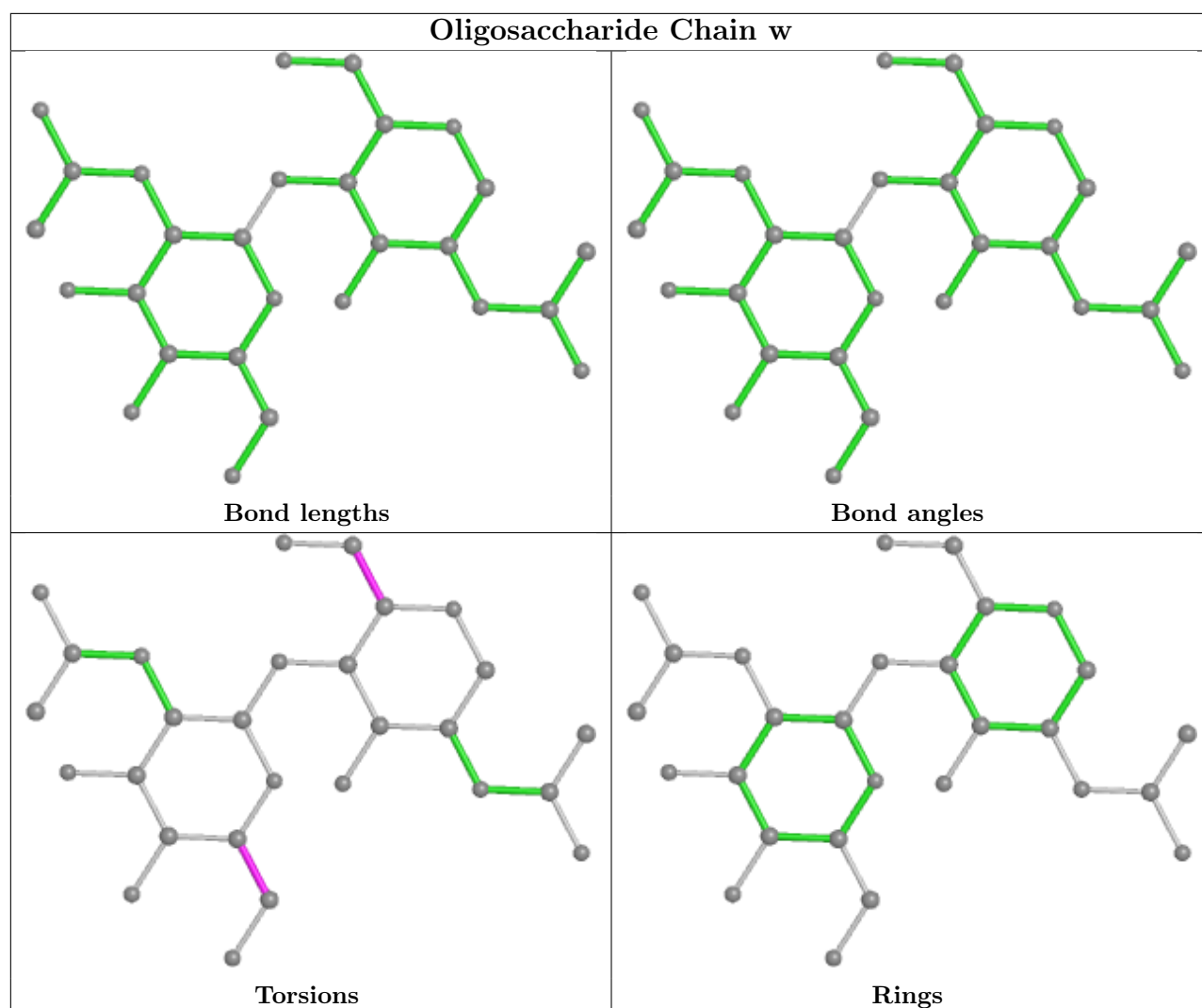


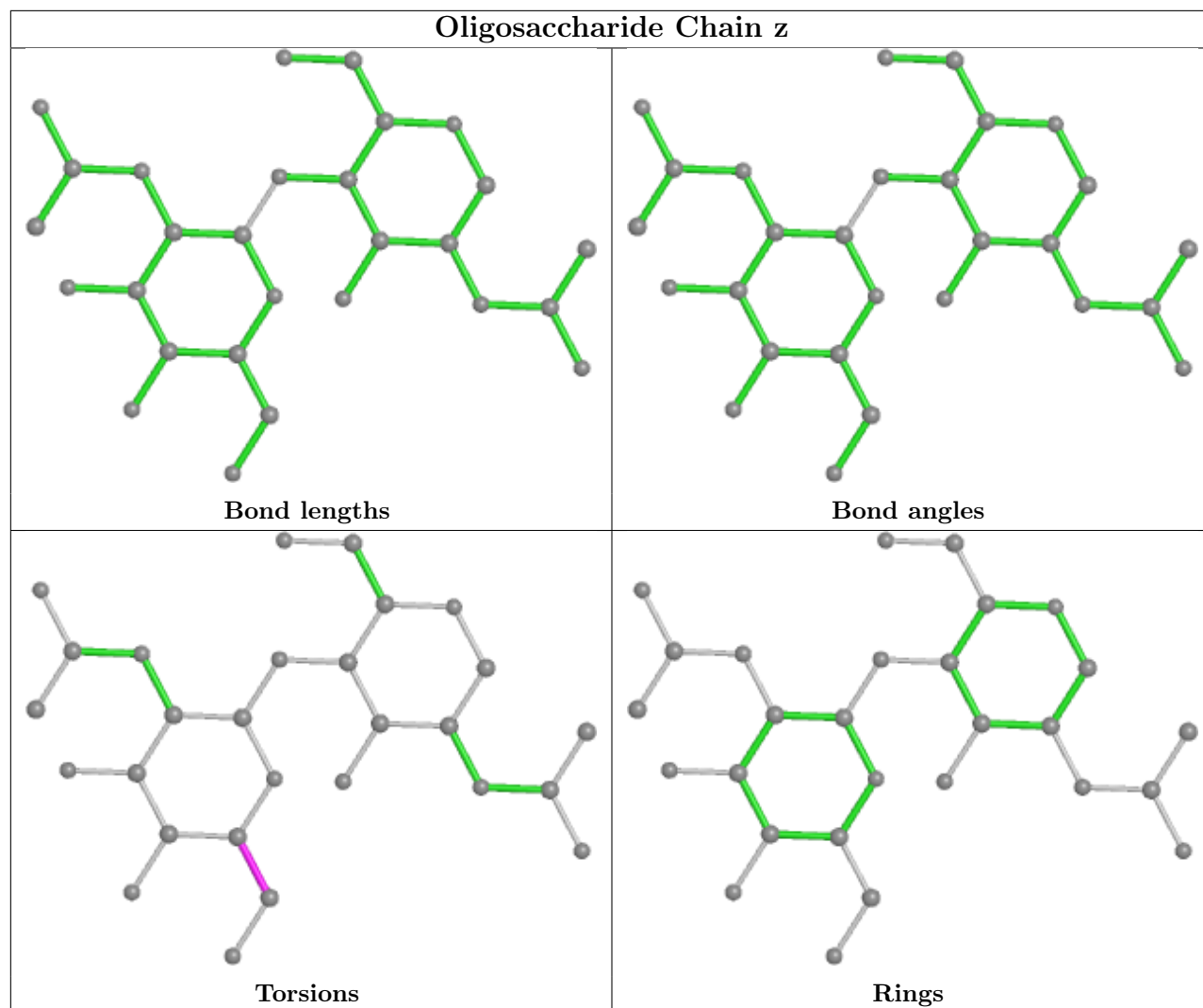


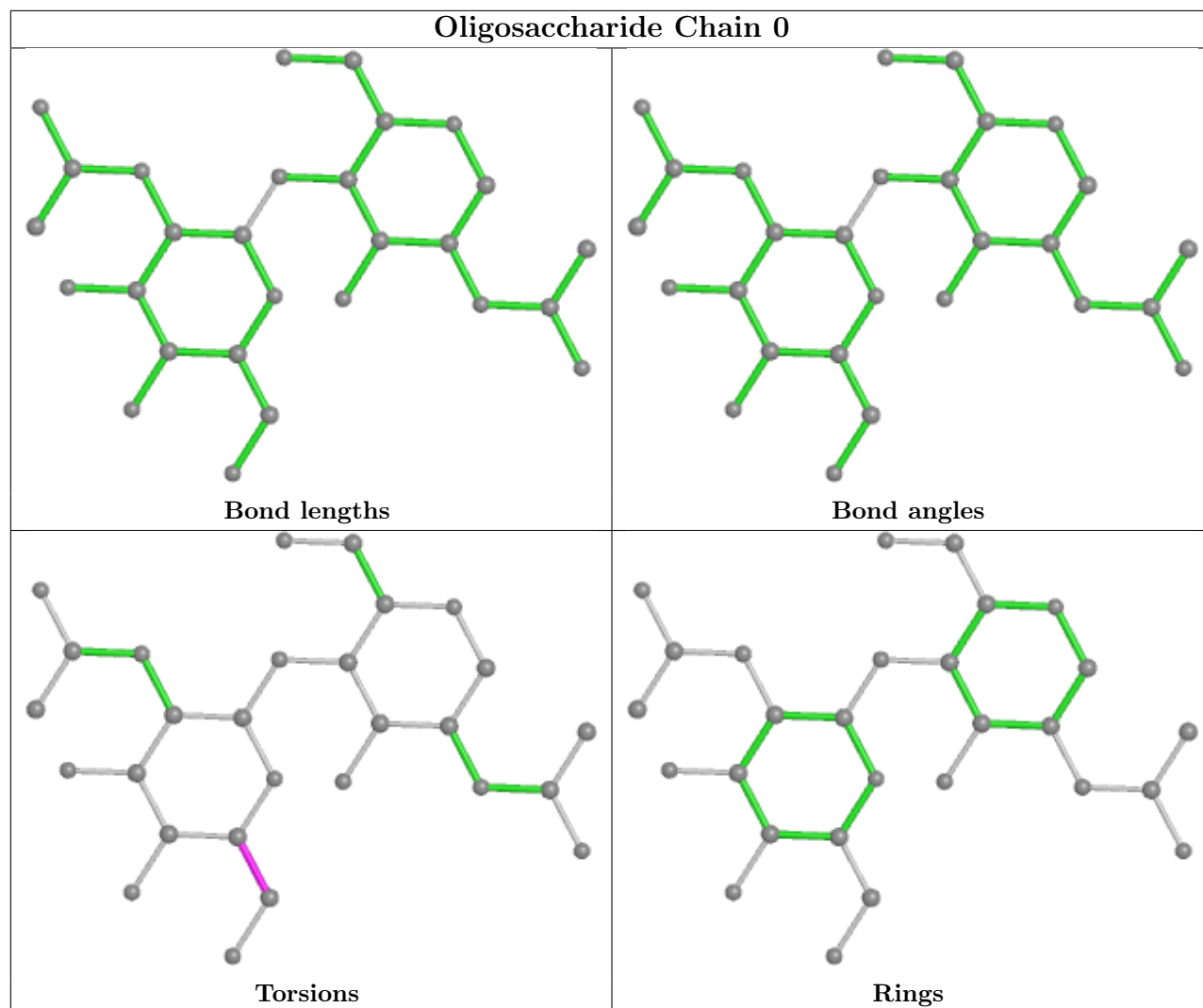


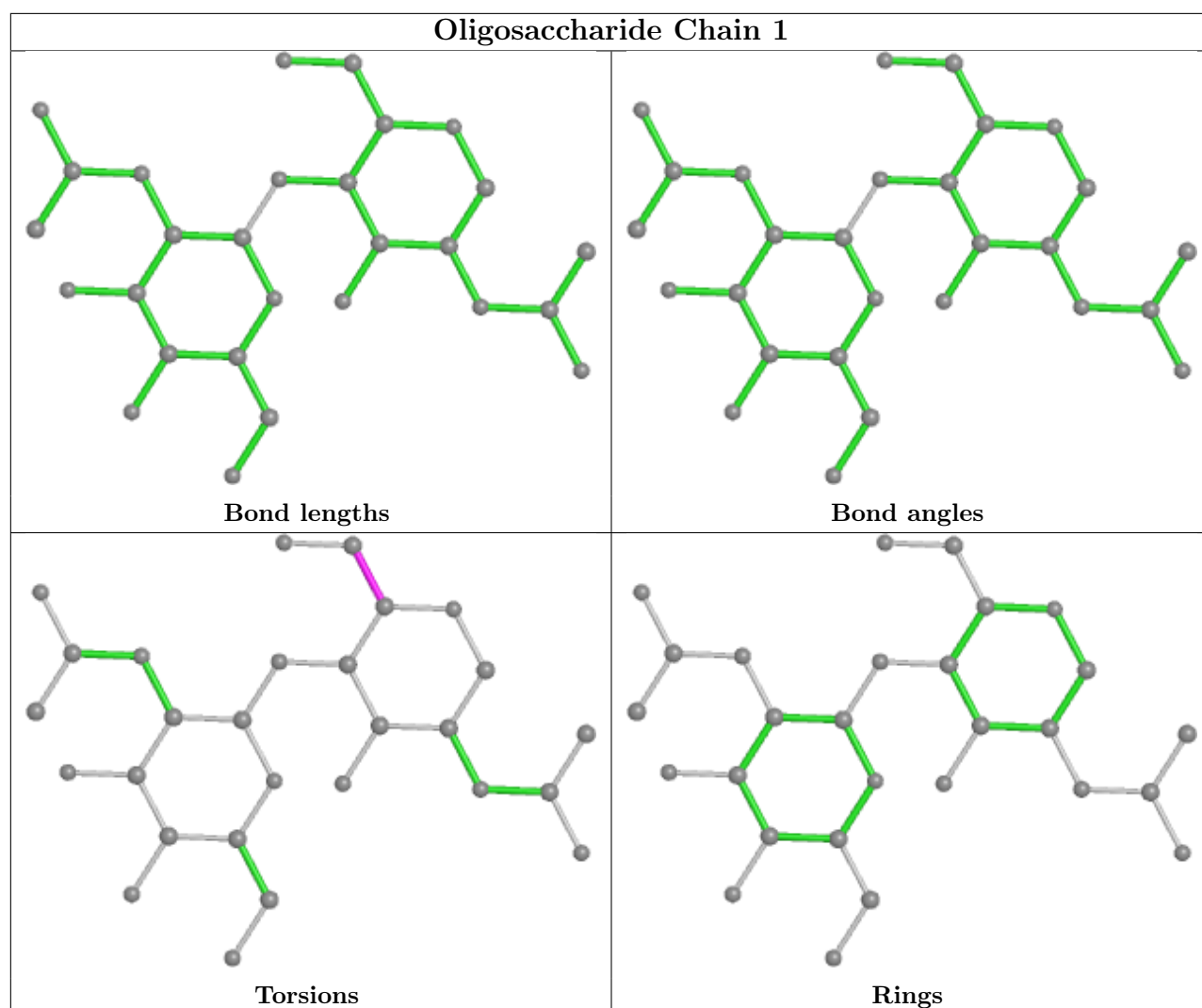


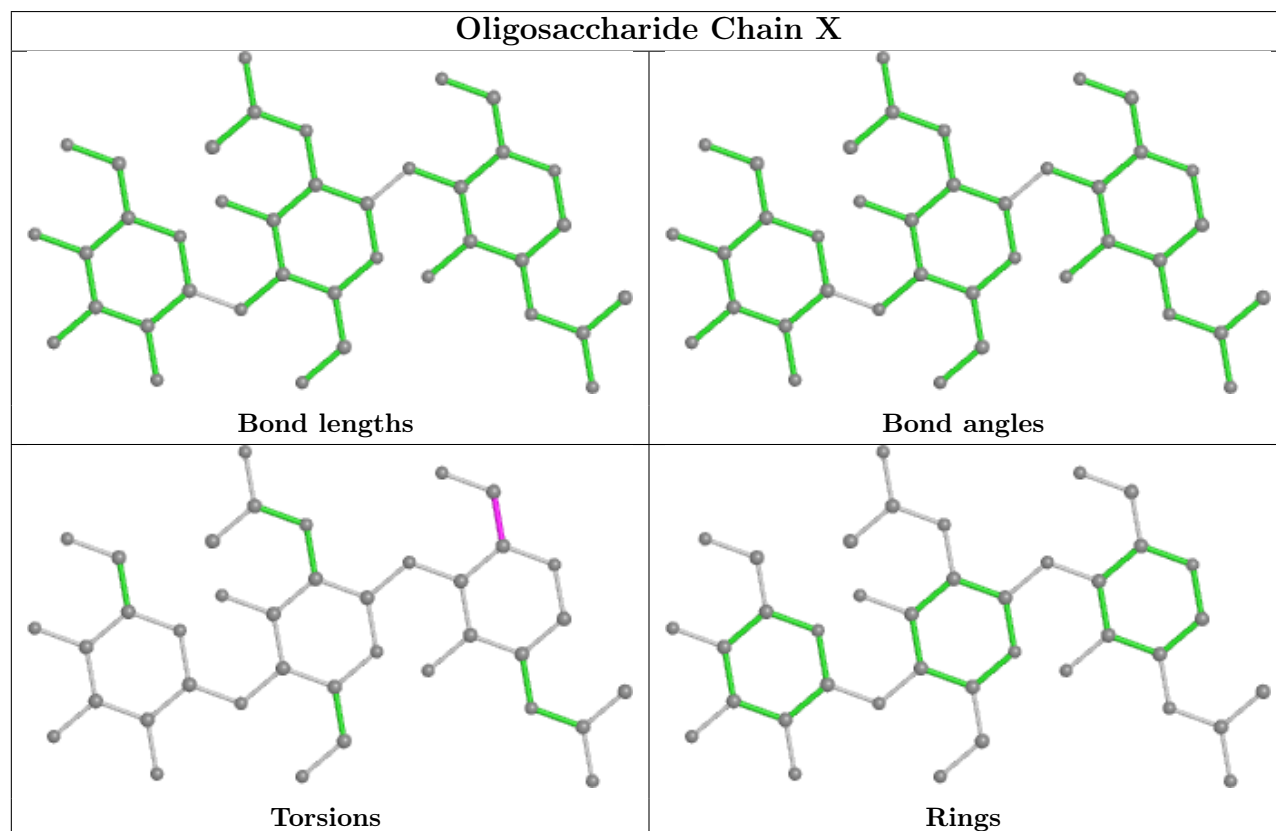
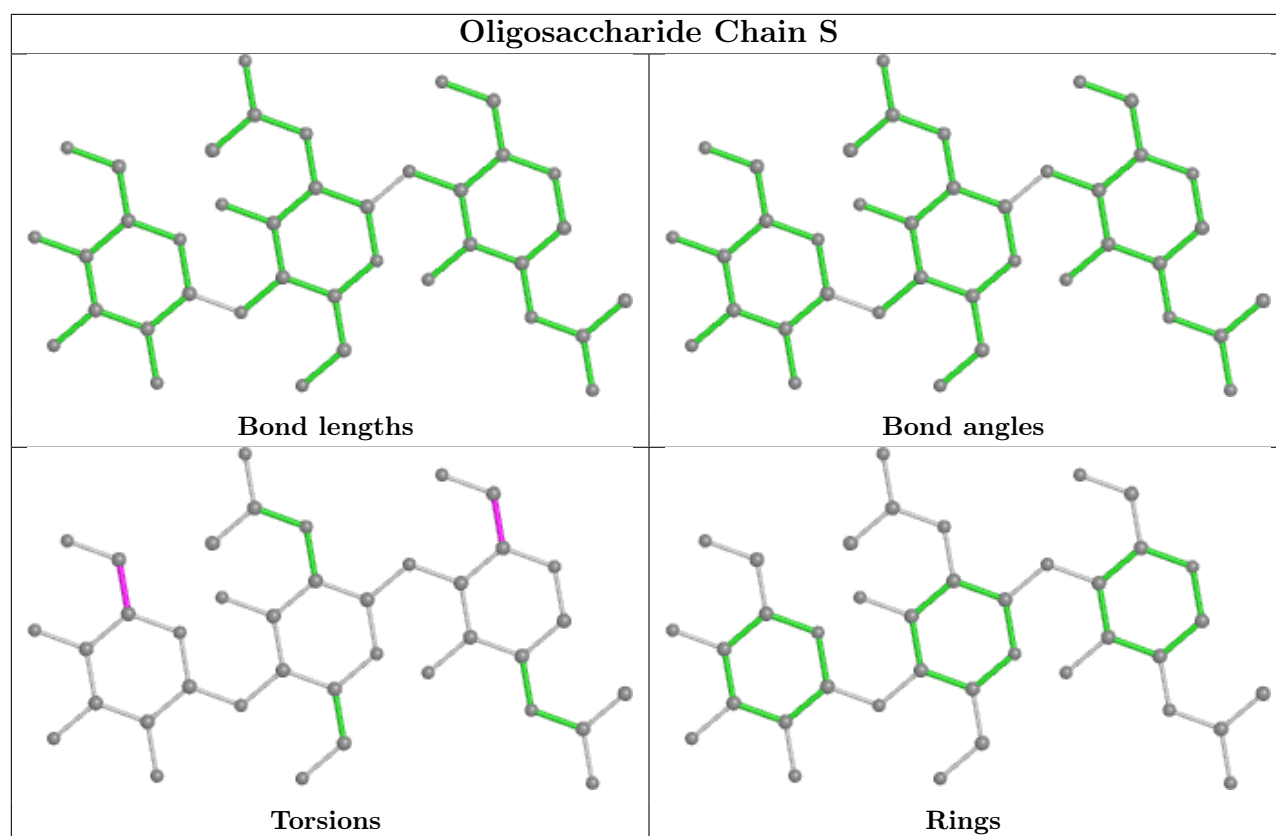


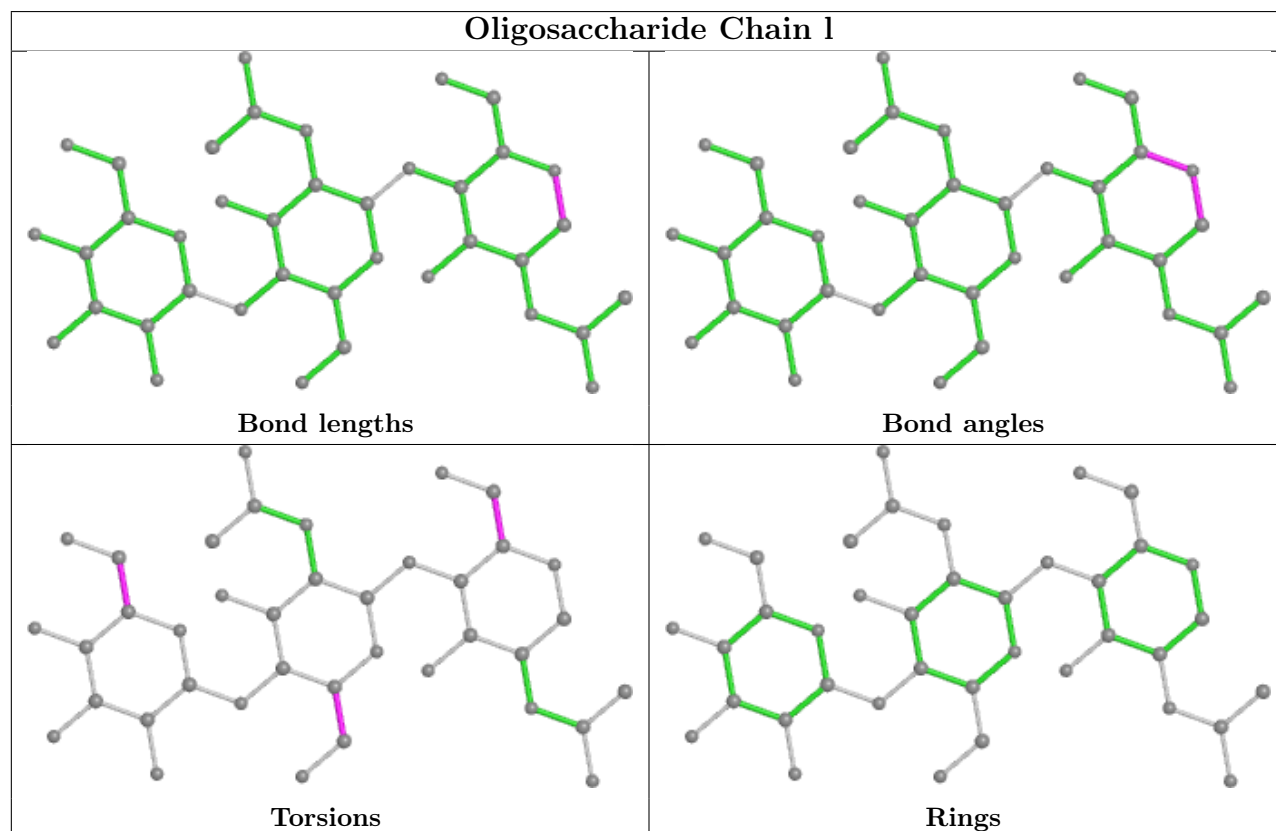
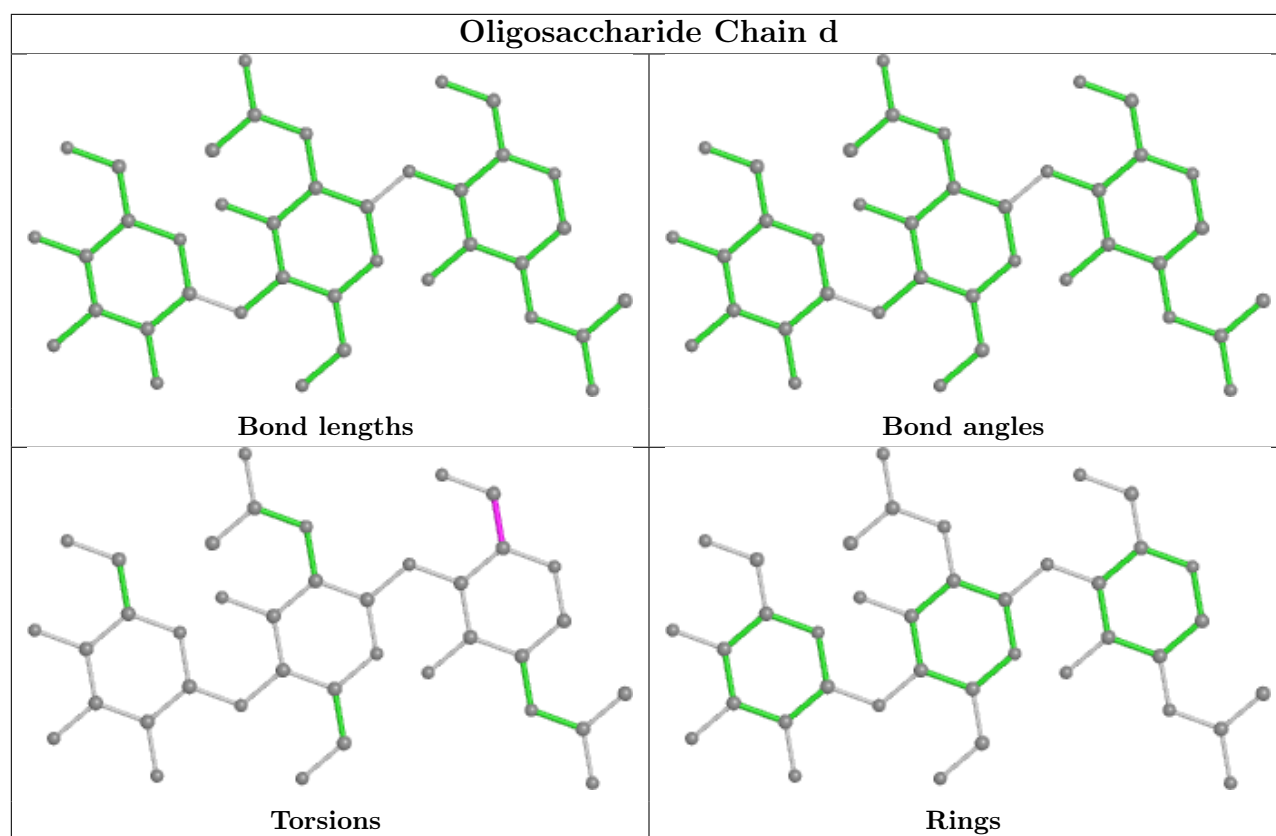


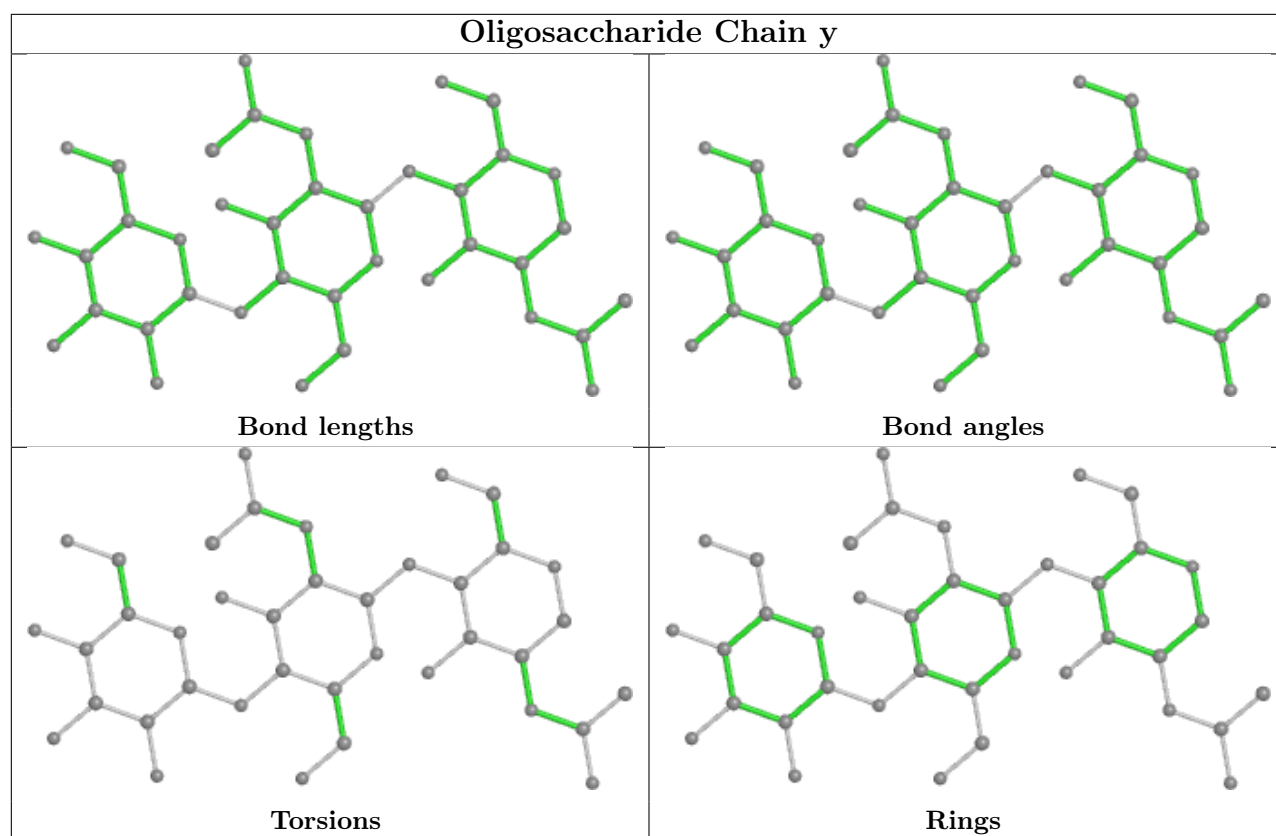


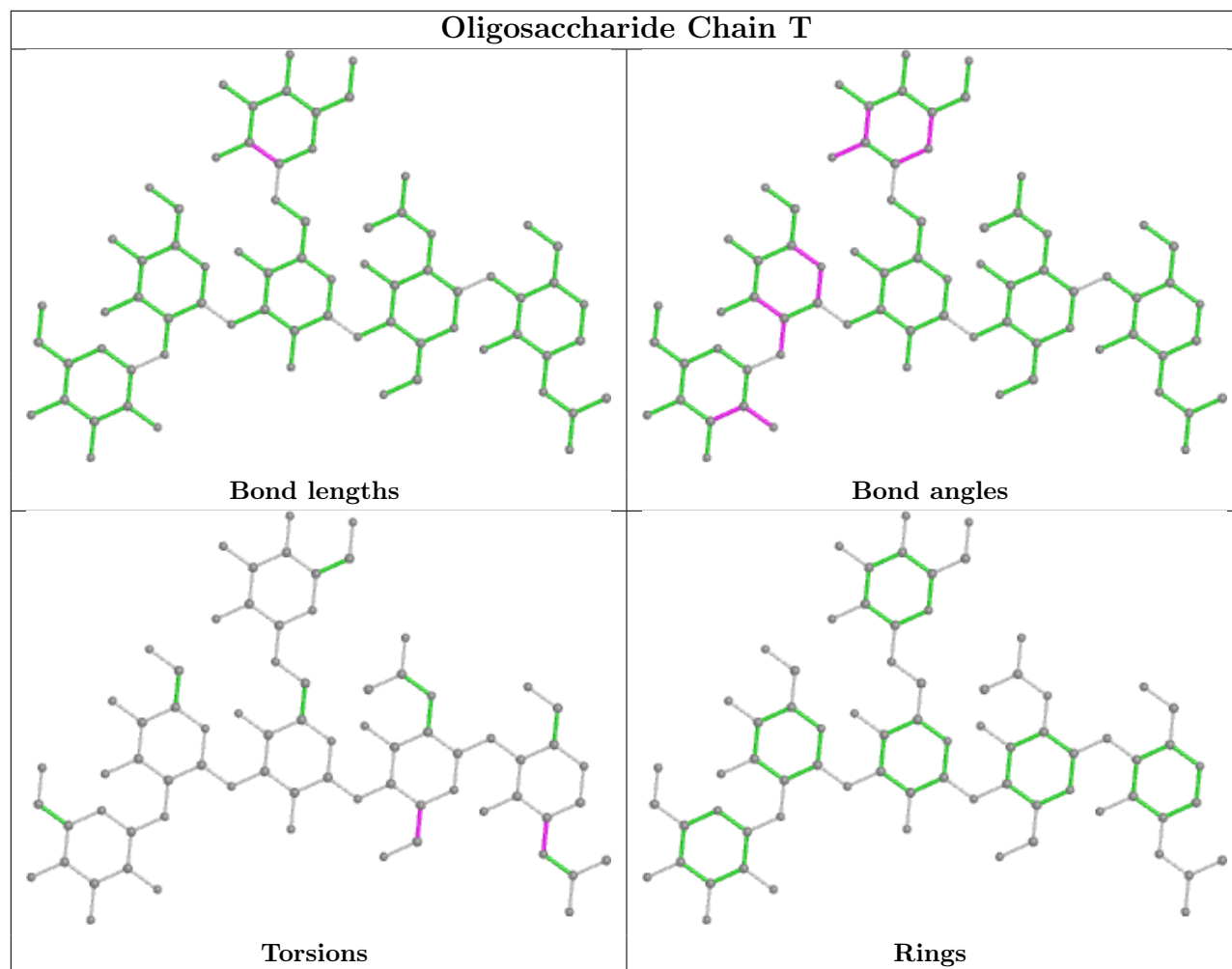


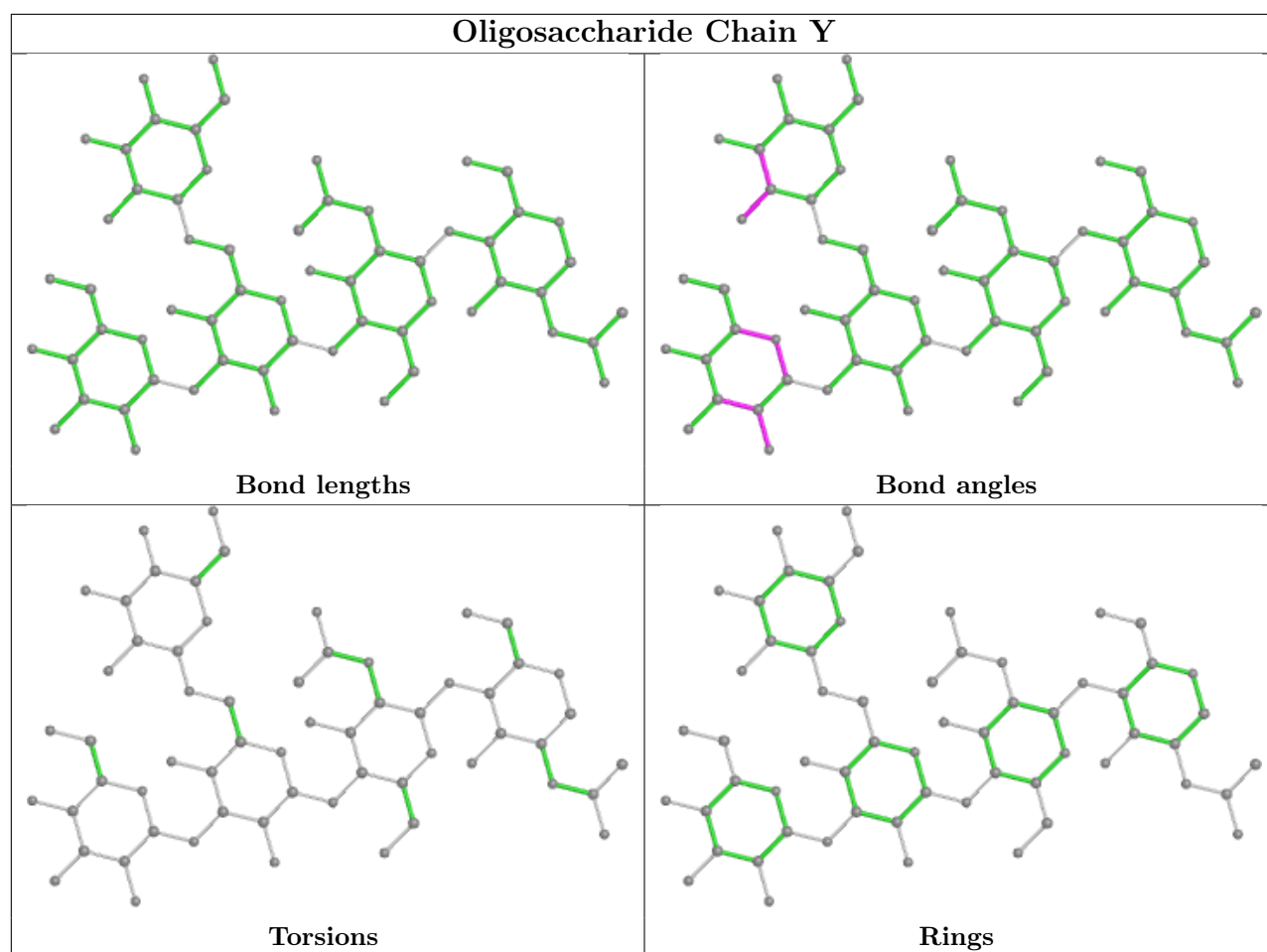


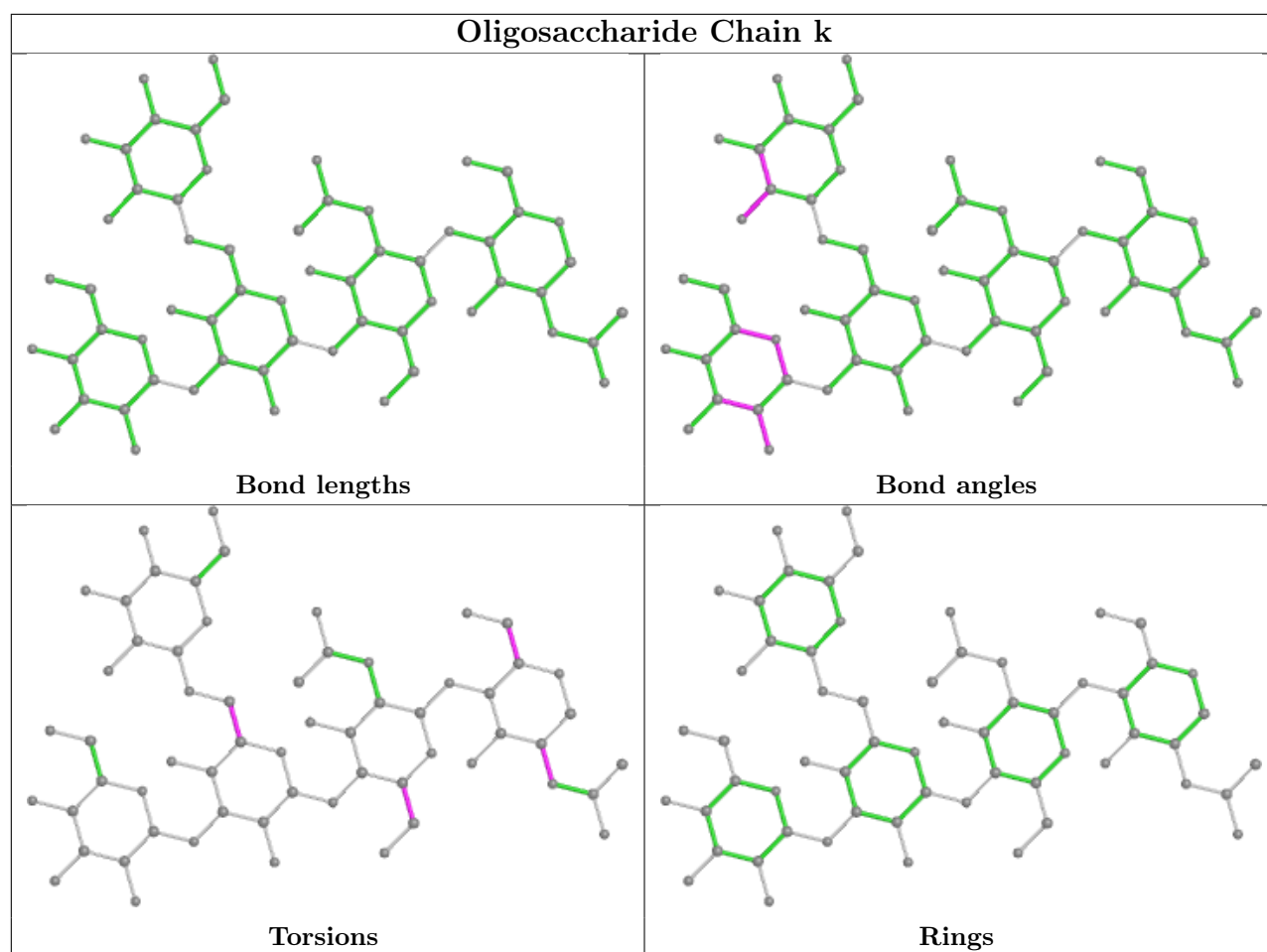


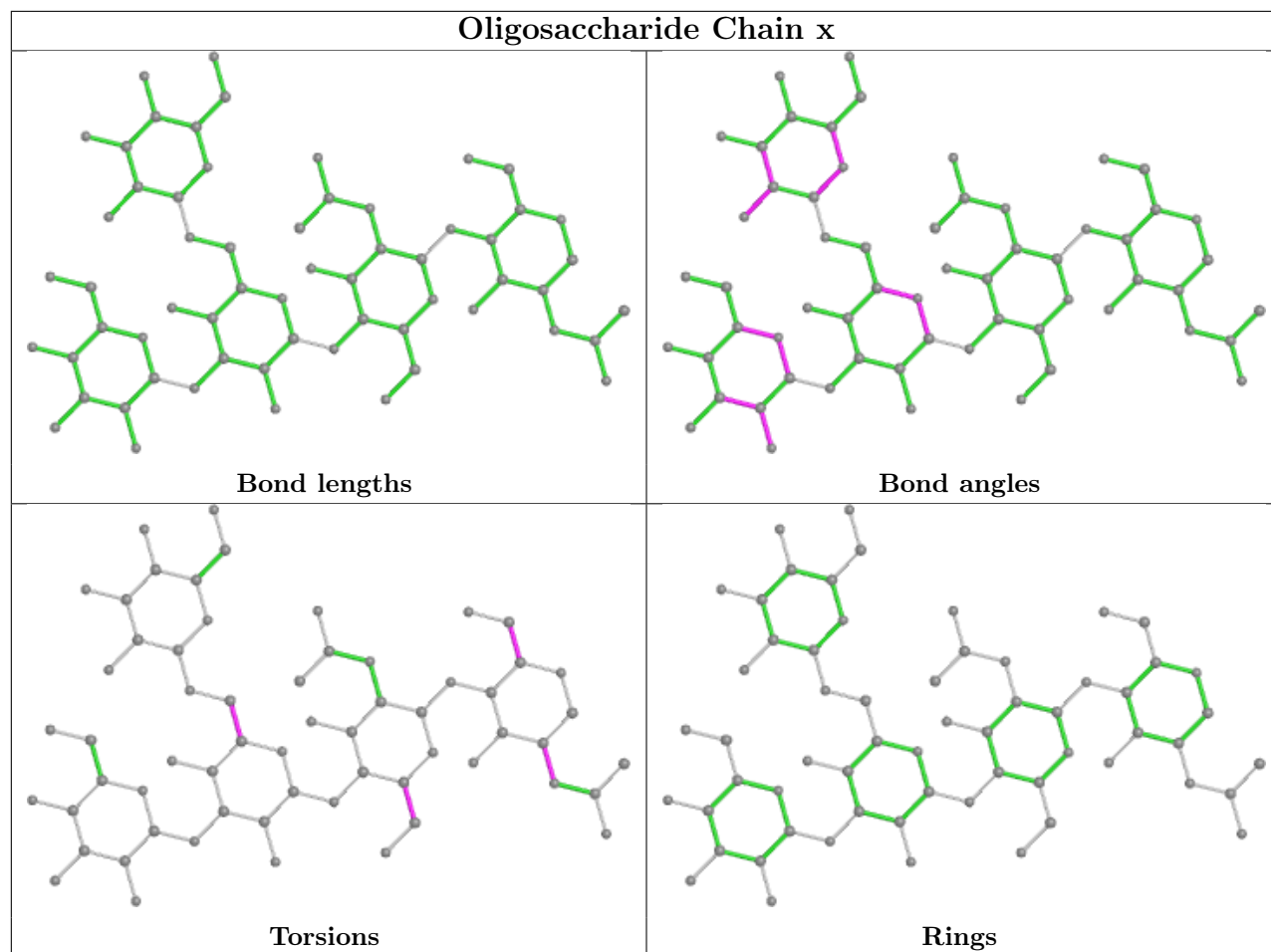


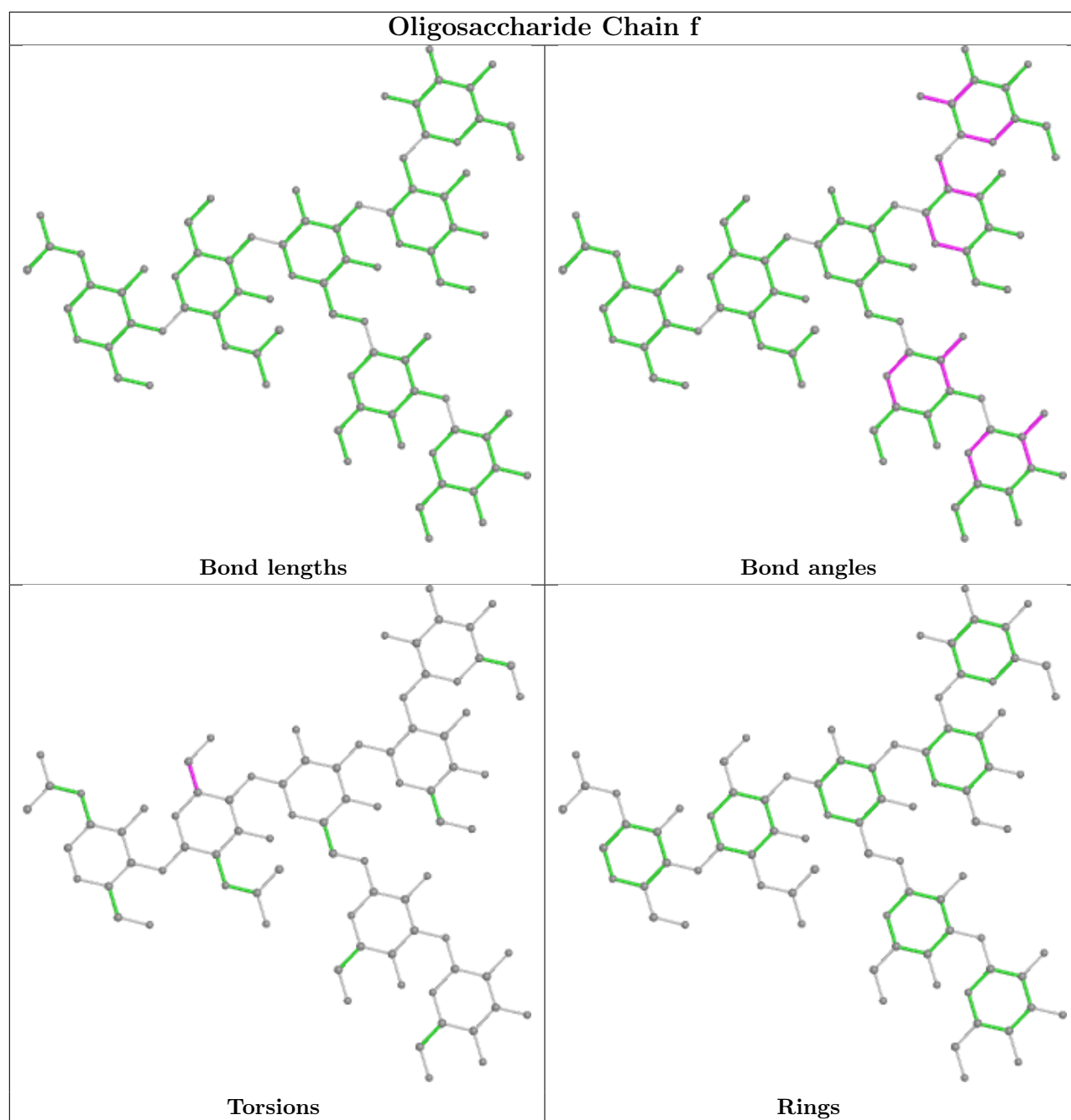


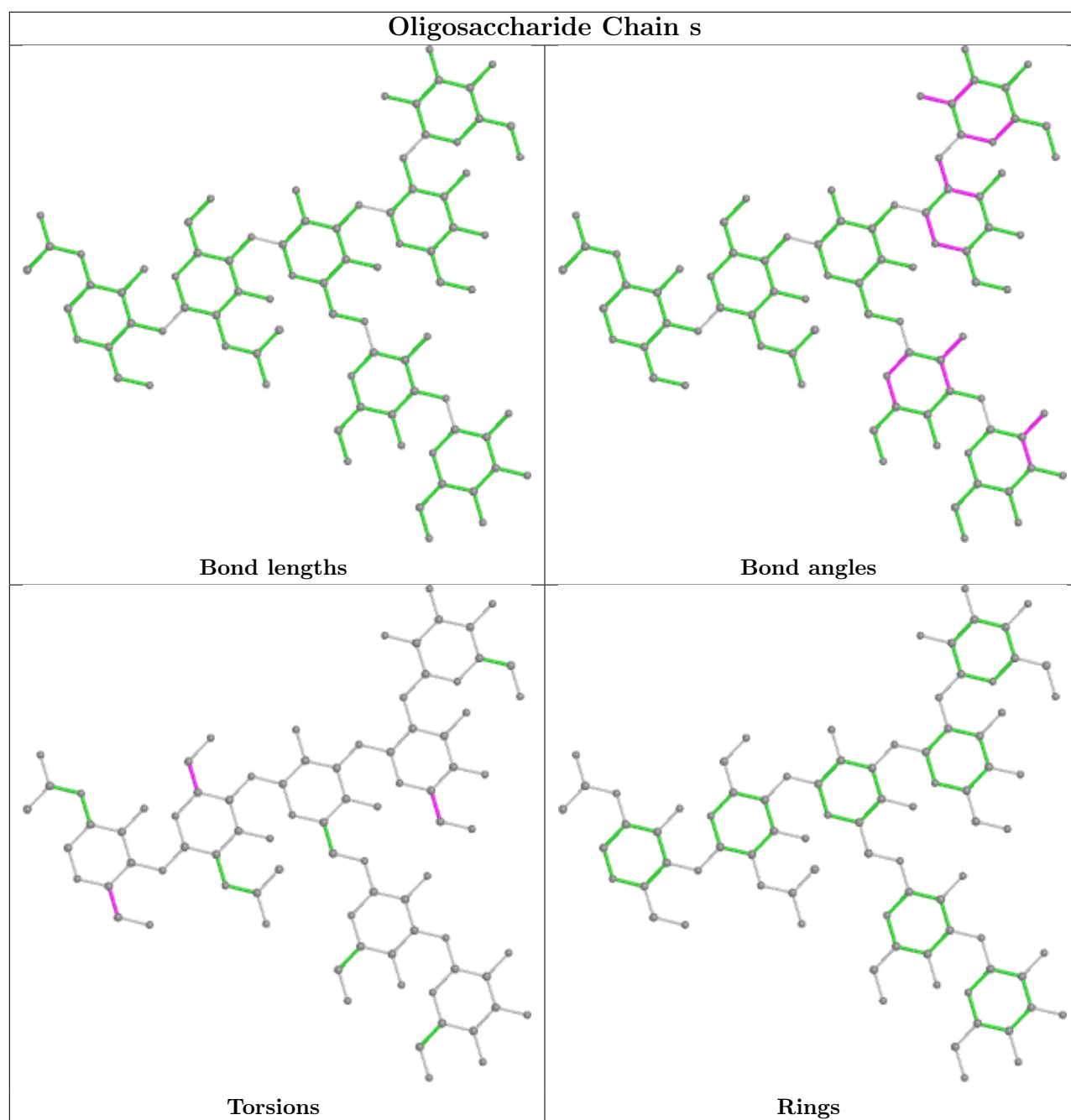


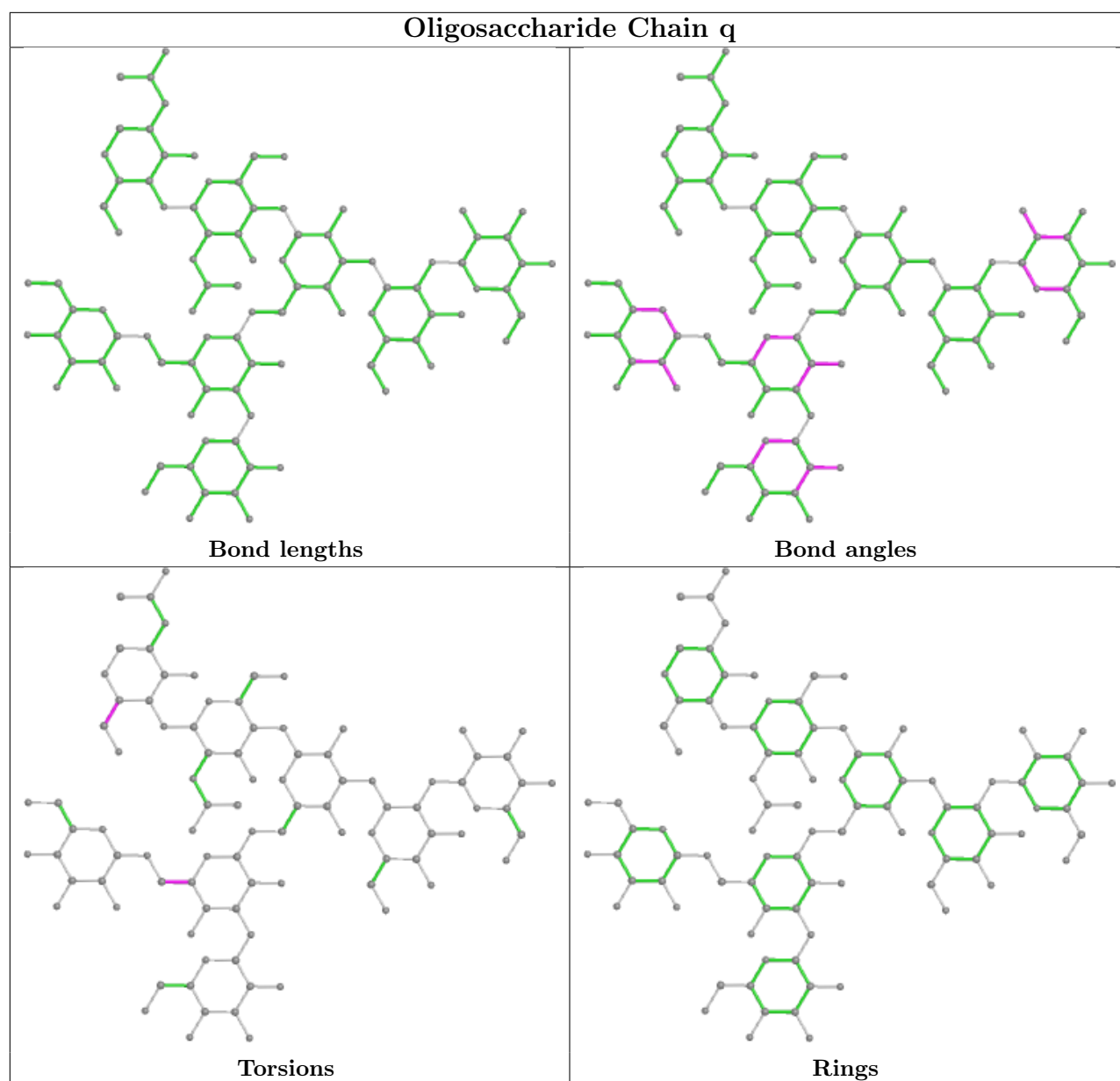












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	C	603	1	14,14,15	0.23	0	17,19,21	0.41	0
11	NAG	A	604	1	14,14,15	0.31	0	17,19,21	0.46	0
11	NAG	C	602	1	14,14,15	0.21	0	17,19,21	0.50	0
11	NAG	D	603	1	14,14,15	1.75	1 (7%)	17,19,21	2.42	2 (11%)
11	NAG	B	703	2	14,14,15	0.20	0	17,19,21	0.42	0
11	NAG	D	604	1	14,14,15	0.33	0	17,19,21	0.34	0
11	NAG	E	702	2	14,14,15	0.28	0	17,19,21	0.44	0
11	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.53	0
11	NAG	A	602	1	14,14,15	0.56	0	17,19,21	1.75	1 (5%)
11	NAG	C	604	1	14,14,15	0.22	0	17,19,21	0.41	0
11	NAG	B	702	2	14,14,15	0.57	0	17,19,21	0.48	0
11	NAG	E	701	2	14,14,15	0.66	0	17,19,21	0.60	0
11	NAG	D	601	1	14,14,15	0.26	0	17,19,21	0.50	0
11	NAG	F	702	2	14,14,15	0.47	0	17,19,21	0.92	1 (5%)
11	NAG	B	701	2	14,14,15	1.11	1 (7%)	17,19,21	1.52	1 (5%)
11	NAG	D	605	1	14,14,15	0.36	0	17,19,21	0.40	0
11	NAG	D	602	1	14,14,15	0.17	0	17,19,21	0.48	0
11	NAG	F	701	2	14,14,15	0.38	0	17,19,21	0.43	0
11	NAG	C	601	1	14,14,15	0.24	0	17,19,21	0.55	0
11	NAG	A	603	1	14,14,15	0.26	0	17,19,21	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	C	603	1	-	2/6/23/26	0/1/1/1
11	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	NAG	C	602	1	-	2/6/23/26	0/1/1/1
11	NAG	D	603	1	-	2/6/23/26	0/1/1/1
11	NAG	B	703	2	-	2/6/23/26	0/1/1/1
11	NAG	D	604	1	-	3/6/23/26	0/1/1/1
11	NAG	E	702	2	-	2/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	NAG	A	602	1	-	2/6/23/26	0/1/1/1
11	NAG	C	604	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	0/6/23/26	0/1/1/1
11	NAG	E	701	2	-	3/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	603	NAG	O5-C1	6.41	1.54	1.43
11	B	701	NAG	O5-C1	3.99	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	603	NAG	C1-O5-C5	8.97	124.34	112.19
11	A	602	NAG	C1-O5-C5	6.50	121.00	112.19
11	B	701	NAG	C1-O5-C5	5.96	120.27	112.19
11	D	603	NAG	C4-C3-C2	-3.32	106.15	111.02
11	F	702	NAG	C1-O5-C5	2.71	115.86	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

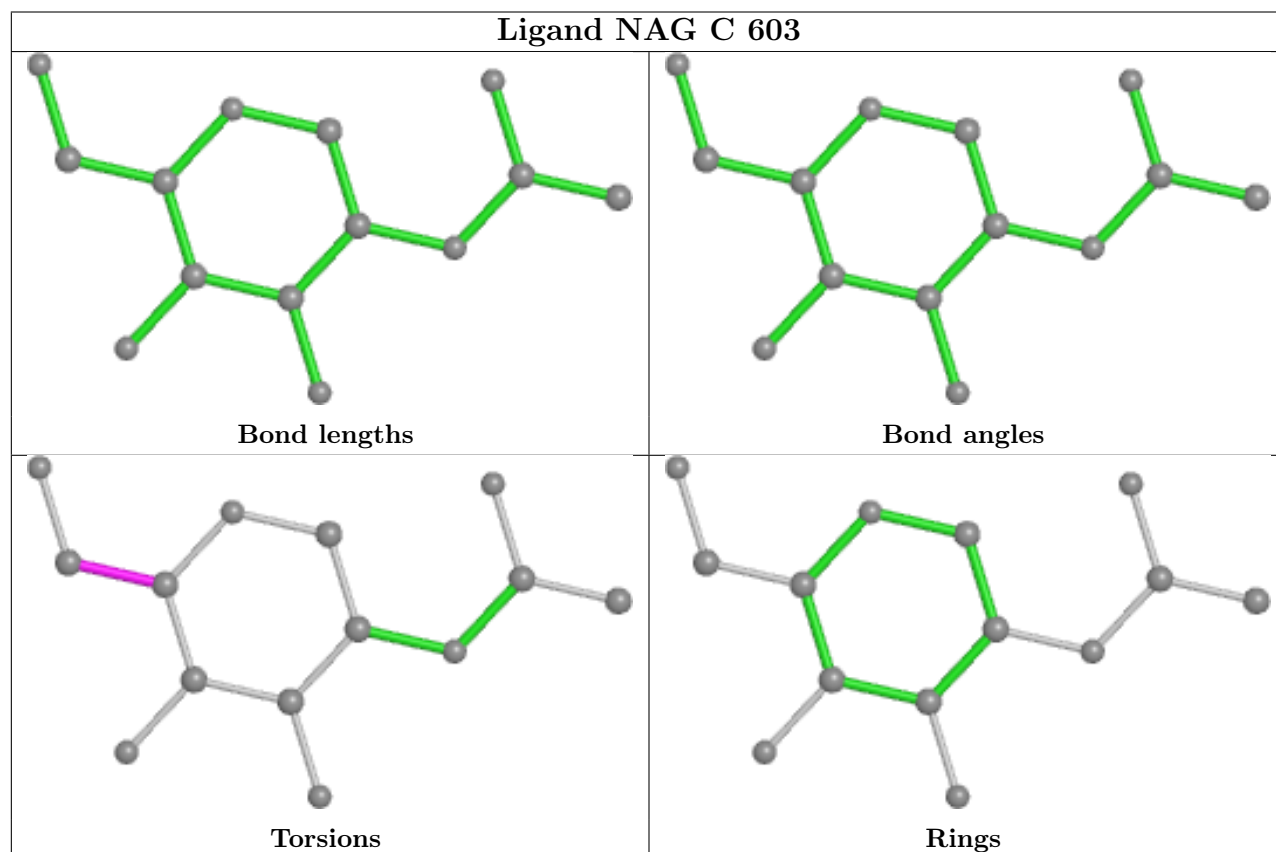
Mol	Chain	Res	Type	Atoms
11	A	602	NAG	O5-C5-C6-O6
11	C	603	NAG	O5-C5-C6-O6
11	D	603	NAG	O5-C5-C6-O6
11	F	701	NAG	O5-C5-C6-O6
11	A	601	NAG	O5-C5-C6-O6

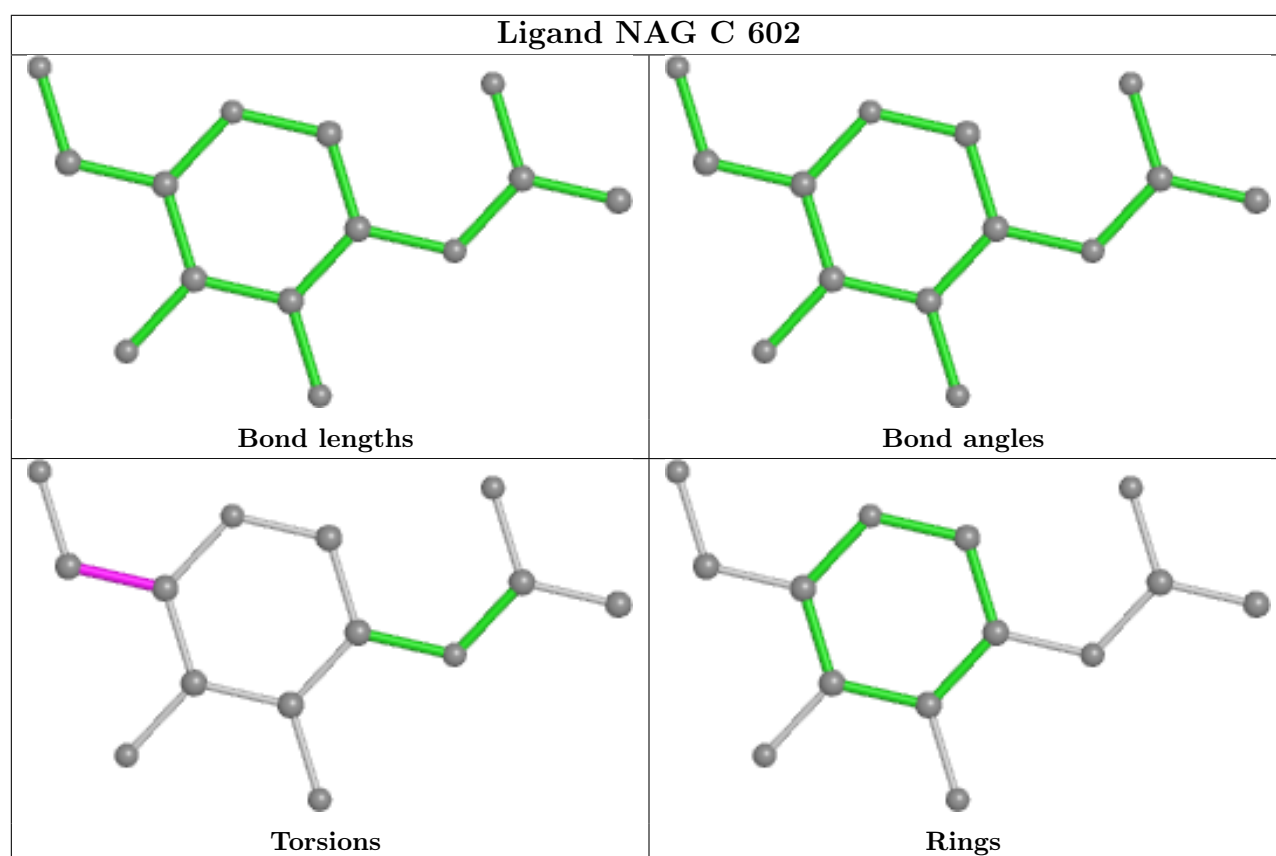
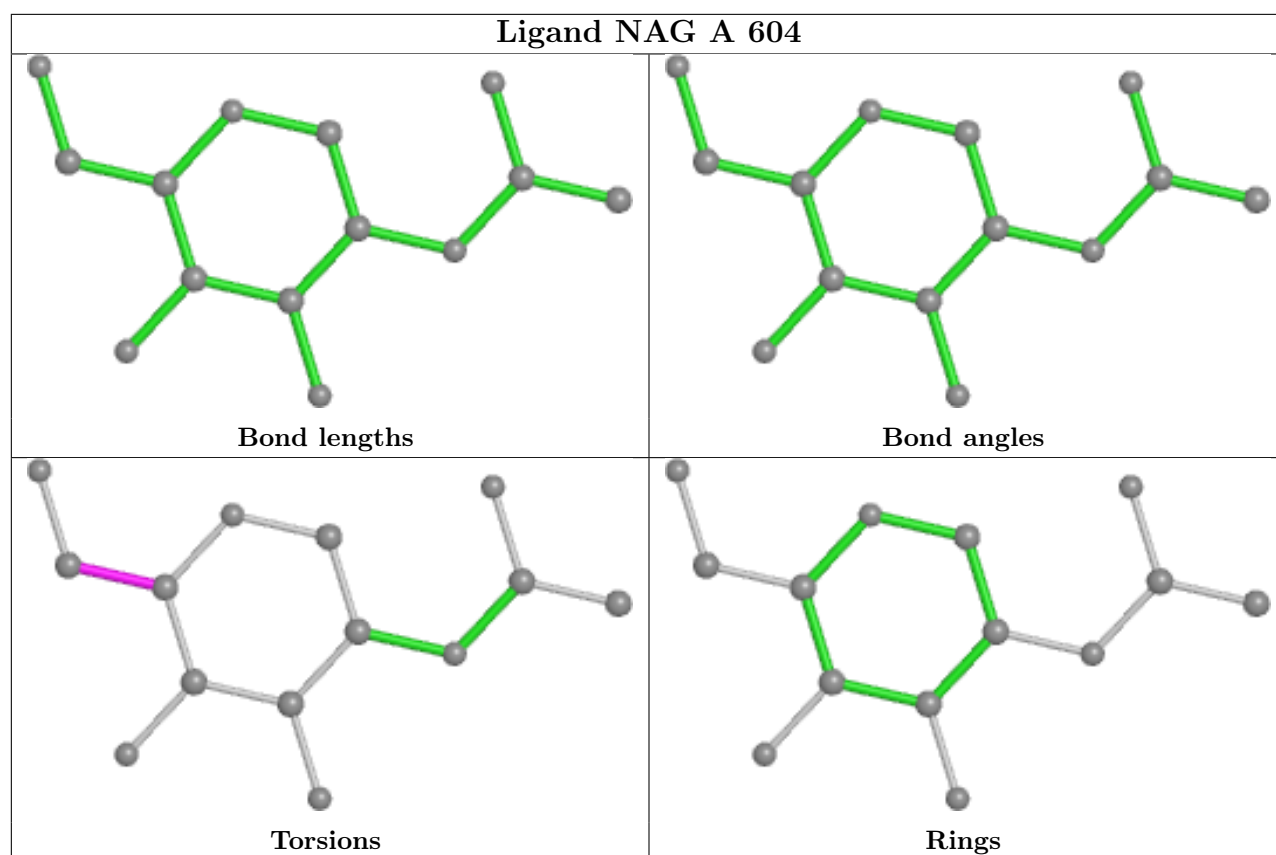
There are no ring outliers.

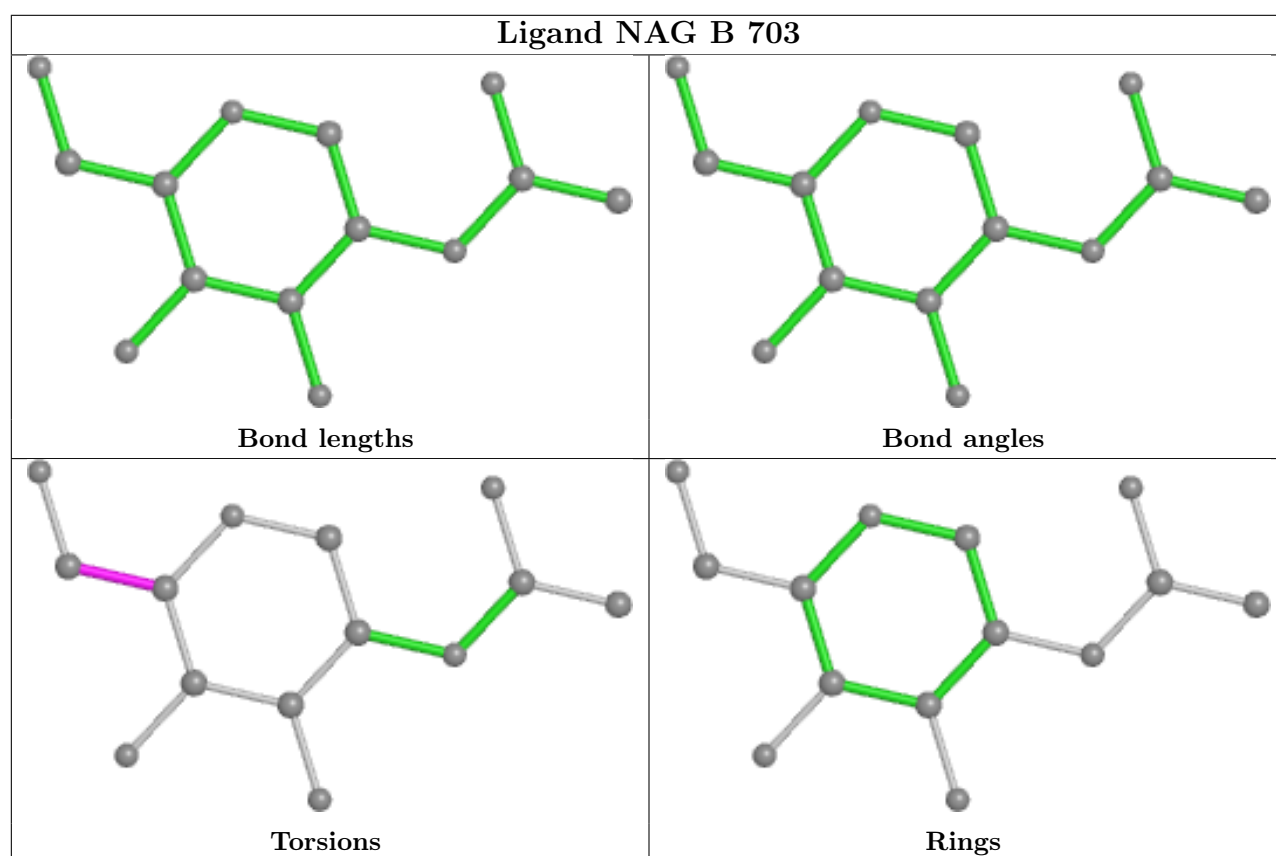
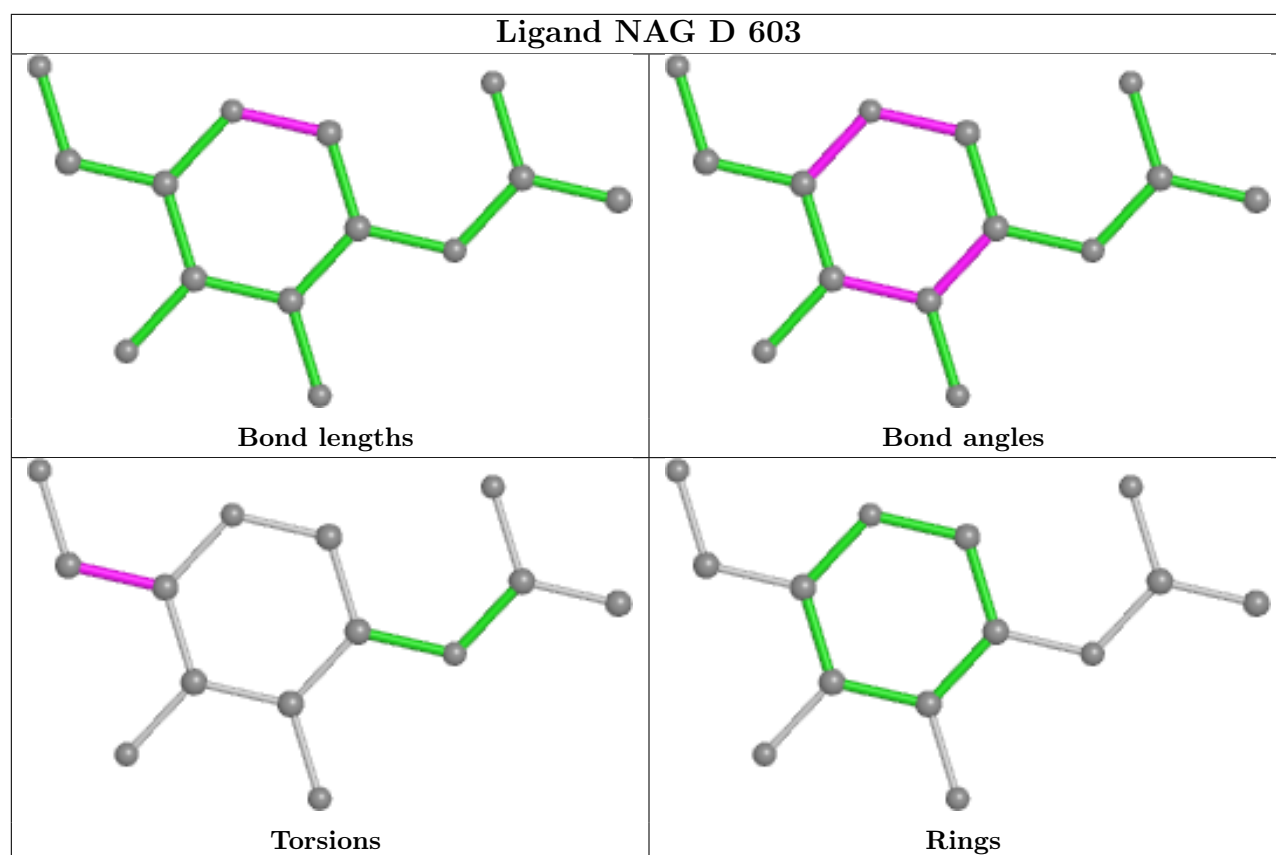
No monomer is involved in short contacts.

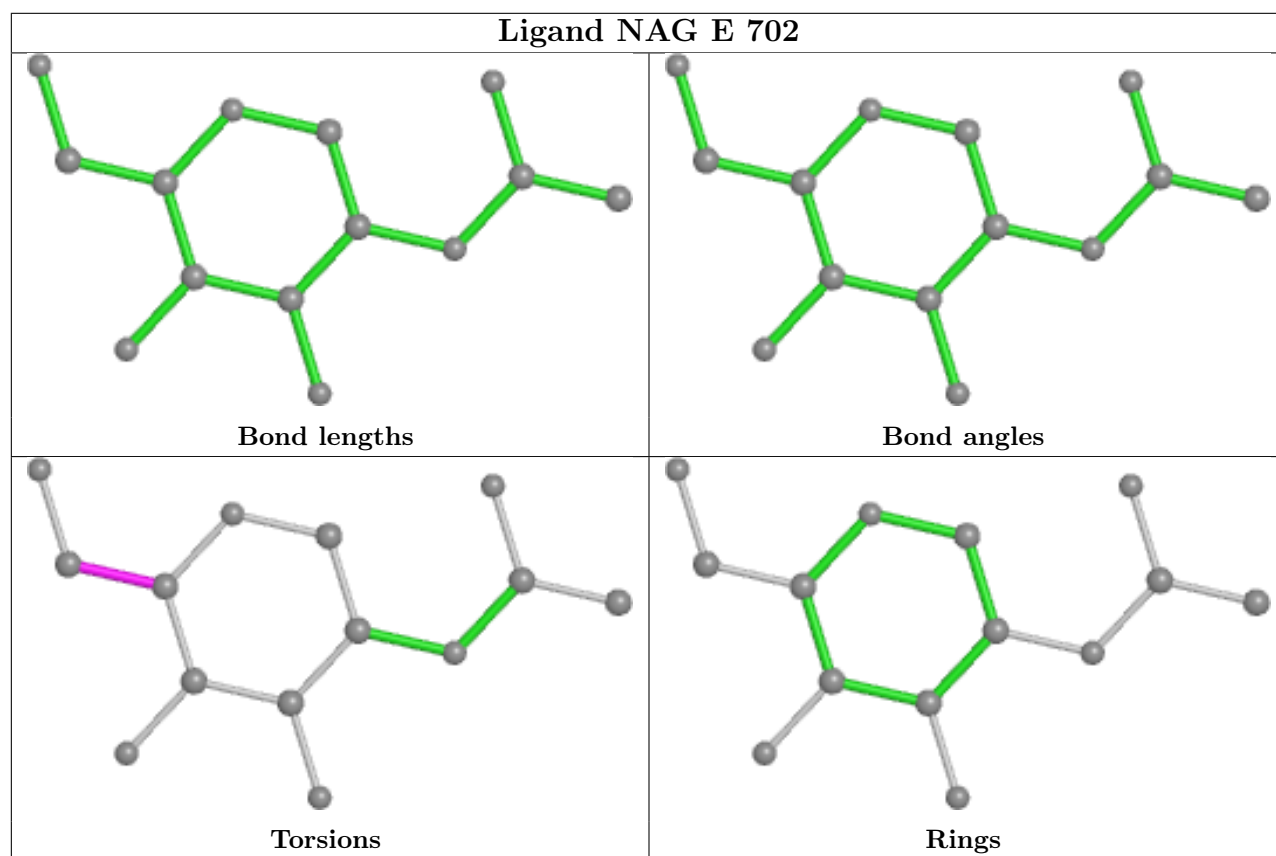
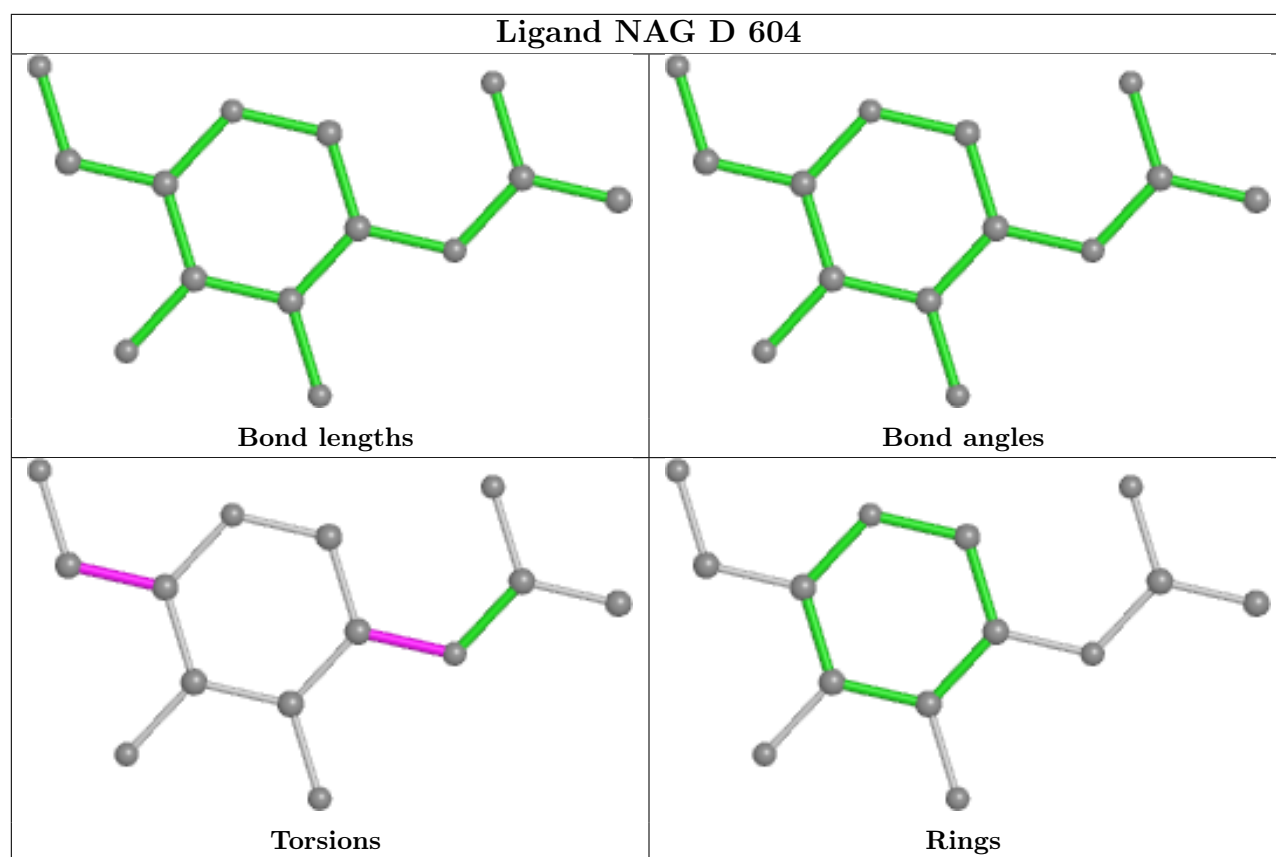
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

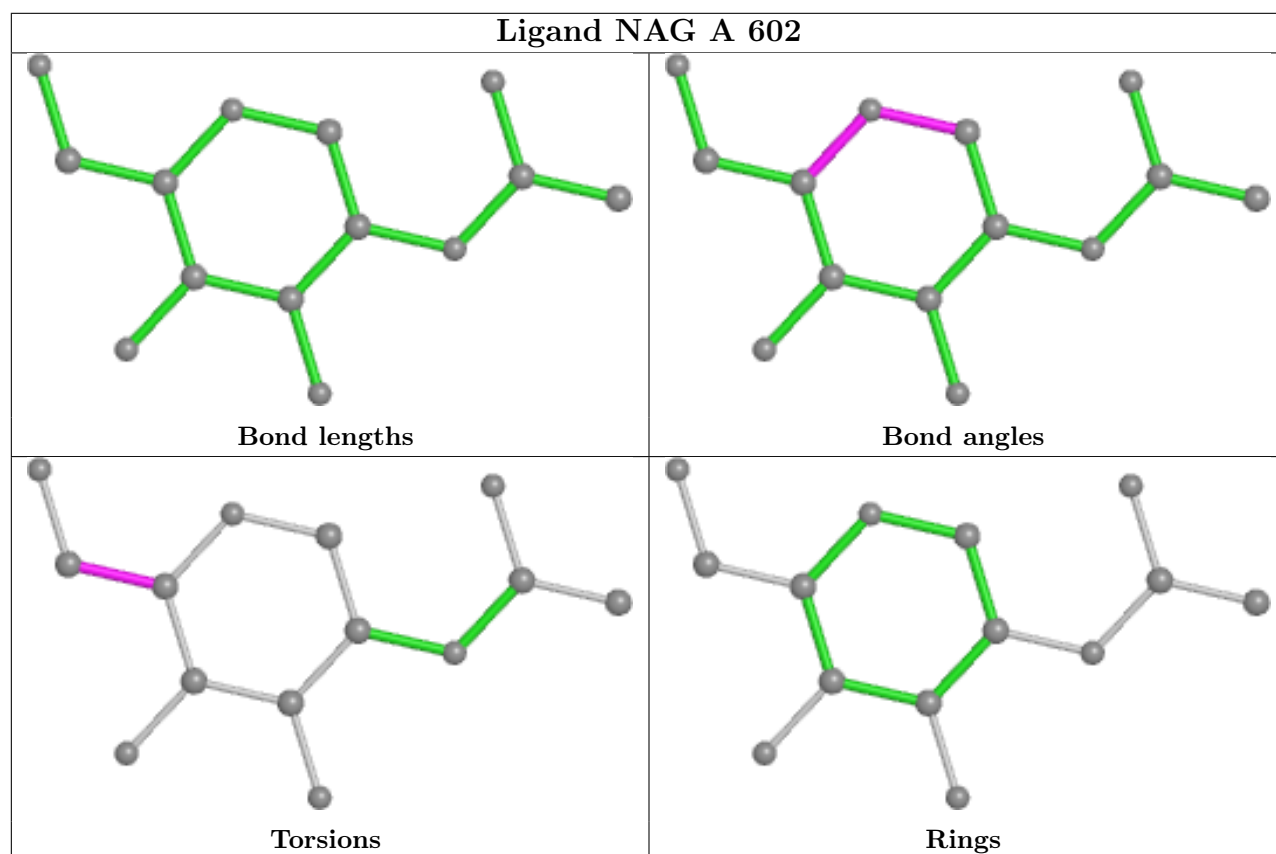
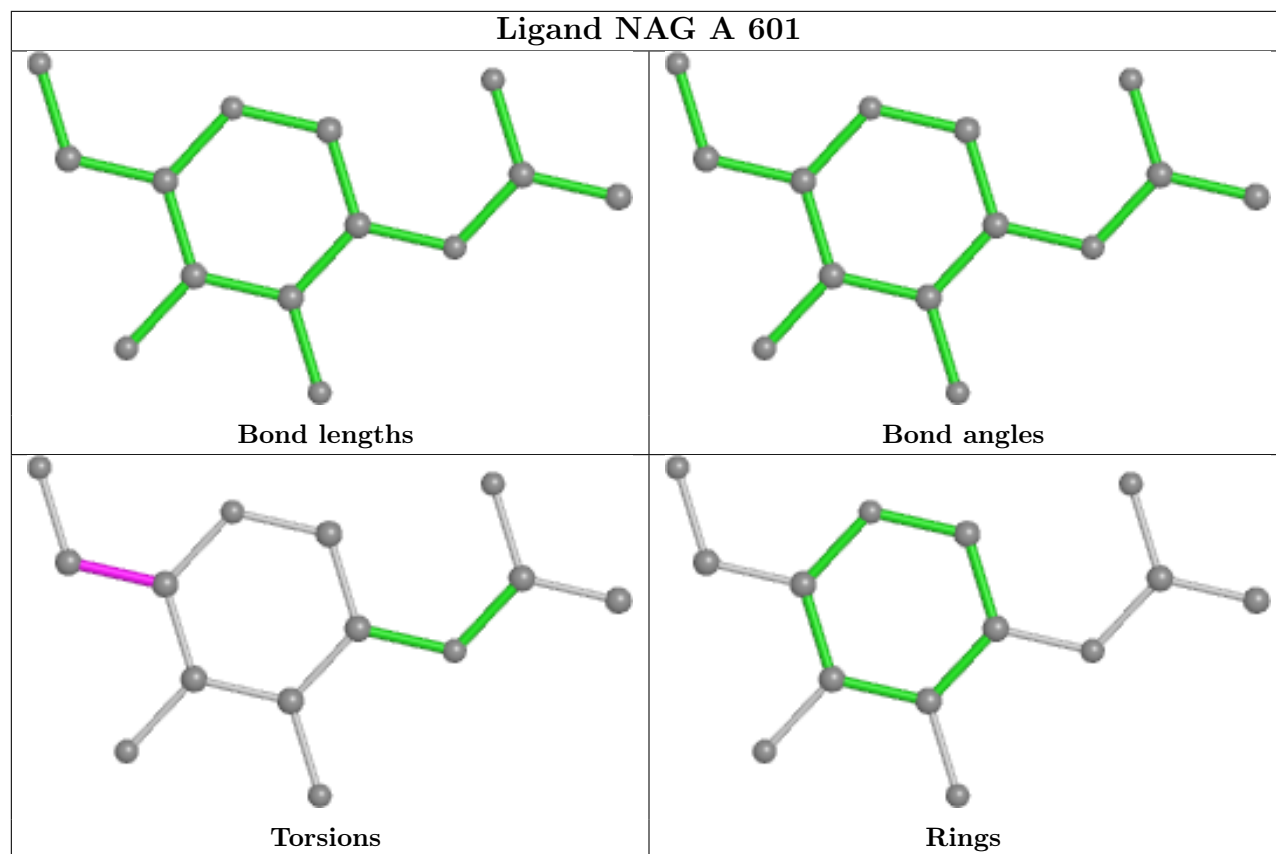
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

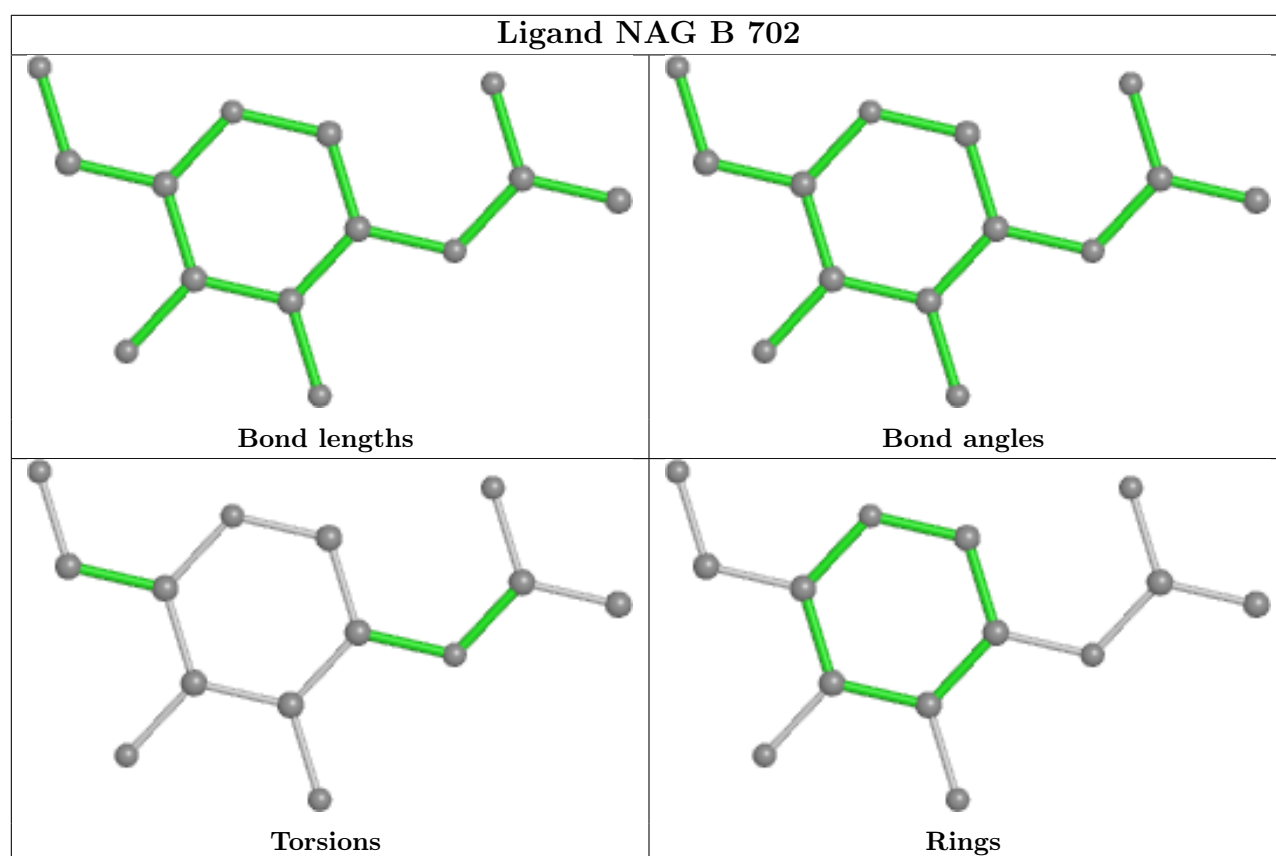
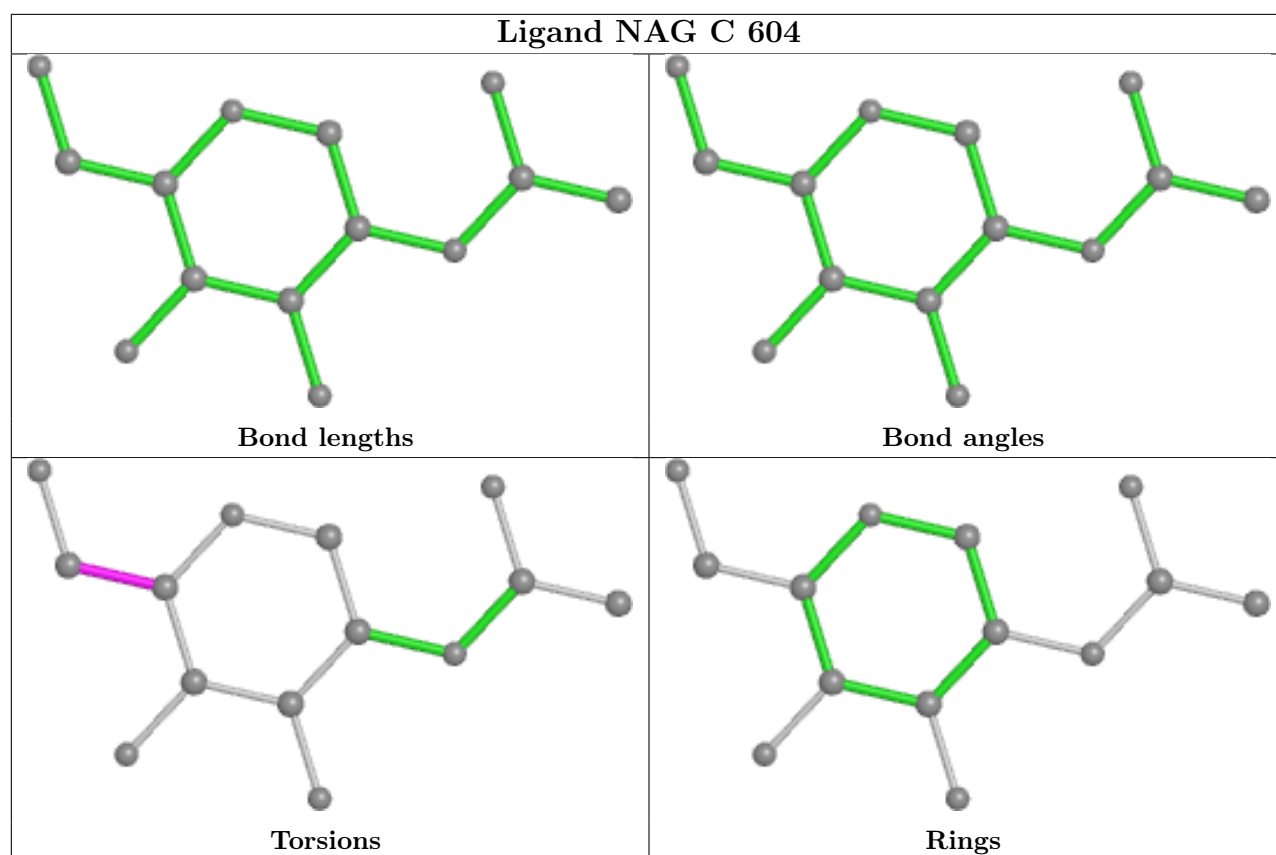


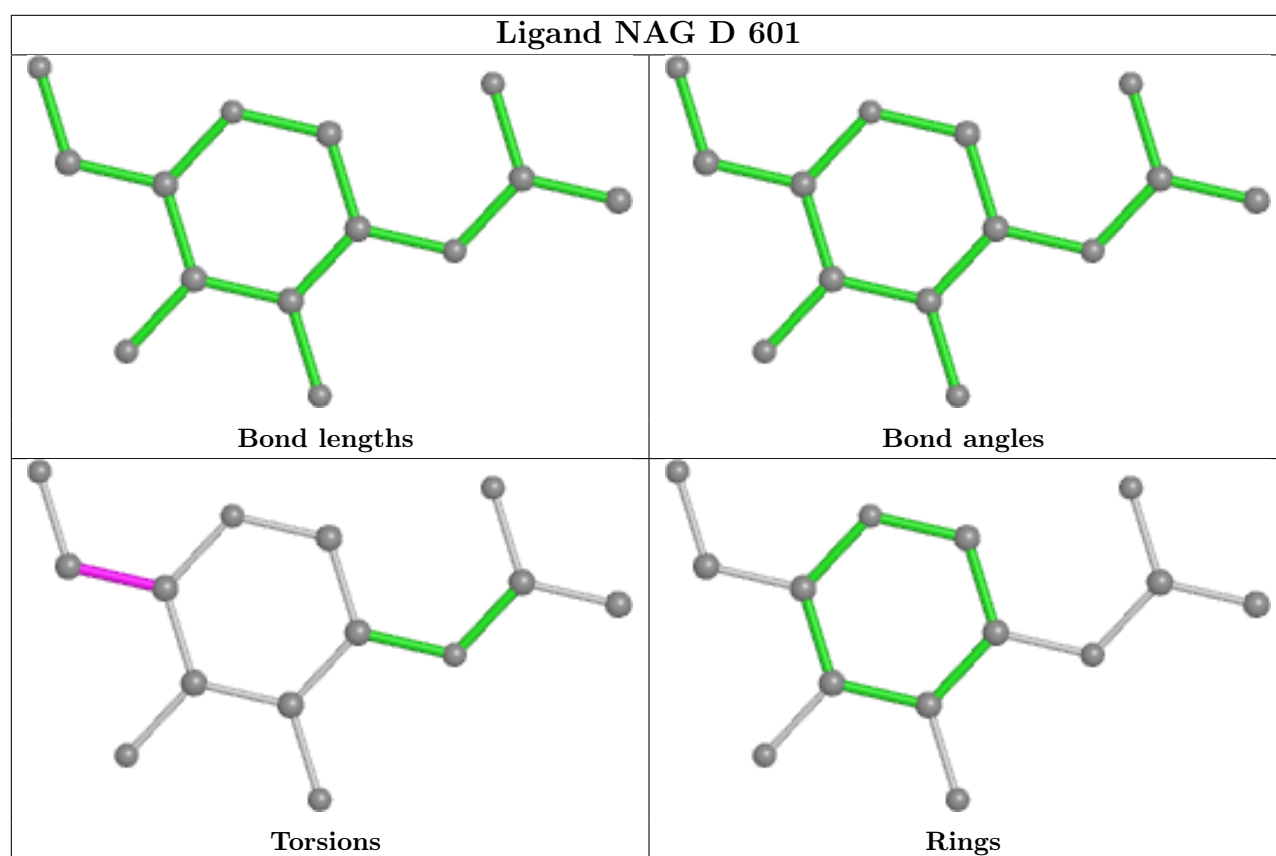
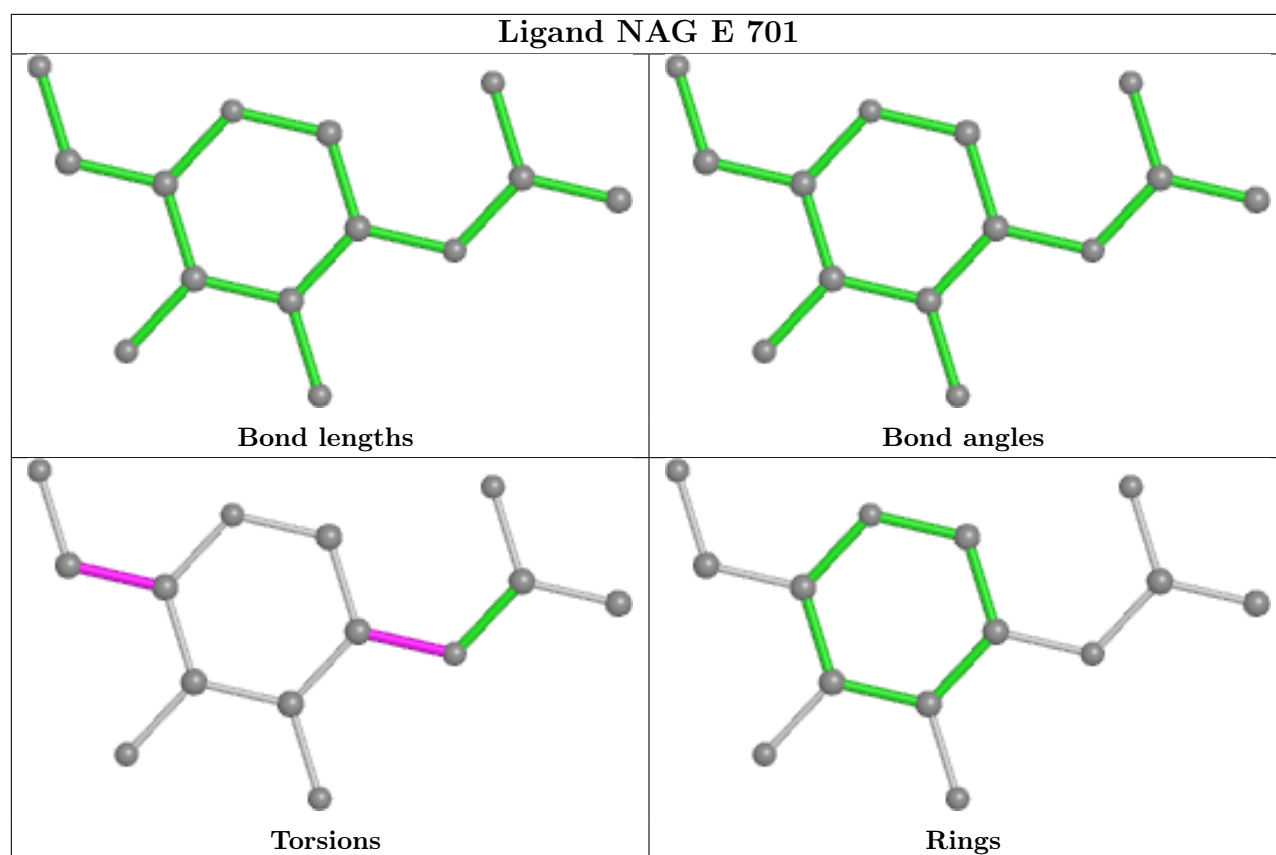


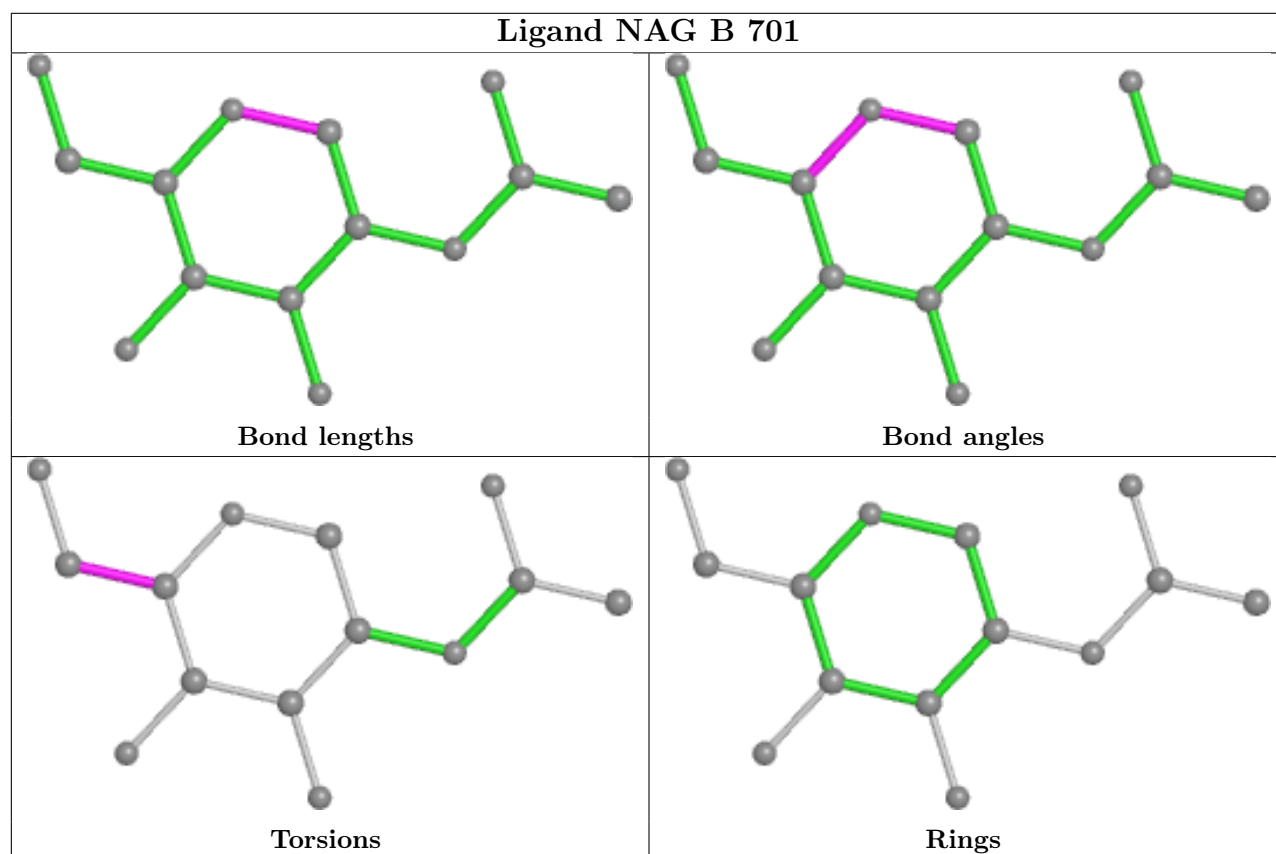
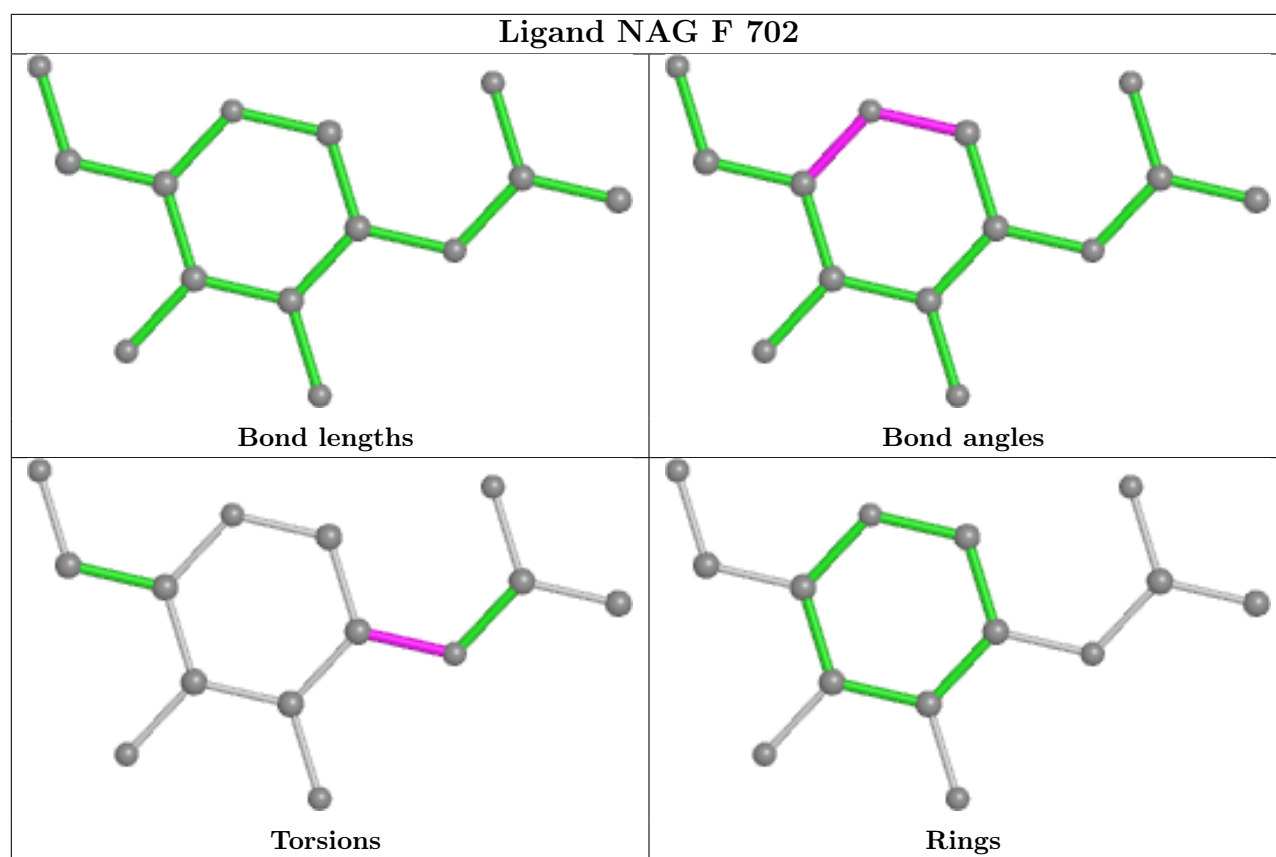


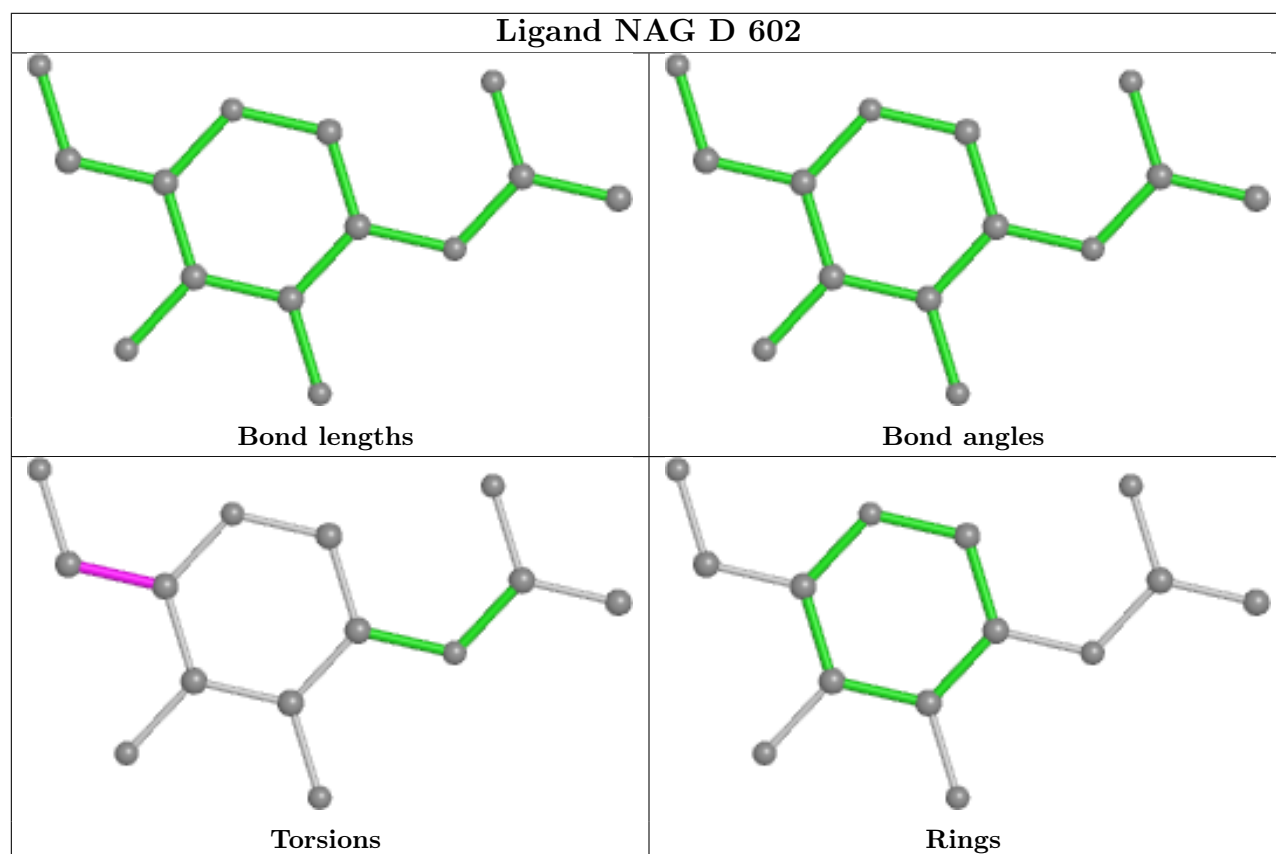
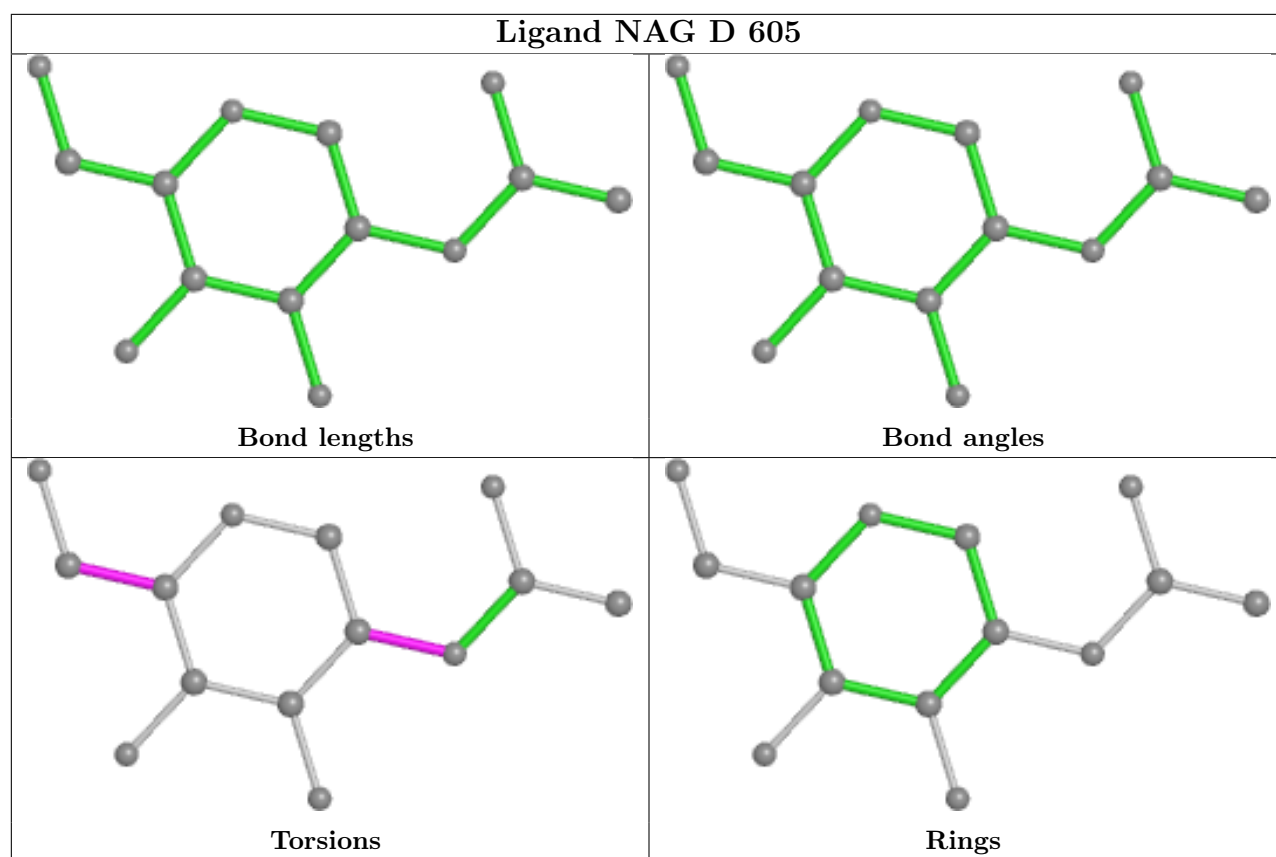


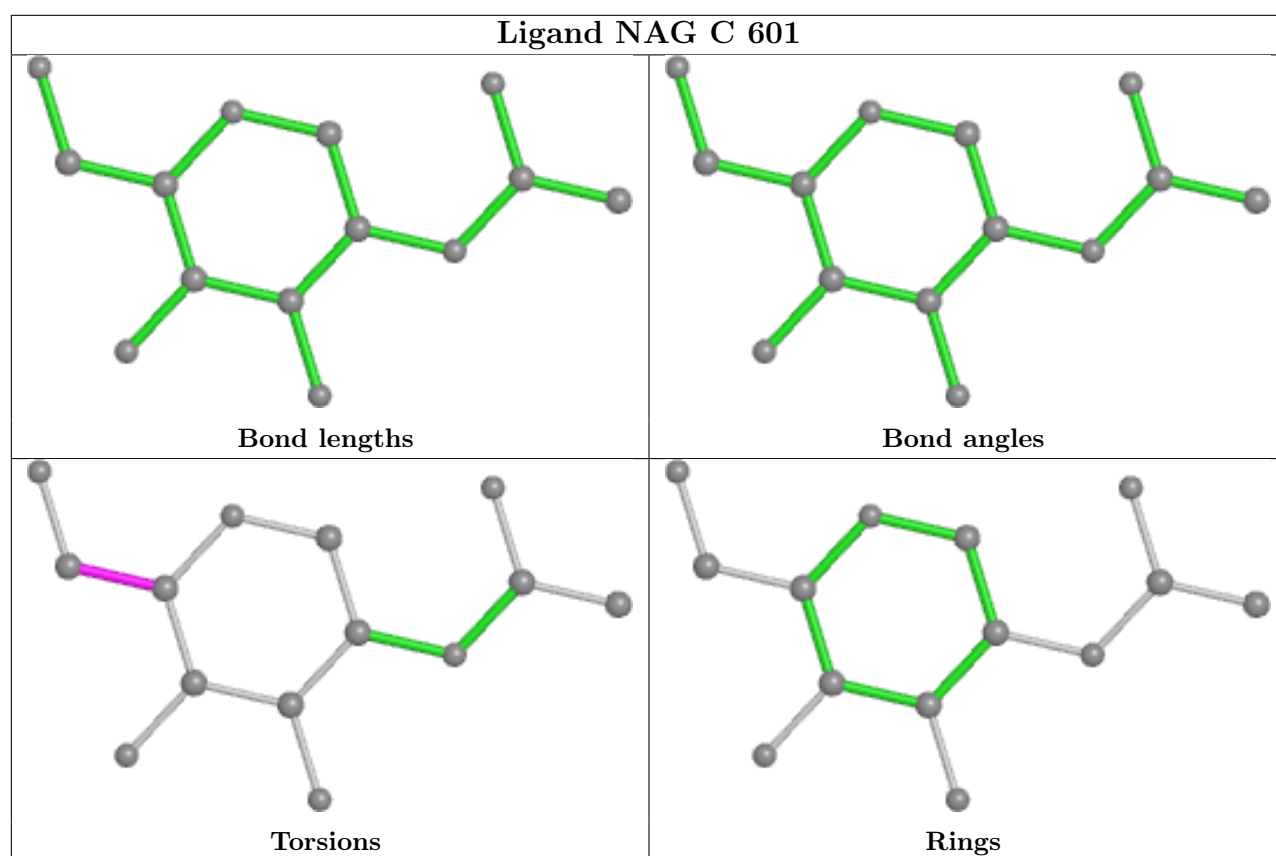
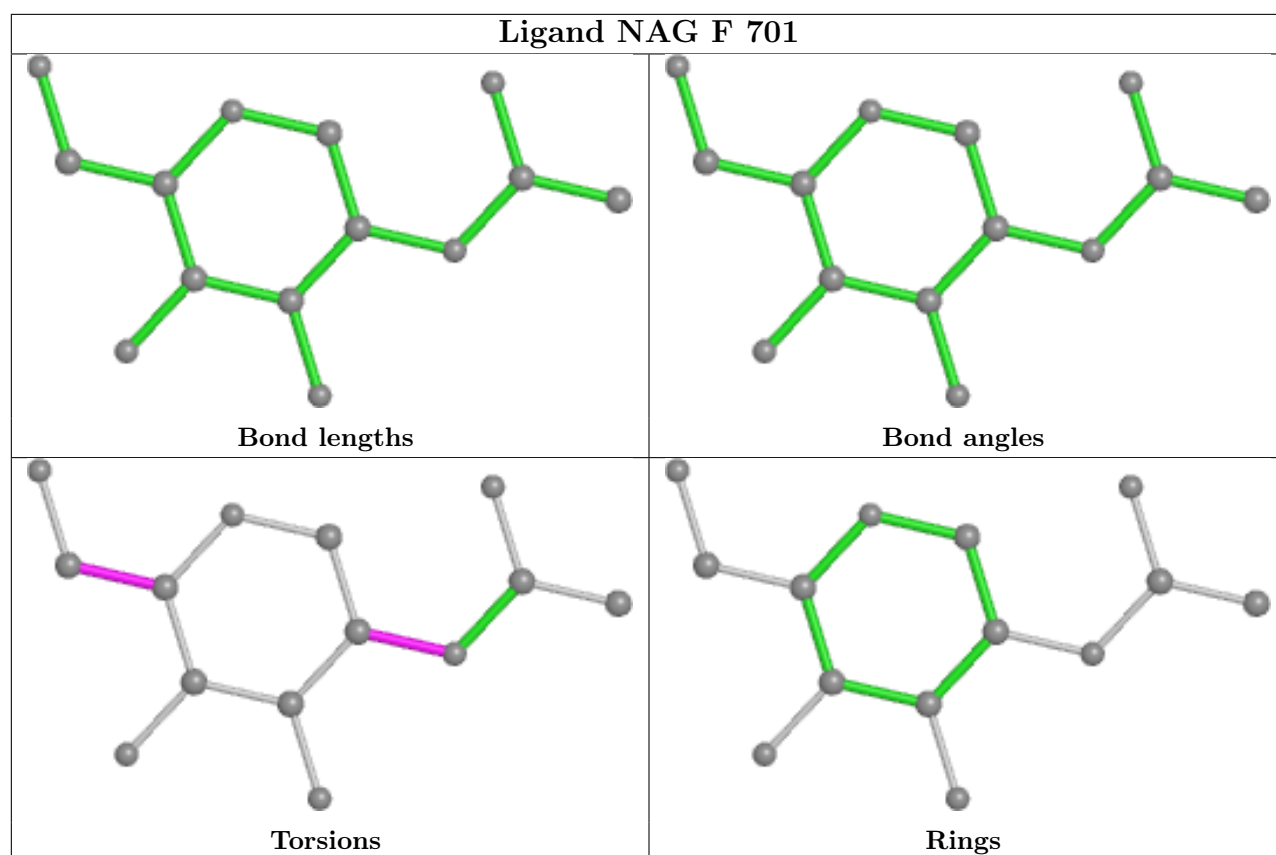


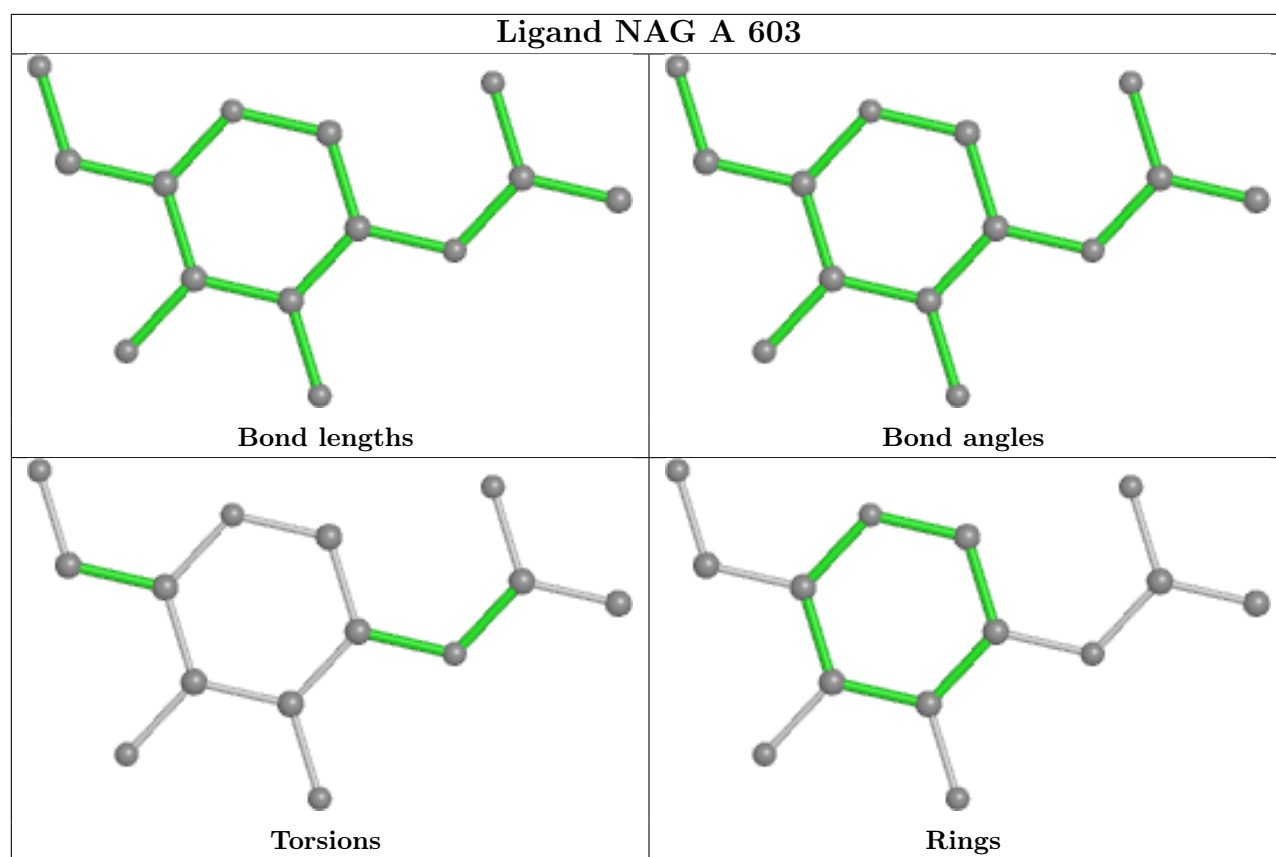












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

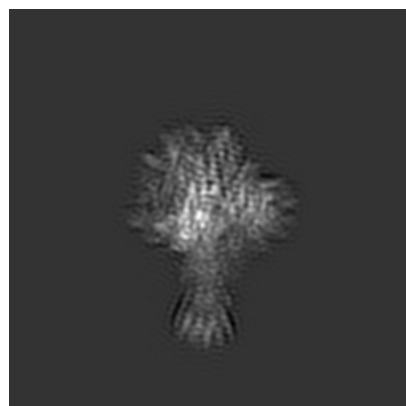
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36649. These allow visual inspection of the internal detail of the map and identification of artifacts.

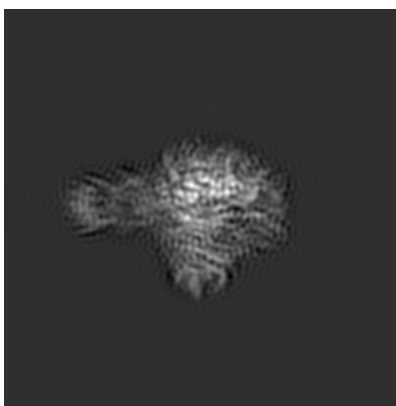
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

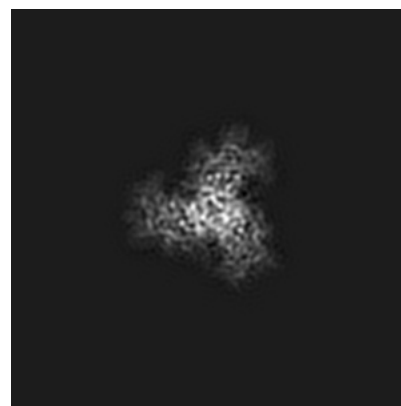
6.1.1 Primary map



X

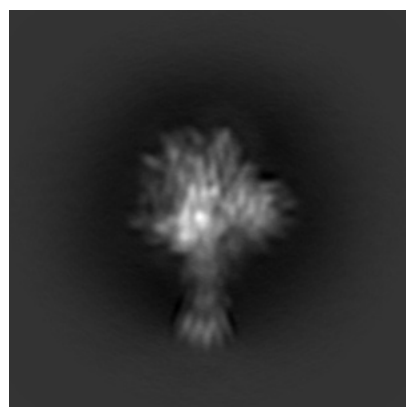


Y

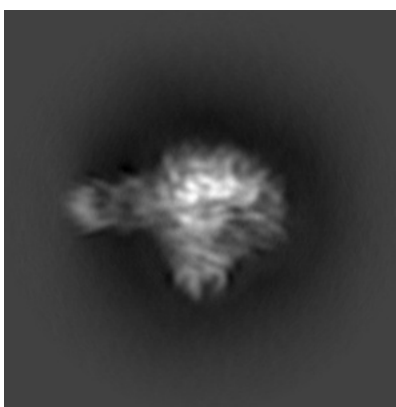


Z

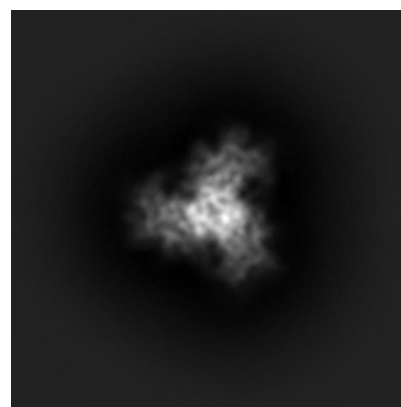
6.1.2 Raw map



X



Y

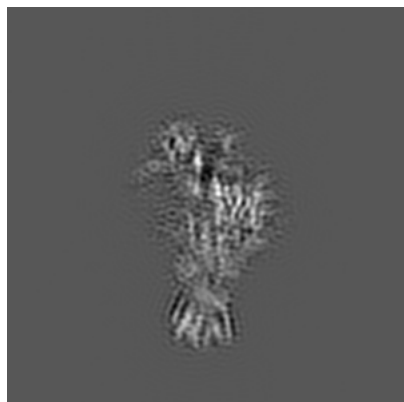


Z

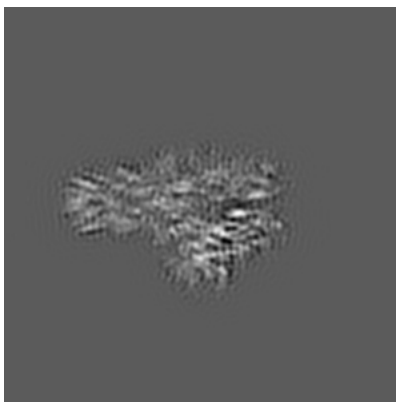
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

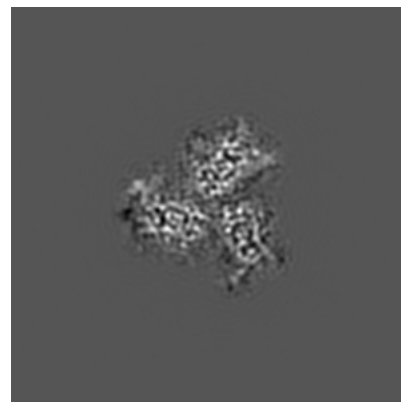
6.2.1 Primary map



X Index: 120

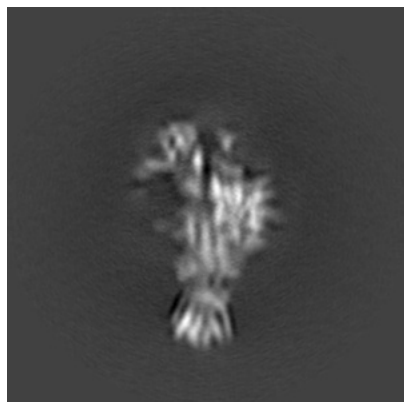


Y Index: 120

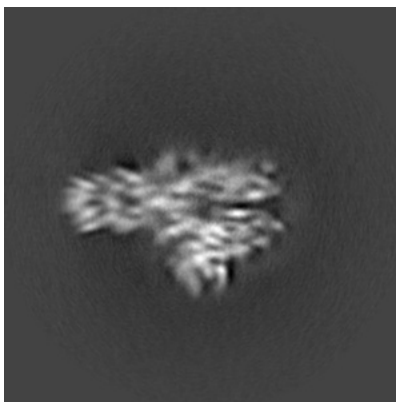


Z Index: 120

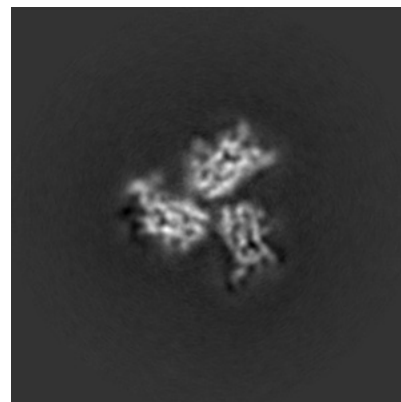
6.2.2 Raw map



X Index: 120



Y Index: 120

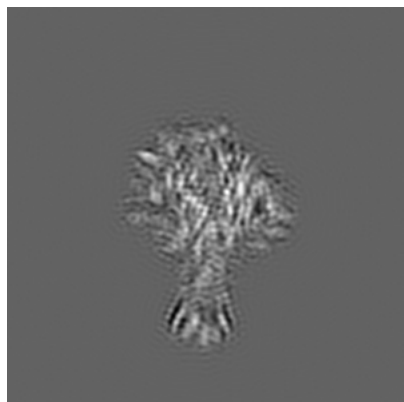


Z Index: 120

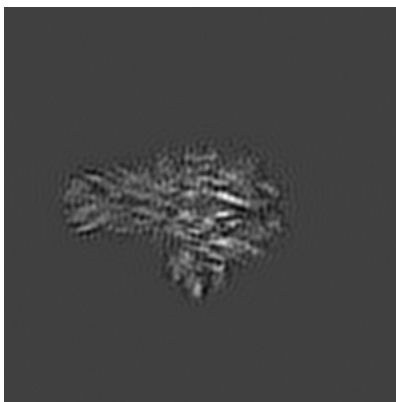
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 129

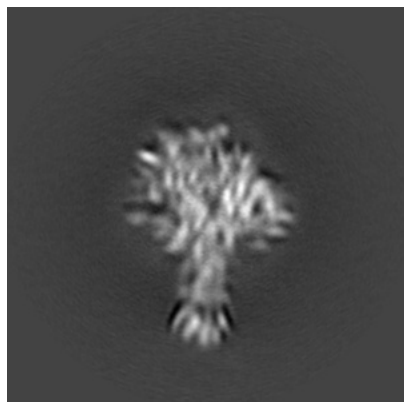


Y Index: 116

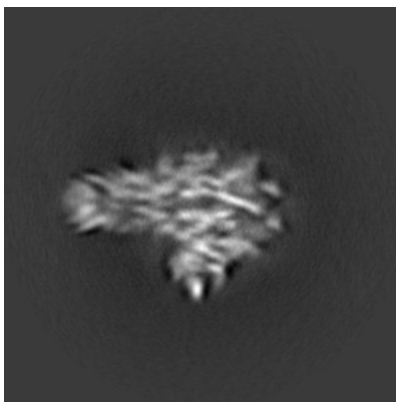


Z Index: 124

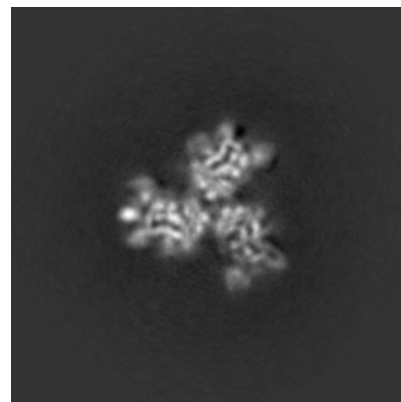
6.3.2 Raw map



X Index: 129



Y Index: 115

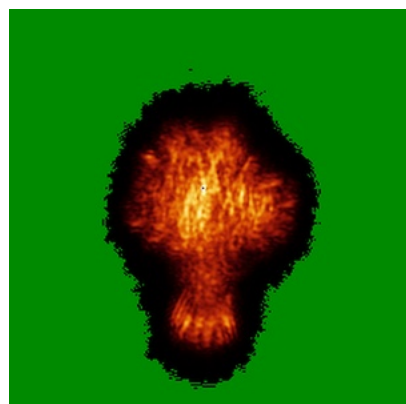


Z Index: 115

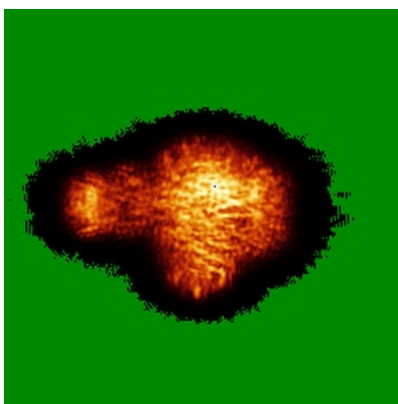
The images above show the largest variance slices of the map in three orthogonal directions.

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

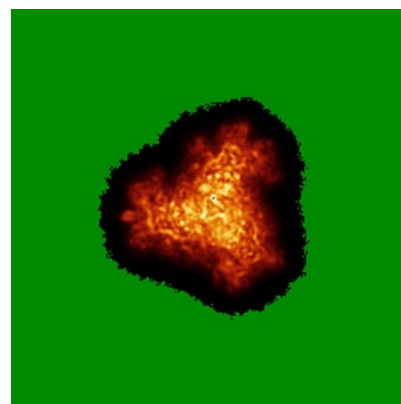
6.4.1 Primary map



X



Y

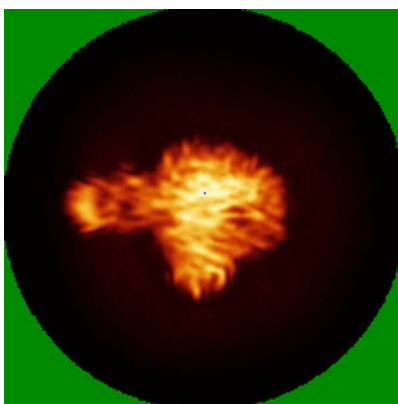


Z

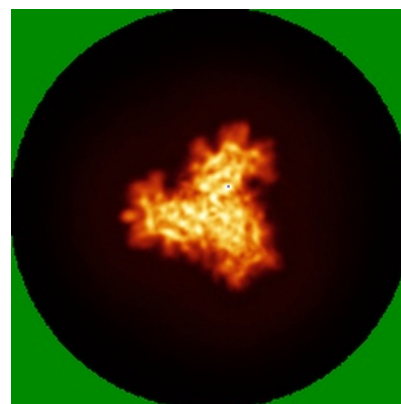
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

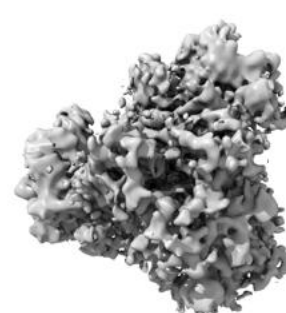
6.5.1 Primary map



X



Y



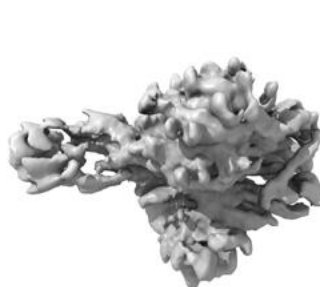
Z

The images above show the 3D surface view of the map at the recommended contour level 4.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

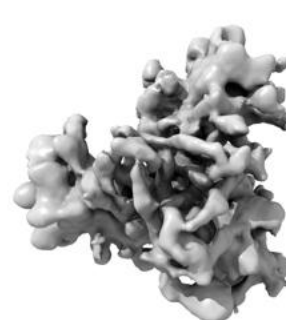
6.5.2 Raw map



X



Y



Z

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

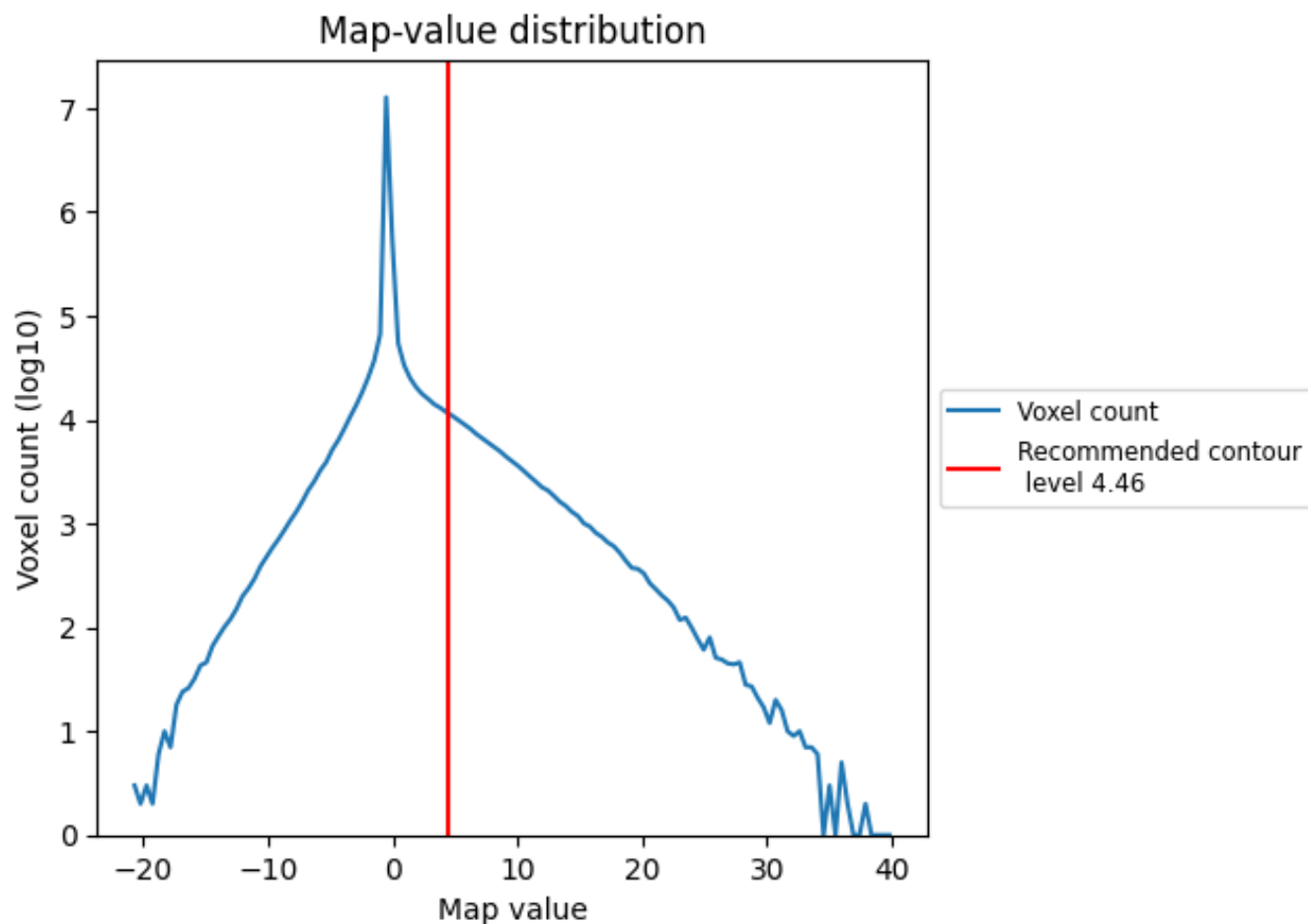
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

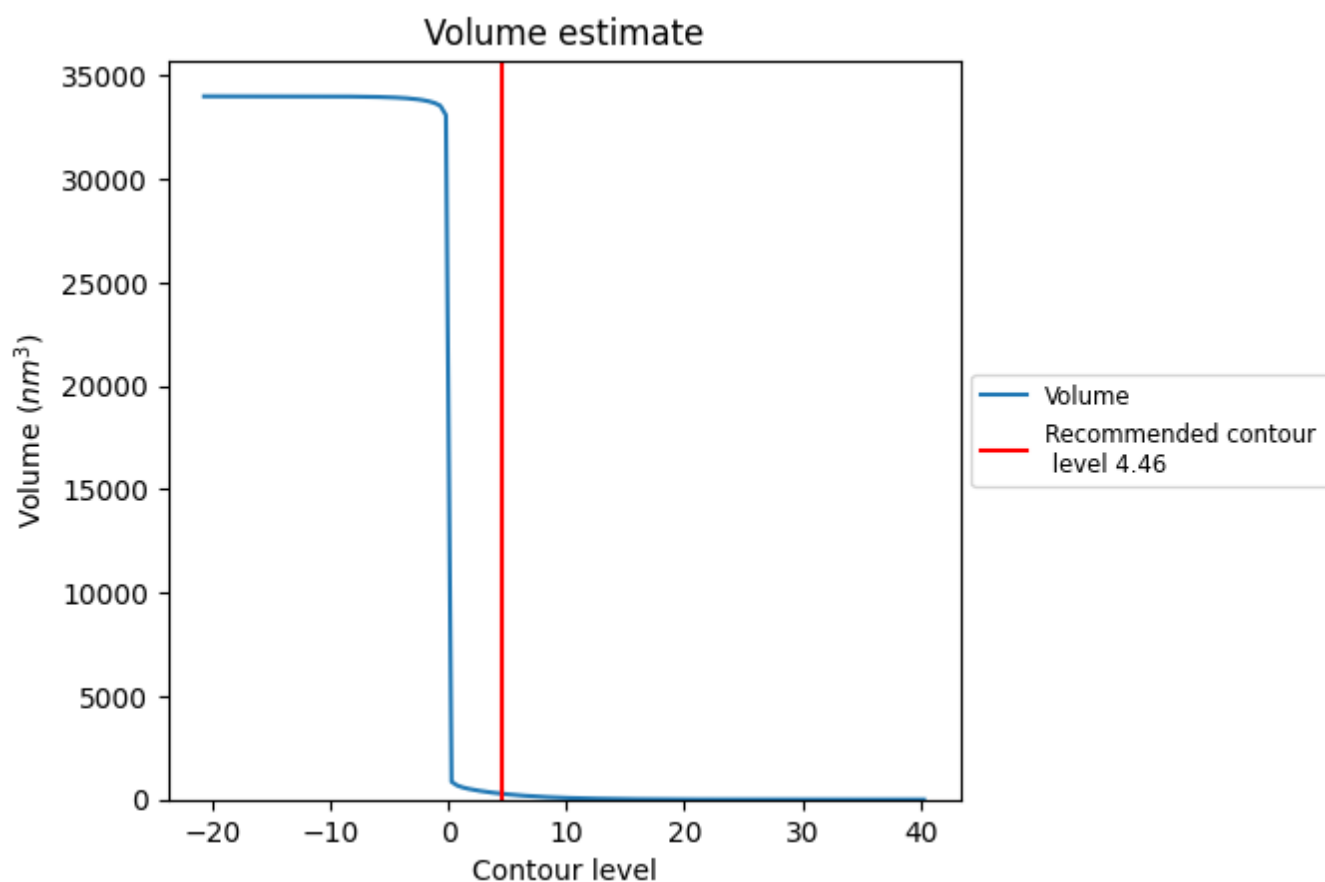
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

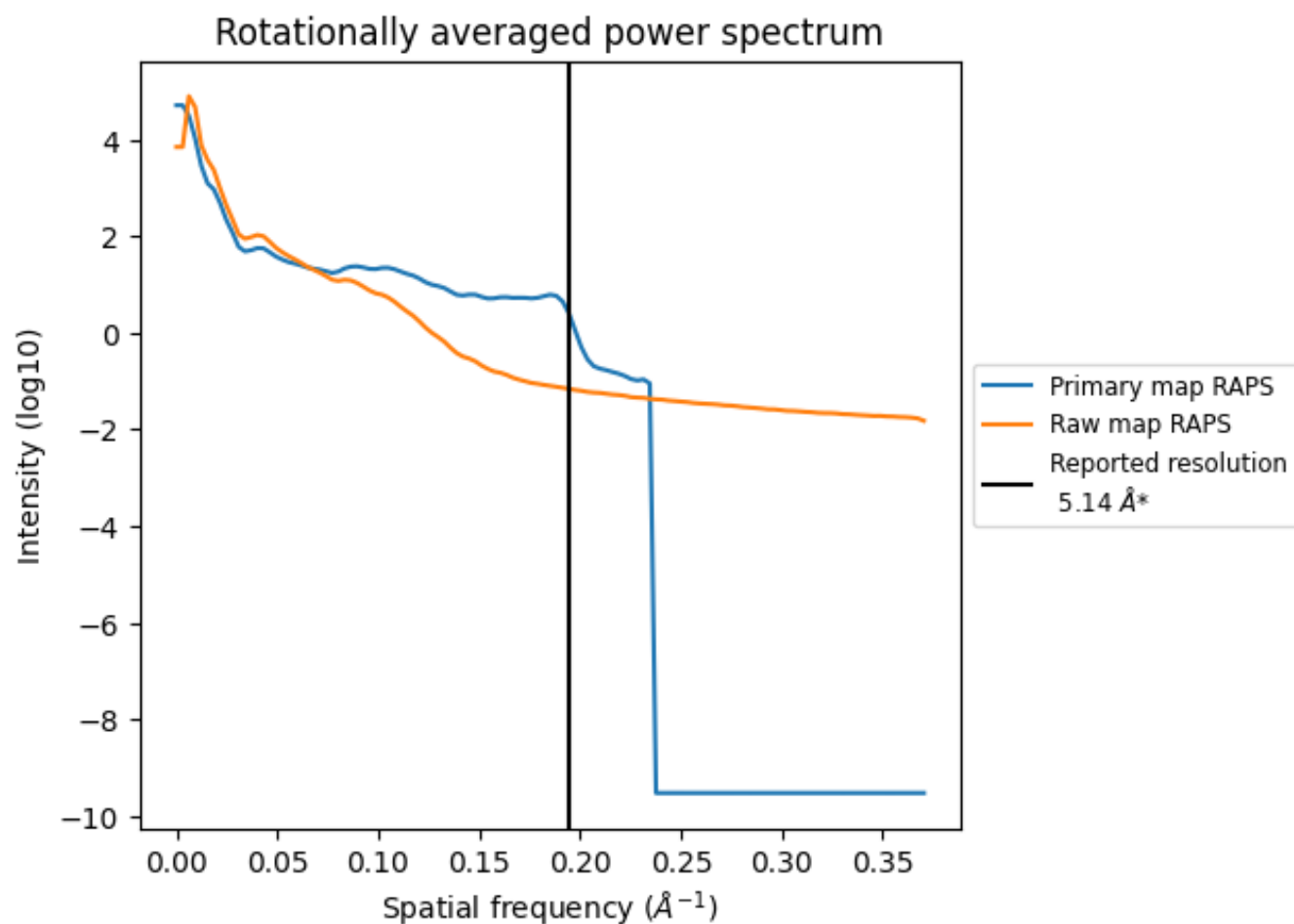
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm^3 ; this corresponds to an approximate mass of 260 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

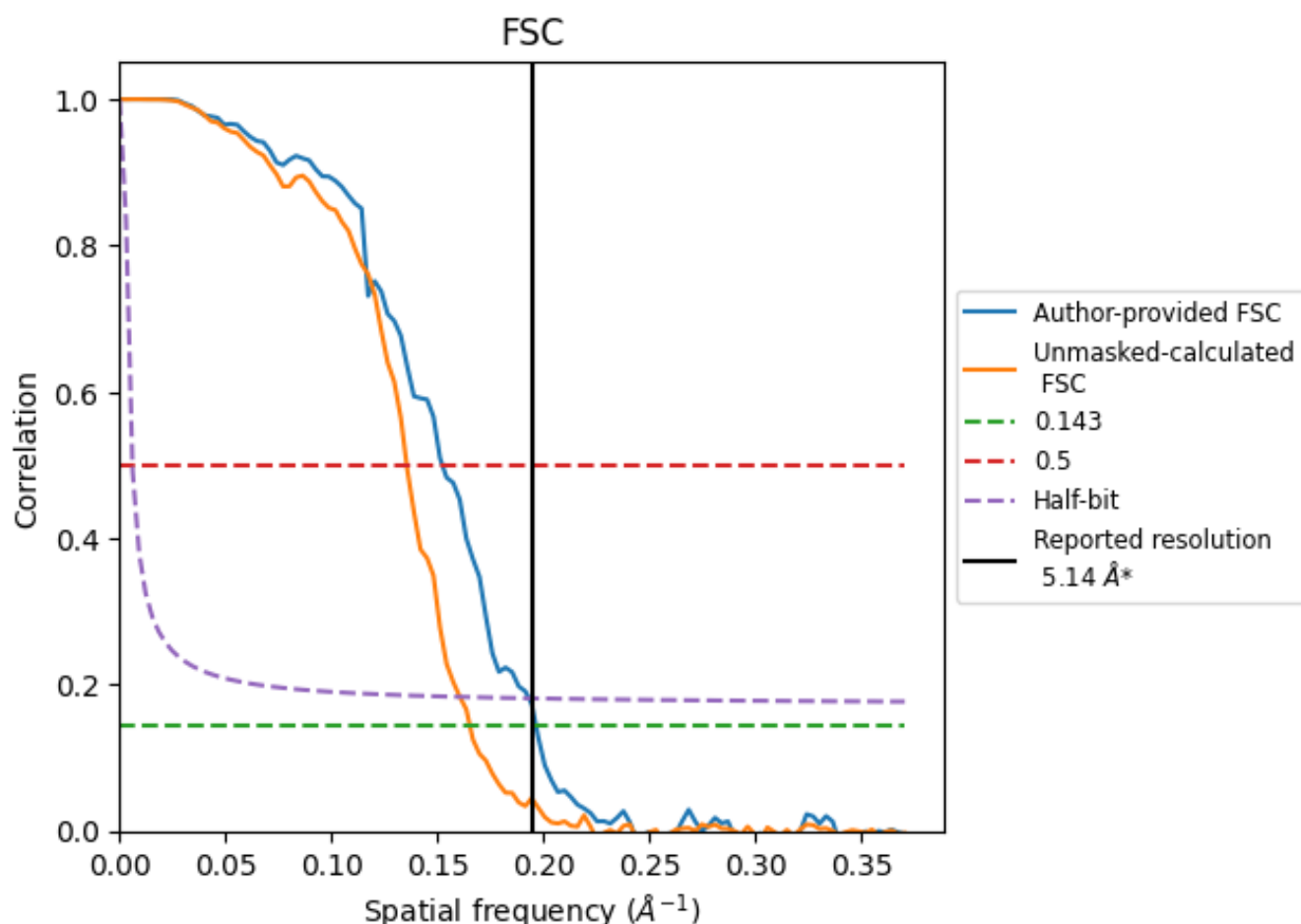


*Reported resolution corresponds to spatial frequency of 0.195 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.195 \AA^{-1}

8.2 Resolution estimates [i](#)

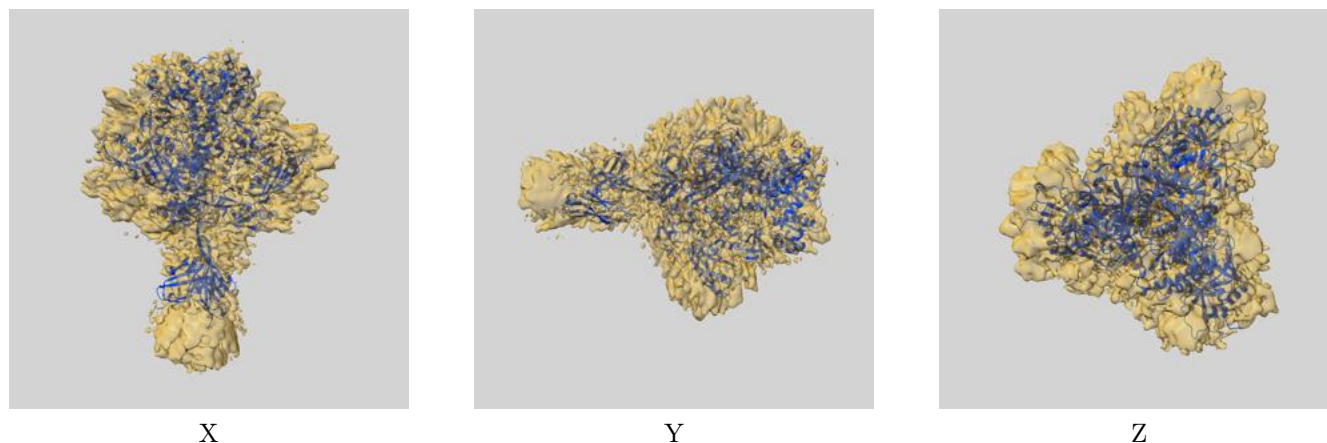
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.14	-	-
Author-provided FSC curve	5.09	6.57	5.18
Unmasked-calculated*	6.05	7.38	6.23

*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 6.05 differs from the reported value 5.14 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36649 and PDB model 8JTM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



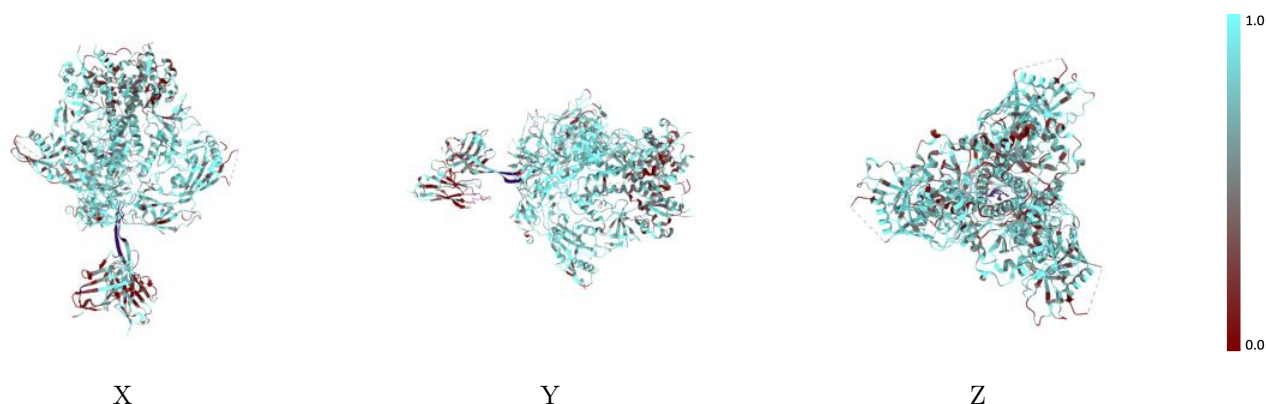
The images above show the 3D surface view of the map at the recommended contour level 4.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



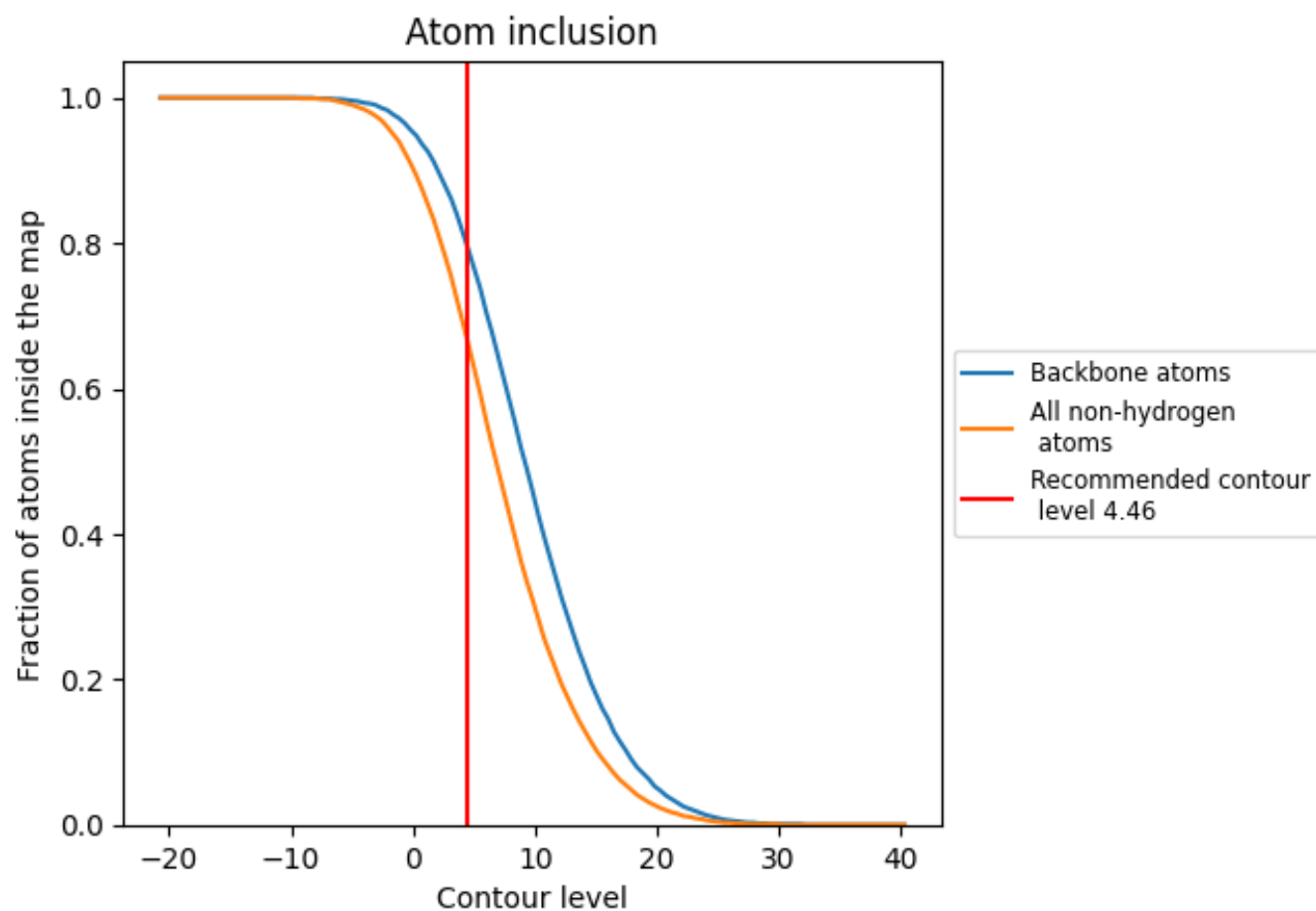
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.46).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 67% 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 (4.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.1660
0	 0.5710	 0.3270
1	 0.0000	 0.1630
A	 0.7050	 0.1830
B	 0.6780	 0.1730
C	 0.7610	 0.2030
D	 0.7400	 0.1840
E	 0.5770	 0.1620
F	 0.5870	 0.1710
J	 0.5390	 0.0980
N	 0.4540	 0.0760
O	 0.3210	 0.0660
P	 0.0710	 0.0320
Q	 0.7500	 0.1920
R	 0.7140	 0.1400
S	 0.5380	 0.0870
T	 0.5690	 0.0800
V	 0.1070	 -0.1920
W	 0.3210	 0.0130
X	 0.1030	 0.0180
Y	 0.3930	 -0.0130
Z	 0.6790	 0.1710
a	 0.6430	 0.2140
b	 0.0000	 -0.0500
c	 0.6070	 0.1800
d	 0.7440	 0.1510
e	 0.7500	 0.2550
f	 0.7710	 0.2120
h	 0.3570	 0.0530
i	 0.6430	 0.1800
j	 0.4290	 -0.0050
k	 0.1800	 -0.0310
l	 0.8210	 0.1640
m	 0.3210	 -0.0050
n	 0.7140	 0.1930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o	 0.0000	 -0.0940
p	 0.3210	 0.1480
q	 0.6810	 0.0920
r	 0.5710	 0.2650
s	 0.7830	 0.1770
u	 0.3210	 -0.0860
v	 0.5710	 0.1860
w	 0.0710	 -0.1570
x	 0.2950	 -0.0580
y	 0.6150	 0.1360
z	 0.7140	 0.0410