



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:07 AM UTC

PDB ID : 6MYX / pdb_00006myx
EMDB ID : EMD-9294
Title : Germline VRC01 antibody recognition of a modified clade C HIV-1 envelope trimer, 3 Fabs bound, sharpened map
Authors : Borst, A.J.; Weidle, C.E.; Gray, M.D.; Frenz, B.; Snijder, J.; Joyce, M.G.; Georgiev, I.S.; Stewart-Jones, G.B.E.; Kwong, P.D.; McGuire, A.T.; DiMaio, F.; Stamatatos, L.; Pancera, M.; Veesler, D.
Deposited on : 2018-11-02
Resolution : 3.80 Å(reported)

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

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

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:

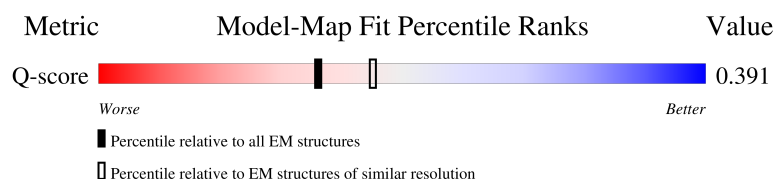
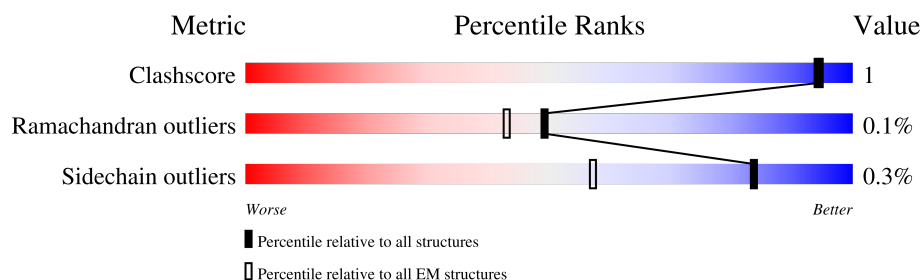
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



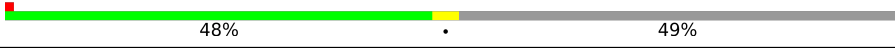
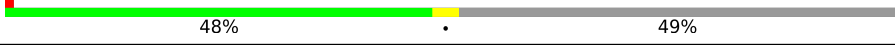
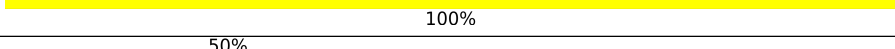
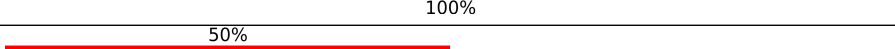
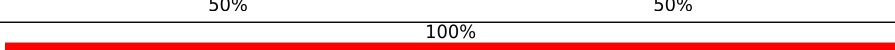
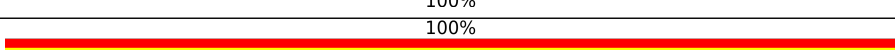
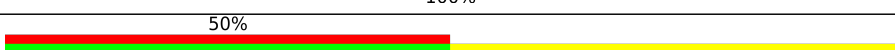
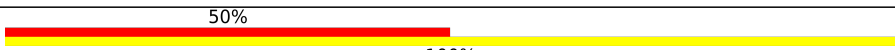
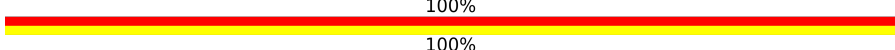
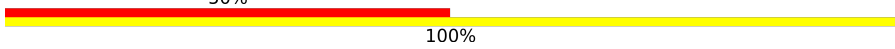
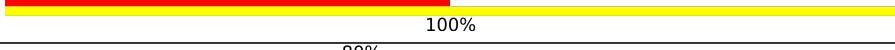
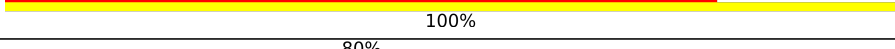
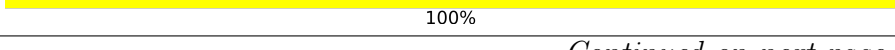
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	626	
1	B	626	
1	E	626	
2	C	229	

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Mol	Chain	Length	Quality of chain
2	F	229	
2	L	229	
3	D	233	
3	G	233	
3	H	233	
4	I	2	
4	J	2	
4	S	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	g	2	
4	i	2	
4	j	2	
4	k	2	
4	l	2	
4	m	2	
4	u	2	
4	w	2	
4	x	2	
4	y	2	
5	K	5	
5	Z	5	

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Mol	Chain	Length	Quality of chain
5	n	5	80% 100%
6	M	6	50% 100%
6	a	6	50% 100%
6	o	6	50% 100%
7	N	3	33% 33% 67%
7	P	3	67% 33% 67%
7	Q	3	67% 100%
7	b	3	67% 33% 67%
7	d	3	67% 33% 67%
7	e	3	67% 100%
7	p	3	33% 33% 67%
7	r	3	67% 33% 67%
7	s	3	67% 100%
8	O	7	43% 100%
8	c	7	43% 100%
8	q	7	43% 100%
9	R	4	50% 100%
9	f	4	50% 100%
9	t	4	50% 100%
10	T	5	60% 100%
10	h	5	60% 100%
10	v	5	60% 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20139 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 426c DS-SOSIP D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	550	Total	C	N	O	S	0	0
			4338	2736	757	811	34		
1	B	550	Total	C	N	O	S	0	0
			4338	2736	757	811	34		
1	E	550	Total	C	N	O	S	0	0
			4338	2736	757	811	34		

- Molecule 2 is a protein called VRC01GL light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	100	Total	C	N	O	S	0	0
			767	485	127	153	2		
2	C	100	Total	C	N	O	S	0	0
			767	485	127	153	2		
2	F	100	Total	C	N	O	S	0	0
			767	485	127	153	2		

- Molecule 3 is a protein called VRC01GL heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	119	Total	C	N	O	S	0	0
			940	591	165	177	7		
3	D	119	Total	C	N	O	S	0	0
			940	591	165	177	7		
3	G	119	Total	C	N	O	S	0	0
			940	591	165	177	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	220	HIS	-	expression tag	UNP S6C4S0
H	221	HIS	-	expression tag	UNP S6C4S0
H	222	HIS	-	expression tag	UNP S6C4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	223	HIS	-	expression tag	UNP S6C4S0
H	224	HIS	-	expression tag	UNP S6C4S0
H	225	HIS	-	expression tag	UNP S6C4S0
D	220	HIS	-	expression tag	UNP S6C4S0
D	221	HIS	-	expression tag	UNP S6C4S0
D	222	HIS	-	expression tag	UNP S6C4S0
D	223	HIS	-	expression tag	UNP S6C4S0
D	224	HIS	-	expression tag	UNP S6C4S0
D	225	HIS	-	expression tag	UNP S6C4S0
G	220	HIS	-	expression tag	UNP S6C4S0
G	221	HIS	-	expression tag	UNP S6C4S0
G	222	HIS	-	expression tag	UNP S6C4S0
G	223	HIS	-	expression tag	UNP S6C4S0
G	224	HIS	-	expression tag	UNP S6C4S0
G	225	HIS	-	expression tag	UNP S6C4S0

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



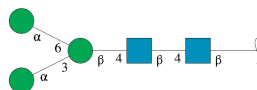
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		

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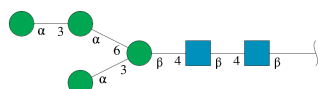
Mol	Chain	Residues	Atoms				AltConf	Trace
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	x	2	Total	C	N	O	0	0
			28	16	2	10		
4	y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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.



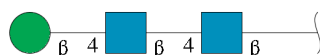
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	5	Total	C	N	O	0	0
			61	34	2	25		
5	Z	5	Total	C	N	O	0	0
			61	34	2	25		
5	n	5	Total	C	N	O	0	0
			61	34	2	25		

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



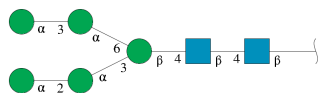
Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	6	Total	C	N	O	0	0
			72	40	2	30		
6	a	6	Total	C	N	O	0	0
			72	40	2	30		
6	o	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 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
7	N	3	Total	C	N	O	0	0
			39	22	2	15		
7	P	3	Total	C	N	O	0	0
			39	22	2	15		
7	Q	3	Total	C	N	O	0	0
			39	22	2	15		
7	b	3	Total	C	N	O	0	0
			39	22	2	15		
7	d	3	Total	C	N	O	0	0
			39	22	2	15		
7	e	3	Total	C	N	O	0	0
			39	22	2	15		
7	p	3	Total	C	N	O	0	0
			39	22	2	15		
7	r	3	Total	C	N	O	0	0
			39	22	2	15		
7	s	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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.



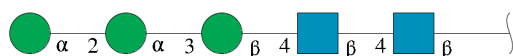
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	7	Total	C	N	O	0	0
			83	46	2	35		
8	c	7	Total	C	N	O	0	0
			83	46	2	35		
8	q	7	Total	C	N	O	0	0
			83	46	2	35		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	4	Total	C	N	O	0	0
			50	28	2	20		
9	f	4	Total	C	N	O	0	0
			50	28	2	20		
9	t	4	Total	C	N	O	0	0
			50	28	2	20		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
10	T	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	v	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	B	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	

Frequency	Percentage
Daily	81%
Weekly	6%
Monthly	12%



Frequency	Percentage
Daily	41%
Weekly	56%
Monthly	3%



Response	Percentage
Doing a good job	41%
Not doing a good job	56%



Frequency	Percentage
Often	41%
Not often	56%



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

Chain J: 



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

Chain S: 



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

Chain U: 

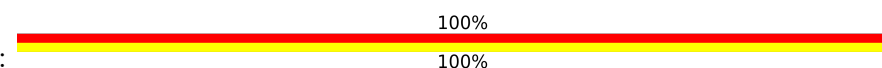


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain W: 



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

Chain X: 



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



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



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



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



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



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



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



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



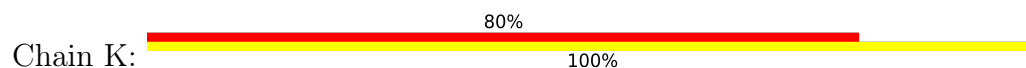
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



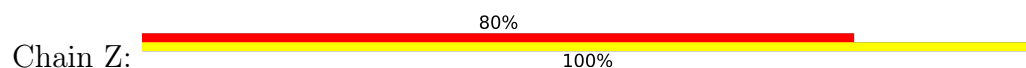
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



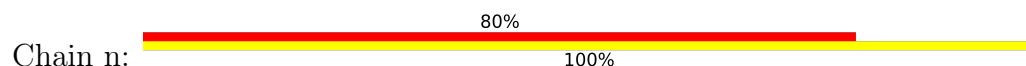
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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 5: 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 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

ido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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

Chain e: 



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

Chain p: 



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

Chain r: 

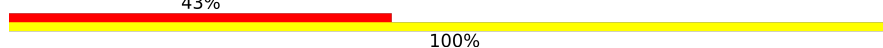


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 

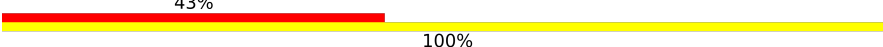


- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 



- Molecule 8: 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

Chain c: 



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



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



- Molecule 9: alpha-D-mannopyranose-(1-3)-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)-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)-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)-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	134443	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 ($e^-/\text{\AA}^2$)	1	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	0.322	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/4423	0.89	40/6004 (0.7%)
1	B	0.68	0/4423	0.89	40/6004 (0.7%)
1	E	0.68	0/4423	0.89	40/6004 (0.7%)
2	C	0.64	0/785	0.94	11/1067 (1.0%)
2	F	0.64	0/785	0.93	11/1067 (1.0%)
2	L	0.64	0/785	0.94	11/1067 (1.0%)
3	D	0.65	0/958	0.75	4/1300 (0.3%)
3	G	0.64	0/958	0.75	4/1300 (0.3%)
3	H	0.64	0/958	0.75	4/1300 (0.3%)
All	All	0.67	0/18498	0.87	165/25113 (0.7%)

There are no bond length outliers.

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ALA	CA-C-N	9.37	126.41	119.66
1	B	436	ALA	C-N-CA	9.37	126.41	119.66
1	E	436	ALA	CA-C-N	9.36	126.40	119.66
1	E	436	ALA	C-N-CA	9.36	126.40	119.66
1	A	436	ALA	CA-C-N	9.35	126.39	119.66
1	A	436	ALA	C-N-CA	9.35	126.39	119.66
1	E	353	PHE	CA-C-N	8.48	128.13	119.56
1	E	353	PHE	C-N-CA	8.48	128.13	119.56
1	A	353	PHE	CA-C-N	8.47	128.12	119.56
1	A	353	PHE	C-N-CA	8.47	128.12	119.56
1	B	353	PHE	CA-C-N	8.44	128.08	119.56
1	B	353	PHE	C-N-CA	8.44	128.08	119.56
1	A	237	GLY	CA-C-N	7.86	127.86	119.76
1	A	237	GLY	C-N-CA	7.86	127.86	119.76
1	E	237	GLY	CA-C-N	7.86	127.86	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	237	GLY	C-N-CA	7.86	127.86	119.76
1	B	237	GLY	CA-C-N	7.85	127.84	119.76
1	B	237	GLY	C-N-CA	7.85	127.84	119.76
1	E	205	CYS	CA-C-N	7.52	127.23	119.56
1	E	205	CYS	C-N-CA	7.52	127.23	119.56
1	A	205	CYS	CA-C-N	7.50	127.21	119.56
1	A	205	CYS	C-N-CA	7.50	127.21	119.56
1	B	205	CYS	CA-C-N	7.48	127.19	119.56
1	B	205	CYS	C-N-CA	7.48	127.19	119.56
1	E	492	GLU	CA-C-N	7.35	126.98	119.56
1	E	492	GLU	C-N-CA	7.35	126.98	119.56
1	B	492	GLU	CA-C-N	7.32	126.95	119.56
1	B	492	GLU	C-N-CA	7.32	126.95	119.56
1	A	492	GLU	CA-C-N	7.30	126.93	119.56
1	A	492	GLU	C-N-CA	7.30	126.93	119.56
2	L	58	ILE	CA-C-N	7.15	127.19	119.89
2	L	58	ILE	C-N-CA	7.15	127.19	119.89
2	C	58	ILE	CA-C-N	7.14	127.18	119.89
2	C	58	ILE	C-N-CA	7.14	127.18	119.89
2	F	58	ILE	CA-C-N	7.12	127.16	119.89
2	F	58	ILE	C-N-CA	7.12	127.16	119.89
1	E	219	ALA	CA-C-N	6.95	127.12	120.31
1	E	219	ALA	C-N-CA	6.95	127.12	120.31
1	A	437	PRO	CA-C-N	6.94	126.86	119.85
1	A	437	PRO	C-N-CA	6.94	126.86	119.85
1	A	219	ALA	CA-C-N	6.94	127.11	120.31
1	A	219	ALA	C-N-CA	6.94	127.11	120.31
1	B	437	PRO	CA-C-N	6.92	126.83	119.85
1	B	437	PRO	C-N-CA	6.92	126.83	119.85
1	B	219	ALA	CA-C-N	6.91	127.08	120.31
1	B	219	ALA	C-N-CA	6.91	127.08	120.31
1	E	437	PRO	CA-C-N	6.90	126.82	119.85
1	E	437	PRO	C-N-CA	6.90	126.82	119.85
1	A	469	ARG	CA-C-N	6.70	126.68	119.78
1	A	469	ARG	C-N-CA	6.70	126.68	119.78
1	B	469	ARG	CA-C-N	6.69	126.67	119.78
1	B	469	ARG	C-N-CA	6.69	126.67	119.78
1	E	469	ARG	CA-C-N	6.69	126.67	119.78
1	E	469	ARG	C-N-CA	6.69	126.67	119.78
1	B	608	VAL	CA-C-N	6.67	126.59	119.85
1	B	608	VAL	C-N-CA	6.67	126.59	119.85
1	A	78	ASP	CA-C-N	6.65	126.79	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASP	C-N-CA	6.65	126.79	119.87
1	E	78	ASP	CA-C-N	6.65	126.78	119.87
1	E	78	ASP	C-N-CA	6.65	126.78	119.87
1	E	608	VAL	CA-C-N	6.64	126.56	119.85
1	E	608	VAL	C-N-CA	6.64	126.56	119.85
1	A	608	VAL	CA-C-N	6.63	126.55	119.85
1	A	608	VAL	C-N-CA	6.63	126.55	119.85
1	B	78	ASP	CA-C-N	6.63	126.77	119.87
1	B	78	ASP	C-N-CA	6.63	126.77	119.87
1	A	182	VAL	CA-C-N	6.57	126.60	119.90
1	A	182	VAL	C-N-CA	6.57	126.60	119.90
1	B	182	VAL	CA-C-N	6.57	126.60	119.90
1	B	182	VAL	C-N-CA	6.57	126.60	119.90
1	E	80	ASN	CA-C-N	6.57	126.55	119.78
1	E	80	ASN	C-N-CA	6.57	126.55	119.78
1	A	80	ASN	CA-C-N	6.55	126.52	119.78
1	A	80	ASN	C-N-CA	6.55	126.52	119.78
1	E	416	LEU	CA-C-N	6.55	126.46	119.85
1	E	416	LEU	C-N-CA	6.55	126.46	119.85
1	B	80	ASN	CA-C-N	6.53	126.51	119.78
1	B	80	ASN	C-N-CA	6.53	126.51	119.78
1	A	416	LEU	CA-C-N	6.53	126.44	119.85
1	A	416	LEU	C-N-CA	6.53	126.44	119.85
1	E	182	VAL	CA-C-N	6.51	126.54	119.90
1	E	182	VAL	C-N-CA	6.51	126.54	119.90
1	B	416	LEU	CA-C-N	6.49	126.40	119.85
1	B	416	LEU	C-N-CA	6.49	126.40	119.85
2	L	14	SER	CA-C-N	6.45	126.48	119.90
2	L	14	SER	C-N-CA	6.45	126.48	119.90
2	C	14	SER	CA-C-N	6.43	126.46	119.90
2	C	14	SER	C-N-CA	6.43	126.46	119.90
2	F	14	SER	CA-C-N	6.42	126.45	119.90
2	F	14	SER	C-N-CA	6.42	126.45	119.90
2	L	43	ALA	CA-C-N	6.36	126.31	119.76
2	L	43	ALA	C-N-CA	6.36	126.31	119.76
2	F	43	ALA	CA-C-N	6.33	126.28	119.76
2	F	43	ALA	C-N-CA	6.33	126.28	119.76
2	C	43	ALA	CA-C-N	6.32	126.27	119.76
2	C	43	ALA	C-N-CA	6.32	126.27	119.76
1	B	213	ILE	CA-C-N	6.24	126.19	119.76
1	B	213	ILE	C-N-CA	6.24	126.19	119.76
1	A	497	ALA	CA-C-N	6.22	127.16	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	ALA	C-N-CA	6.22	127.16	120.13
1	B	497	ALA	CA-C-N	6.22	127.16	120.13
1	B	497	ALA	C-N-CA	6.22	127.16	120.13
1	E	497	ALA	CA-C-N	6.22	127.16	120.13
1	E	497	ALA	C-N-CA	6.22	127.16	120.13
1	A	213	ILE	CA-C-N	6.21	126.16	119.76
1	A	213	ILE	C-N-CA	6.21	126.16	119.76
1	E	213	ILE	CA-C-N	6.21	126.16	119.76
1	E	213	ILE	C-N-CA	6.21	126.16	119.76
3	H	13	LYS	CA-C-N	6.20	126.23	119.90
3	H	13	LYS	C-N-CA	6.20	126.23	119.90
3	D	13	LYS	CA-C-N	6.12	126.15	119.90
3	D	13	LYS	C-N-CA	6.12	126.15	119.90
1	B	75	VAL	CA-C-N	6.09	126.03	119.76
1	B	75	VAL	C-N-CA	6.09	126.03	119.76
3	G	13	LYS	CA-C-N	6.09	126.11	119.90
3	G	13	LYS	C-N-CA	6.09	126.11	119.90
1	E	75	VAL	CA-C-N	6.09	126.03	119.76
1	E	75	VAL	C-N-CA	6.09	126.03	119.76
1	A	75	VAL	CA-C-N	6.08	126.02	119.76
1	A	75	VAL	C-N-CA	6.08	126.02	119.76
1	B	312	GLY	CA-C-N	6.01	127.35	119.84
1	B	312	GLY	C-N-CA	6.01	127.35	119.84
1	E	312	GLY	CA-C-N	6.00	127.34	119.84
1	E	312	GLY	C-N-CA	6.00	127.34	119.84
2	F	79	GLU	CA-C-N	5.99	126.42	119.47
2	F	79	GLU	C-N-CA	5.99	126.42	119.47
2	C	79	GLU	CA-C-N	5.97	126.40	119.47
2	C	79	GLU	C-N-CA	5.97	126.40	119.47
2	L	79	GLU	CA-C-N	5.97	126.40	119.47
2	L	79	GLU	C-N-CA	5.97	126.40	119.47
1	A	312	GLY	CA-C-N	5.95	127.28	119.84
1	A	312	GLY	C-N-CA	5.95	127.28	119.84
3	D	40	ALA	CA-C-N	5.62	126.86	119.84
3	D	40	ALA	C-N-CA	5.62	126.86	119.84
3	H	40	ALA	CA-C-N	5.61	126.85	119.84
3	H	40	ALA	C-N-CA	5.61	126.85	119.84
3	G	40	ALA	CA-C-N	5.60	126.84	119.84
3	G	40	ALA	C-N-CA	5.60	126.84	119.84
1	E	427	TRP	CB-CA-C	-5.59	110.11	116.54
1	A	427	TRP	CB-CA-C	-5.57	110.14	116.54
1	B	427	TRP	CB-CA-C	-5.56	110.14	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	ASP	CA-C-N	5.33	126.51	119.84
1	E	211	ASP	C-N-CA	5.33	126.51	119.84
1	A	211	ASP	CA-C-N	5.33	126.50	119.84
1	A	211	ASP	C-N-CA	5.33	126.50	119.84
1	B	211	ASP	CA-C-N	5.32	126.49	119.84
1	B	211	ASP	C-N-CA	5.32	126.49	119.84
1	B	123	THR	CA-C-N	5.32	125.78	120.04
1	B	123	THR	C-N-CA	5.32	125.78	120.04
1	A	123	THR	CA-C-N	5.30	125.76	120.04
1	A	123	THR	C-N-CA	5.30	125.76	120.04
1	E	123	THR	CA-C-N	5.30	125.76	120.04
1	E	123	THR	C-N-CA	5.30	125.76	120.04
2	F	39	LYS	CA-C-N	5.26	126.42	119.84
2	F	39	LYS	C-N-CA	5.26	126.42	119.84
2	C	39	LYS	CA-C-N	5.25	126.41	119.84
2	C	39	LYS	C-N-CA	5.25	126.41	119.84
2	L	39	LYS	CA-C-N	5.23	126.38	119.84
2	L	39	LYS	C-N-CA	5.23	126.38	119.84
2	C	91	TYR	CB-CA-C	-5.15	110.66	116.63
2	L	91	TYR	CB-CA-C	-5.12	110.69	116.63
1	A	300	ASN	N-CA-C	5.12	117.17	109.23
2	F	91	TYR	CB-CA-C	-5.12	110.69	116.63
1	E	300	ASN	N-CA-C	5.11	117.14	109.23
1	B	300	ASN	N-CA-C	5.09	117.11	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4280	13	0
1	B	4338	0	4280	14	0
1	E	4338	0	4280	13	0
2	C	767	0	740	0	0
2	F	767	0	740	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	767	0	740	1	0
3	D	940	0	887	3	0
3	G	940	0	887	3	0
3	H	940	0	887	3	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	g	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	k	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	u	28	0	25	0	0
4	w	28	0	25	0	0
4	x	28	0	25	0	0
4	y	28	0	25	0	0
5	K	61	0	49	0	0
5	Z	61	0	49	0	0
5	n	61	0	49	0	0
6	M	72	0	57	0	0
6	a	72	0	57	0	0
6	o	72	0	57	0	0
7	N	39	0	33	0	0
7	P	39	0	33	0	0
7	Q	39	0	33	0	0
7	b	39	0	33	0	0
7	d	39	0	33	0	0
7	e	39	0	33	0	0
7	p	39	0	33	0	0
7	r	39	0	33	0	0
7	s	39	0	33	0	0
8	O	83	0	66	0	0
8	c	83	0	66	0	0
8	q	83	0	66	0	0
9	R	50	0	41	0	0
9	f	50	0	41	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	t	50	0	41	0	0
10	T	61	0	50	0	0
10	h	61	0	50	0	0
10	v	61	0	50	0	0
11	A	56	0	52	0	0
11	B	56	0	52	0	0
11	E	56	0	52	0	0
All	All	20139	0	19413	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:OD1	1:B:574:LYS:NZ	2.30	0.64
1:E:107:ASP:OD1	1:E:574:LYS:NZ	2.30	0.64
1:A:107:ASP:OD1	1:A:574:LYS:NZ	2.30	0.64
1:B:123:THR:N	1:B:124:PRO:CD	2.67	0.58
1:A:123:THR:N	1:A:124:PRO:CD	2.67	0.57
1:B:117:LYS:N	1:B:118:PRO:CD	2.68	0.57
1:E:123:THR:N	1:E:124:PRO:CD	2.67	0.57
1:A:117:LYS:N	1:A:118:PRO:CD	2.68	0.56
1:A:123:THR:N	1:A:124:PRO:HD2	2.21	0.56
1:E:117:LYS:N	1:E:118:PRO:CD	2.68	0.56
1:E:275:LYS:NZ	3:G:99:ASP:OD1	2.39	0.55
1:B:123:THR:N	1:B:124:PRO:HD2	2.21	0.55
1:E:123:THR:N	1:E:124:PRO:HD2	2.21	0.55
1:B:275:LYS:NZ	3:D:99:ASP:OD1	2.39	0.54
1:A:275:LYS:NZ	3:H:99:ASP:OD1	2.39	0.53
1:B:490:LYS:NZ	1:B:492:GLU:OE2	2.43	0.52
1:A:490:LYS:NZ	1:A:492:GLU:OE2	2.43	0.50
1:E:490:LYS:NZ	1:E:492:GLU:OE2	2.43	0.50
1:A:117:LYS:N	1:A:118:PRO:HD2	2.29	0.48
1:B:117:LYS:N	1:B:118:PRO:HD2	2.29	0.48
1:E:117:LYS:N	1:E:118:PRO:HD2	2.28	0.48
1:B:49:LYS:NZ	1:B:99:ASP:OD2	2.38	0.47
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.51	0.46
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.51	0.46
3:G:47:TRP:CZ2	3:G:49:GLY:HA2	2.51	0.46
1:A:49:LYS:NZ	1:A:99:ASP:OD2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASN:OD1	1:B:230:ASN:C	2.60	0.45
1:A:55:ALA:O	1:A:56:SER:C	2.61	0.44
1:B:289:ASN:OD1	1:B:289:ASN:N	2.50	0.44
1:A:230:ASN:C	1:A:230:ASN:OD1	2.60	0.44
1:E:392:ASN:OD1	1:E:393:ASP:N	2.50	0.44
1:A:392:ASN:OD1	1:A:393:ASP:N	2.50	0.43
1:B:392:ASN:OD1	1:B:393:ASP:N	2.50	0.43
1:B:133:ASN:O	1:B:134:VAL:C	2.62	0.43
1:B:55:ALA:O	1:B:56:SER:C	2.60	0.43
1:E:426:MET:HB3	1:E:427:TRP:CE3	2.55	0.42
1:E:133:ASN:O	1:E:134:VAL:C	2.62	0.42
1:E:230:ASN:OD1	1:E:230:ASN:C	2.60	0.42
1:B:426:MET:HB3	1:B:427:TRP:CE3	2.55	0.42
1:A:426:MET:HB3	1:A:427:TRP:CE3	2.54	0.41
1:A:133:ASN:O	1:A:134:VAL:C	2.62	0.41
2:L:58:ILE:HA	2:L:59:PRO:HD3	1.88	0.41
1:E:55:ALA:O	1:E:56:SER:C	2.60	0.41
2:F:39:LYS:HA	2:F:40:PRO:HD3	1.94	0.41
3:H:12:LYS:O	3:H:111:VAL:HA	2.21	0.40
3:D:12:LYS:O	3:D:111:VAL:HA	2.21	0.40
1:E:289:ASN:OD1	1:E:289:ASN:N	2.50	0.40
3:G:13:LYS:HA	3:G:14:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/626 (86%)	522 (97%)	15 (3%)	1 (0%)	43	73
1	B	538/626 (86%)	522 (97%)	15 (3%)	1 (0%)	43	73
1	E	538/626 (86%)	522 (97%)	15 (3%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	98/229 (43%)	93 (95%)	5 (5%)	0	100	100
2	F	98/229 (43%)	93 (95%)	5 (5%)	0	100	100
2	L	98/229 (43%)	93 (95%)	5 (5%)	0	100	100
3	D	117/233 (50%)	112 (96%)	5 (4%)	0	100	100
3	G	117/233 (50%)	112 (96%)	5 (4%)	0	100	100
3	H	117/233 (50%)	112 (96%)	5 (4%)	0	100	100
All	All	2259/3264 (69%)	2181 (96%)	75 (3%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	B	258	GLN
1	E	258	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/554 (88%)	487 (100%)	2 (0%)	84	83
1	B	489/554 (88%)	487 (100%)	2 (0%)	84	83
1	E	489/554 (88%)	487 (100%)	2 (0%)	84	83
2	C	83/197 (42%)	83 (100%)	0	100	100
2	F	83/197 (42%)	83 (100%)	0	100	100
2	L	83/197 (42%)	83 (100%)	0	100	100
3	D	98/198 (50%)	98 (100%)	0	100	100
3	G	98/198 (50%)	98 (100%)	0	100	100
3	H	98/198 (50%)	98 (100%)	0	100	100
All	All	2010/2847 (71%)	2004 (100%)	6 (0%)	84	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	A	637	ASN
1	B	337	ASN
1	B	637	ASN
1	E	337	ASN
1	E	637	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	HIS
1	E	216	HIS
3	G	101	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	H	1	3	7,8,9	0.67	0	9,10,12	1.22	1 (11%)
3	PCA	G	1	3	7,8,9	0.68	0	9,10,12	1.22	1 (11%)
3	PCA	D	1	3	7,8,9	0.68	0	9,10,12	1.23	1 (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
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1
3	PCA	G	1	3	-	0/0/11/13	0/1/1/1
3	PCA	D	1	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	PCA	CB-CA-C	-2.18	109.67	112.66
3	H	1	PCA	CB-CA-C	-2.15	109.70	112.66
3	G	1	PCA	CB-CA-C	-2.15	109.71	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

144 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
4	NAG	I	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	I	2	4	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.75	0	17,19,21	0.85	0
4	NAG	J	2	4	14,14,15	0.74	0	17,19,21	1.08	1 (5%)
5	NAG	K	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	0.98	0
5	NAG	K	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.71	2 (11%)
5	BMA	K	3	5	11,11,12	1.71	3 (27%)	15,15,17	1.27	2 (13%)
5	MAN	K	4	5	11,11,12	1.79	2 (18%)	15,15,17	0.92	0
5	MAN	K	5	5	11,11,12	1.80	2 (18%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	M	2	6	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
6	BMA	M	3	6	11,11,12	1.85	3 (27%)	15,15,17	0.92	0
6	MAN	M	4	6	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
6	MAN	M	5	6	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)
6	MAN	M	6	6	11,11,12	1.79	2 (18%)	15,15,17	0.94	1 (6%)
7	NAG	N	1	7,1	14,14,15	0.79	0	17,19,21	0.94	0
7	NAG	N	2	7	14,14,15	0.80	0	17,19,21	1.07	1 (5%)
7	BMA	N	3	7	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)
8	NAG	O	1	8,1	14,14,15	0.79	1 (7%)	17,19,21	1.01	0
8	NAG	O	2	8	14,14,15	0.78	1 (7%)	17,19,21	1.01	0
8	BMA	O	3	8	11,11,12	2.00	4 (36%)	15,15,17	1.29	2 (13%)
8	MAN	O	4	8	11,11,12	1.59	2 (18%)	15,15,17	0.85	0
8	MAN	O	5	8	11,11,12	1.82	2 (18%)	15,15,17	0.95	1 (6%)
8	MAN	O	6	8	11,11,12	1.83	2 (18%)	15,15,17	0.91	1 (6%)
8	MAN	O	7	8	11,11,12	1.81	2 (18%)	15,15,17	0.92	1 (6%)
7	NAG	P	1	7,1	14,14,15	0.79	0	17,19,21	0.91	0
7	NAG	P	2	7	14,14,15	0.85	0	17,19,21	1.48	2 (11%)
7	BMA	P	3	7	11,11,12	1.84	2 (18%)	15,15,17	1.01	1 (6%)
7	NAG	Q	1	7,1	14,14,15	1.04	1 (7%)	17,19,21	1.00	0
7	NAG	Q	2	7	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
7	BMA	Q	3	7	11,11,12	1.83	2 (18%)	15,15,17	0.93	1 (6%)
9	NAG	R	1	9,1	14,14,15	0.78	1 (7%)	17,19,21	0.92	0
9	NAG	R	2	9	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
9	BMA	R	3	9	11,11,12	1.79	2 (18%)	15,15,17	1.04	1 (6%)
9	MAN	R	4	9	11,11,12	1.80	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	S	1	4,1	14,14,15	0.78	0	17,19,21	0.91	0
4	NAG	S	2	4	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
10	NAG	T	1	1,10	14,14,15	0.81	1 (7%)	17,19,21	0.91	0
10	NAG	T	2	10	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
10	BMA	T	3	10	11,11,12	1.86	2 (18%)	15,15,17	1.05	1 (6%)
10	MAN	T	4	10	11,11,12	1.68	2 (18%)	15,15,17	0.92	1 (6%)
10	MAN	T	5	10	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)
4	NAG	U	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	U	2	4	14,14,15	0.72	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	V	1	4,1	14,14,15	0.72	0	17,19,21	0.82	0
4	NAG	V	2	4	14,14,15	0.75	0	17,19,21	1.15	1 (5%)
4	NAG	W	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	W	2	4	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
4	NAG	X	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	X	2	4	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
4	NAG	Y	1	4,1	14,14,15	0.75	0	17,19,21	0.85	0
4	NAG	Y	2	4	14,14,15	0.74	0	17,19,21	1.08	1 (5%)
5	NAG	Z	1	1,5	14,14,15	0.80	1 (7%)	17,19,21	0.97	0
5	NAG	Z	2	5	14,14,15	0.85	1 (7%)	17,19,21	1.72	2 (11%)
5	BMA	Z	3	5	11,11,12	1.70	3 (27%)	15,15,17	1.27	2 (13%)
5	MAN	Z	4	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	0
5	MAN	Z	5	5	11,11,12	1.80	2 (18%)	15,15,17	1.06	1 (6%)
6	NAG	a	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.03	1 (5%)
6	NAG	a	2	6	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
6	BMA	a	3	6	11,11,12	1.83	3 (27%)	15,15,17	0.92	0
6	MAN	a	4	6	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
6	MAN	a	5	6	11,11,12	1.83	2 (18%)	15,15,17	0.93	1 (6%)
6	MAN	a	6	6	11,11,12	1.79	2 (18%)	15,15,17	0.94	1 (6%)
7	NAG	b	1	7,1	14,14,15	0.79	0	17,19,21	0.94	0
7	NAG	b	2	7	14,14,15	0.80	0	17,19,21	1.07	1 (5%)
7	BMA	b	3	7	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)
8	NAG	c	1	8,1	14,14,15	0.79	1 (7%)	17,19,21	1.00	0
8	NAG	c	2	8	14,14,15	0.78	1 (7%)	17,19,21	1.00	0
8	BMA	c	3	8	11,11,12	2.00	4 (36%)	15,15,17	1.29	2 (13%)
8	MAN	c	4	8	11,11,12	1.60	2 (18%)	15,15,17	0.85	0
8	MAN	c	5	8	11,11,12	1.82	2 (18%)	15,15,17	0.95	1 (6%)
8	MAN	c	6	8	11,11,12	1.83	2 (18%)	15,15,17	0.91	1 (6%)
8	MAN	c	7	8	11,11,12	1.82	2 (18%)	15,15,17	0.92	1 (6%)
7	NAG	d	1	7,1	14,14,15	0.78	0	17,19,21	0.91	0
7	NAG	d	2	7	14,14,15	0.86	0	17,19,21	1.48	2 (11%)
7	BMA	d	3	7	11,11,12	1.83	2 (18%)	15,15,17	1.01	1 (6%)
7	NAG	e	1	7,1	14,14,15	1.05	1 (7%)	17,19,21	1.00	0
7	NAG	e	2	7	14,14,15	0.82	0	17,19,21	1.04	1 (5%)
7	BMA	e	3	7	11,11,12	1.85	2 (18%)	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	f	1	9,1	14,14,15	0.78	1 (7%)	17,19,21	0.92	0
9	NAG	f	2	9	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
9	BMA	f	3	9	11,11,12	1.80	2 (18%)	15,15,17	1.03	1 (6%)
9	MAN	f	4	9	11,11,12	1.81	2 (18%)	15,15,17	0.93	1 (6%)
4	NAG	g	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	0.91	0
4	NAG	g	2	4	14,14,15	0.73	0	17,19,21	1.09	1 (5%)
10	NAG	h	1	1,10	14,14,15	0.80	1 (7%)	17,19,21	0.91	0
10	NAG	h	2	10	14,14,15	0.76	0	17,19,21	1.02	1 (5%)
10	BMA	h	3	10	11,11,12	1.86	2 (18%)	15,15,17	1.04	1 (6%)
10	MAN	h	4	10	11,11,12	1.68	2 (18%)	15,15,17	0.92	1 (6%)
10	MAN	h	5	10	11,11,12	1.81	2 (18%)	15,15,17	0.93	1 (6%)
4	NAG	i	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	i	2	4	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
4	NAG	j	1	4,1	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	j	2	4	14,14,15	0.75	0	17,19,21	1.15	1 (5%)
4	NAG	k	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	k	2	4	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
4	NAG	l	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	l	2	4	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
4	NAG	m	1	4,1	14,14,15	0.76	0	17,19,21	0.85	0
4	NAG	m	2	4	14,14,15	0.75	0	17,19,21	1.08	1 (5%)
5	NAG	n	1	1,5	14,14,15	0.80	1 (7%)	17,19,21	0.97	0
5	NAG	n	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.72	2 (11%)
5	BMA	n	3	5	11,11,12	1.70	3 (27%)	15,15,17	1.28	2 (13%)
5	MAN	n	4	5	11,11,12	1.80	2 (18%)	15,15,17	0.92	0
5	MAN	n	5	5	11,11,12	1.79	2 (18%)	15,15,17	1.06	1 (6%)
6	NAG	o	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	o	2	6	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
6	BMA	o	3	6	11,11,12	1.85	3 (27%)	15,15,17	0.93	0
6	MAN	o	4	6	11,11,12	1.80	2 (18%)	15,15,17	1.08	1 (6%)
6	MAN	o	5	6	11,11,12	1.83	2 (18%)	15,15,17	0.92	1 (6%)
6	MAN	o	6	6	11,11,12	1.79	2 (18%)	15,15,17	0.94	1 (6%)
7	NAG	p	1	7,1	14,14,15	0.79	0	17,19,21	0.94	0
7	NAG	p	2	7	14,14,15	0.79	0	17,19,21	1.07	1 (5%)
7	BMA	p	3	7	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	q	1	8,1	14,14,15	0.80	1 (7%)	17,19,21	1.01	0
8	NAG	q	2	8	14,14,15	0.78	1 (7%)	17,19,21	1.01	0
8	BMA	q	3	8	11,11,12	1.99	4 (36%)	15,15,17	1.29	2 (13%)
8	MAN	q	4	8	11,11,12	1.60	2 (18%)	15,15,17	0.85	0
8	MAN	q	5	8	11,11,12	1.82	2 (18%)	15,15,17	0.95	1 (6%)
8	MAN	q	6	8	11,11,12	1.84	2 (18%)	15,15,17	0.91	1 (6%)
8	MAN	q	7	8	11,11,12	1.81	2 (18%)	15,15,17	0.92	1 (6%)
7	NAG	r	1	7,1	14,14,15	0.79	0	17,19,21	0.92	0
7	NAG	r	2	7	14,14,15	0.85	0	17,19,21	1.48	2 (11%)
7	BMA	r	3	7	11,11,12	1.83	2 (18%)	15,15,17	1.01	1 (6%)
7	NAG	s	1	7,1	14,14,15	1.05	1 (7%)	17,19,21	1.00	0
7	NAG	s	2	7	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
7	BMA	s	3	7	11,11,12	1.84	2 (18%)	15,15,17	0.93	1 (6%)
9	NAG	t	1	9,1	14,14,15	0.78	1 (7%)	17,19,21	0.92	0
9	NAG	t	2	9	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
9	BMA	t	3	9	11,11,12	1.80	2 (18%)	15,15,17	1.04	1 (6%)
9	MAN	t	4	9	11,11,12	1.80	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	u	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	0.92	0
4	NAG	u	2	4	14,14,15	0.71	0	17,19,21	1.10	1 (5%)
10	NAG	v	1	1,10	14,14,15	0.81	1 (7%)	17,19,21	0.90	0
10	NAG	v	2	10	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
10	BMA	v	3	10	11,11,12	1.87	2 (18%)	15,15,17	1.05	1 (6%)
10	MAN	v	4	10	11,11,12	1.68	2 (18%)	15,15,17	0.92	1 (6%)
10	MAN	v	5	10	11,11,12	1.82	2 (18%)	15,15,17	0.93	1 (6%)
4	NAG	w	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	w	2	4	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
4	NAG	x	1	4,1	14,14,15	0.74	0	17,19,21	0.82	0
4	NAG	x	2	4	14,14,15	0.76	0	17,19,21	1.14	1 (5%)
4	NAG	y	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	y	2	4	14,14,15	0.71	0	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	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	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1
6	MAN	M	4	6	-	2/2/19/22	0/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
6	MAN	M	6	6	-	2/2/19/22	0/1/1/1
7	NAG	N	1	7,1	-	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	-	1/2/19/22	0/1/1/1
8	NAG	O	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	BMA	O	3	8	-	1/2/19/22	0/1/1/1
8	MAN	O	4	8	-	2/2/19/22	0/1/1/1
8	MAN	O	5	8	-	2/2/19/22	0/1/1/1
8	MAN	O	6	8	-	2/2/19/22	0/1/1/1
8	MAN	O	7	8	-	2/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
9	NAG	R	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	BMA	R	3	9	-	2/2/19/22	0/1/1/1
9	MAN	R	4	9	-	2/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
10	NAG	T	1	1,10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	T	2	10	-	0/6/23/26	0/1/1/1
10	BMA	T	3	10	-	2/2/19/22	0/1/1/1
10	MAN	T	4	10	-	2/2/19/22	0/1/1/1
10	MAN	T	5	10	-	1/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	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
5	BMA	Z	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	5	5	-	2/2/19/22	0/1/1/1
6	NAG	a	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	2/2/19/22	0/1/1/1
6	MAN	a	4	6	-	2/2/19/22	0/1/1/1
6	MAN	a	5	6	-	2/2/19/22	0/1/1/1
6	MAN	a	6	6	-	2/2/19/22	0/1/1/1
7	NAG	b	1	7,1	-	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	-	1/2/19/22	0/1/1/1
8	NAG	c	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	1/6/23/26	0/1/1/1
8	BMA	c	3	8	-	1/2/19/22	0/1/1/1
8	MAN	c	4	8	-	2/2/19/22	0/1/1/1
8	MAN	c	5	8	-	2/2/19/22	0/1/1/1
8	MAN	c	6	8	-	2/2/19/22	0/1/1/1
8	MAN	c	7	8	-	2/2/19/22	0/1/1/1
7	NAG	d	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
7	BMA	d	3	7	-	1/2/19/22	0/1/1/1

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

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

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	3	BMA	O2-C2	-4.25	1.34	1.43
7	r	3	BMA	O2-C2	-4.22	1.34	1.43
7	b	3	BMA	O2-C2	-4.22	1.34	1.43
7	N	3	BMA	O2-C2	-4.22	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	3	BMA	O2-C2	-4.21	1.34	1.43
7	d	3	BMA	O2-C2	-4.20	1.34	1.43
7	e	3	BMA	O2-C2	-4.15	1.34	1.43
6	M	5	MAN	O2-C2	-4.14	1.34	1.43
6	o	5	MAN	O2-C2	-4.14	1.34	1.43
8	O	7	MAN	O2-C2	-4.14	1.34	1.43
6	a	5	MAN	O2-C2	-4.14	1.34	1.43
8	q	7	MAN	O2-C2	-4.13	1.34	1.43
8	c	7	MAN	O2-C2	-4.13	1.34	1.43
10	v	3	BMA	O2-C2	-4.11	1.34	1.43
5	n	5	MAN	O2-C2	-4.10	1.34	1.43
10	T	3	BMA	O2-C2	-4.10	1.34	1.43
9	t	4	MAN	O2-C2	-4.08	1.34	1.43
10	h	3	BMA	O2-C2	-4.08	1.34	1.43
5	Z	5	MAN	O2-C2	-4.08	1.34	1.43
5	K	5	MAN	O2-C2	-4.08	1.34	1.43
10	T	5	MAN	O2-C2	-4.07	1.34	1.43
7	s	3	BMA	O2-C2	-4.07	1.34	1.43
10	h	5	MAN	O2-C2	-4.07	1.34	1.43
7	Q	3	BMA	O2-C2	-4.07	1.34	1.43
8	O	5	MAN	O2-C2	-4.06	1.34	1.43
10	v	5	MAN	O2-C2	-4.05	1.34	1.43
9	f	4	MAN	O2-C2	-4.05	1.34	1.43
9	t	3	BMA	O2-C2	-4.05	1.34	1.43
8	q	5	MAN	O2-C2	-4.05	1.34	1.43
9	R	4	MAN	O2-C2	-4.05	1.34	1.43
8	c	5	MAN	O2-C2	-4.04	1.34	1.43
9	f	3	BMA	O2-C2	-4.03	1.34	1.43
9	R	3	BMA	O2-C2	-4.02	1.34	1.43
6	M	4	MAN	O2-C2	-3.99	1.35	1.43
6	a	4	MAN	O2-C2	-3.98	1.35	1.43
6	o	4	MAN	O2-C2	-3.95	1.35	1.43
6	M	6	MAN	O2-C2	-3.94	1.35	1.43
6	a	6	MAN	O2-C2	-3.93	1.35	1.43
6	o	6	MAN	O2-C2	-3.92	1.35	1.43
5	Z	4	MAN	O2-C2	-3.88	1.35	1.43
8	q	6	MAN	O2-C2	-3.88	1.35	1.43
5	n	4	MAN	O2-C2	-3.88	1.35	1.43
8	c	6	MAN	O2-C2	-3.87	1.35	1.43
5	K	4	MAN	O2-C2	-3.87	1.35	1.43
8	O	6	MAN	O2-C2	-3.86	1.35	1.43
10	h	4	MAN	O2-C2	-3.58	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	v	4	MAN	O2-C2	-3.57	1.35	1.43
10	T	4	MAN	O2-C2	-3.56	1.35	1.43
8	O	3	BMA	O2-C2	-3.55	1.35	1.43
6	o	3	BMA	O2-C2	-3.54	1.35	1.43
6	M	3	BMA	O2-C2	-3.54	1.35	1.43
8	q	3	BMA	O2-C2	-3.52	1.36	1.43
6	a	3	BMA	O2-C2	-3.52	1.36	1.43
8	c	3	BMA	O2-C2	-3.52	1.36	1.43
8	c	4	MAN	O2-C2	-3.26	1.36	1.43
8	q	4	MAN	O2-C2	-3.24	1.36	1.43
8	O	4	MAN	O2-C2	-3.23	1.36	1.43
8	q	3	BMA	O5-C1	3.22	1.49	1.43
8	c	3	BMA	O5-C1	3.22	1.49	1.43
8	O	3	BMA	O5-C1	3.20	1.49	1.43
5	Z	3	BMA	O2-C2	-3.18	1.36	1.43
5	K	3	BMA	O2-C2	-3.18	1.36	1.43
5	n	3	BMA	O2-C2	-3.18	1.36	1.43
8	c	3	BMA	C6-C5	2.88	1.61	1.51
7	s	1	NAG	C3-C2	-2.88	1.46	1.52
8	O	3	BMA	C6-C5	2.87	1.61	1.51
7	e	1	NAG	C3-C2	-2.86	1.46	1.52
5	Z	4	MAN	C2-C3	-2.86	1.48	1.52
8	q	3	BMA	C6-C5	2.85	1.61	1.51
5	n	4	MAN	C2-C3	-2.83	1.48	1.52
7	Q	1	NAG	C3-C2	-2.82	1.46	1.52
5	K	4	MAN	C2-C3	-2.80	1.48	1.52
8	q	6	MAN	C2-C3	-2.78	1.48	1.52
6	M	3	BMA	C6-C5	2.78	1.61	1.51
6	o	3	BMA	C6-C5	2.77	1.61	1.51
6	a	3	BMA	C6-C5	2.76	1.61	1.51
8	O	6	MAN	C2-C3	-2.76	1.48	1.52
8	c	6	MAN	C2-C3	-2.73	1.48	1.52
8	c	5	MAN	C2-C3	-2.67	1.48	1.52
8	q	5	MAN	C2-C3	-2.66	1.48	1.52
6	o	3	BMA	O5-C1	2.65	1.48	1.43
8	O	5	MAN	C2-C3	-2.62	1.48	1.52
6	M	3	BMA	O5-C1	2.62	1.48	1.43
6	M	6	MAN	C2-C3	-2.58	1.48	1.52
6	a	6	MAN	C2-C3	-2.58	1.48	1.52
6	o	6	MAN	C2-C3	-2.57	1.48	1.52
6	a	3	BMA	O5-C1	2.57	1.48	1.43
5	Z	3	BMA	C6-C5	2.56	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n	3	BMA	C6-C5	2.54	1.60	1.51
10	v	3	BMA	C2-C3	-2.54	1.48	1.52
8	c	7	MAN	C2-C3	-2.52	1.48	1.52
10	v	5	MAN	C2-C3	-2.52	1.48	1.52
10	h	3	BMA	C2-C3	-2.52	1.48	1.52
7	Q	3	BMA	C2-C3	-2.52	1.48	1.52
5	K	3	BMA	C6-C5	2.52	1.60	1.51
10	T	3	BMA	C2-C3	-2.51	1.48	1.52
6	a	5	MAN	C2-C3	-2.51	1.48	1.52
7	s	3	BMA	C2-C3	-2.50	1.48	1.52
8	q	7	MAN	C2-C3	-2.50	1.48	1.52
10	T	5	MAN	C2-C3	-2.50	1.48	1.52
6	o	5	MAN	C2-C3	-2.49	1.48	1.52
10	h	5	MAN	C2-C3	-2.49	1.48	1.52
6	M	5	MAN	C2-C3	-2.48	1.48	1.52
7	e	3	BMA	C2-C3	-2.48	1.48	1.52
8	O	7	MAN	C2-C3	-2.46	1.48	1.52
9	f	4	MAN	C2-C3	-2.44	1.48	1.52
7	P	3	BMA	C2-C3	-2.42	1.48	1.52
9	R	4	MAN	C2-C3	-2.42	1.48	1.52
7	d	3	BMA	C2-C3	-2.40	1.48	1.52
9	t	4	MAN	C2-C3	-2.39	1.48	1.52
5	K	3	BMA	O5-C1	2.38	1.47	1.43
7	r	3	BMA	C2-C3	-2.38	1.48	1.52
5	n	3	BMA	O5-C1	2.37	1.47	1.43
6	a	4	MAN	C2-C3	-2.33	1.48	1.52
6	o	4	MAN	C2-C3	-2.31	1.48	1.52
6	M	4	MAN	C2-C3	-2.31	1.49	1.52
5	Z	3	BMA	O5-C1	2.31	1.47	1.43
7	N	3	BMA	C2-C3	-2.28	1.49	1.52
7	b	3	BMA	C2-C3	-2.27	1.49	1.52
7	p	3	BMA	C2-C3	-2.24	1.49	1.52
5	K	5	MAN	C2-C3	-2.23	1.49	1.52
5	Z	5	MAN	C2-C3	-2.23	1.49	1.52
5	n	5	MAN	C2-C3	-2.21	1.49	1.52
6	o	1	NAG	C3-C2	-2.21	1.47	1.52
6	M	1	NAG	C3-C2	-2.20	1.47	1.52
9	t	1	NAG	C3-C2	-2.20	1.47	1.52
9	R	1	NAG	C3-C2	-2.20	1.47	1.52
6	a	1	NAG	C3-C2	-2.20	1.47	1.52
9	f	1	NAG	C3-C2	-2.19	1.47	1.52
8	q	4	MAN	C2-C3	-2.19	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	t	3	BMA	C2-C3	-2.19	1.49	1.52
8	c	4	MAN	C2-C3	-2.18	1.49	1.52
8	O	4	MAN	C2-C3	-2.18	1.49	1.52
9	f	3	BMA	C2-C3	-2.18	1.49	1.52
5	Z	1	NAG	C3-C2	-2.18	1.48	1.52
9	R	3	BMA	C2-C3	-2.17	1.49	1.52
5	n	1	NAG	C3-C2	-2.16	1.48	1.52
10	v	4	MAN	C2-C3	-2.15	1.49	1.52
10	T	4	MAN	C2-C3	-2.14	1.49	1.52
10	v	1	NAG	C3-C2	-2.14	1.48	1.52
10	T	1	NAG	C3-C2	-2.14	1.48	1.52
5	K	1	NAG	C3-C2	-2.13	1.48	1.52
8	q	2	NAG	C3-C2	-2.13	1.48	1.52
10	h	4	MAN	C2-C3	-2.13	1.49	1.52
10	h	1	NAG	C3-C2	-2.13	1.48	1.52
4	k	1	NAG	C3-C2	-2.12	1.48	1.52
8	c	2	NAG	C3-C2	-2.11	1.48	1.52
4	W	1	NAG	C3-C2	-2.11	1.48	1.52
8	q	1	NAG	C3-C2	-2.10	1.48	1.52
8	c	1	NAG	C3-C2	-2.10	1.48	1.52
4	w	1	NAG	C3-C2	-2.09	1.48	1.52
4	i	1	NAG	C3-C2	-2.09	1.48	1.52
8	O	1	NAG	C3-C2	-2.09	1.48	1.52
4	U	1	NAG	C3-C2	-2.09	1.48	1.52
8	O	2	NAG	C3-C2	-2.08	1.48	1.52
4	y	1	NAG	C3-C2	-2.08	1.48	1.52
8	O	3	BMA	C2-C3	-2.07	1.49	1.52
4	X	1	NAG	C3-C2	-2.07	1.48	1.52
8	c	3	BMA	C2-C3	-2.07	1.49	1.52
4	I	1	NAG	C3-C2	-2.06	1.48	1.52
5	Z	2	NAG	C3-C2	-2.05	1.48	1.52
4	l	1	NAG	C3-C2	-2.05	1.48	1.52
8	q	3	BMA	C2-C3	-2.03	1.49	1.52
5	n	2	NAG	C3-C2	-2.03	1.48	1.52
4	u	1	NAG	C3-C2	-2.02	1.48	1.52
5	K	2	NAG	C3-C2	-2.02	1.48	1.52
4	g	1	NAG	C3-C2	-2.00	1.48	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	n	2	NAG	C4-C3-C2	-5.36	103.16	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	C4-C3-C2	-5.35	103.18	111.02
5	Z	2	NAG	C4-C3-C2	-5.34	103.20	111.02
7	r	2	NAG	C4-C3-C2	-4.12	104.97	111.02
7	d	2	NAG	C4-C3-C2	-4.12	104.98	111.02
7	P	2	NAG	C4-C3-C2	-4.12	104.99	111.02
4	j	2	NAG	C4-C3-C2	-3.11	106.47	111.02
4	V	2	NAG	C4-C3-C2	-3.08	106.50	111.02
4	x	2	NAG	C4-C3-C2	-3.08	106.50	111.02
4	I	2	NAG	C4-C3-C2	-3.07	106.51	111.02
4	u	2	NAG	C4-C3-C2	-3.06	106.53	111.02
4	X	2	NAG	C4-C3-C2	-3.06	106.53	111.02
4	l	2	NAG	C4-C3-C2	-3.05	106.54	111.02
4	S	2	NAG	C4-C3-C2	-3.03	106.58	111.02
4	m	2	NAG	C4-C3-C2	-3.02	106.59	111.02
4	g	2	NAG	C4-C3-C2	-3.02	106.59	111.02
4	Y	2	NAG	C4-C3-C2	-3.02	106.60	111.02
4	J	2	NAG	C4-C3-C2	-3.01	106.61	111.02
5	K	3	BMA	C2-C3-C4	-2.97	105.63	110.86
5	n	3	BMA	C2-C3-C4	-2.97	105.63	110.86
5	Z	3	BMA	C2-C3-C4	-2.96	105.66	110.86
4	W	2	NAG	C4-C3-C2	-2.87	106.82	111.02
4	y	2	NAG	C4-C3-C2	-2.86	106.82	111.02
4	k	2	NAG	C4-C3-C2	-2.84	106.85	111.02
8	q	3	BMA	C2-C3-C4	-2.81	105.92	110.86
8	c	3	BMA	C2-C3-C4	-2.81	105.92	110.86
8	O	3	BMA	C2-C3-C4	-2.81	105.92	110.86
9	R	3	BMA	C2-C3-C4	-2.75	106.03	110.86
9	t	3	BMA	C2-C3-C4	-2.74	106.04	110.86
9	f	3	BMA	C2-C3-C4	-2.73	106.06	110.86
4	i	2	NAG	C4-C3-C2	-2.68	107.09	111.02
4	U	2	NAG	C4-C3-C2	-2.68	107.10	111.02
7	b	2	NAG	C4-C3-C2	-2.67	107.10	111.02
4	w	2	NAG	C4-C3-C2	-2.66	107.12	111.02
7	N	2	NAG	C4-C3-C2	-2.65	107.13	111.02
7	p	2	NAG	C4-C3-C2	-2.64	107.14	111.02
8	q	3	BMA	C1-C2-C3	2.63	113.48	109.64
5	n	2	NAG	O5-C5-C4	-2.62	104.44	110.83
5	K	2	NAG	O5-C5-C4	-2.62	104.46	110.83
8	O	3	BMA	C1-C2-C3	2.61	113.44	109.64
8	c	3	BMA	C1-C2-C3	2.61	113.44	109.64
5	Z	2	NAG	O5-C5-C4	-2.61	104.48	110.83
5	n	3	BMA	C1-C2-C3	2.59	113.42	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	3	BMA	C1-C2-C3	2.58	113.40	109.64
10	T	3	BMA	C2-C3-C4	-2.58	106.33	110.86
5	Z	3	BMA	C1-C2-C3	2.57	113.38	109.64
10	v	3	BMA	C2-C3-C4	-2.56	106.36	110.86
5	n	5	MAN	C2-C3-C4	-2.55	106.37	110.86
10	h	3	BMA	C2-C3-C4	-2.55	106.37	110.86
6	a	1	NAG	C4-C3-C2	-2.55	107.28	111.02
6	M	1	NAG	C4-C3-C2	-2.55	107.28	111.02
6	o	1	NAG	C4-C3-C2	-2.54	107.29	111.02
5	Z	5	MAN	C2-C3-C4	-2.54	106.39	110.86
5	K	5	MAN	C2-C3-C4	-2.54	106.39	110.86
9	R	2	NAG	C4-C3-C2	-2.53	107.30	111.02
9	t	2	NAG	C4-C3-C2	-2.53	107.31	111.02
9	f	2	NAG	C4-C3-C2	-2.53	107.31	111.02
4	k	1	NAG	C4-C3-C2	-2.49	107.37	111.02
4	W	1	NAG	C4-C3-C2	-2.49	107.37	111.02
4	y	1	NAG	C4-C3-C2	-2.47	107.39	111.02
4	l	1	NAG	C4-C3-C2	-2.42	107.47	111.02
4	I	1	NAG	C4-C3-C2	-2.40	107.50	111.02
4	X	1	NAG	C4-C3-C2	-2.40	107.50	111.02
10	T	2	NAG	C4-C3-C2	-2.37	107.55	111.02
10	h	2	NAG	C4-C3-C2	-2.36	107.56	111.02
10	v	2	NAG	C4-C3-C2	-2.35	107.57	111.02
7	e	2	NAG	C4-C3-C2	-2.33	107.60	111.02
7	Q	2	NAG	C4-C3-C2	-2.32	107.62	111.02
7	d	3	BMA	C2-C3-C4	-2.32	106.79	110.86
6	M	4	MAN	C2-C3-C4	-2.32	106.79	110.86
7	P	3	BMA	C2-C3-C4	-2.31	106.79	110.86
6	o	4	MAN	C2-C3-C4	-2.31	106.80	110.86
6	a	4	MAN	C2-C3-C4	-2.31	106.80	110.86
7	s	2	NAG	C4-C3-C2	-2.31	107.64	111.02
7	r	3	BMA	C2-C3-C4	-2.30	106.82	110.86
7	P	2	NAG	O5-C5-C4	-2.23	105.39	110.83
7	d	2	NAG	O5-C5-C4	-2.23	105.40	110.83
7	r	2	NAG	O5-C5-C4	-2.22	105.42	110.83
7	b	3	BMA	C2-C3-C4	-2.22	106.96	110.86
7	p	3	BMA	C2-C3-C4	-2.21	106.98	110.86
4	U	1	NAG	C4-C3-C2	-2.20	107.79	111.02
7	N	3	BMA	C2-C3-C4	-2.20	106.99	110.86
4	i	1	NAG	C4-C3-C2	-2.17	107.84	111.02
4	w	1	NAG	C4-C3-C2	-2.16	107.85	111.02
8	c	6	MAN	C2-C3-C4	-2.15	107.07	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	2	NAG	C4-C3-C2	-2.15	107.87	111.02
6	M	5	MAN	C2-C3-C4	-2.14	107.09	110.86
8	O	6	MAN	C2-C3-C4	-2.14	107.10	110.86
8	q	6	MAN	C2-C3-C4	-2.13	107.11	110.86
8	O	5	MAN	C2-C3-C4	-2.13	107.11	110.86
6	o	2	NAG	C4-C3-C2	-2.13	107.90	111.02
6	a	5	MAN	C2-C3-C4	-2.12	107.13	110.86
6	a	2	NAG	C4-C3-C2	-2.12	107.91	111.02
8	c	5	MAN	C2-C3-C4	-2.12	107.14	110.86
6	o	5	MAN	C2-C3-C4	-2.11	107.15	110.86
8	q	5	MAN	C2-C3-C4	-2.11	107.16	110.86
9	t	4	MAN	C2-C3-C4	-2.08	107.19	110.86
8	O	7	MAN	C2-C3-C4	-2.08	107.20	110.86
7	Q	3	BMA	C2-C3-C4	-2.08	107.21	110.86
7	e	3	BMA	C2-C3-C4	-2.08	107.21	110.86
8	q	7	MAN	C2-C3-C4	-2.07	107.22	110.86
10	T	5	MAN	C2-C3-C4	-2.07	107.22	110.86
7	s	3	BMA	C2-C3-C4	-2.07	107.23	110.86
9	R	4	MAN	C2-C3-C4	-2.06	107.23	110.86
8	c	7	MAN	C2-C3-C4	-2.06	107.24	110.86
10	T	4	MAN	C2-C3-C4	-2.05	107.25	110.86
10	h	4	MAN	C2-C3-C4	-2.05	107.26	110.86
10	h	5	MAN	C2-C3-C4	-2.05	107.26	110.86
10	v	5	MAN	C2-C3-C4	-2.05	107.26	110.86
10	v	4	MAN	C2-C3-C4	-2.04	107.27	110.86
9	f	4	MAN	C2-C3-C4	-2.04	107.27	110.86
6	o	6	MAN	C2-C3-C4	-2.04	107.28	110.86
6	M	6	MAN	C2-C3-C4	-2.03	107.28	110.86
6	a	6	MAN	C2-C3-C4	-2.03	107.29	110.86

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	6	MAN	C4-C5-C6-O6
6	a	6	MAN	C4-C5-C6-O6
6	o	6	MAN	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	M	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	a	2	NAG	C4-C5-C6-O6
6	a	5	MAN	C4-C5-C6-O6
6	o	2	NAG	C4-C5-C6-O6
6	o	5	MAN	C4-C5-C6-O6
6	M	6	MAN	O5-C5-C6-O6
6	a	6	MAN	O5-C5-C6-O6
6	o	6	MAN	O5-C5-C6-O6
9	R	3	BMA	O5-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
9	f	3	BMA	O5-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
10	h	1	NAG	O5-C5-C6-O6
10	v	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	k	2	NAG	O5-C5-C6-O6
4	x	2	NAG	O5-C5-C6-O6
4	y	2	NAG	O5-C5-C6-O6
6	M	5	MAN	O5-C5-C6-O6
6	a	5	MAN	O5-C5-C6-O6
6	o	5	MAN	O5-C5-C6-O6
10	T	4	MAN	O5-C5-C6-O6
10	h	4	MAN	O5-C5-C6-O6
10	v	4	MAN	O5-C5-C6-O6
8	O	5	MAN	C4-C5-C6-O6
8	c	5	MAN	C4-C5-C6-O6
8	q	5	MAN	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
9	R	4	MAN	O5-C5-C6-O6
9	f	4	MAN	O5-C5-C6-O6
9	t	4	MAN	O5-C5-C6-O6
9	R	3	BMA	C4-C5-C6-O6
9	f	3	BMA	C4-C5-C6-O6
9	t	3	BMA	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
5	Z	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	n	5	MAN	O5-C5-C6-O6
6	M	4	MAN	O5-C5-C6-O6
6	a	4	MAN	O5-C5-C6-O6
6	o	4	MAN	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	k	2	NAG	C4-C5-C6-O6
4	y	2	NAG	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
5	n	3	BMA	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	o	2	NAG	O5-C5-C6-O6
8	O	6	MAN	O5-C5-C6-O6
8	c	6	MAN	O5-C5-C6-O6
8	q	6	MAN	O5-C5-C6-O6
10	T	3	BMA	O5-C5-C6-O6
10	h	3	BMA	O5-C5-C6-O6
10	v	3	BMA	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	u	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	w	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	n	3	BMA	O5-C5-C6-O6
8	O	5	MAN	O5-C5-C6-O6
8	c	5	MAN	O5-C5-C6-O6
8	q	5	MAN	O5-C5-C6-O6
8	O	6	MAN	C4-C5-C6-O6
8	c	6	MAN	C4-C5-C6-O6
8	q	6	MAN	C4-C5-C6-O6
7	N	3	BMA	O5-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
7	p	3	BMA	O5-C5-C6-O6
8	O	7	MAN	O5-C5-C6-O6
8	q	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	M	4	MAN	C4-C5-C6-O6
6	a	4	MAN	C4-C5-C6-O6
6	o	4	MAN	C4-C5-C6-O6
8	c	7	MAN	O5-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
10	h	1	NAG	C4-C5-C6-O6
10	v	1	NAG	C4-C5-C6-O6
10	T	5	MAN	O5-C5-C6-O6
10	h	5	MAN	O5-C5-C6-O6
10	v	5	MAN	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	l	2	NAG	C4-C5-C6-O6
10	h	4	MAN	C4-C5-C6-O6
10	v	4	MAN	C4-C5-C6-O6
10	T	4	MAN	C4-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
7	r	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	x	2	NAG	C4-C5-C6-O6
8	O	4	MAN	O5-C5-C6-O6
8	c	4	MAN	O5-C5-C6-O6
8	q	4	MAN	O5-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
7	s	3	BMA	O5-C5-C6-O6
6	o	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	d	3	BMA	O5-C5-C6-O6
7	r	3	BMA	O5-C5-C6-O6
9	R	4	MAN	C4-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	f	2	NAG	C4-C5-C6-O6
9	f	4	MAN	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	r	1	NAG	O5-C5-C6-O6
9	t	4	MAN	C4-C5-C6-O6
7	d	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
8	O	3	BMA	C4-C5-C6-O6
8	c	3	BMA	C4-C5-C6-O6
8	q	3	BMA	C4-C5-C6-O6
7	r	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	y	1	NAG	O5-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	u	2	NAG	C4-C5-C6-O6
10	v	3	BMA	C4-C5-C6-O6
10	T	3	BMA	C4-C5-C6-O6
10	h	3	BMA	C4-C5-C6-O6
6	M	3	BMA	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
6	o	3	BMA	O5-C5-C6-O6
5	Z	5	MAN	C4-C5-C6-O6
5	K	5	MAN	C4-C5-C6-O6
5	n	5	MAN	C4-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
8	q	1	NAG	C4-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
6	o	3	BMA	C4-C5-C6-O6
8	O	2	NAG	C1-C2-N2-C7
8	c	2	NAG	C1-C2-N2-C7
8	q	2	NAG	C1-C2-N2-C7
9	R	1	NAG	O5-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6

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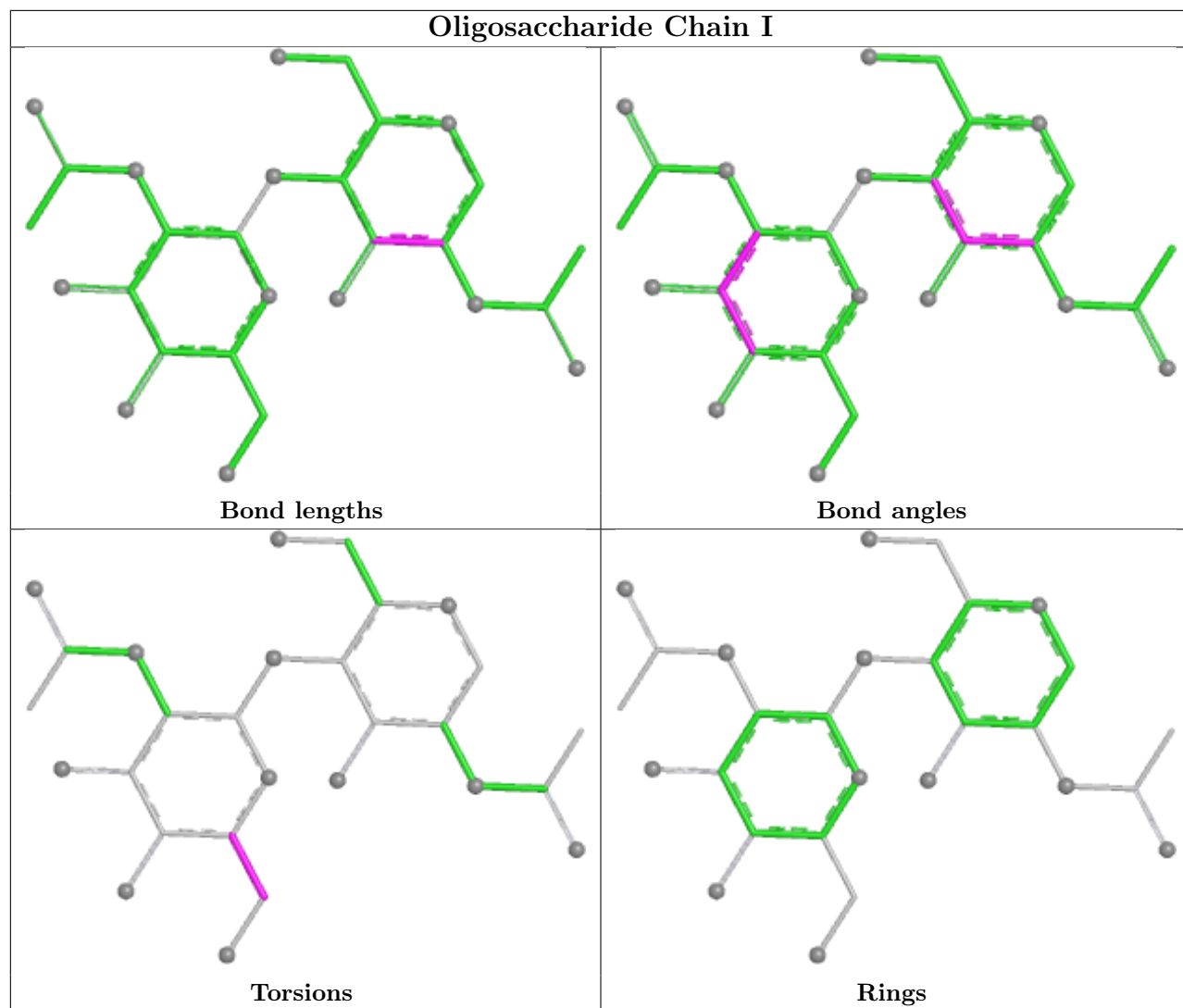
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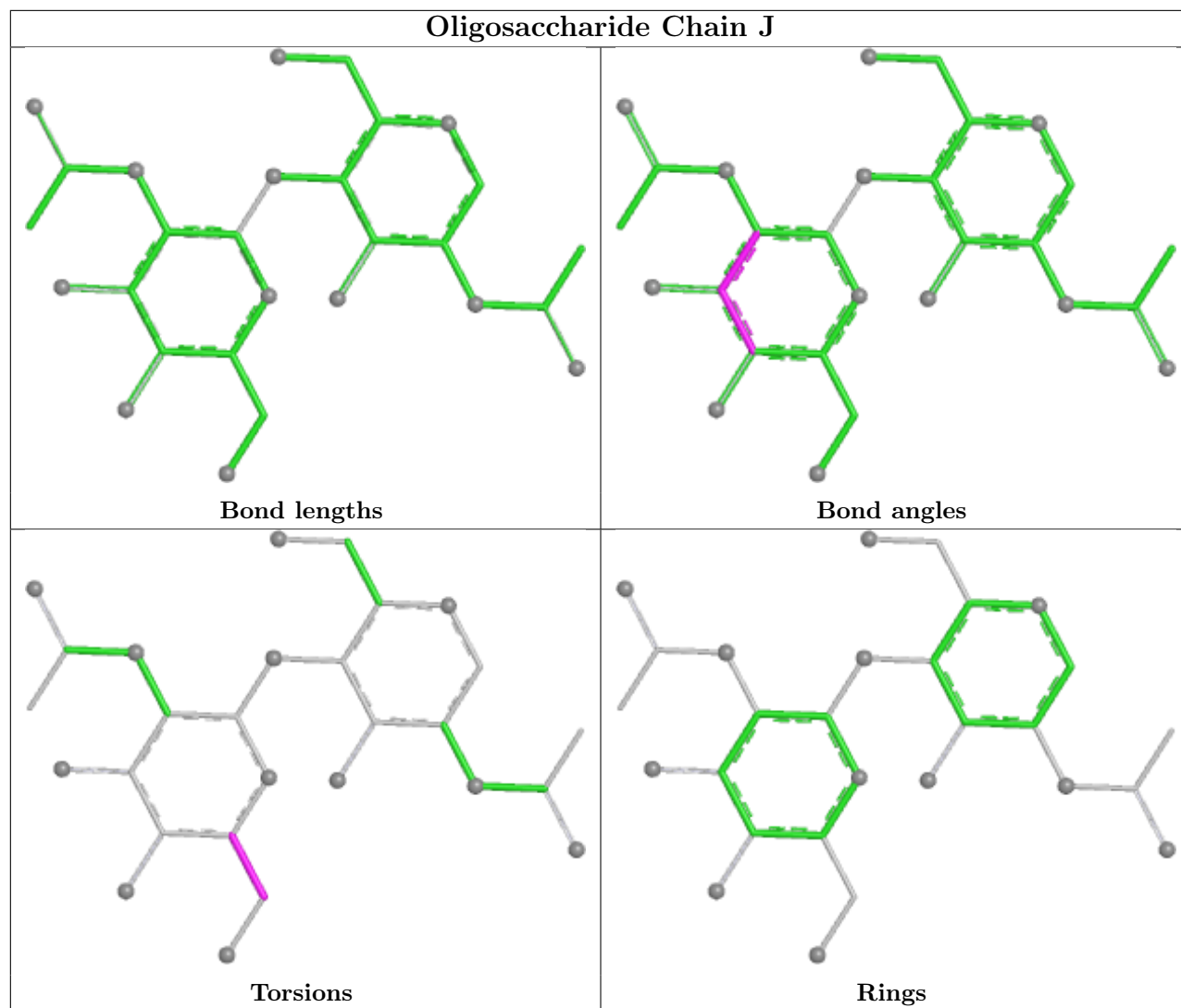
Mol	Chain	Res	Type	Atoms
9	t	1	NAG	O5-C5-C6-O6
8	O	7	MAN	C4-C5-C6-O6
8	q	7	MAN	C4-C5-C6-O6
4	w	2	NAG	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
8	c	7	MAN	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
8	O	4	MAN	C4-C5-C6-O6
8	c	4	MAN	C4-C5-C6-O6
8	q	4	MAN	C4-C5-C6-O6

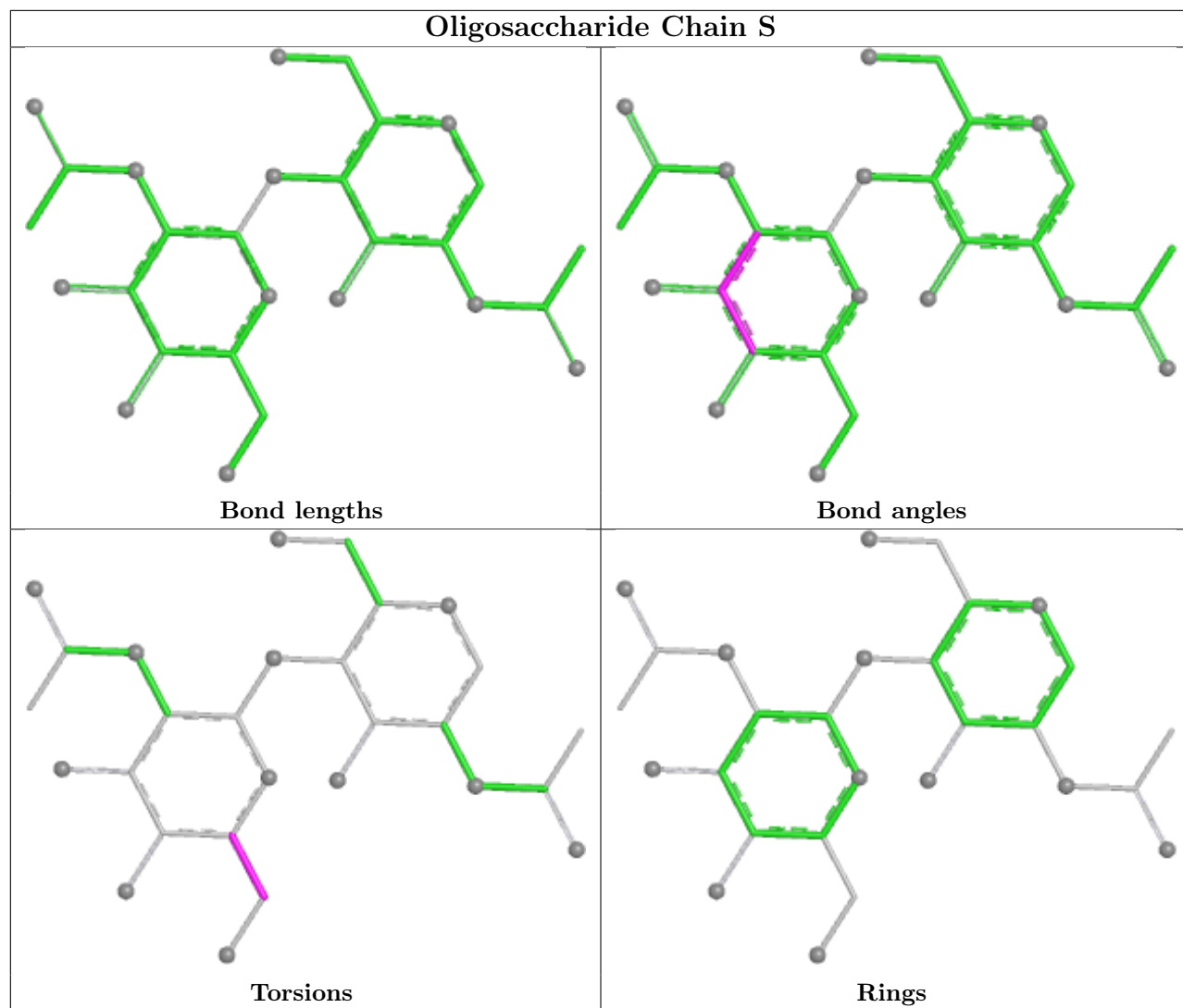
There are no ring outliers.

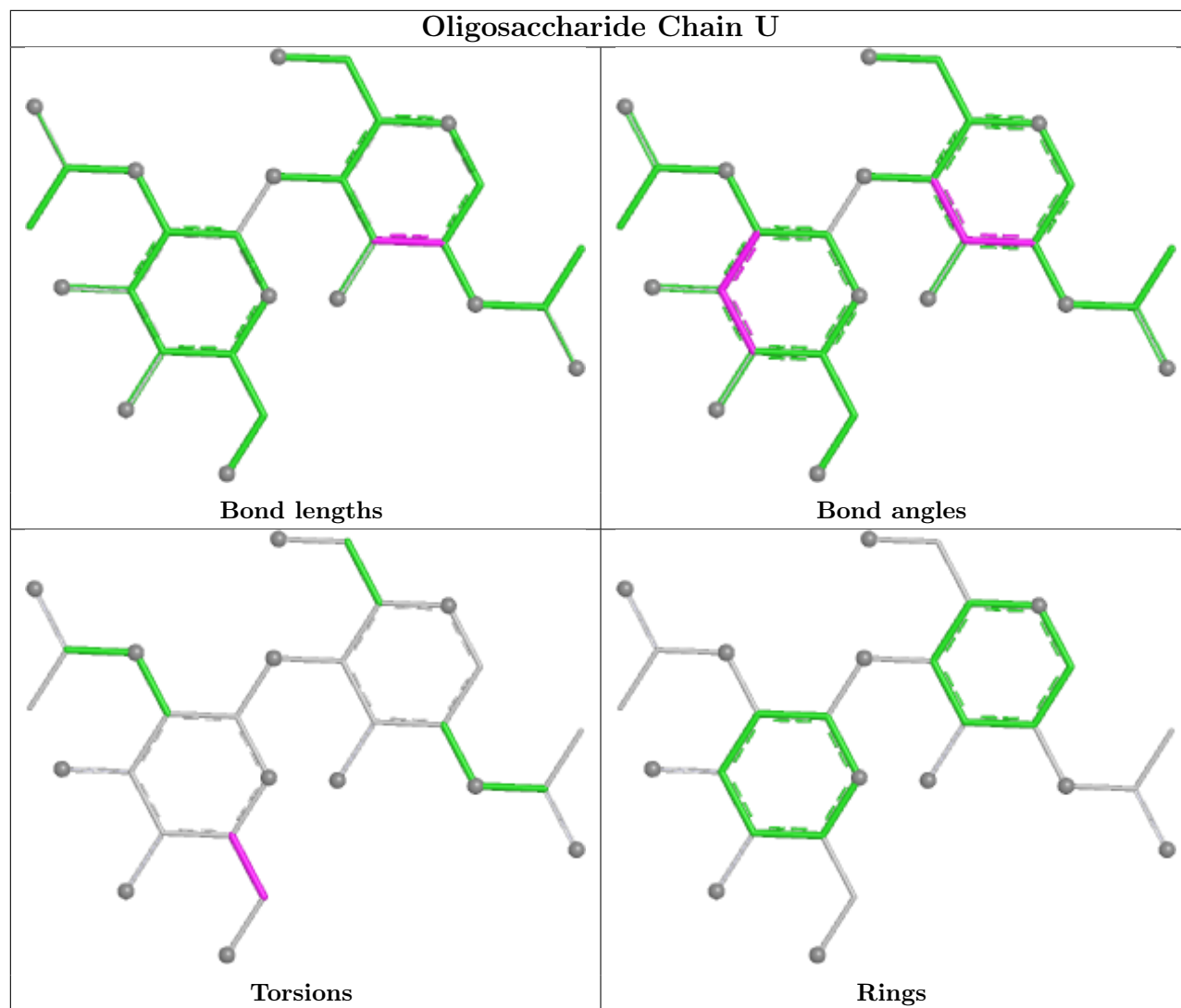
No monomer is involved in short contacts.

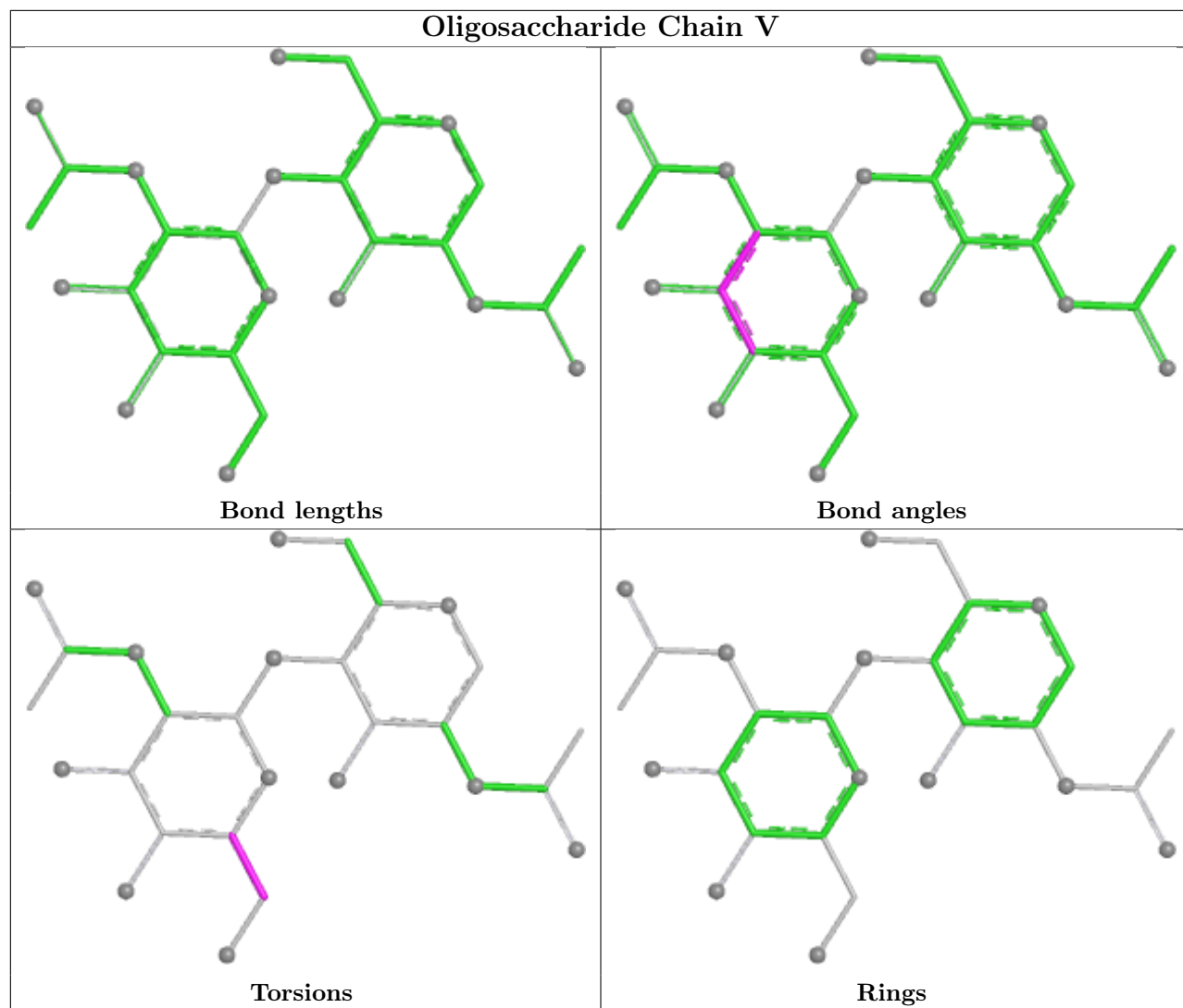
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

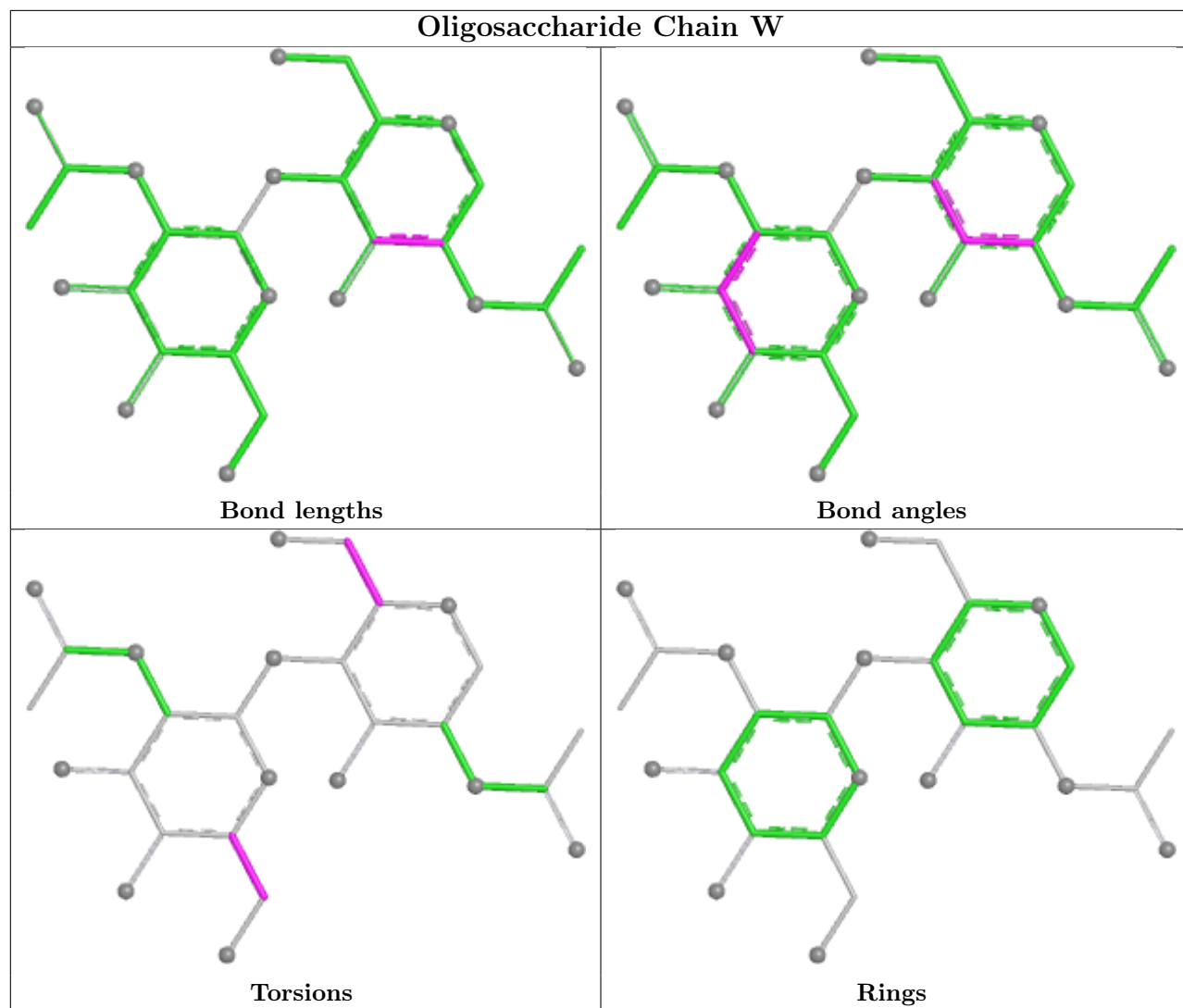


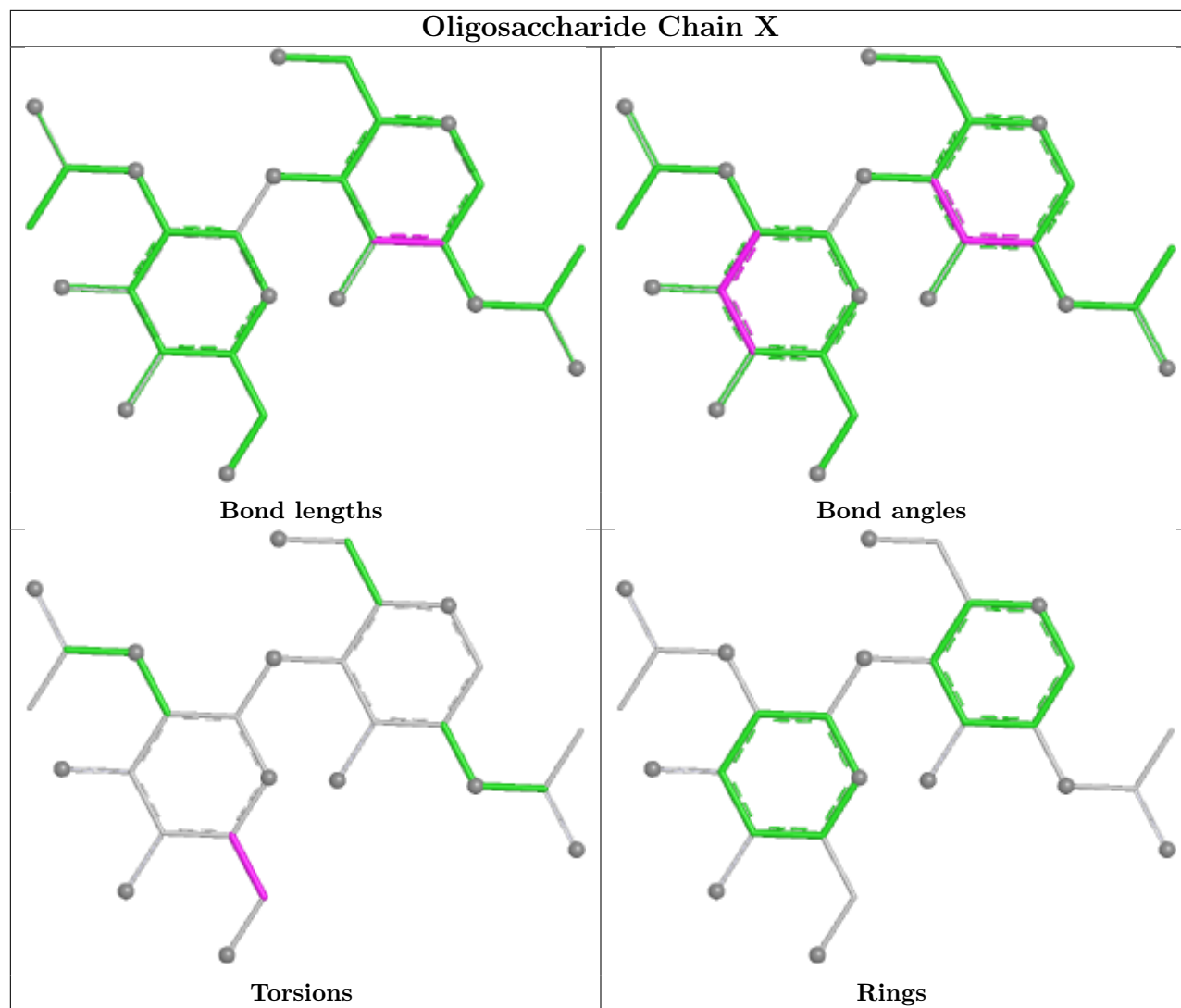


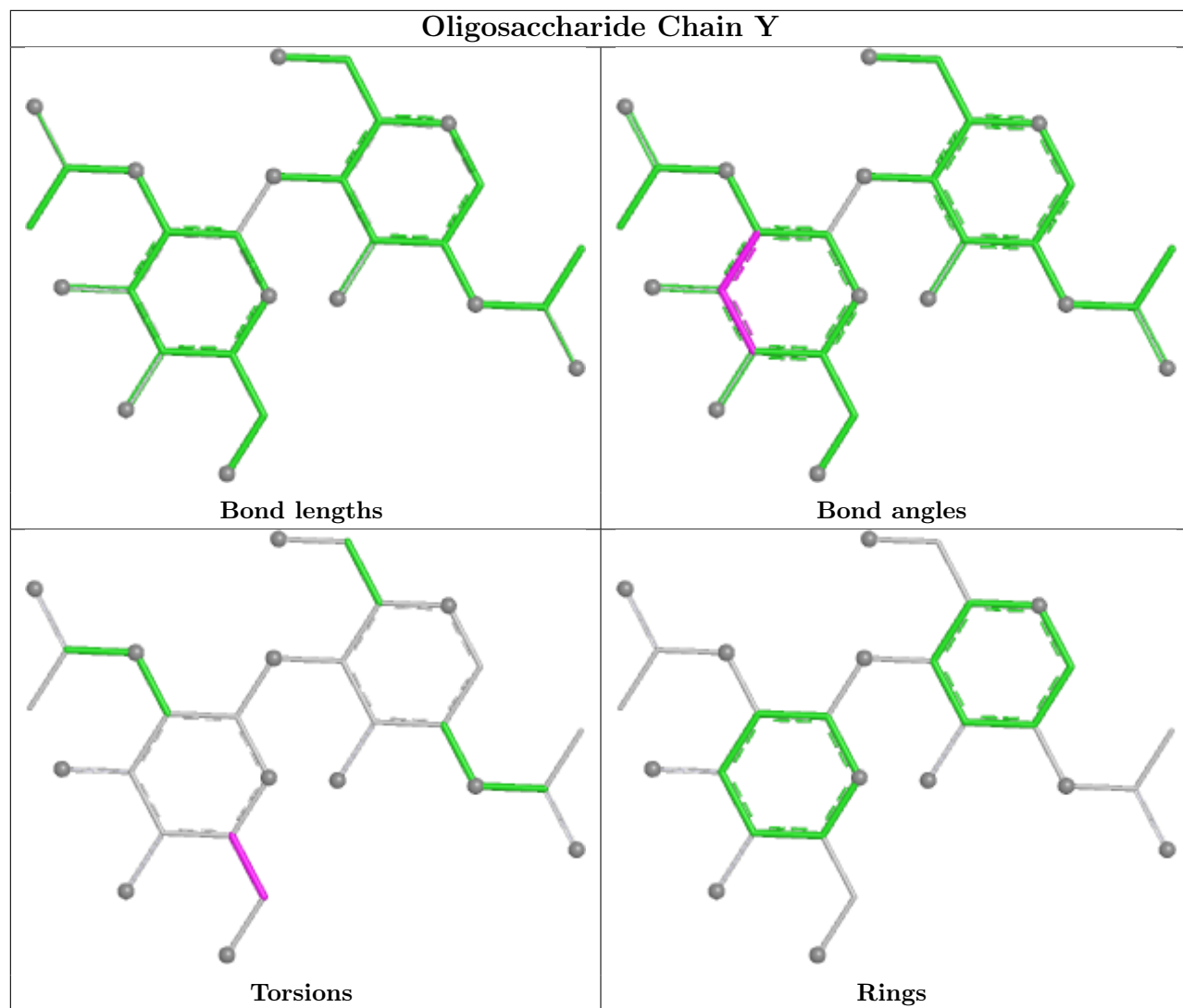


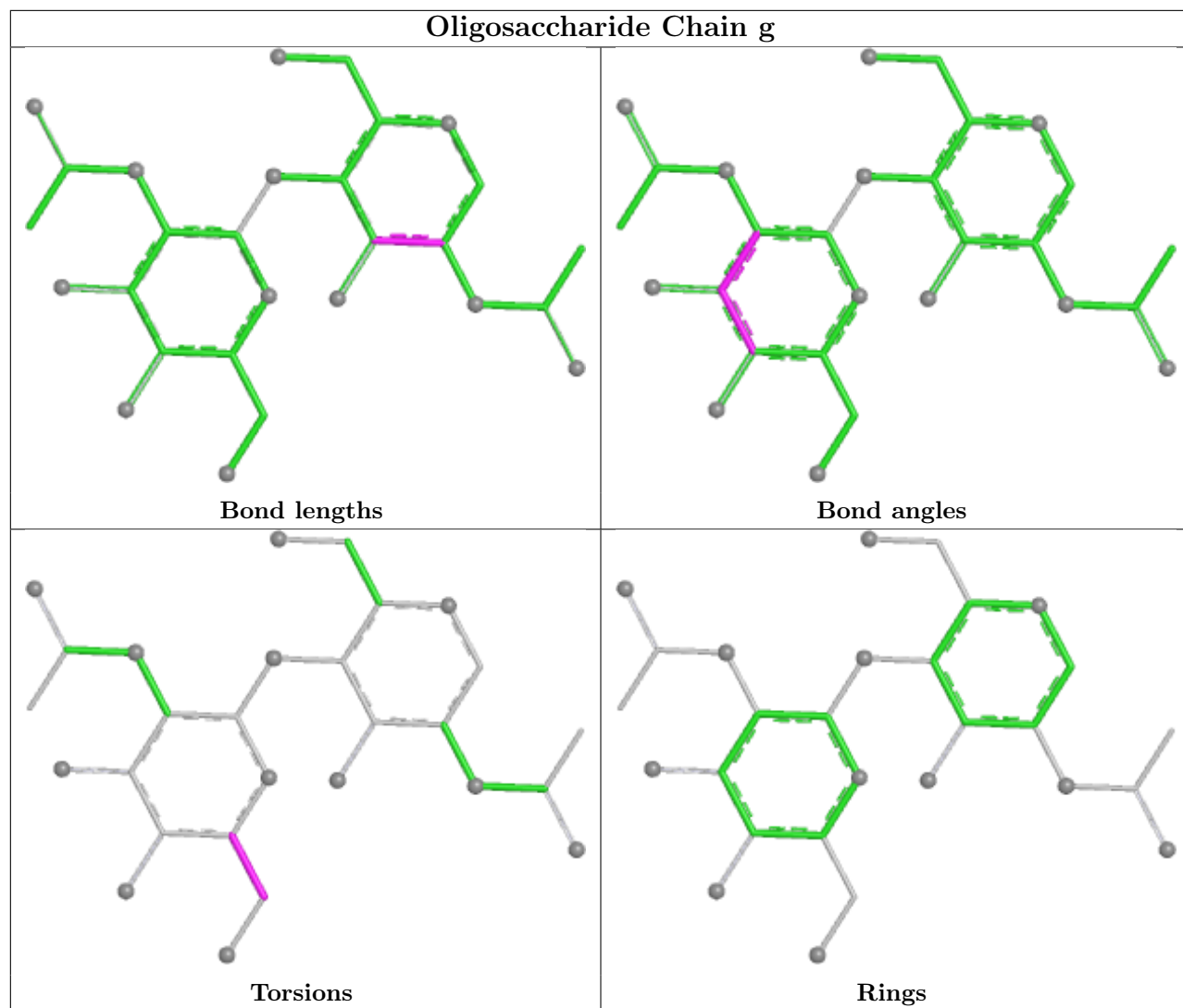


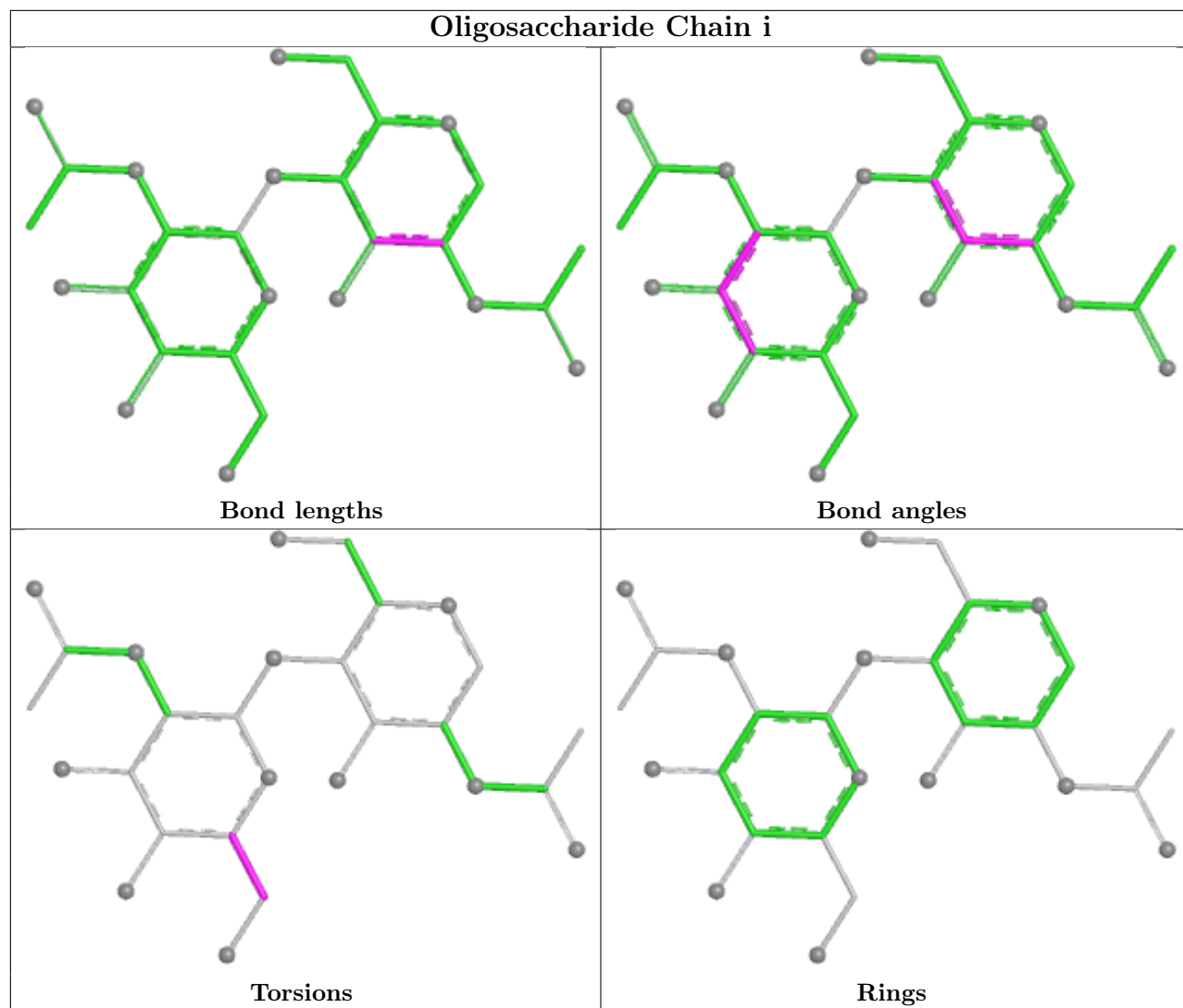


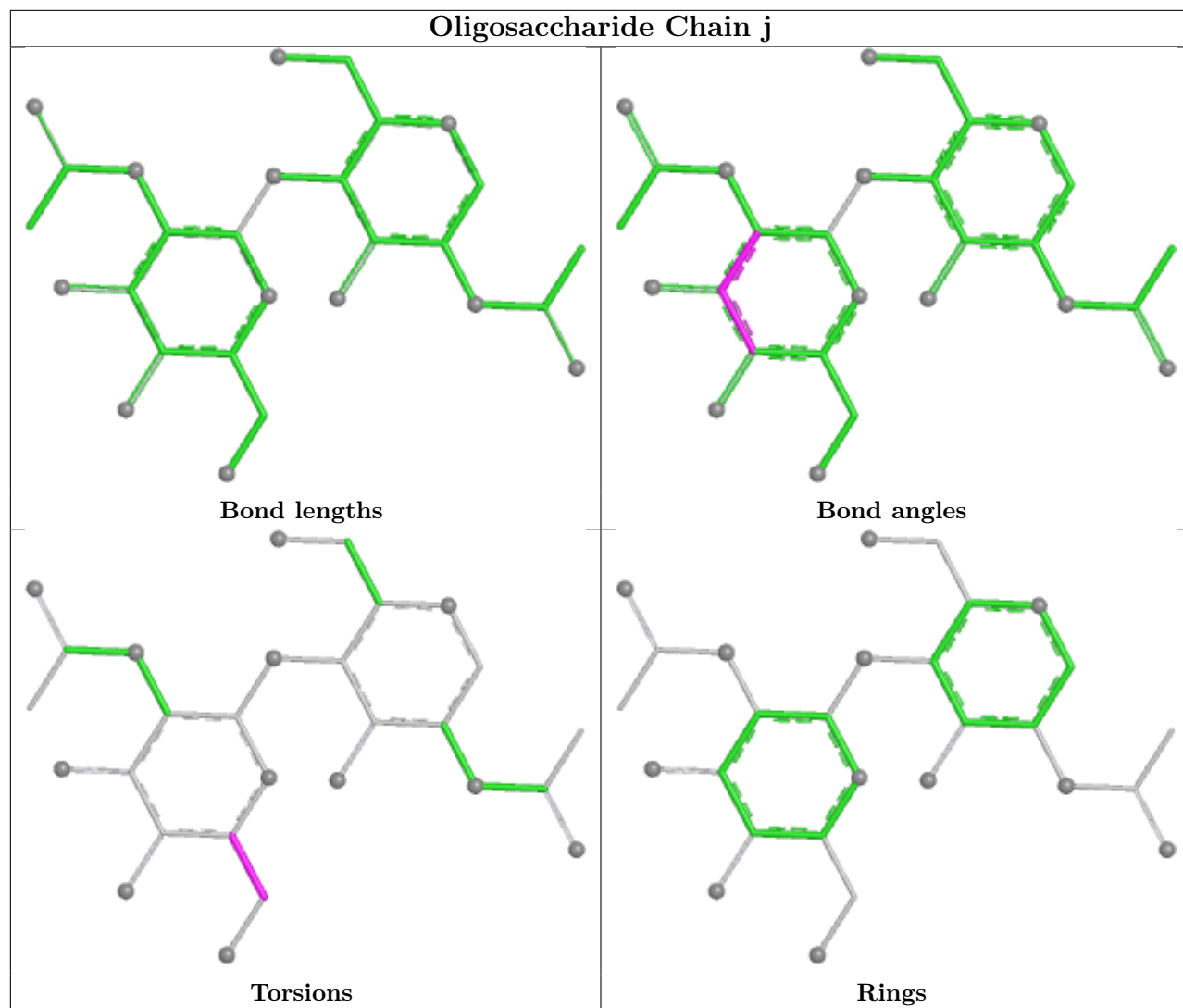


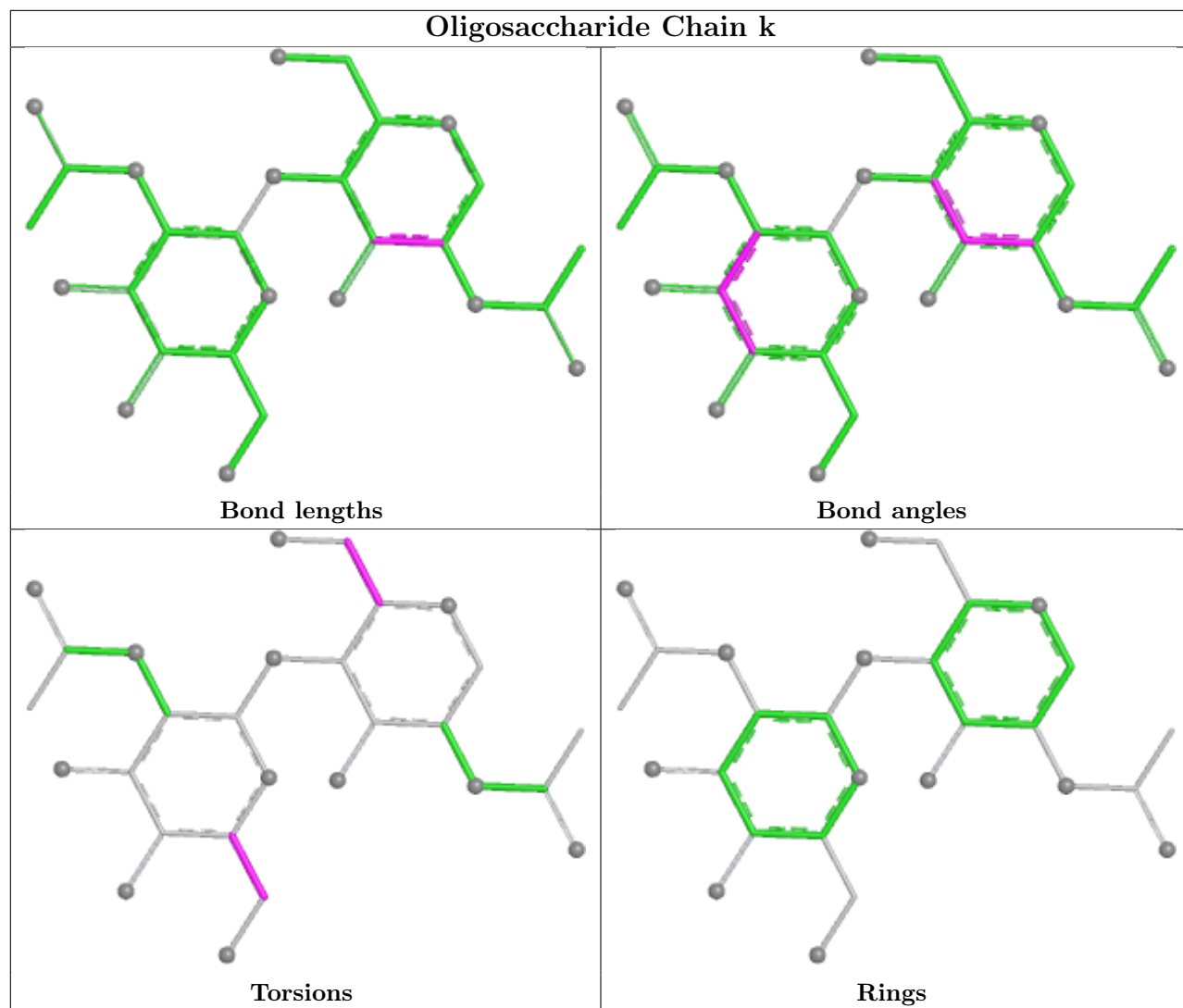


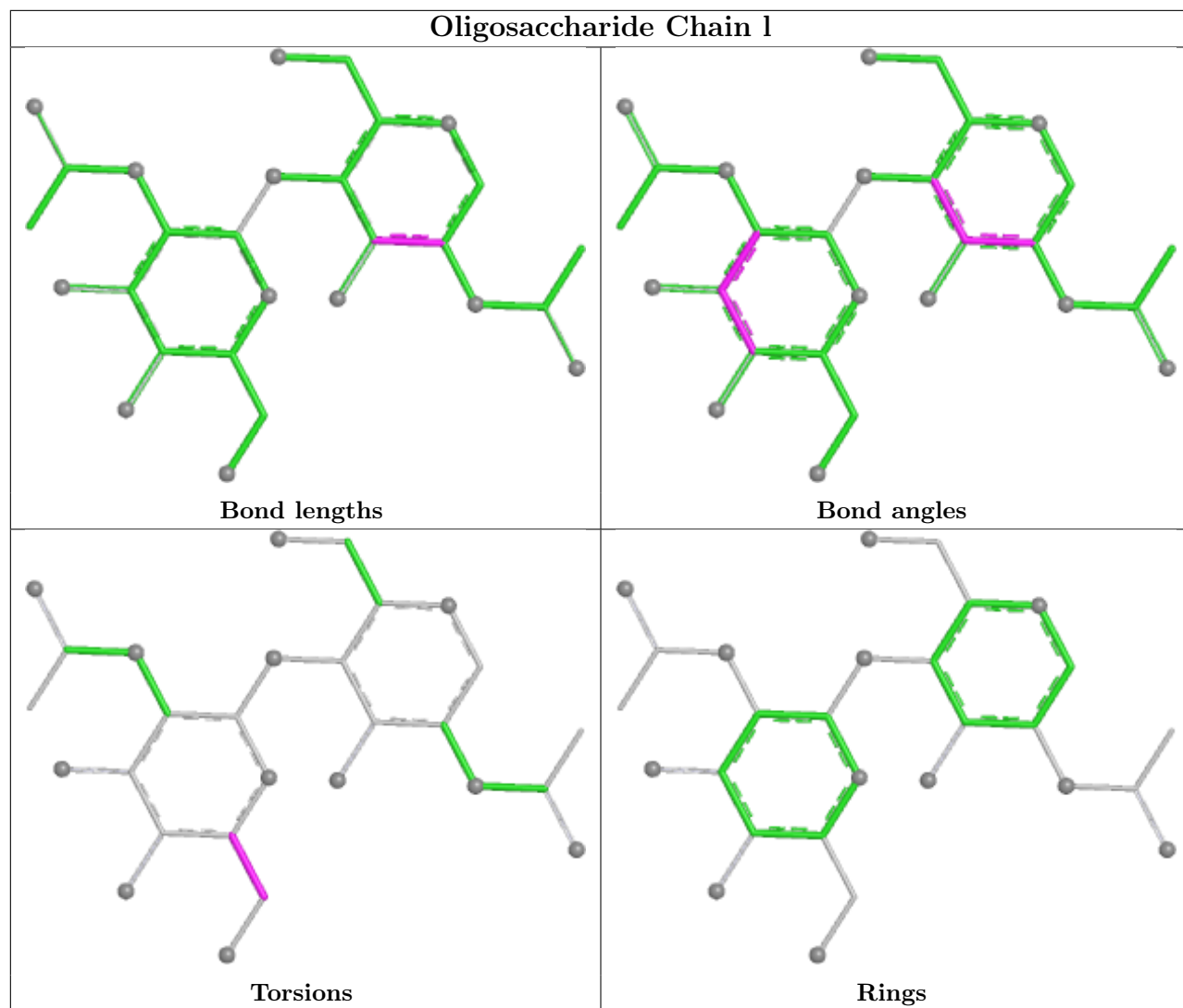


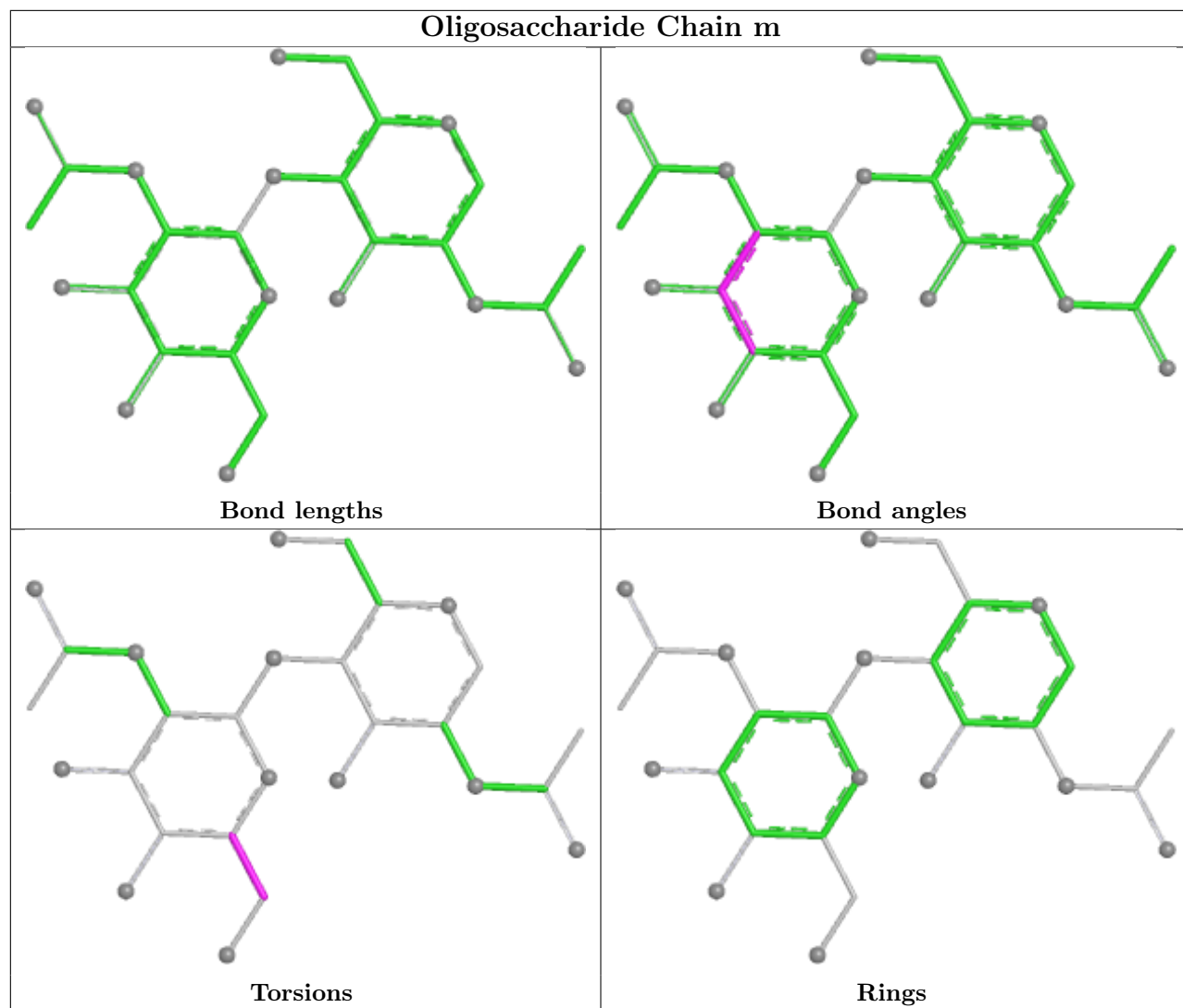


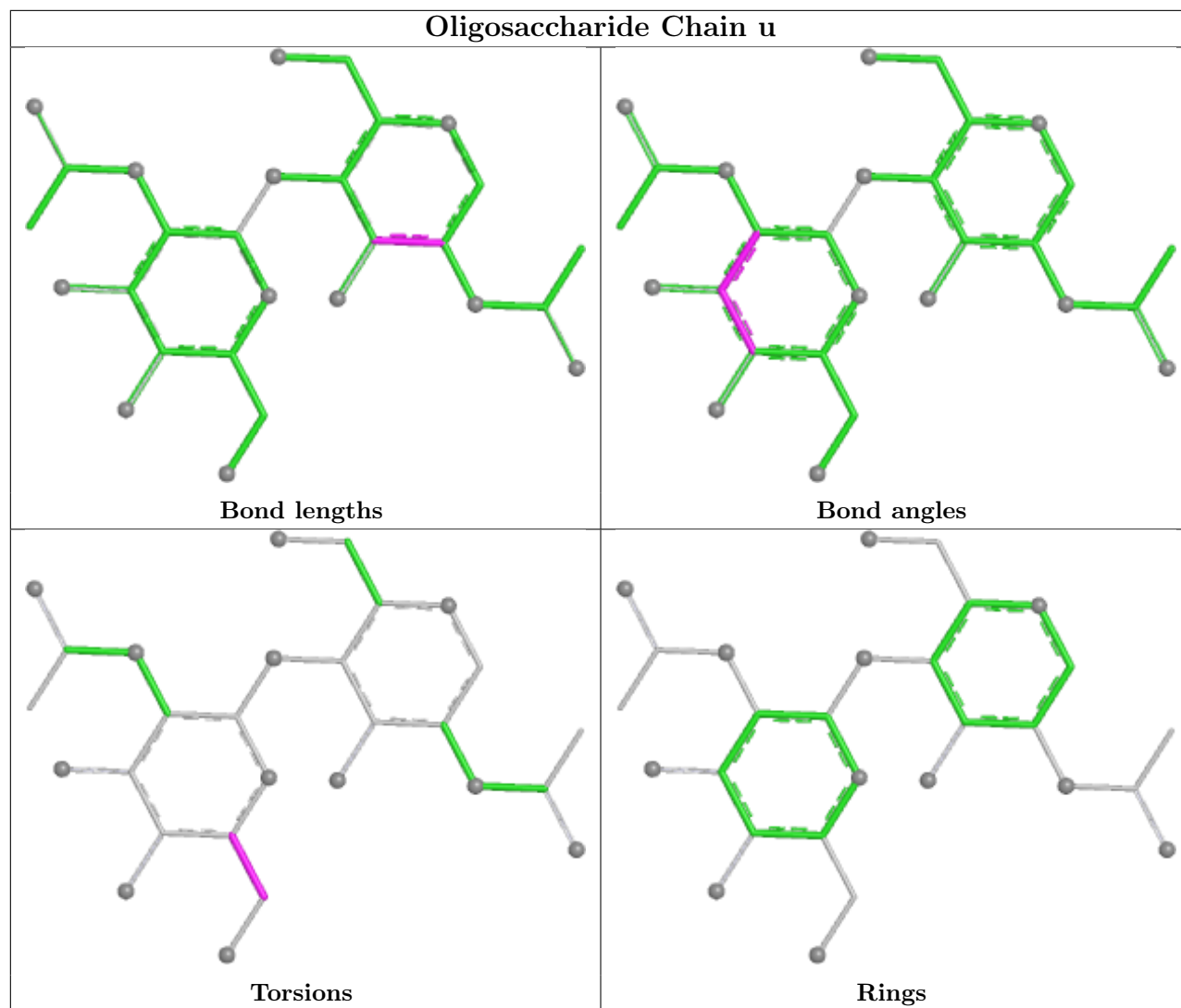


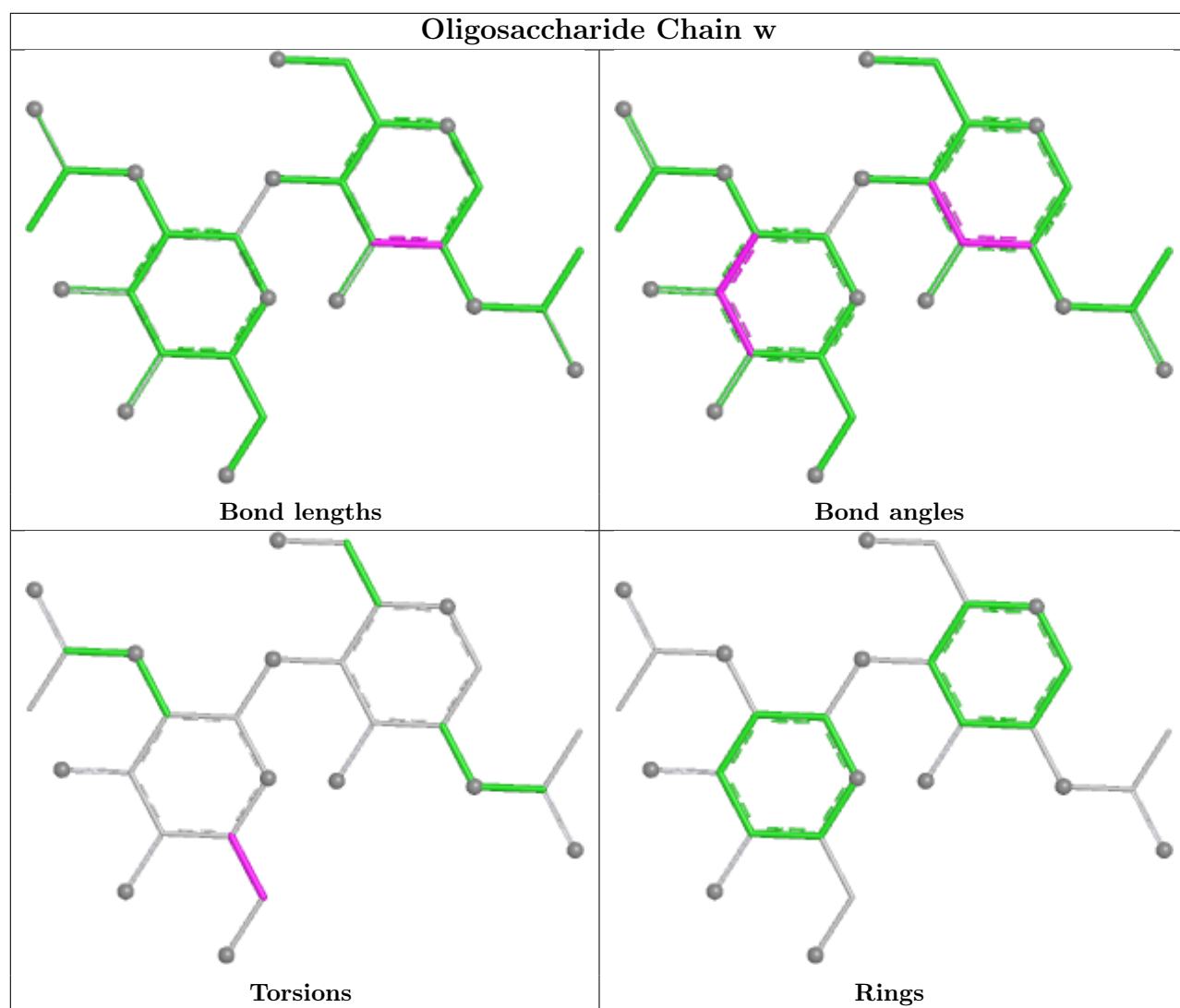


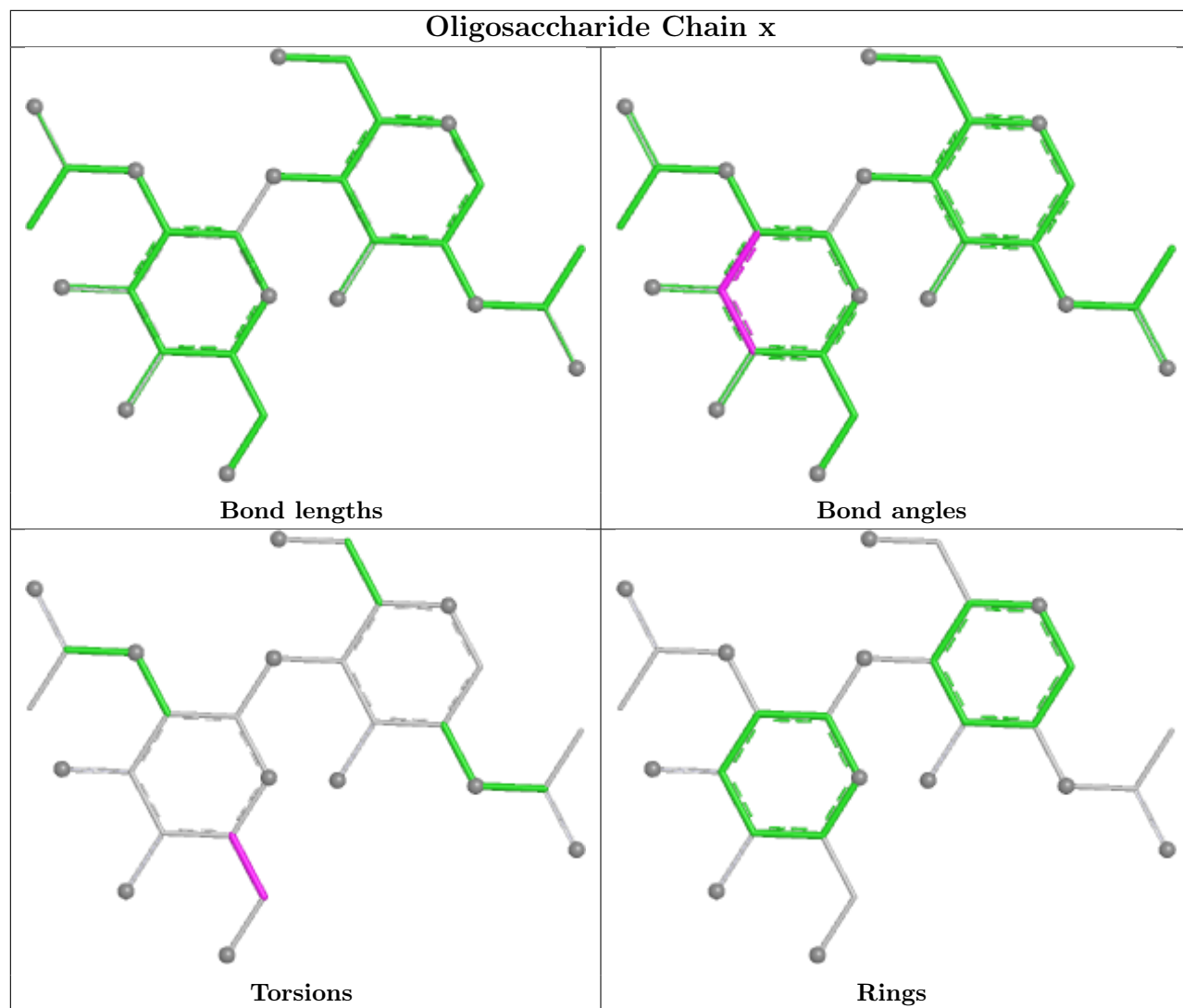


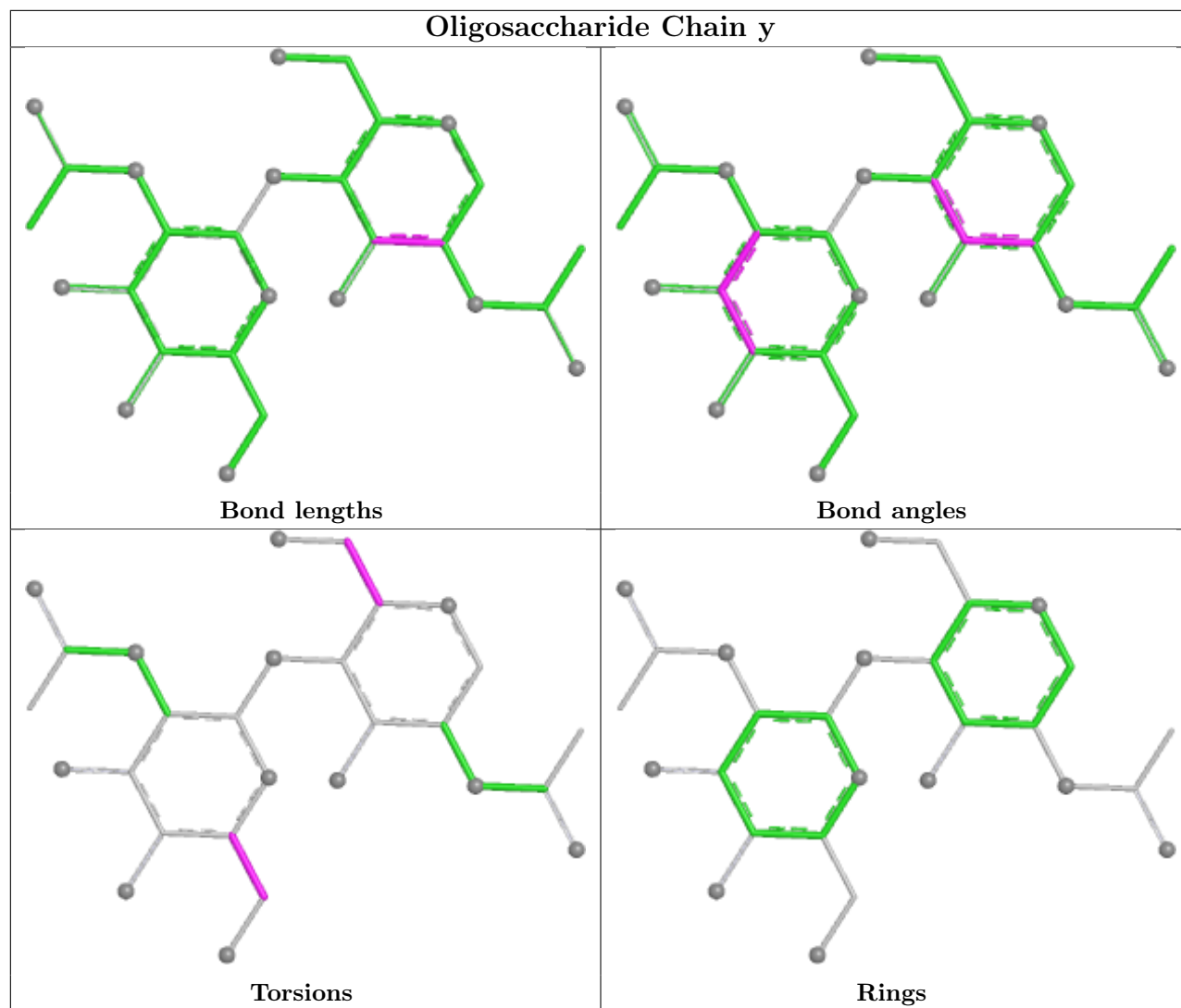


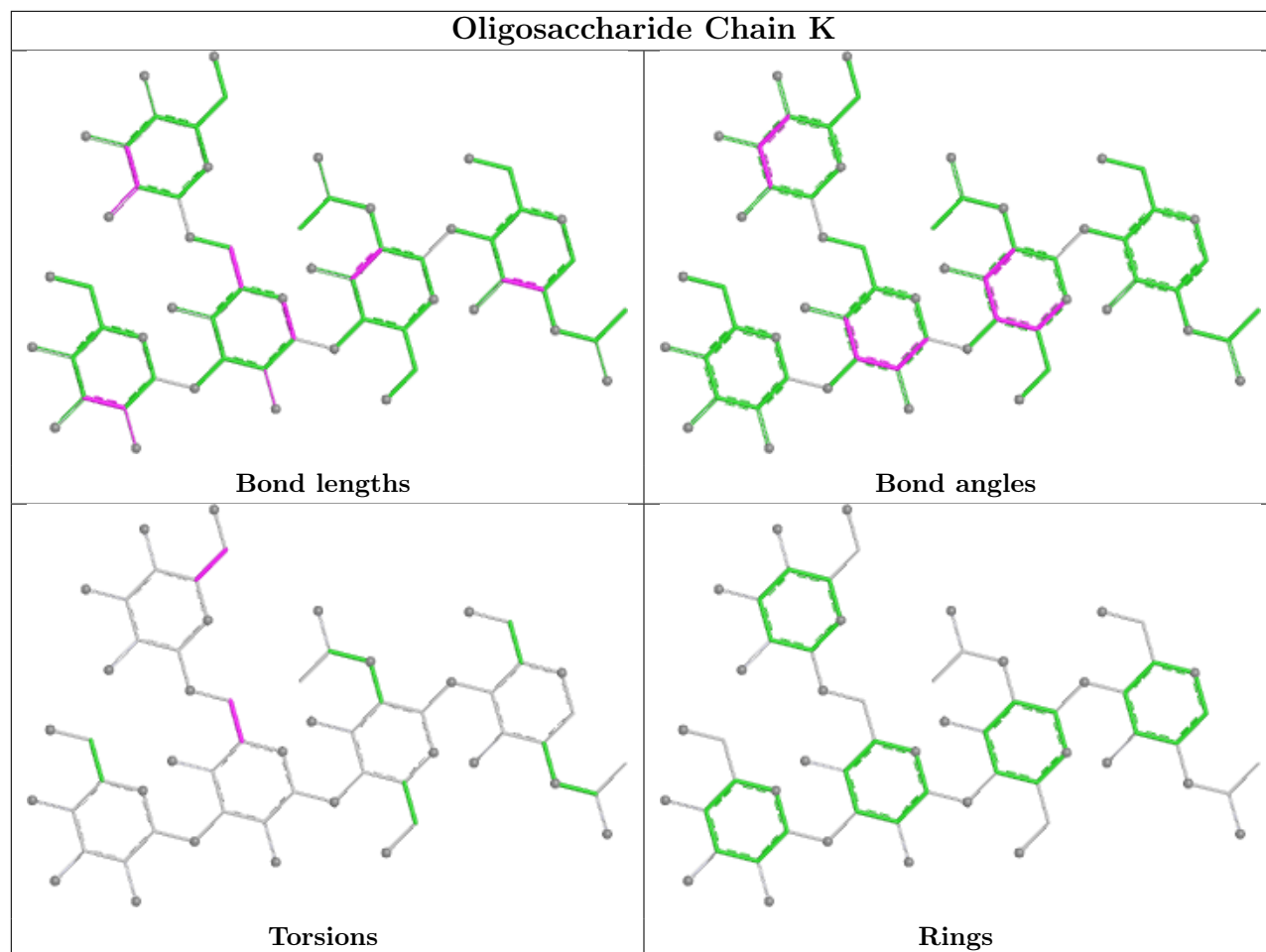


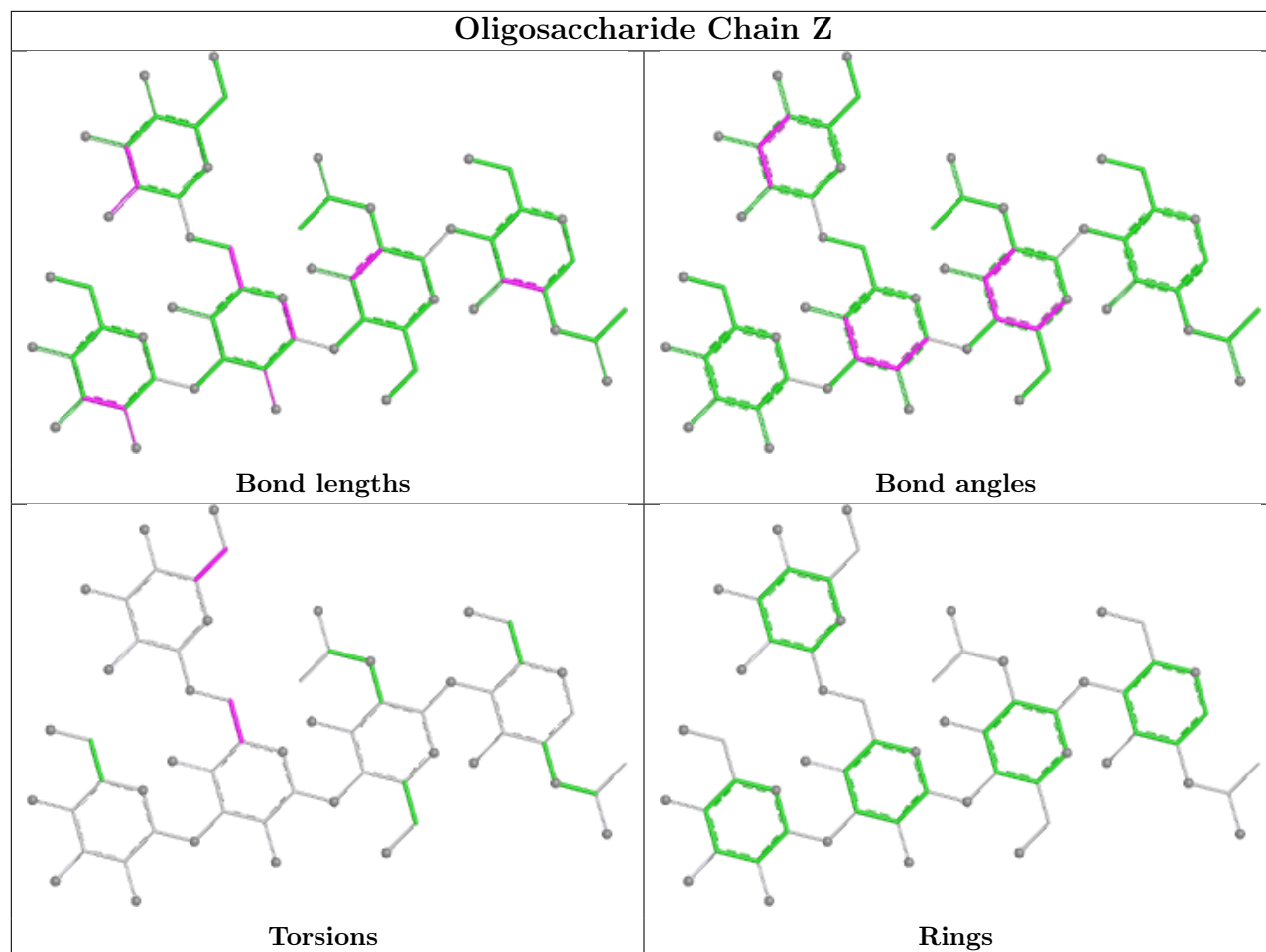


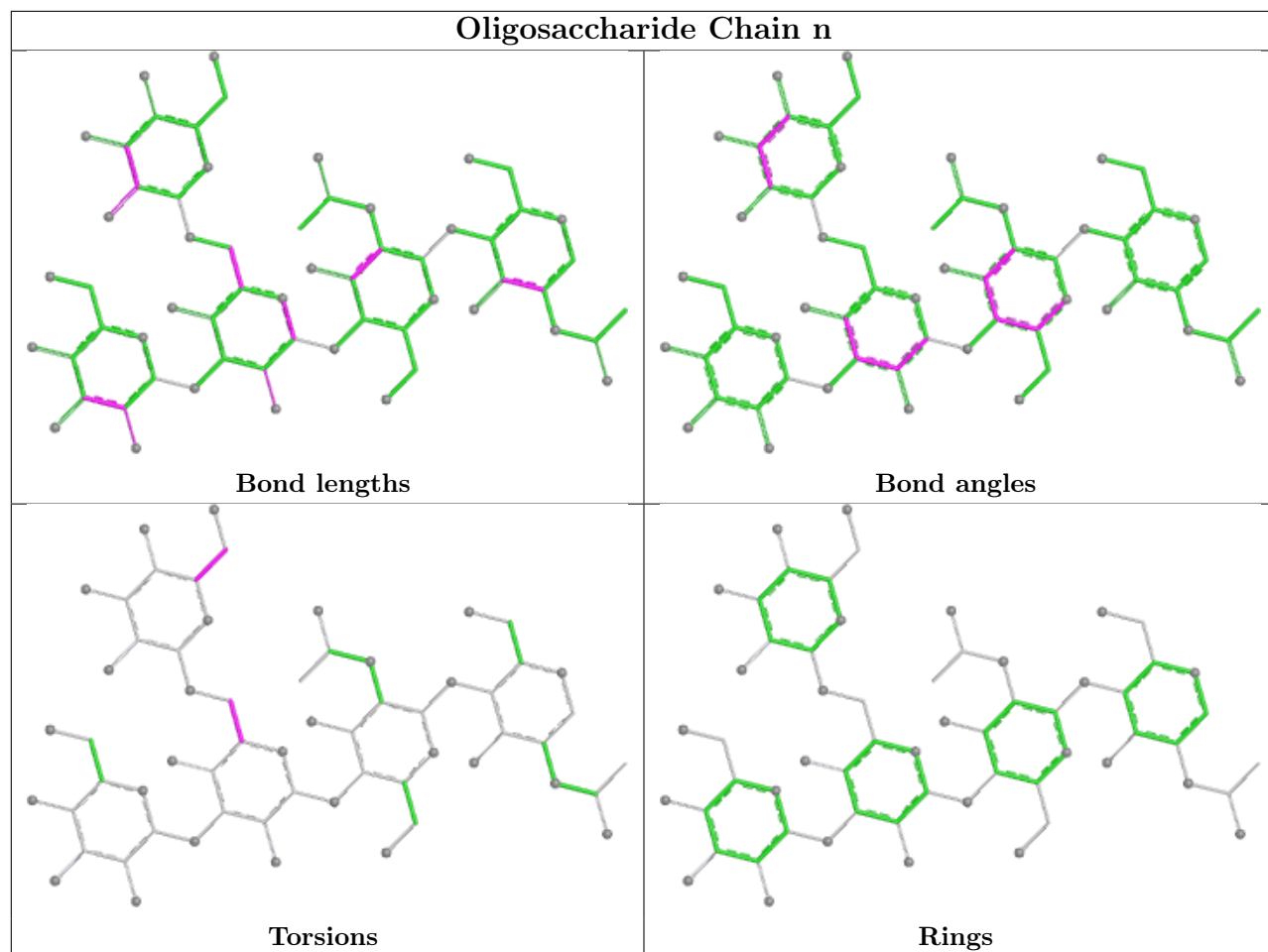


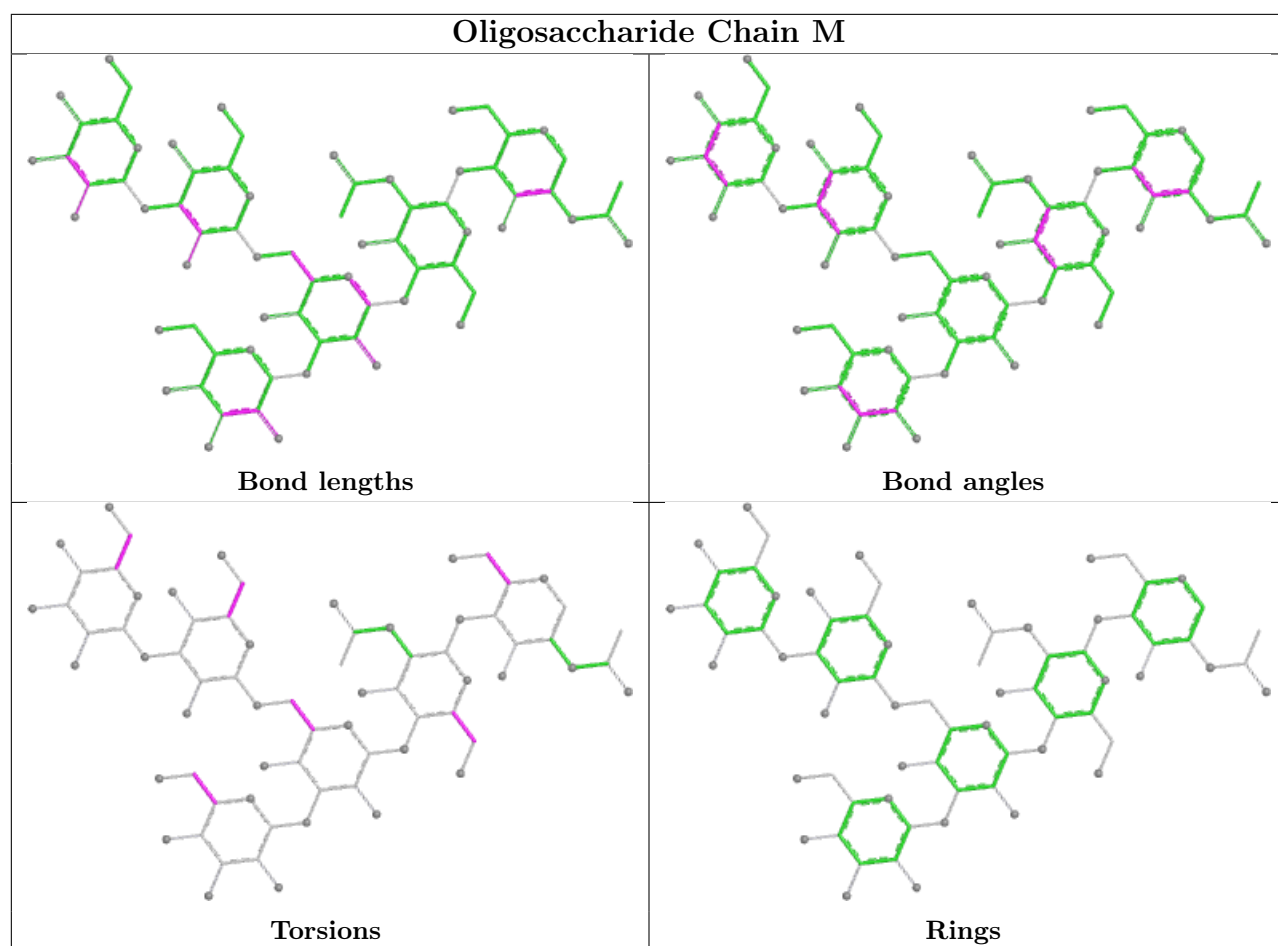


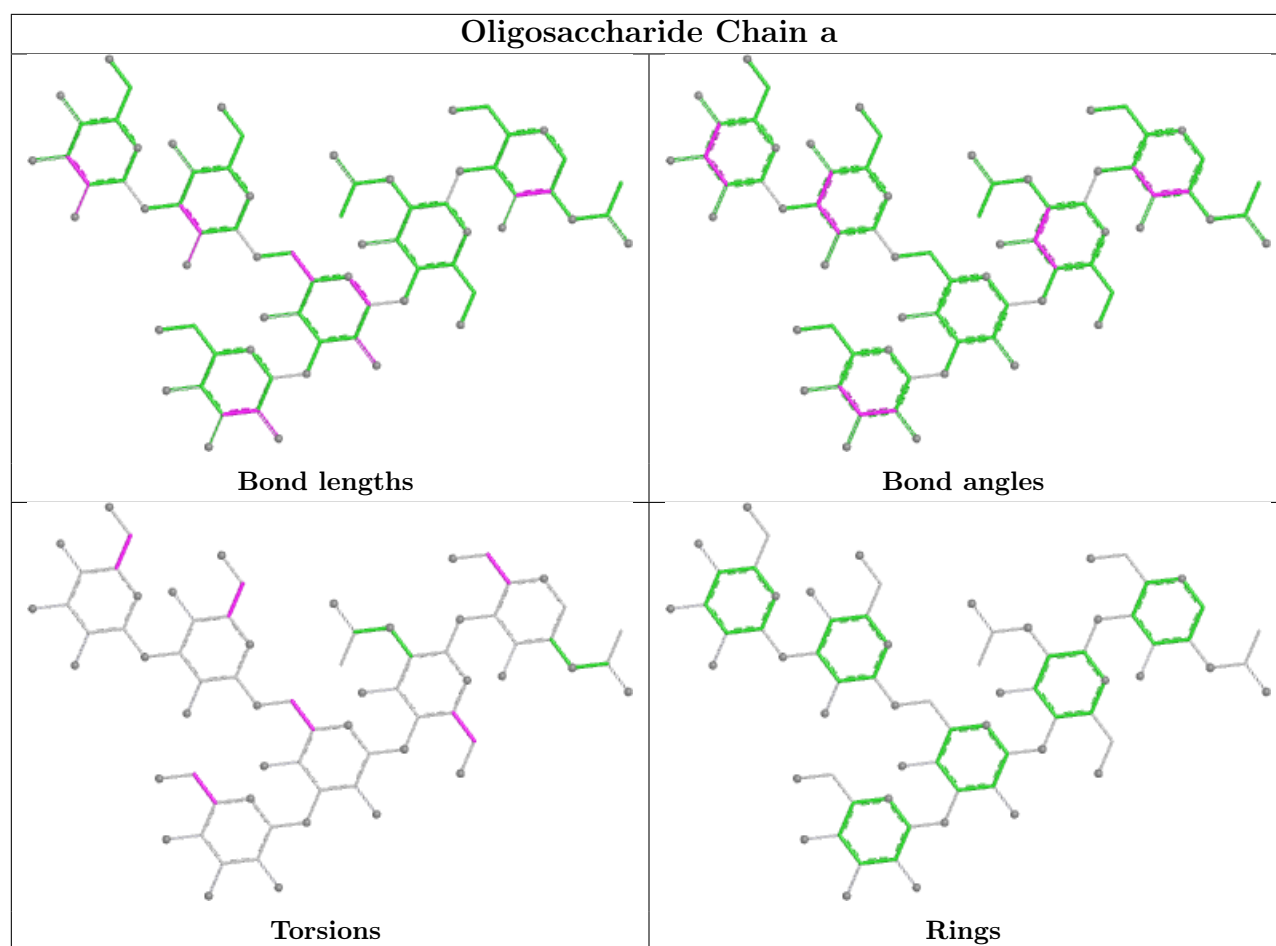


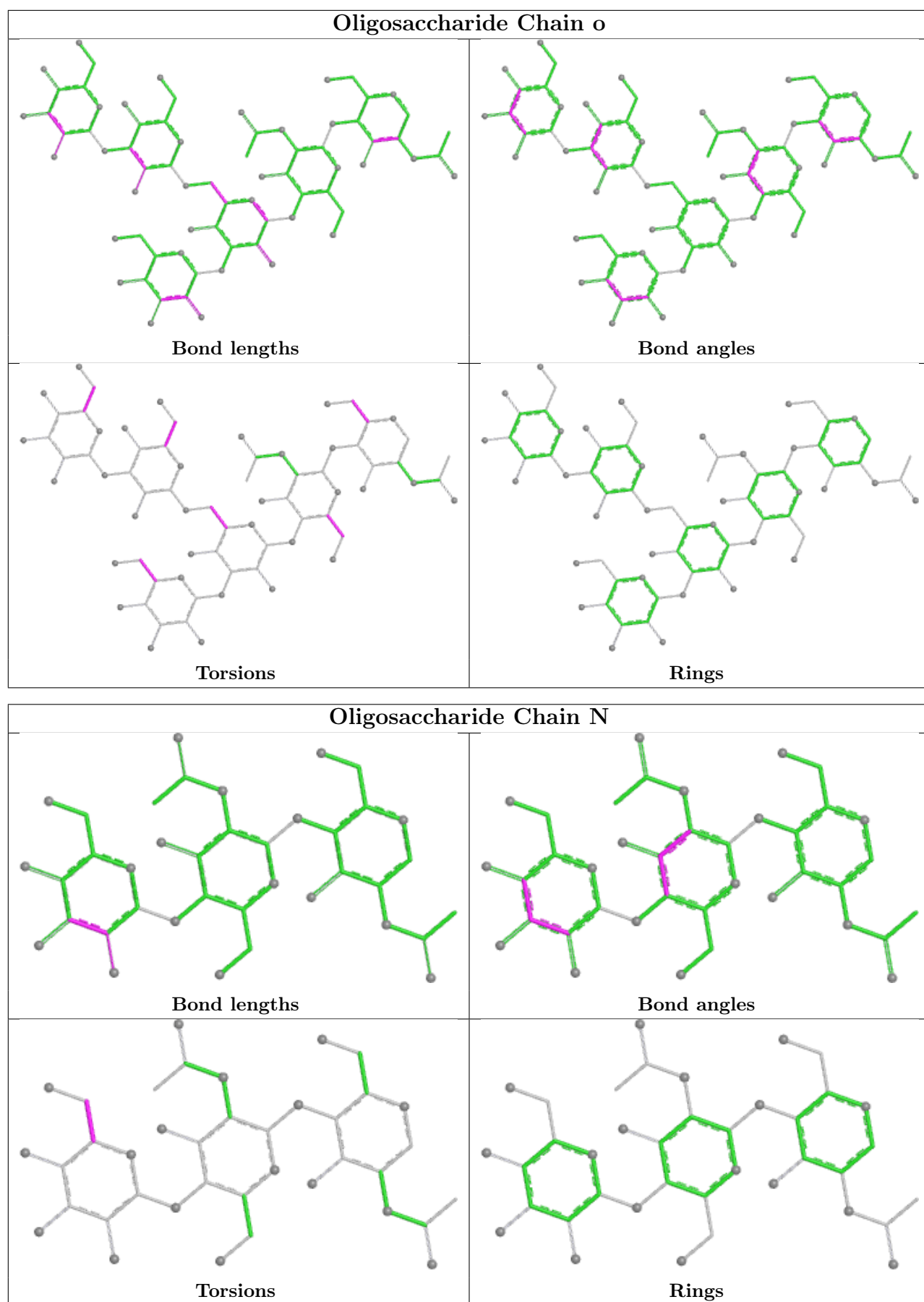


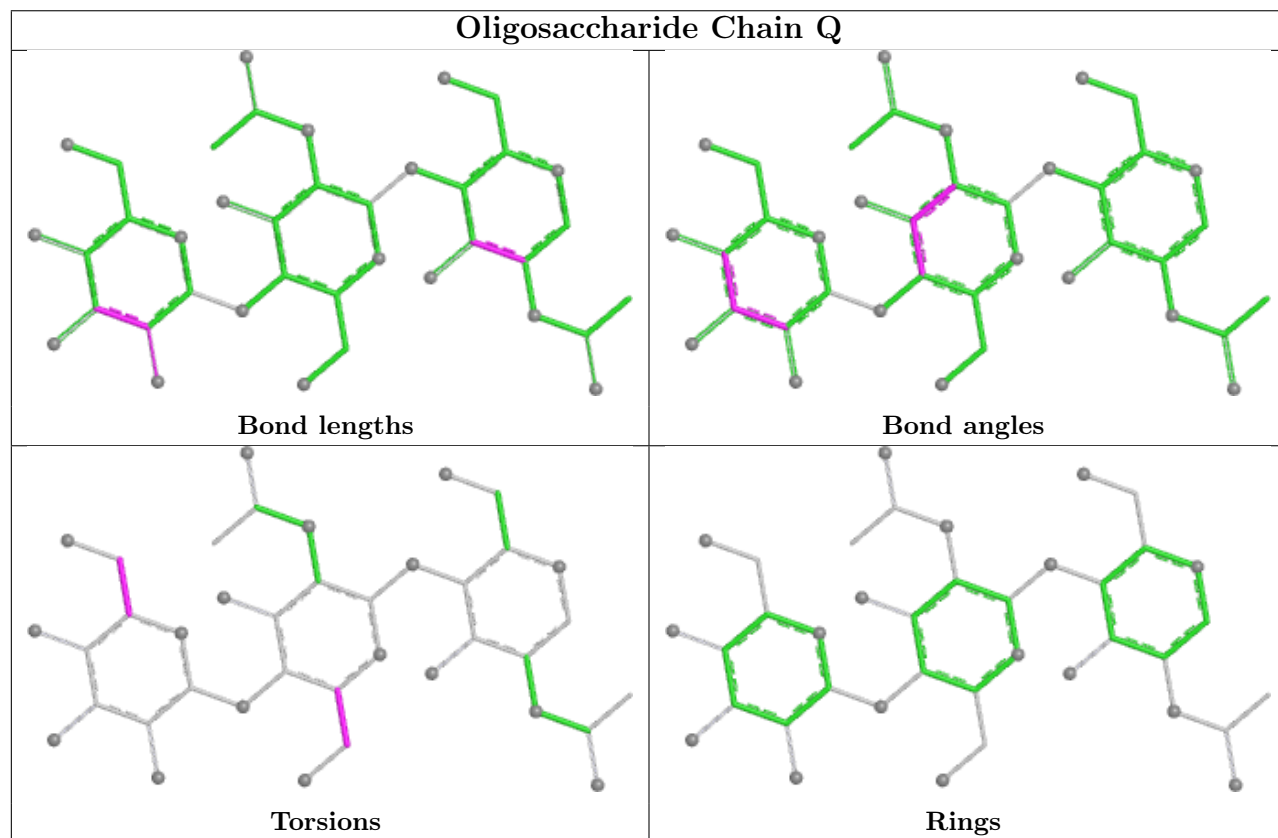
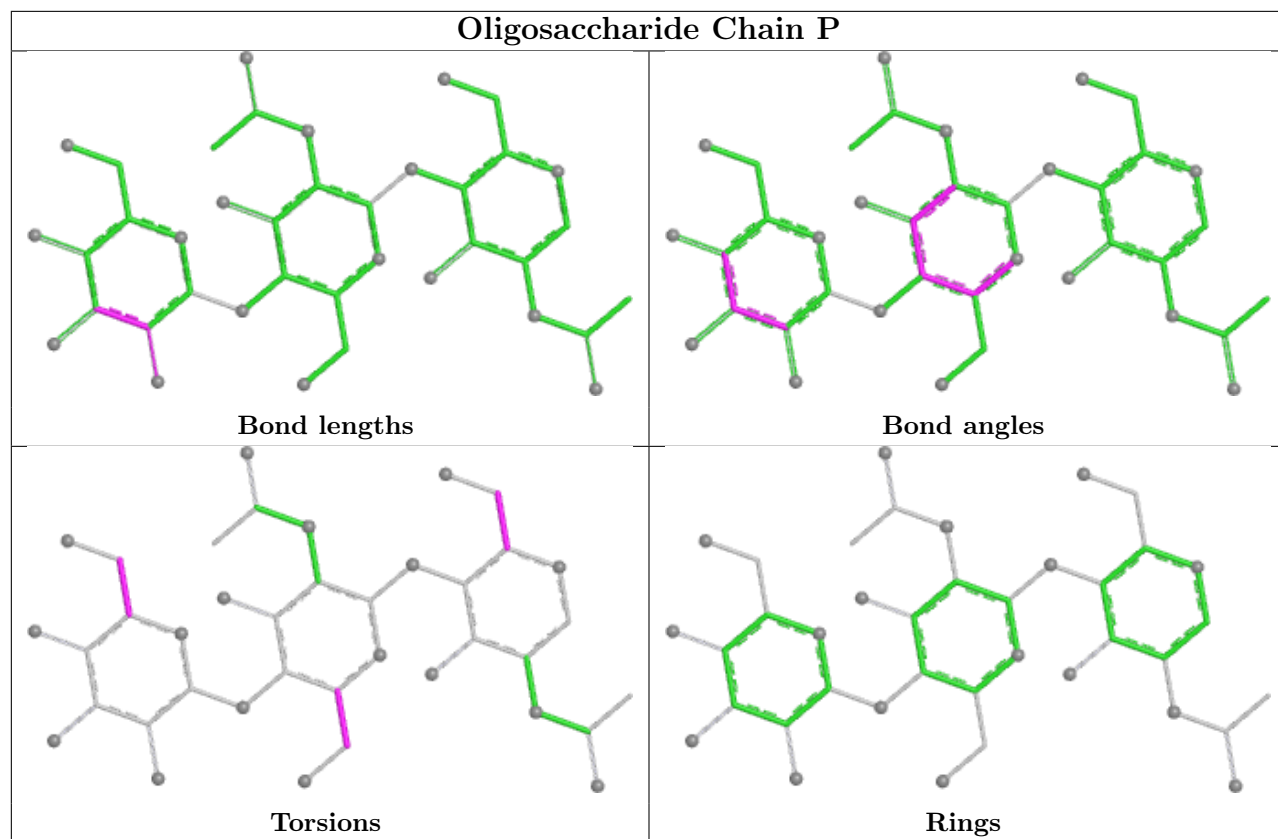


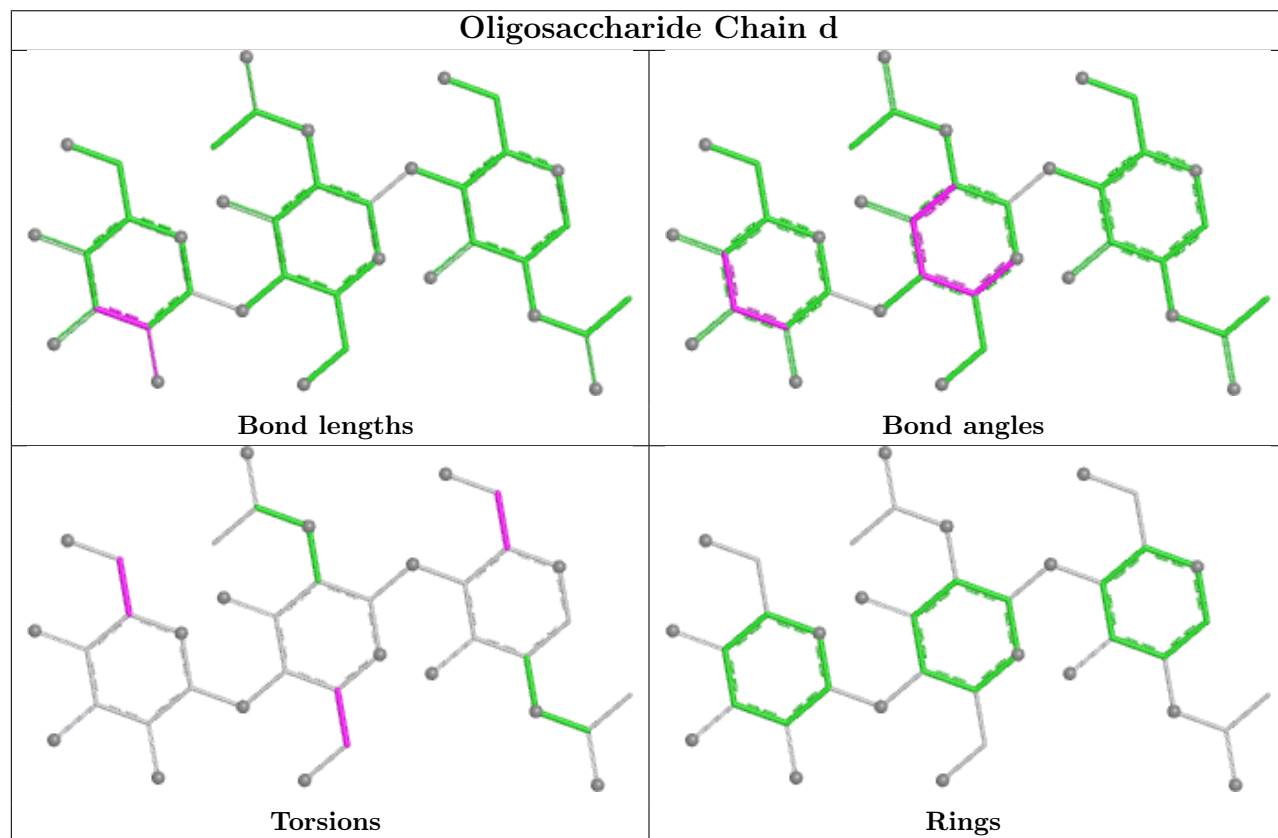
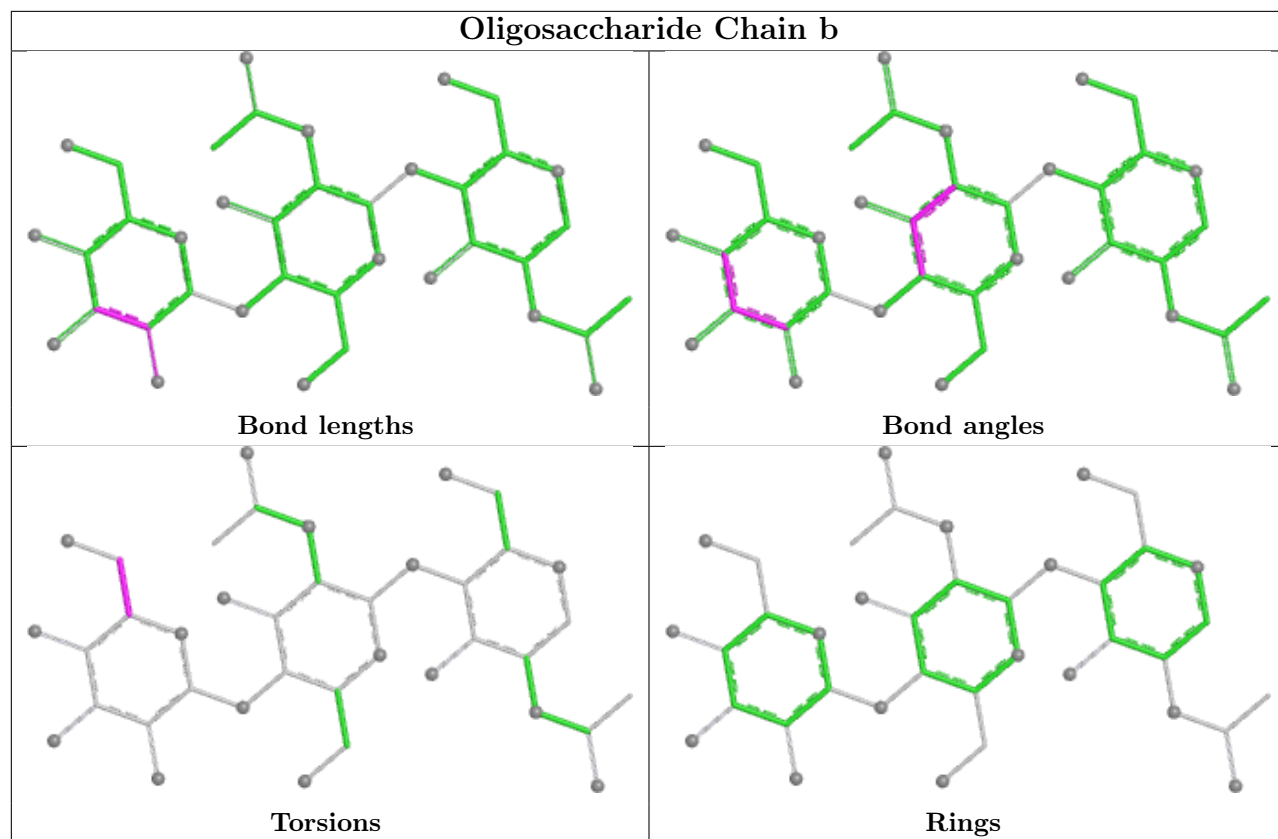


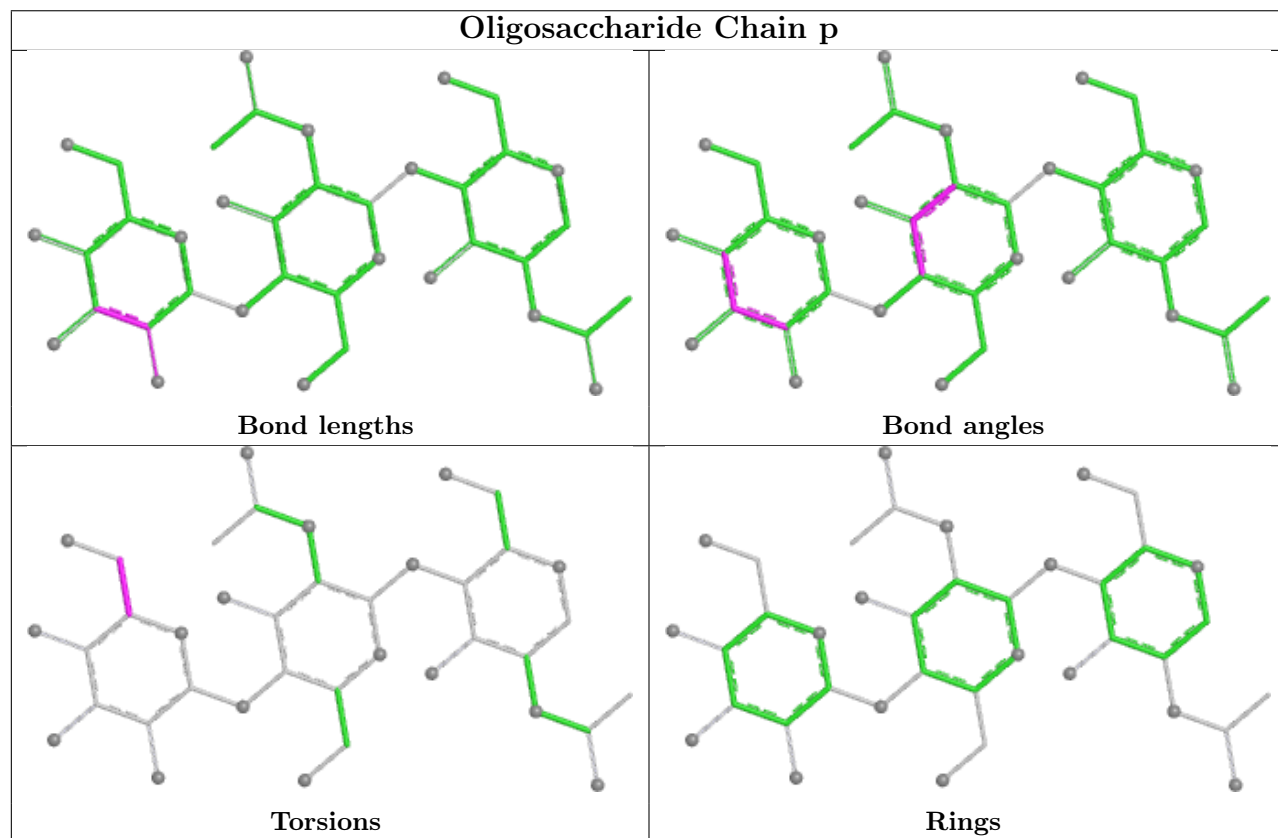
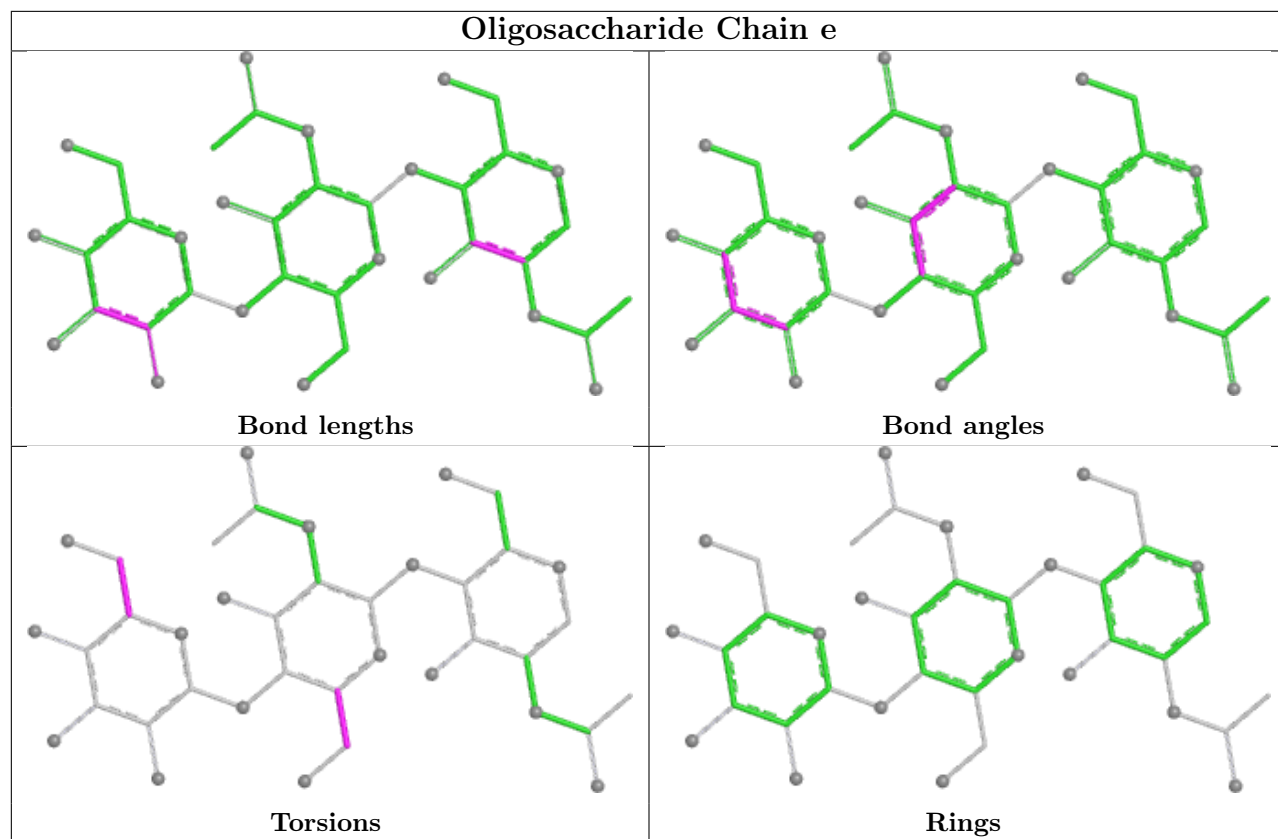


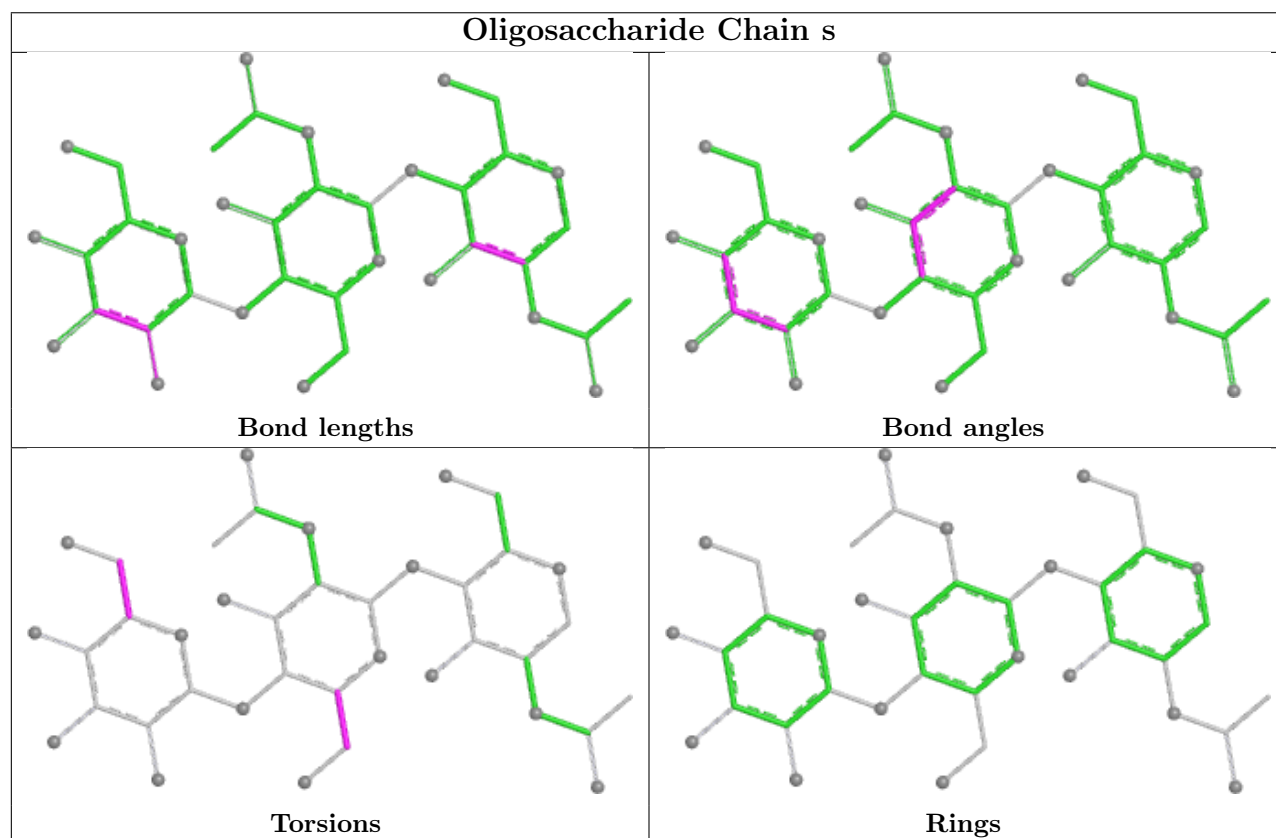
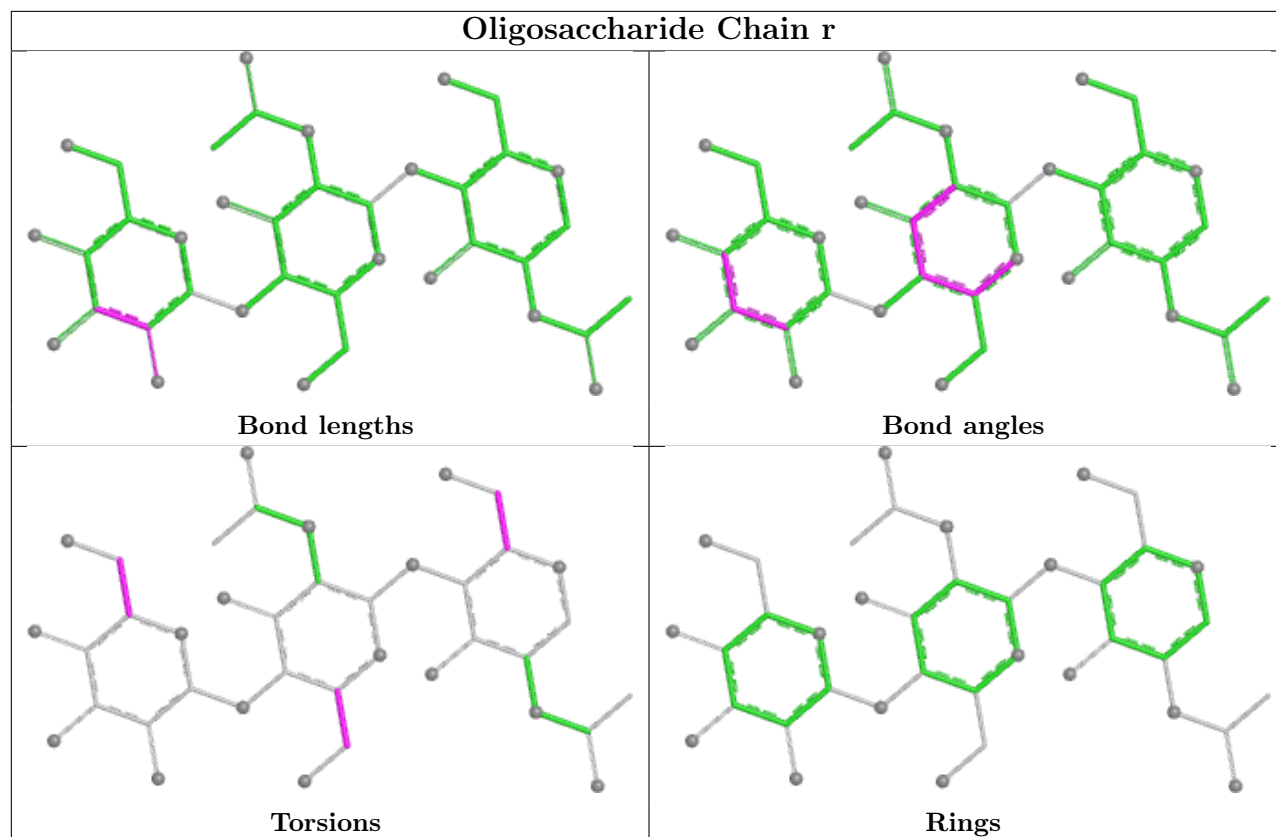


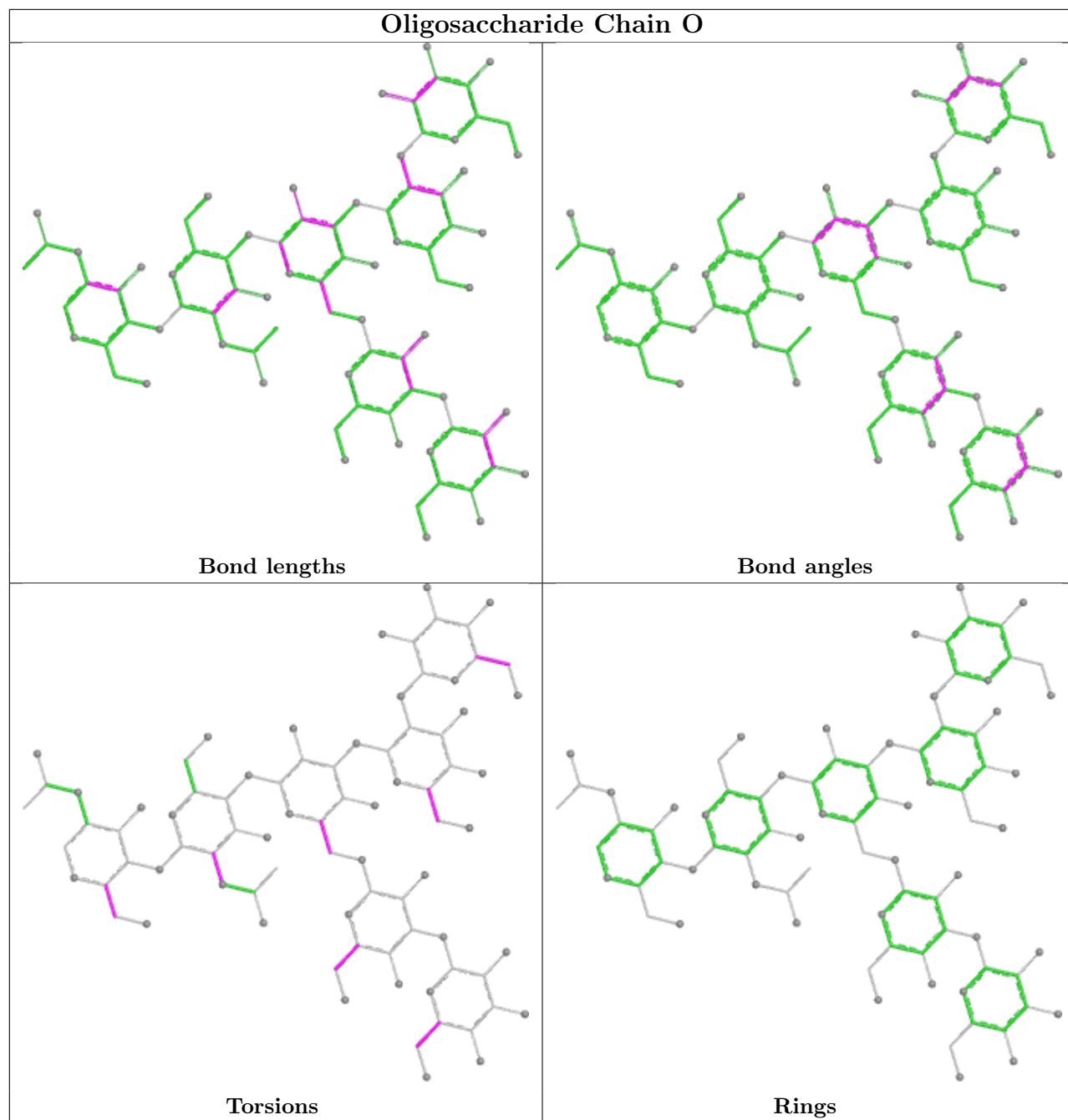


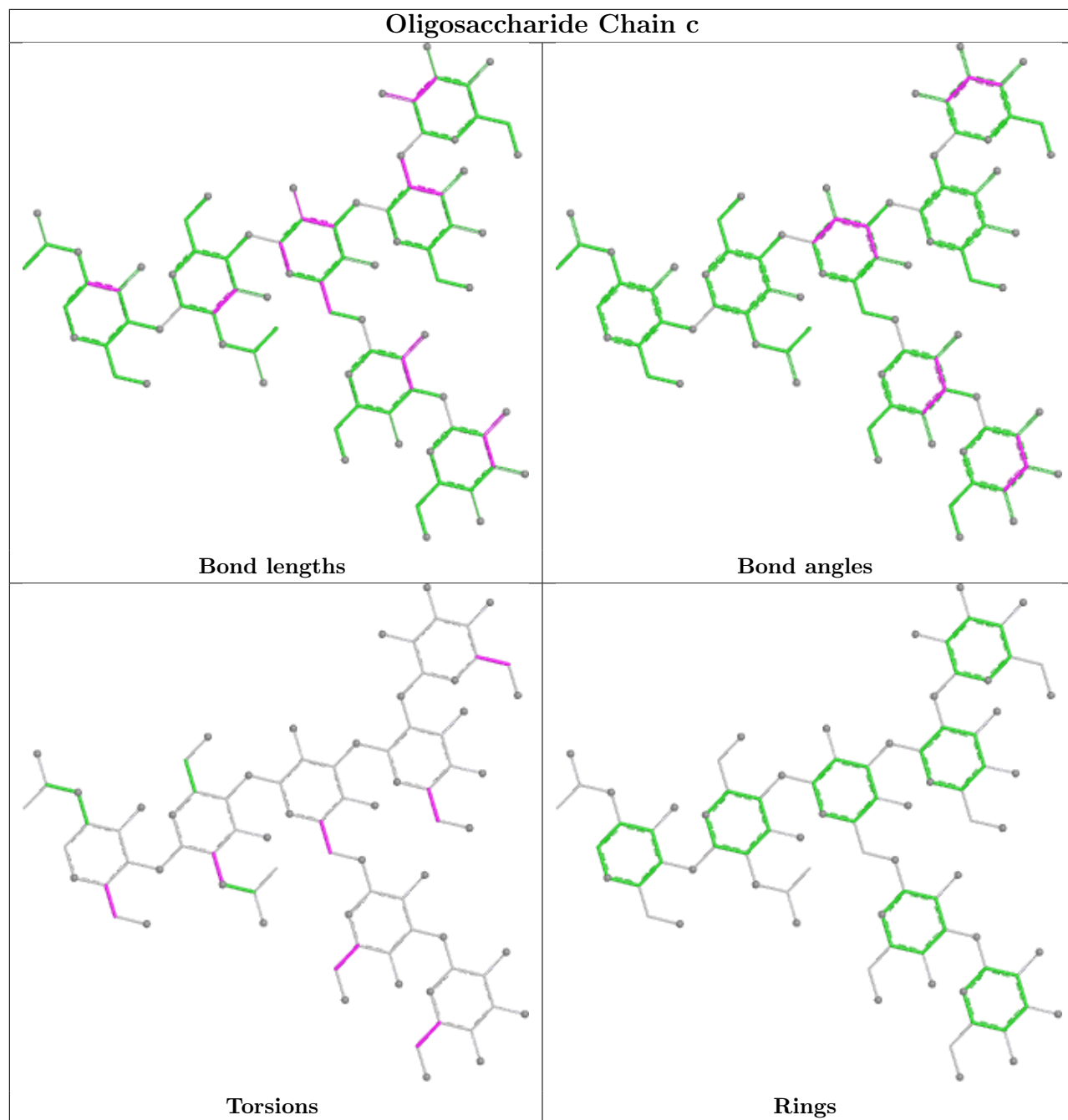


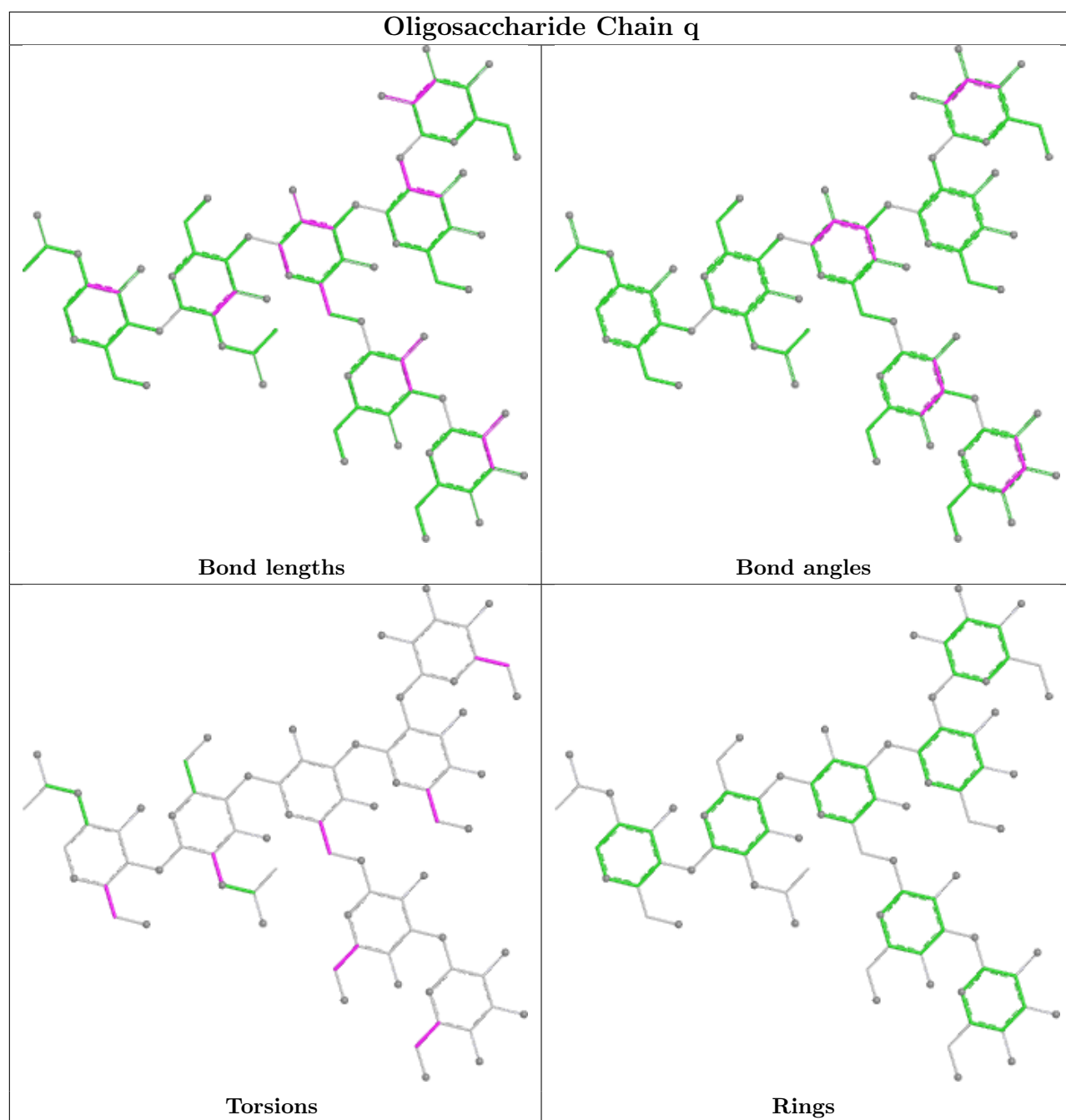


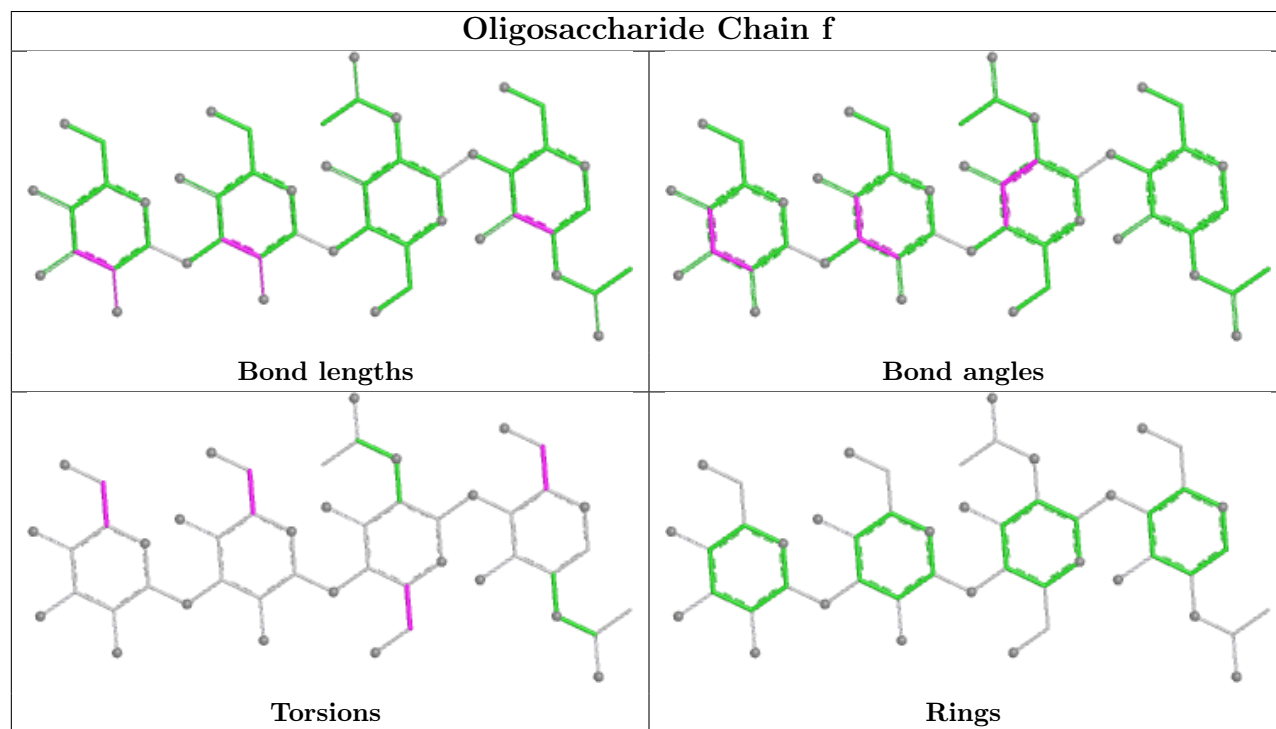
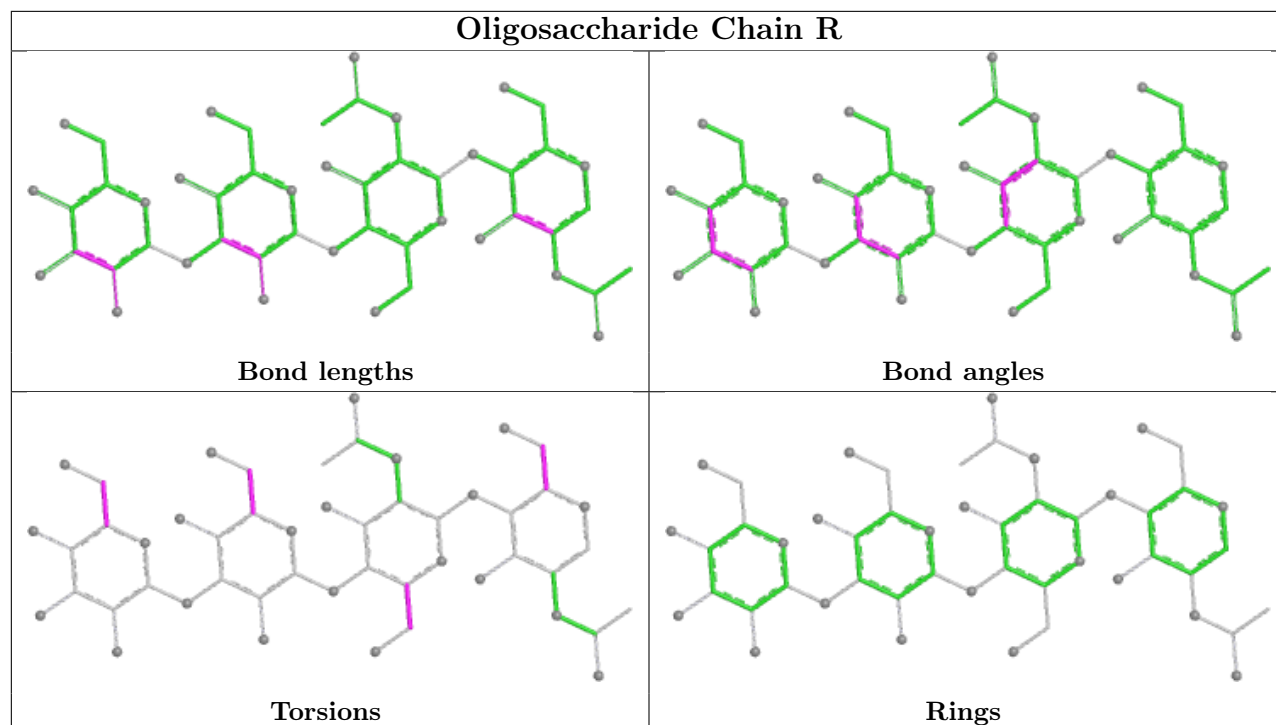


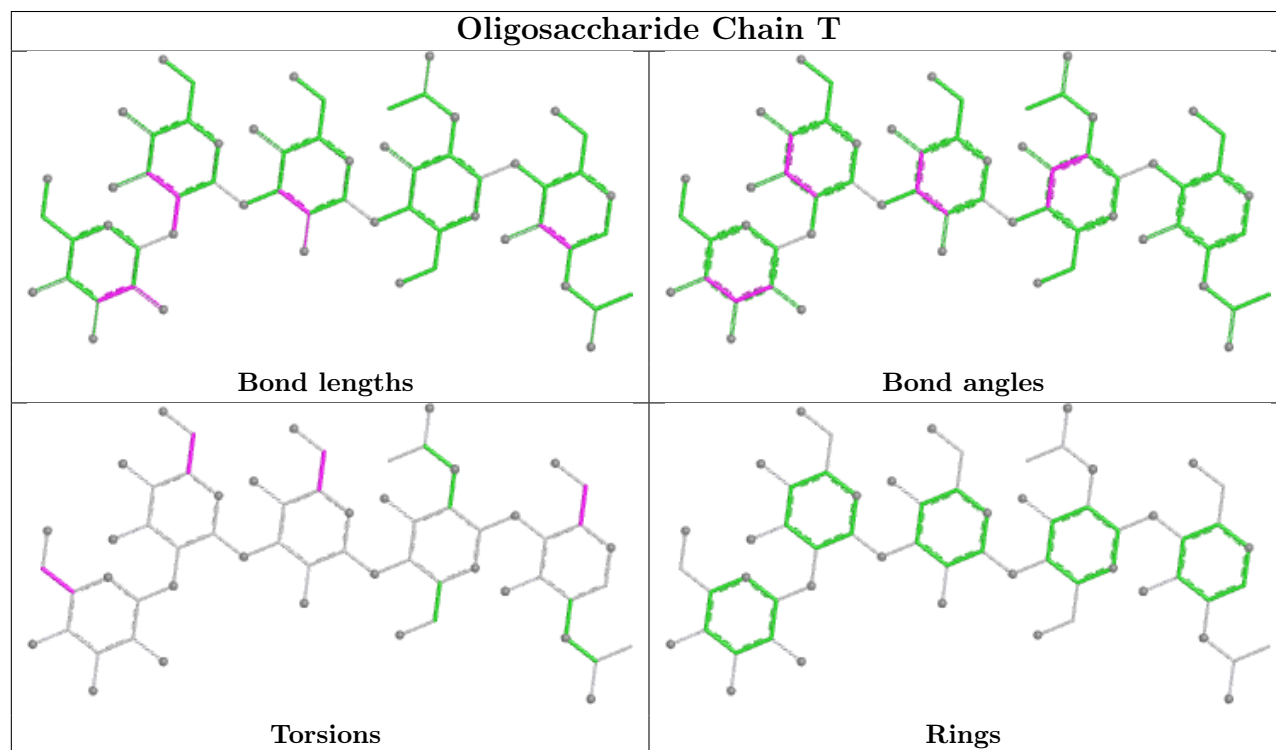
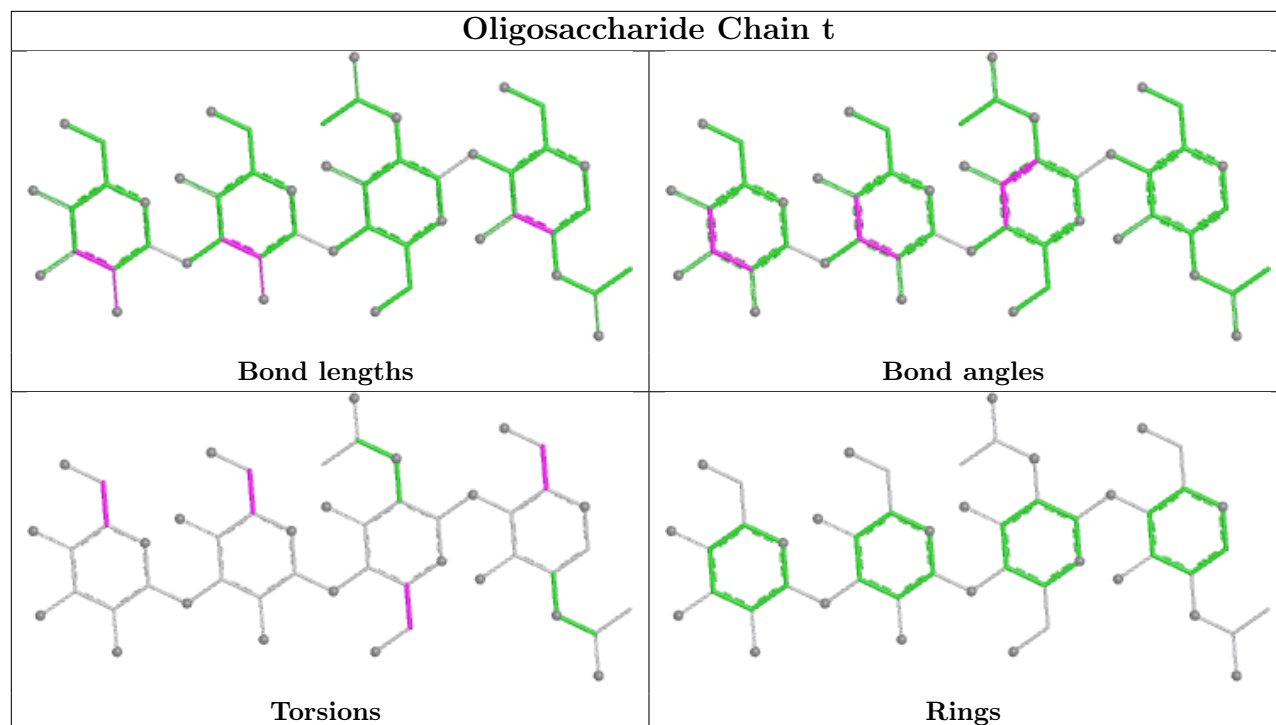


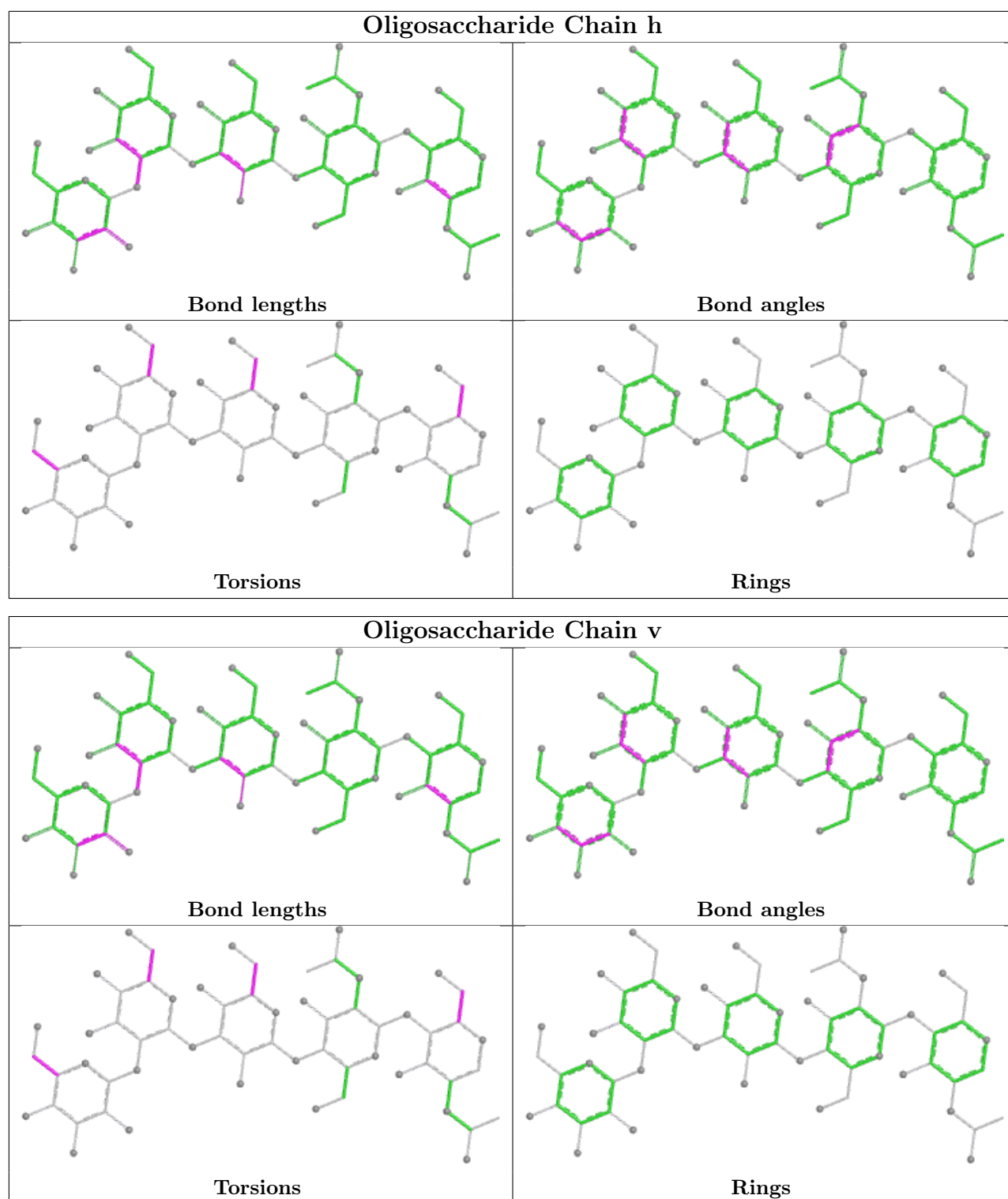












5.6 Ligand geometry [i](#)

12 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	A	738	1	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
11	NAG	E	748	1	14,14,15	0.80	0	17,19,21	1.07	1 (5%)
11	NAG	A	748	1	14,14,15	0.81	1 (7%)	17,19,21	1.06	1 (5%)
11	NAG	E	747	1	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
11	NAG	A	744	1	14,14,15	0.84	0	17,19,21	0.81	0
11	NAG	B	748	1	14,14,15	0.80	0	17,19,21	1.07	1 (5%)
11	NAG	E	744	1	14,14,15	0.84	0	17,19,21	0.81	0
11	NAG	B	747	1	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
11	NAG	A	747	1	14,14,15	0.82	0	17,19,21	0.99	1 (5%)
11	NAG	E	738	1	14,14,15	0.79	0	17,19,21	0.94	1 (5%)
11	NAG	B	744	1	14,14,15	0.82	0	17,19,21	0.80	0
11	NAG	B	738	1	14,14,15	0.78	0	17,19,21	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	738	1	-	2/6/23/26	0/1/1/1
11	NAG	E	748	1	-	1/6/23/26	0/1/1/1
11	NAG	A	748	1	-	1/6/23/26	0/1/1/1
11	NAG	E	747	1	-	4/6/23/26	0/1/1/1
11	NAG	A	744	1	-	1/6/23/26	0/1/1/1
11	NAG	B	748	1	-	1/6/23/26	0/1/1/1
11	NAG	E	744	1	-	1/6/23/26	0/1/1/1
11	NAG	B	747	1	-	4/6/23/26	0/1/1/1
11	NAG	A	747	1	-	4/6/23/26	0/1/1/1
11	NAG	E	738	1	-	2/6/23/26	0/1/1/1
11	NAG	B	744	1	-	1/6/23/26	0/1/1/1
11	NAG	B	738	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	748	NAG	C3-C2	-2.02	1.48	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	748	NAG	C4-C3-C2	-3.12	106.45	111.02
11	E	748	NAG	C4-C3-C2	-3.11	106.46	111.02
11	A	748	NAG	C4-C3-C2	-3.09	106.49	111.02
11	A	747	NAG	C4-C3-C2	-2.94	106.70	111.02
11	E	747	NAG	C4-C3-C2	-2.93	106.72	111.02
11	B	747	NAG	C4-C3-C2	-2.92	106.73	111.02
11	B	738	NAG	C4-C3-C2	-2.63	107.17	111.02
11	E	738	NAG	C4-C3-C2	-2.61	107.19	111.02
11	A	738	NAG	C4-C3-C2	-2.60	107.21	111.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	747	NAG	O5-C5-C6-O6
11	B	747	NAG	O5-C5-C6-O6
11	E	747	NAG	O5-C5-C6-O6
11	A	738	NAG	O5-C5-C6-O6
11	E	738	NAG	O5-C5-C6-O6
11	B	738	NAG	O5-C5-C6-O6
11	A	748	NAG	O5-C5-C6-O6
11	B	748	NAG	O5-C5-C6-O6
11	E	748	NAG	O5-C5-C6-O6
11	A	744	NAG	O5-C5-C6-O6
11	B	744	NAG	O5-C5-C6-O6
11	E	744	NAG	O5-C5-C6-O6
11	A	747	NAG	C1-C2-N2-C7
11	B	747	NAG	C1-C2-N2-C7
11	E	747	NAG	C1-C2-N2-C7
11	A	747	NAG	C3-C2-N2-C7
11	B	747	NAG	C3-C2-N2-C7
11	E	747	NAG	C3-C2-N2-C7
11	B	747	NAG	C4-C5-C6-O6
11	A	747	NAG	C4-C5-C6-O6
11	E	747	NAG	C4-C5-C6-O6
11	A	738	NAG	C4-C5-C6-O6
11	B	738	NAG	C4-C5-C6-O6
11	E	738	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

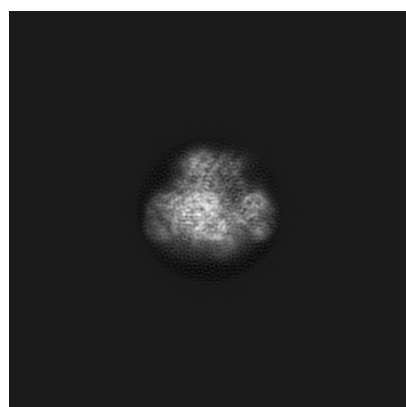
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9294. These allow visual inspection of the internal detail of the map and identification of artifacts.

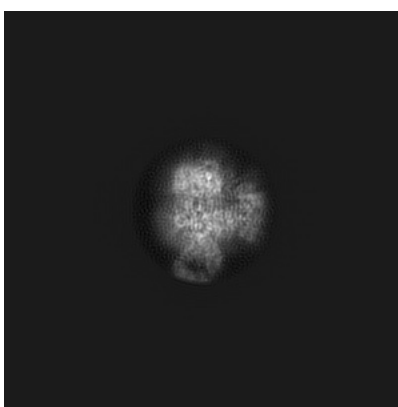
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

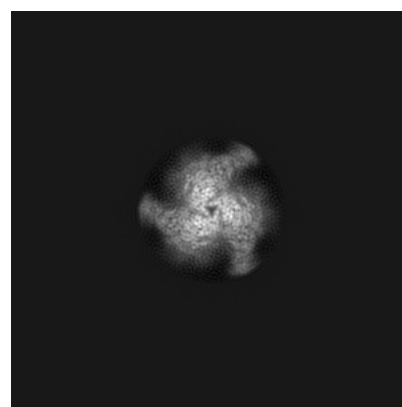
6.1.1 Primary map



X



Y

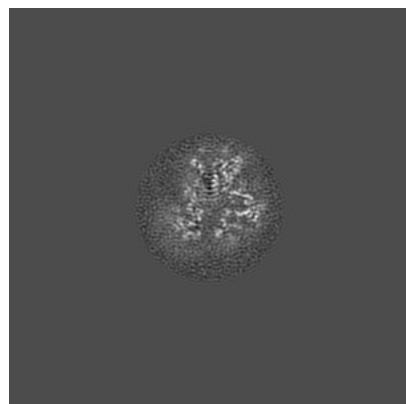


Z

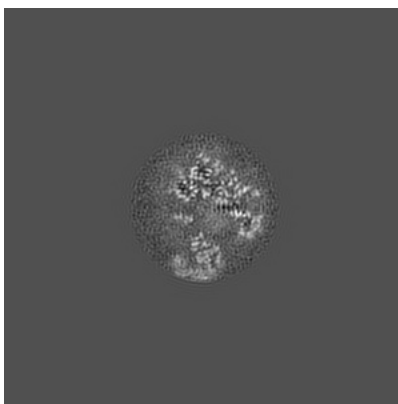
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

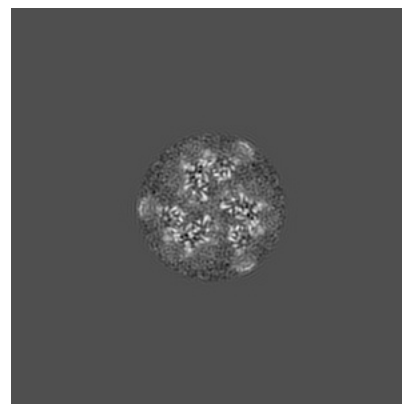
6.2.1 Primary map



X Index: 160



Y Index: 160

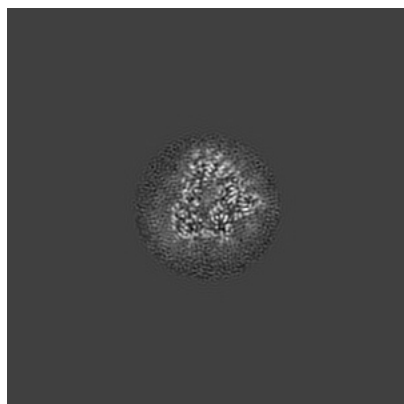


Z Index: 160

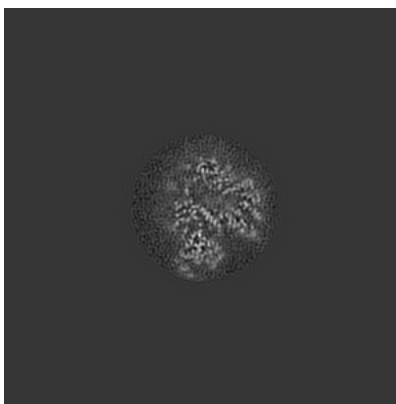
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

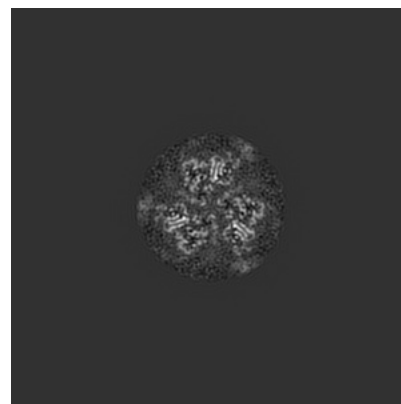
6.3.1 Primary map



X Index: 153



Y Index: 151

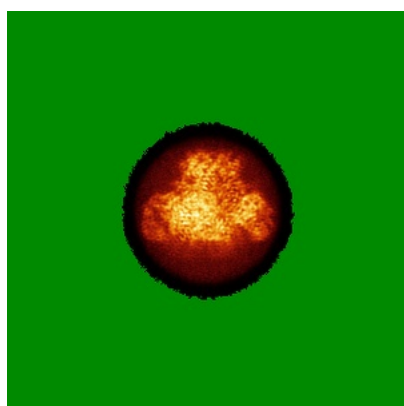


Z Index: 156

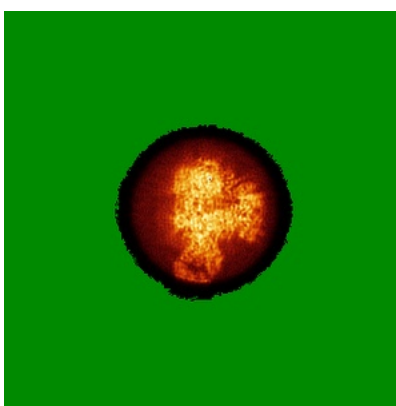
The images above show the largest variance slices of the map in three orthogonal directions.

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

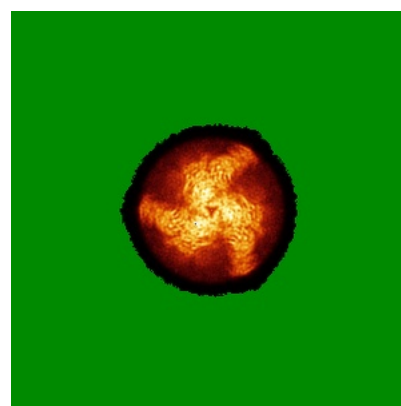
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

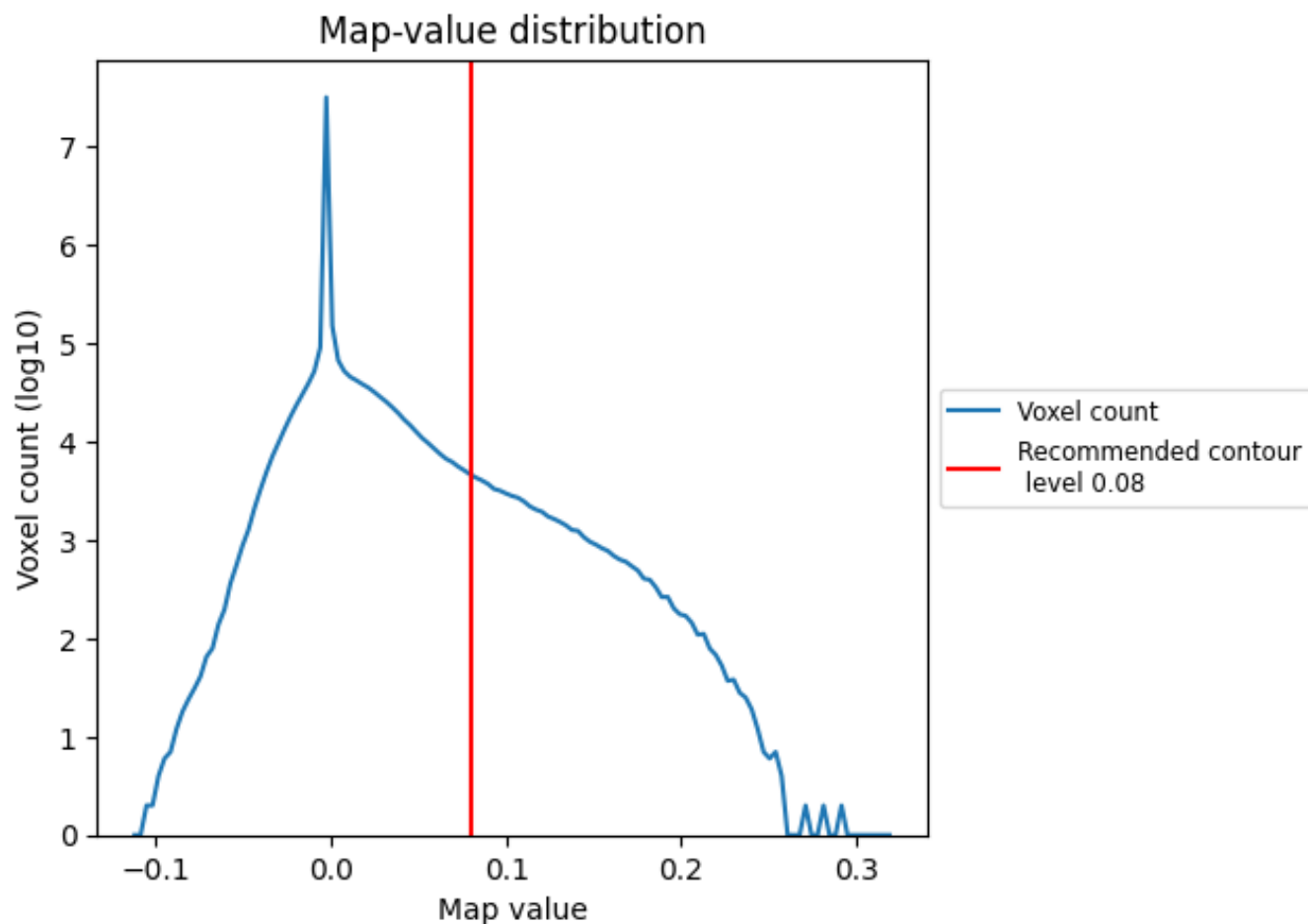
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

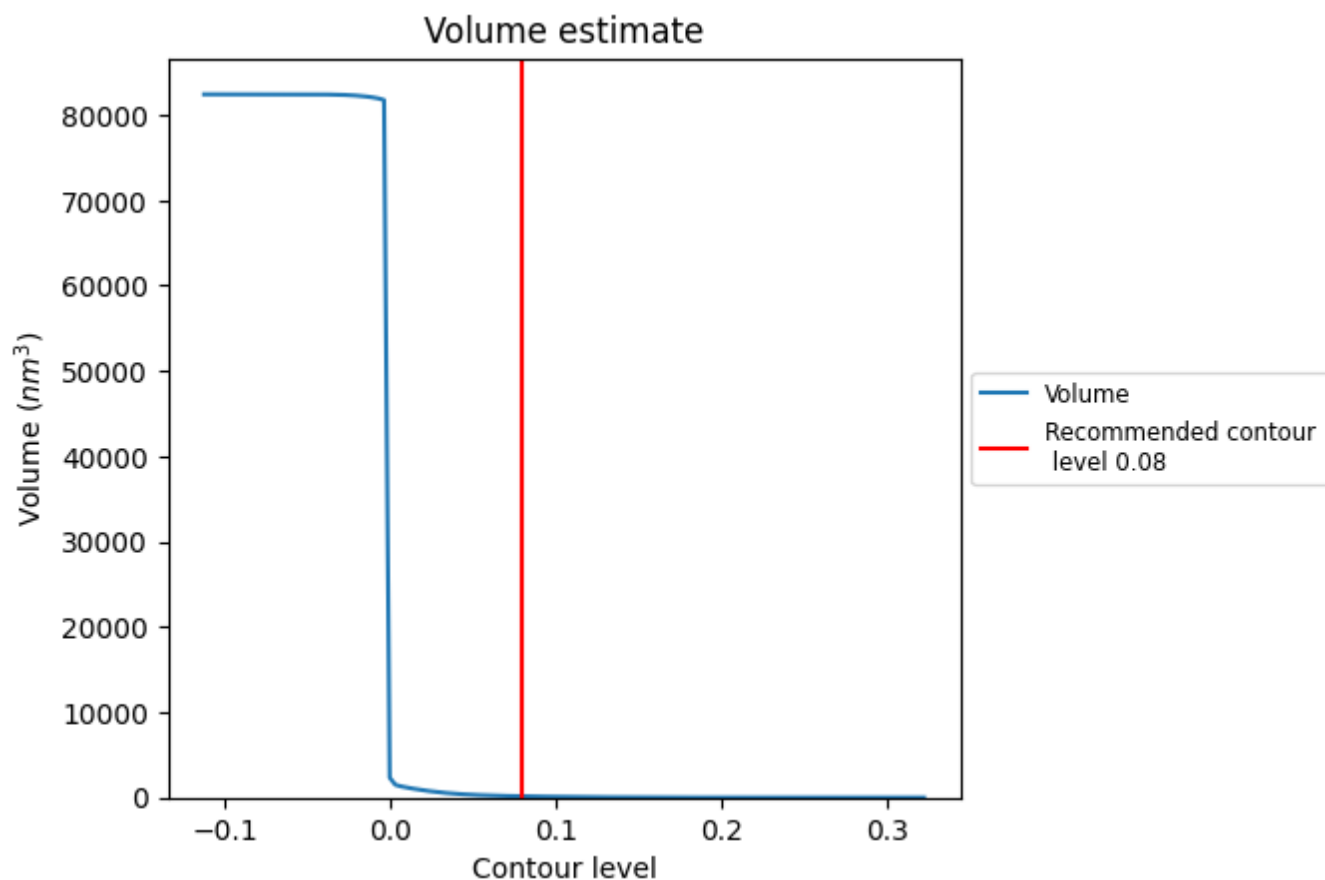
This section contains the results of statistical analysis of the map.

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.

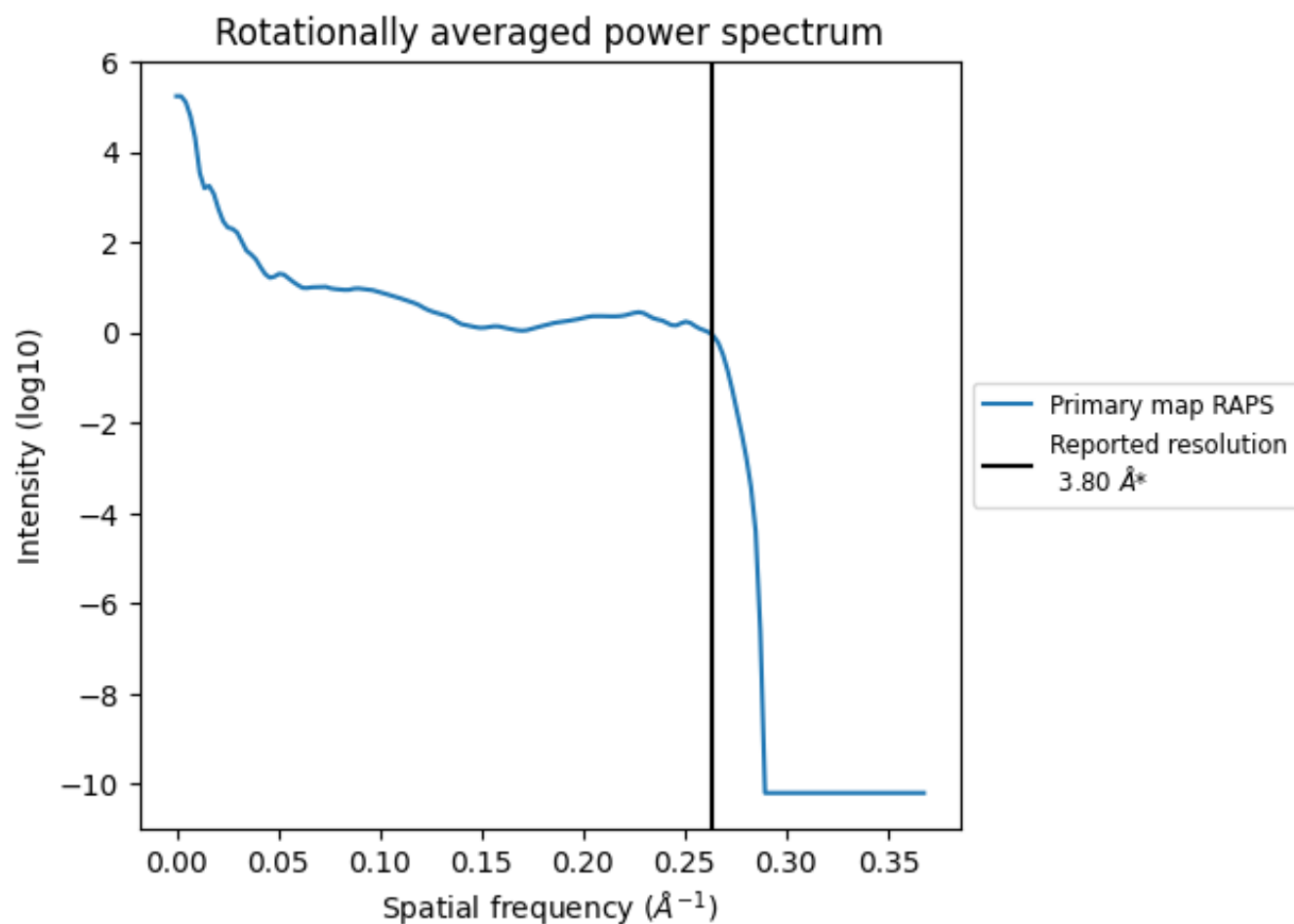
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 134 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 0.263 $\text{\AA}^{-1}$

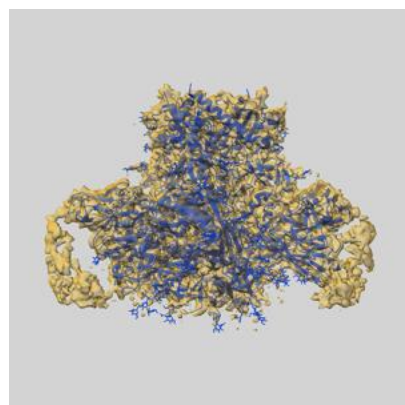
8 Fourier-Shell correlation

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

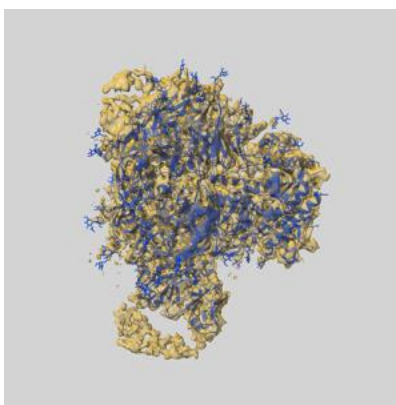
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9294 and PDB model 6MYY. Per-residue inclusion information can be found in section [3](#) on page [11](#).

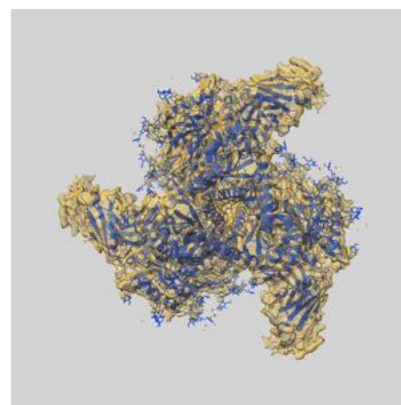
9.1 Map-model overlay [i](#)



X



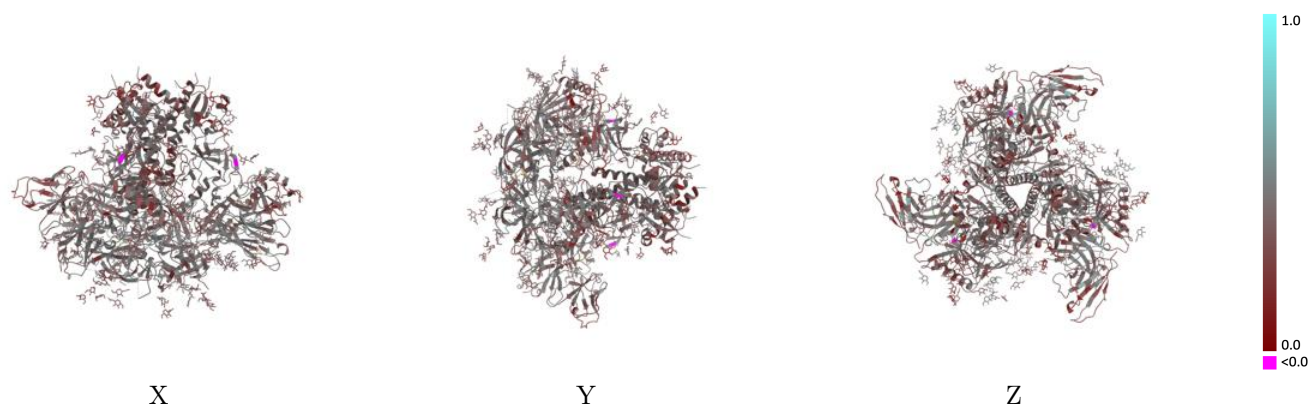
Y



Z

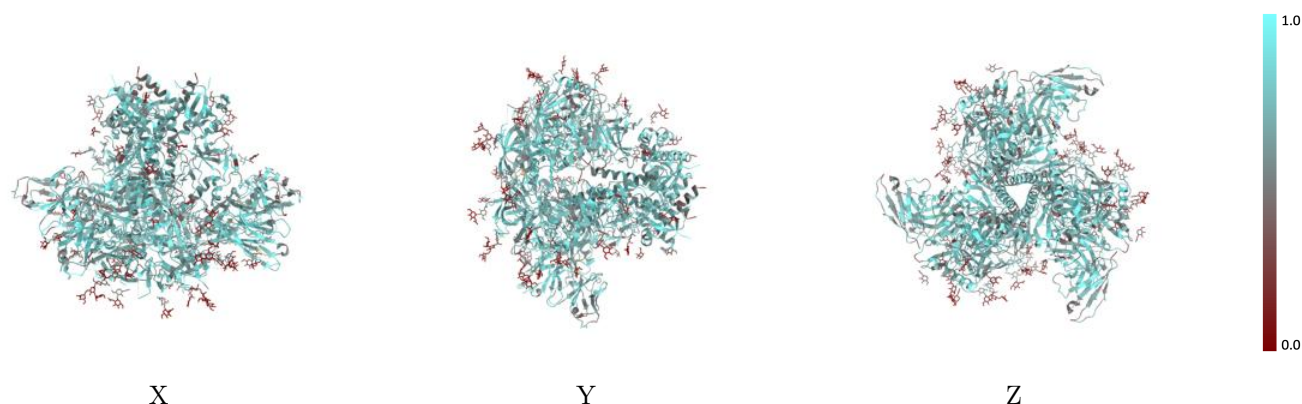
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



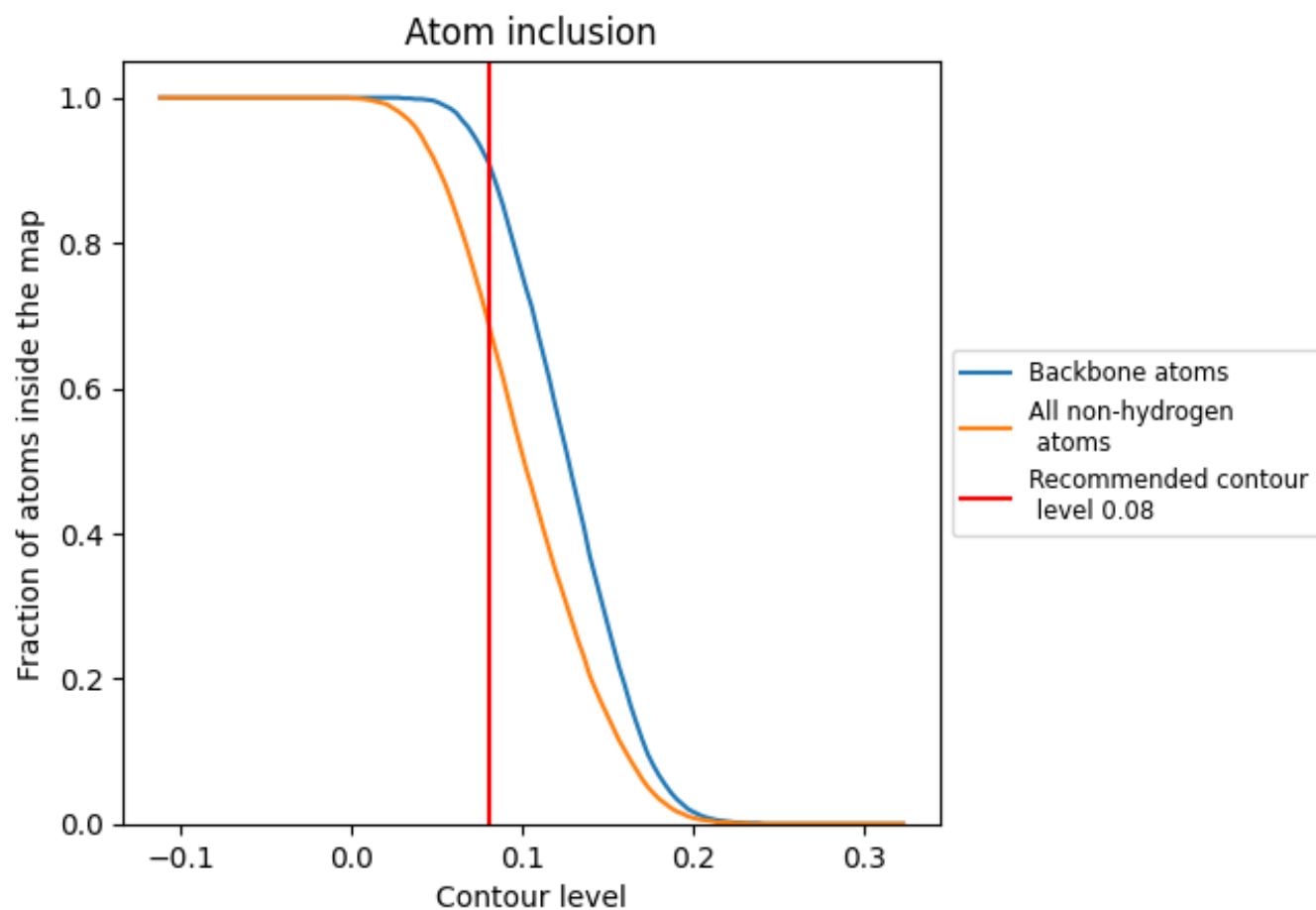
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 69% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.3910
A	 0.7160	 0.3910
B	 0.7160	 0.3920
C	 0.6710	 0.3520
D	 0.7970	 0.4410
E	 0.7130	 0.3890
F	 0.6650	 0.3510
G	 0.7940	 0.4430
H	 0.7990	 0.4420
I	 0.2140	 0.3100
J	 0.2140	 0.3460
K	 0.2950	 0.3540
L	 0.6710	 0.3510
M	 0.4440	 0.4060
N	 0.4360	 0.4040
O	 0.4460	 0.3650
P	 0.4100	 0.2780
Q	 0.2560	 0.3450
R	 0.3800	 0.4120
S	 0.3570	 0.4220
T	 0.4100	 0.3840
U	 0.2500	 0.3550
V	 0.4290	 0.2740
W	 0.2140	 0.3210
X	 0.1790	 0.3070
Y	 0.2140	 0.3470
Z	 0.3110	 0.3560
a	 0.4720	 0.4140
b	 0.3850	 0.3900
c	 0.4460	 0.3640
d	 0.4100	 0.2880
e	 0.2560	 0.3390
f	 0.3800	 0.4060
g	 0.3570	 0.4120
h	 0.4260	 0.3930



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Chain	Atom inclusion	Q-score
i	 0.2500	 0.3480
j	 0.4290	 0.2850
k	 0.2140	 0.2970
l	 0.2140	 0.2970
m	 0.2140	 0.3410
n	 0.2950	 0.3570
o	 0.4720	 0.4060
p	 0.4360	 0.3940
q	 0.4340	 0.3610
r	 0.3590	 0.2890
s	 0.2310	 0.3480
t	 0.3200	 0.3980
u	 0.3570	 0.4160
v	 0.3770	 0.3900
w	 0.2860	 0.3510
x	 0.4290	 0.2770
y	 0.2140	 0.3030