



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 11:19 AM EDT

PDB ID : 6BFU
EMDB ID : EMD-7094
Title : Glycan shield and fusion activation of a deltacoronavirus spike glycoprotein fine-tuned for enteric infections
Authors : Xiong, X.; Tortorici, M.A.; Snijder, S.; Yoshioka, C.; Walls, A.C.; Li, W.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); McGuire, A.T.; Rey, F.A.; Bosch, B.J.; Veisler, D.
Deposited on : 2017-10-27
Resolution : 3.50 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

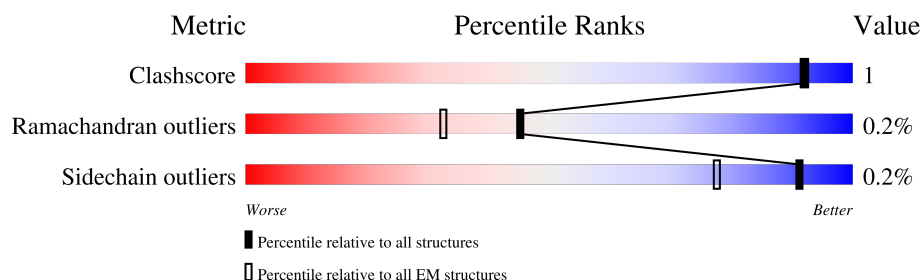
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

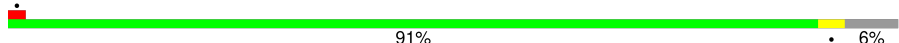


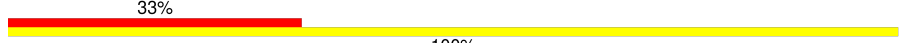

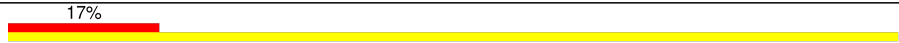
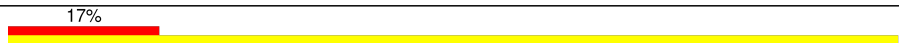
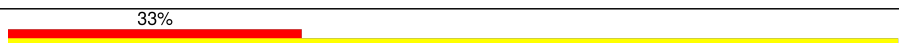
The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1024	 91% 6%
1	B	1024	 92% 6%
1	C	1024	 91% 6%
2	D	6	 33% 100%
2	F	6	 33% 100%
2	O	6	 17% 100%
2	Q	6	 17% 100%
2	S	6	 33% 100%

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Mol	Chain	Length	Quality of chain
2	b	6	17% 100%
2	d	6	33% 100%
2	f	6	33% 100%
2	o	6	17% 100%
3	E	3	33% 100%
3	H	3	67% 100%
3	J	3	67% 100%
3	K	3	33% 100%
3	L	3	33% 100%
3	M	3	33% 100%
3	N	3	100%
3	R	3	33% 100%
3	U	3	67% 100%
3	W	3	67% 100%
3	X	3	33% 100%
3	Y	3	33% 100%
3	Z	3	33% 100%
3	a	3	100%
3	e	3	33% 100%
3	h	3	67% 100%
3	j	3	67% 100%
3	k	3	33% 100%
3	l	3	33% 100%
3	m	3	33% 100%
3	n	3	100%

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Mol	Chain	Length	Quality of chain
4	G	2	<div><div>50%</div><div>100%</div></div>
4	P	2	<div><div>50%</div><div>100%</div></div>
4	T	2	<div><div>50%</div><div>100%</div></div>
4	c	2	<div><div>50%</div><div>100%</div></div>
4	g	2	<div><div>50%</div><div>100%</div></div>
4	p	2	<div><div>50%</div><div>100%</div></div>
5	I	5	<div><div>60%</div><div>100%</div></div>
5	V	5	<div><div>60%</div><div>100%</div></div>
5	i	5	<div><div>60%</div><div>100%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	964	Total	C	N	O	S	0	0
			7442	4681	1254	1464	43		
1	B	964	Total	C	N	O	S	0	0
			7442	4681	1254	1464	43		
1	C	964	Total	C	N	O	S	0	0
			7442	4681	1254	1464	43		

There are 66 discrepancies between the modelled and reference sequences:

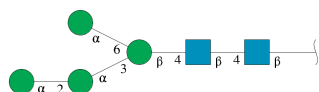
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP A0A140ES81
A	-1	LYS	-	expression tag	UNP A0A140ES81
A	0	LEU	-	expression tag	UNP A0A140ES81
A	1	CYS	-	expression tag	UNP A0A140ES81
A	2	ILE	-	expression tag	UNP A0A140ES81
A	3	LEU	-	expression tag	UNP A0A140ES81
A	4	LEU	-	expression tag	UNP A0A140ES81
A	5	ALA	-	expression tag	UNP A0A140ES81
A	6	VAL	-	expression tag	UNP A0A140ES81
A	7	VAL	-	expression tag	UNP A0A140ES81
A	8	ALA	-	expression tag	UNP A0A140ES81
A	9	PHE	-	expression tag	UNP A0A140ES81
A	10	VAL	-	expression tag	UNP A0A140ES81
A	11	GLY	-	expression tag	UNP A0A140ES81
A	12	LEU	-	expression tag	UNP A0A140ES81
A	13	SER	-	expression tag	UNP A0A140ES81
A	14	LEU	-	expression tag	UNP A0A140ES81
A	15	GLY	-	expression tag	UNP A0A140ES81
A	16	ARG	-	expression tag	UNP A0A140ES81
A	17	SER	-	expression tag	UNP A0A140ES81
A	18	LEU	-	expression tag	UNP A0A140ES81
A	907	PRO	SER	conflict	UNP A0A140ES81
B	-2	MET	-	expression tag	UNP A0A140ES81
B	-1	LYS	-	expression tag	UNP A0A140ES81

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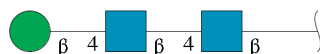
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP A0A140ES81
B	1	CYS	-	expression tag	UNP A0A140ES81
B	2	ILE	-	expression tag	UNP A0A140ES81
B	3	LEU	-	expression tag	UNP A0A140ES81
B	4	LEU	-	expression tag	UNP A0A140ES81
B	5	ALA	-	expression tag	UNP A0A140ES81
B	6	VAL	-	expression tag	UNP A0A140ES81
B	7	VAL	-	expression tag	UNP A0A140ES81
B	8	ALA	-	expression tag	UNP A0A140ES81
B	9	PHE	-	expression tag	UNP A0A140ES81
B	10	VAL	-	expression tag	UNP A0A140ES81
B	11	GLY	-	expression tag	UNP A0A140ES81
B	12	LEU	-	expression tag	UNP A0A140ES81
B	13	SER	-	expression tag	UNP A0A140ES81
B	14	LEU	-	expression tag	UNP A0A140ES81
B	15	GLY	-	expression tag	UNP A0A140ES81
B	16	ARG	-	expression tag	UNP A0A140ES81
B	17	SER	-	expression tag	UNP A0A140ES81
B	18	LEU	-	expression tag	UNP A0A140ES81
B	907	PRO	SER	conflict	UNP A0A140ES81
C	-2	MET	-	expression tag	UNP A0A140ES81
C	-1	LYS	-	expression tag	UNP A0A140ES81
C	0	LEU	-	expression tag	UNP A0A140ES81
C	1	CYS	-	expression tag	UNP A0A140ES81
C	2	ILE	-	expression tag	UNP A0A140ES81
C	3	LEU	-	expression tag	UNP A0A140ES81
C	4	LEU	-	expression tag	UNP A0A140ES81
C	5	ALA	-	expression tag	UNP A0A140ES81
C	6	VAL	-	expression tag	UNP A0A140ES81
C	7	VAL	-	expression tag	UNP A0A140ES81
C	8	ALA	-	expression tag	UNP A0A140ES81
C	9	PHE	-	expression tag	UNP A0A140ES81
C	10	VAL	-	expression tag	UNP A0A140ES81
C	11	GLY	-	expression tag	UNP A0A140ES81
C	12	LEU	-	expression tag	UNP A0A140ES81
C	13	SER	-	expression tag	UNP A0A140ES81
C	14	LEU	-	expression tag	UNP A0A140ES81
C	15	GLY	-	expression tag	UNP A0A140ES81
C	16	ARG	-	expression tag	UNP A0A140ES81
C	17	SER	-	expression tag	UNP A0A140ES81
C	18	LEU	-	expression tag	UNP A0A140ES81
C	907	PRO	SER	conflict	UNP A0A140ES81

- Molecule 2 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
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	F	6	Total	C	N	O	0	0
			72	40	2	30		
2	O	6	Total	C	N	O	0	0
			72	40	2	30		
2	Q	6	Total	C	N	O	0	0
			72	40	2	30		
2	S	6	Total	C	N	O	0	0
			72	40	2	30		
2	b	6	Total	C	N	O	0	0
			72	40	2	30		
2	d	6	Total	C	N	O	0	0
			72	40	2	30		
2	f	6	Total	C	N	O	0	0
			72	40	2	30		
2	o	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 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.



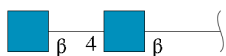
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

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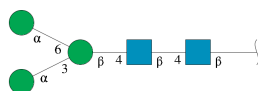
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Y	3	Total	C	N	O	0	0
			39	22	2	15		
3	Z	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	e	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		
3	k	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	m	3	Total	C	N	O	0	0
			39	22	2	15		
3	n	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	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	I	5	Total	C	N	O	0	0
			61	34	2	25		
5	V	5	Total	C	N	O	0	0
			61	34	2	25		
5	i	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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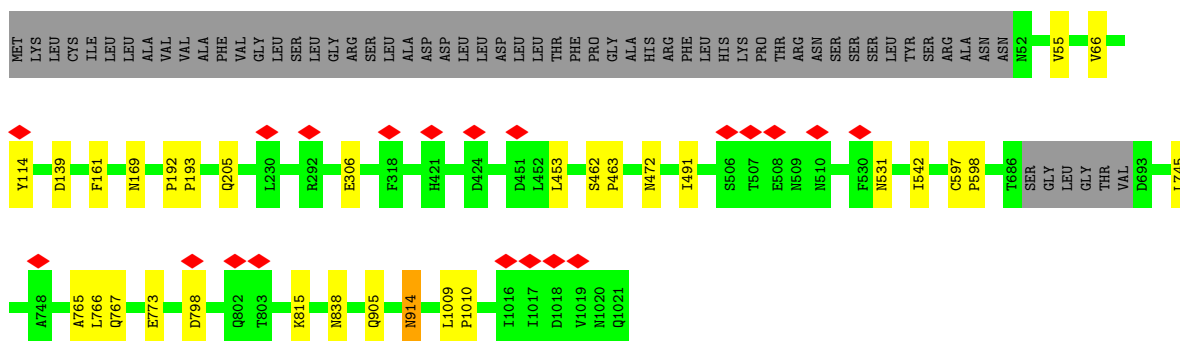
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots [i](#)


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

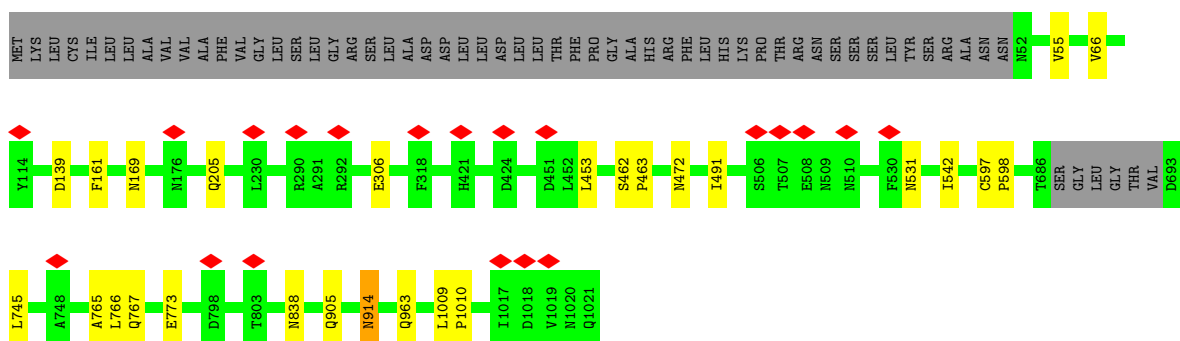
- Molecule 1: Spike protein

Chain A:  91% 6%




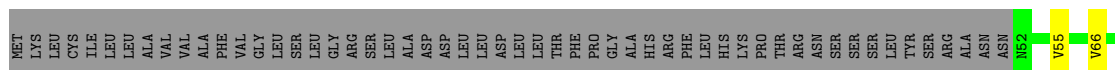
- Molecule 1: Spike protein

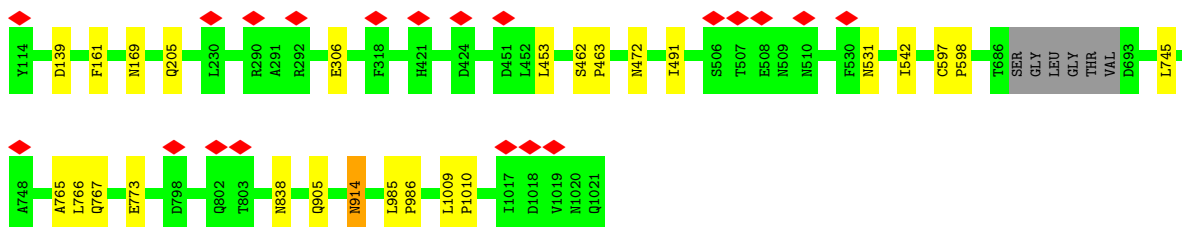
Chain B:  92% 6%



- Molecule 1: Spike protein

Chain C:  91% 6%





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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



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

Chain N:  100%

NAG1
NAG2
BMA3

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

Chain R:  33%  100%

NAG1
NAG2
BMA3

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

Chain U:  67%  100%

NAG1
NAG2
BMA3

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

Chain W:  67%  100%

NAG1
NAG2
BMA3

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

Chain X:  33%  100%

NAG1
NAG2
BMA3

- Molecule 3: 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%

NAG1
NAG2
BMA3

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



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



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



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



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



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



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



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



- Molecule 3: beta-D-mannopyranose-(1-4)-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 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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	455710	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.75	1/7578 (0.0%)	0.55	1/10337 (0.0%)
1	B	0.75	1/7578 (0.0%)	0.55	1/10337 (0.0%)
1	C	0.75	1/7578 (0.0%)	0.55	1/10337 (0.0%)
All	All	0.75	3/22734 (0.0%)	0.55	3/31011 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	GLU	CD-OE2	-5.25	1.19	1.25
1	B	306	GLU	CD-OE2	-5.18	1.20	1.25
1	C	306	GLU	CD-OE2	-5.11	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	LEU	CD1-CG-CD2	7.17	132.02	110.50
1	A	453	LEU	CD1-CG-CD2	7.16	131.99	110.50
1	C	453	LEU	CD1-CG-CD2	7.15	131.96	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7442	0	7293	24	0
1	B	7442	0	7293	22	0
1	C	7442	0	7293	22	0
2	D	72	0	58	0	0
2	F	72	0	58	0	0
2	O	72	0	58	0	0
2	Q	72	0	58	0	0
2	S	72	0	58	0	0
2	b	72	0	58	0	0
2	d	72	0	58	0	0
2	f	72	0	58	0	0
2	o	72	0	58	0	0
3	E	39	0	33	0	0
3	H	39	0	33	0	0
3	J	39	0	33	0	0
3	K	39	0	33	0	0
3	L	39	0	33	0	0
3	M	39	0	33	0	0
3	N	39	0	33	0	0
3	R	39	0	33	0	0
3	U	39	0	33	0	0
3	W	39	0	33	0	0
3	X	39	0	33	0	0
3	Y	39	0	33	0	0
3	Z	39	0	33	0	0
3	a	39	0	33	0	0
3	e	39	0	33	0	0
3	h	39	0	33	0	0
3	j	39	0	33	0	0
3	k	39	0	33	0	0
3	l	39	0	33	0	0
3	m	39	0	33	0	0
3	n	39	0	33	0	0
4	G	28	0	25	0	0
4	P	28	0	25	0	0
4	T	28	0	25	0	0
4	c	28	0	25	0	0
4	g	28	0	25	0	0
4	p	28	0	25	0	0
5	I	61	0	49	0	0
5	V	61	0	49	0	0
5	i	61	0	49	0	0
6	A	112	0	104	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	112	0	104	0	0
6	C	112	0	104	0	0
All	All	24480	0	23703	68	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 (68) 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:C:169:ASN:OD1	1:C:169:ASN:O	2.01	0.79
1:A:169:ASN:O	1:A:169:ASN:OD1	2.00	0.78
1:B:169:ASN:O	1:B:169:ASN:OD1	2.01	0.78
1:A:773:GLU:OE1	1:A:773:GLU:N	2.20	0.74
1:B:914:ASN:OD1	1:B:914:ASN:O	2.06	0.74
1:C:914:ASN:O	1:C:914:ASN:OD1	2.06	0.74
1:A:914:ASN:O	1:A:914:ASN:OD1	2.06	0.73
1:C:55:VAL:HG12	1:C:55:VAL:O	1.91	0.70
1:A:55:VAL:O	1:A:55:VAL:HG12	1.91	0.69
1:C:773:GLU:OE1	1:C:773:GLU:N	2.20	0.69
1:B:55:VAL:HG12	1:B:55:VAL:O	1.91	0.69
1:B:773:GLU:OE1	1:B:773:GLU:N	2.20	0.67
1:C:205:GLN:N	1:C:205:GLN:OE1	2.29	0.64
1:A:205:GLN:N	1:A:205:GLN:OE1	2.29	0.63
1:A:914:ASN:O	1:A:914:ASN:CG	2.37	0.62
1:B:914:ASN:O	1:B:914:ASN:CG	2.37	0.62
1:C:914:ASN:O	1:C:914:ASN:CG	2.37	0.62
1:B:205:GLN:N	1:B:205:GLN:OE1	2.29	0.62
1:B:472:ASN:O	1:B:472:ASN:OD1	2.21	0.58
1:C:472:ASN:O	1:C:472:ASN:OD1	2.21	0.58
1:A:472:ASN:OD1	1:A:472:ASN:O	2.21	0.58
1:A:905:GLN:HG2	1:A:905:GLN:O	2.06	0.56
1:B:905:GLN:O	1:B:905:GLN:HG2	2.06	0.56
1:C:905:GLN:O	1:C:905:GLN:HG2	2.06	0.56
1:B:161:PHE:O	1:B:161:PHE:CD2	2.59	0.55
1:C:161:PHE:CD2	1:C:161:PHE:O	2.59	0.55
1:A:161:PHE:O	1:A:161:PHE:CD2	2.59	0.55
1:C:161:PHE:O	1:C:161:PHE:CG	2.60	0.54
1:A:161:PHE:O	1:A:161:PHE:CG	2.60	0.54
1:C:55:VAL:O	1:C:55:VAL:CG1	2.57	0.53
1:A:55:VAL:O	1:A:55:VAL:CG1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:O	1:B:55:VAL:CG1	2.57	0.52
1:B:161:PHE:O	1:B:161:PHE:CG	2.60	0.52
1:A:597:CYS:HB3	1:A:598:PRO:HD3	1.93	0.51
1:C:597:CYS:HB3	1:C:598:PRO:HD3	1.92	0.51
1:B:597:CYS:HB3	1:B:598:PRO:HD3	1.93	0.50
1:B:491:ILE:HD12	1:B:491:ILE:N	2.27	0.49
1:C:1009:LEU:N	1:C:1010:PRO:CD	2.75	0.49
1:A:491:ILE:HD12	1:A:491:ILE:N	2.28	0.49
1:A:1009:LEU:N	1:A:1010:PRO:CD	2.75	0.49
1:B:1009:LEU:N	1:B:1010:PRO:CD	2.75	0.49
1:C:491:ILE:HD12	1:C:491:ILE:N	2.27	0.49
1:B:542:ILE:C	1:B:542:ILE:HD12	2.36	0.46
1:A:542:ILE:HD12	1:A:542:ILE:C	2.36	0.45
1:C:542:ILE:C	1:C:542:ILE:HD12	2.36	0.45
1:A:66:VAL:HG12	1:A:66:VAL:O	2.17	0.45
1:B:66:VAL:HG12	1:B:66:VAL:O	2.17	0.45
1:A:765:ALA:O	1:A:767:GLN:N	2.50	0.44
1:C:765:ALA:O	1:C:767:GLN:N	2.51	0.44
1:B:745:LEU:N	1:B:745:LEU:HD12	2.33	0.43
1:B:765:ALA:O	1:B:767:GLN:N	2.50	0.43
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.89	0.43
1:A:745:LEU:HD12	1:A:745:LEU:N	2.33	0.43
1:C:66:VAL:HG12	1:C:66:VAL:O	2.17	0.43
1:A:838:ASN:C	1:A:838:ASN:OD1	2.57	0.42
1:C:745:LEU:HD12	1:C:745:LEU:N	2.33	0.42
1:A:462:SER:HB2	1:A:463:PRO:HD2	2.02	0.42
1:B:462:SER:HB2	1:B:463:PRO:HD2	2.02	0.42
1:A:745:LEU:N	1:A:745:LEU:CD1	2.83	0.41
1:B:963:GLN:OE1	1:B:963:GLN:N	2.40	0.41
1:C:462:SER:HB2	1:C:463:PRO:HD2	2.02	0.41
1:B:745:LEU:N	1:B:745:LEU:CD1	2.83	0.41
1:C:745:LEU:N	1:C:745:LEU:CD1	2.83	0.41
1:C:838:ASN:C	1:C:838:ASN:OD1	2.57	0.41
1:A:114:TYR:CE1	6:A:1099:NAG:H82	2.56	0.41
1:B:838:ASN:OD1	1:B:838:ASN:C	2.57	0.40
1:C:985:LEU:HA	1:C:986:PRO:HD3	1.95	0.40
1:A:798:ASP:OD2	1:A:815:LYS:NZ	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	960/1024 (94%)	927 (97%)	31 (3%)	2 (0%)	44	75
1	B	960/1024 (94%)	927 (97%)	31 (3%)	2 (0%)	44	75
1	C	960/1024 (94%)	927 (97%)	31 (3%)	2 (0%)	44	75
All	All	2880/3072 (94%)	2781 (97%)	93 (3%)	6 (0%)	45	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	766	LEU
1	B	766	LEU
1	C	766	LEU
1	A	139	ASP
1	B	139	ASP
1	C	139	ASP

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	847/897 (94%)	845 (100%)	2 (0%)	92	97
1	B	847/897 (94%)	845 (100%)	2 (0%)	92	97
1	C	847/897 (94%)	845 (100%)	2 (0%)	92	97
All	All	2541/2691 (94%)	2535 (100%)	6 (0%)	91	97

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

Mol	Chain	Res	Type
1	A	531	ASN
1	A	914	ASN
1	B	531	ASN
1	B	914	ASN
1	C	531	ASN
1	C	914	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	610	GLN
1	A	712	GLN
1	B	610	GLN
1	B	712	GLN
1	C	610	GLN
1	C	712	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 ⓘ

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	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	1.92	2 (14%)	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	2	2	14,14,15	2.13	5 (35%)	17,19,21	1.33	2 (11%)
2	BMA	D	3	2	11,11,12	1.84	1 (9%)	15,15,17	0.74	0
2	MAN	D	4	2	11,11,12	1.67	2 (18%)	15,15,17	0.72	0
2	MAN	D	5	2	11,11,12	1.85	2 (18%)	15,15,17	0.76	0
2	MAN	D	6	2	11,11,12	1.82	2 (18%)	15,15,17	0.77	0
3	NAG	E	1	1,3	14,14,15	2.04	3 (21%)	17,19,21	1.14	1 (5%)
3	NAG	E	2	3	14,14,15	2.02	3 (21%)	17,19,21	1.29	2 (11%)
3	BMA	E	3	3	11,11,12	1.84	2 (18%)	15,15,17	0.76	0
2	NAG	F	1	1,2	14,14,15	1.93	2 (14%)	17,19,21	1.15	1 (5%)
2	NAG	F	2	2	14,14,15	2.01	2 (14%)	17,19,21	1.28	2 (11%)
2	BMA	F	3	2	11,11,12	1.84	1 (9%)	15,15,17	0.70	0
2	MAN	F	4	2	11,11,12	1.64	2 (18%)	15,15,17	0.74	0
2	MAN	F	5	2	11,11,12	1.85	3 (27%)	15,15,17	0.82	0
2	MAN	F	6	2	11,11,12	1.84	3 (27%)	15,15,17	0.82	0
4	NAG	G	1	1,4	14,14,15	1.98	2 (14%)	17,19,21	1.16	1 (5%)
4	NAG	G	2	4	14,14,15	2.02	1 (7%)	17,19,21	1.25	3 (17%)
3	NAG	H	1	1,3	14,14,15	2.07	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	H	2	3	14,14,15	2.12	4 (28%)	17,19,21	1.47	3 (17%)
3	BMA	H	3	3	11,11,12	1.85	2 (18%)	15,15,17	0.79	0
5	NAG	I	1	1,5	14,14,15	2.01	2 (14%)	17,19,21	1.05	1 (5%)
5	NAG	I	2	5	14,14,15	2.05	3 (21%)	17,19,21	1.38	3 (17%)
5	BMA	I	3	5	11,11,12	1.85	2 (18%)	15,15,17	0.80	0
5	MAN	I	4	5	11,11,12	1.88	4 (36%)	15,15,17	0.83	0
5	MAN	I	5	5	11,11,12	1.84	3 (27%)	15,15,17	0.78	0
3	NAG	J	1	1,3	14,14,15	2.04	2 (14%)	17,19,21	1.16	1 (5%)
3	NAG	J	2	3	14,14,15	2.11	4 (28%)	17,19,21	1.33	2 (11%)
3	BMA	J	3	3	11,11,12	1.85	3 (27%)	15,15,17	0.77	0
3	NAG	K	1	1,3	14,14,15	2.04	3 (21%)	17,19,21	1.26	2 (11%)
3	NAG	K	2	3	14,14,15	2.04	2 (14%)	17,19,21	1.29	1 (5%)
3	BMA	K	3	3	11,11,12	1.87	3 (27%)	15,15,17	0.73	0
3	NAG	L	1	1,3	14,14,15	1.98	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	L	2	3	14,14,15	2.11	3 (21%)	17,19,21	1.40	2 (11%)
3	BMA	L	3	3	11,11,12	1.85	3 (27%)	15,15,17	0.80	0
3	NAG	M	1	1,3	14,14,15	2.01	1 (7%)	17,19,21	1.12	1 (5%)
3	NAG	M	2	3	14,14,15	2.10	4 (28%)	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	M	3	3	11,11,12	1.84	2 (18%)	15,15,17	0.80	0
3	NAG	N	1	1,3	14,14,15	1.97	2 (14%)	17,19,21	1.32	2 (11%)
3	NAG	N	2	3	14,14,15	2.06	2 (14%)	17,19,21	1.18	1 (5%)
3	BMA	N	3	3	11,11,12	1.82	4 (36%)	15,15,17	0.78	0
2	NAG	O	1	1,2	14,14,15	1.95	1 (7%)	17,19,21	1.30	2 (11%)
2	NAG	O	2	2	14,14,15	2.01	2 (14%)	17,19,21	1.30	2 (11%)
2	BMA	O	3	2	11,11,12	1.83	1 (9%)	15,15,17	0.74	0
2	MAN	O	4	2	11,11,12	1.61	2 (18%)	15,15,17	0.72	0
2	MAN	O	5	2	11,11,12	1.86	3 (27%)	15,15,17	0.80	0
2	MAN	O	6	2	11,11,12	1.83	2 (18%)	15,15,17	0.81	0
4	NAG	P	1	1,4	14,14,15	2.01	2 (14%)	17,19,21	1.10	1 (5%)
4	NAG	P	2	4	14,14,15	2.05	2 (14%)	17,19,21	1.28	2 (11%)
2	NAG	Q	1	1,2	14,14,15	1.90	2 (14%)	17,19,21	1.30	3 (17%)
2	NAG	Q	2	2	14,14,15	2.11	3 (21%)	17,19,21	1.34	2 (11%)
2	BMA	Q	3	2	11,11,12	1.83	1 (9%)	15,15,17	0.74	0
2	MAN	Q	4	2	11,11,12	1.67	2 (18%)	15,15,17	0.72	0
2	MAN	Q	5	2	11,11,12	1.82	2 (18%)	15,15,17	0.76	0
2	MAN	Q	6	2	11,11,12	1.82	2 (18%)	15,15,17	0.77	0
3	NAG	R	1	1,3	14,14,15	2.03	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	R	2	3	14,14,15	2.01	2 (14%)	17,19,21	1.27	2 (11%)
3	BMA	R	3	3	11,11,12	1.84	2 (18%)	15,15,17	0.76	0
2	NAG	S	1	1,2	14,14,15	1.93	2 (14%)	17,19,21	1.14	1 (5%)
2	NAG	S	2	2	14,14,15	2.02	2 (14%)	17,19,21	1.28	2 (11%)
2	BMA	S	3	2	11,11,12	1.85	1 (9%)	15,15,17	0.70	0
2	MAN	S	4	2	11,11,12	1.64	2 (18%)	15,15,17	0.74	0
2	MAN	S	5	2	11,11,12	1.85	2 (18%)	15,15,17	0.82	0
2	MAN	S	6	2	11,11,12	1.83	2 (18%)	15,15,17	0.81	0
4	NAG	T	1	1,4	14,14,15	2.00	2 (14%)	17,19,21	1.16	1 (5%)
4	NAG	T	2	4	14,14,15	2.04	1 (7%)	17,19,21	1.25	2 (11%)
3	NAG	U	1	1,3	14,14,15	2.09	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	U	2	3	14,14,15	2.14	4 (28%)	17,19,21	1.47	3 (17%)
3	BMA	U	3	3	11,11,12	1.85	3 (27%)	15,15,17	0.79	0
5	NAG	V	1	1,5	14,14,15	2.03	3 (21%)	17,19,21	1.04	1 (5%)
5	NAG	V	2	5	14,14,15	2.05	3 (21%)	17,19,21	1.38	3 (17%)
5	BMA	V	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	V	4	5	11,11,12	1.86	4 (36%)	15,15,17	0.82	0
5	MAN	V	5	5	11,11,12	1.84	3 (27%)	15,15,17	0.78	0
3	NAG	W	1	1,3	14,14,15	2.05	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	W	2	3	14,14,15	2.13	5 (35%)	17,19,21	1.34	2 (11%)
3	BMA	W	3	3	11,11,12	1.84	3 (27%)	15,15,17	0.77	0
3	NAG	X	1	1,3	14,14,15	2.03	3 (21%)	17,19,21	1.27	2 (11%)
3	NAG	X	2	3	14,14,15	2.05	3 (21%)	17,19,21	1.29	1 (5%)
3	BMA	X	3	3	11,11,12	1.86	3 (27%)	15,15,17	0.73	0
3	NAG	Y	1	1,3	14,14,15	1.99	2 (14%)	17,19,21	1.19	1 (5%)
3	NAG	Y	2	3	14,14,15	2.11	3 (21%)	17,19,21	1.40	2 (11%)
3	BMA	Y	3	3	11,11,12	1.85	2 (18%)	15,15,17	0.80	0
3	NAG	Z	1	1,3	14,14,15	2.03	1 (7%)	17,19,21	1.13	1 (5%)
3	NAG	Z	2	3	14,14,15	2.10	3 (21%)	17,19,21	1.42	2 (11%)
3	BMA	Z	3	3	11,11,12	1.85	3 (27%)	15,15,17	0.81	0
3	NAG	a	1	1,3	14,14,15	1.96	2 (14%)	17,19,21	1.33	2 (11%)
3	NAG	a	2	3	14,14,15	2.06	2 (14%)	17,19,21	1.19	2 (11%)
3	BMA	a	3	3	11,11,12	1.83	4 (36%)	15,15,17	0.79	0
2	NAG	b	1	1,2	14,14,15	1.93	1 (7%)	17,19,21	1.29	2 (11%)
2	NAG	b	2	2	14,14,15	1.99	2 (14%)	17,19,21	1.29	2 (11%)
2	BMA	b	3	2	11,11,12	1.83	1 (9%)	15,15,17	0.75	0
2	MAN	b	4	2	11,11,12	1.61	2 (18%)	15,15,17	0.72	0
2	MAN	b	5	2	11,11,12	1.84	3 (27%)	15,15,17	0.81	0
2	MAN	b	6	2	11,11,12	1.84	2 (18%)	15,15,17	0.82	0
4	NAG	c	1	1,4	14,14,15	2.01	2 (14%)	17,19,21	1.11	1 (5%)
4	NAG	c	2	4	14,14,15	2.05	2 (14%)	17,19,21	1.27	2 (11%)
2	NAG	d	1	1,2	14,14,15	1.92	2 (14%)	17,19,21	1.31	3 (17%)
2	NAG	d	2	2	14,14,15	2.13	4 (28%)	17,19,21	1.32	2 (11%)
2	BMA	d	3	2	11,11,12	1.83	1 (9%)	15,15,17	0.74	0
2	MAN	d	4	2	11,11,12	1.67	2 (18%)	15,15,17	0.72	0
2	MAN	d	5	2	11,11,12	1.84	2 (18%)	15,15,17	0.76	0
2	MAN	d	6	2	11,11,12	1.81	2 (18%)	15,15,17	0.77	0
3	NAG	e	1	1,3	14,14,15	2.04	2 (14%)	17,19,21	1.15	1 (5%)
3	NAG	e	2	3	14,14,15	1.99	2 (14%)	17,19,21	1.27	2 (11%)
3	BMA	e	3	3	11,11,12	1.84	2 (18%)	15,15,17	0.76	0
2	NAG	f	1	1,2	14,14,15	1.93	2 (14%)	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	f	2	2	14,14,15	2.03	2 (14%)	17,19,21	1.28	2 (11%)
2	BMA	f	3	2	11,11,12	1.84	1 (9%)	15,15,17	0.70	0
2	MAN	f	4	2	11,11,12	1.63	2 (18%)	15,15,17	0.74	0
2	MAN	f	5	2	11,11,12	1.84	2 (18%)	15,15,17	0.81	0
2	MAN	f	6	2	11,11,12	1.84	3 (27%)	15,15,17	0.81	0
4	NAG	g	1	1,4	14,14,15	1.98	2 (14%)	17,19,21	1.16	1 (5%)
4	NAG	g	2	4	14,14,15	2.04	2 (14%)	17,19,21	1.24	2 (11%)
3	NAG	h	1	1,3	14,14,15	2.09	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	h	2	3	14,14,15	2.12	3 (21%)	17,19,21	1.47	3 (17%)
3	BMA	h	3	3	11,11,12	1.86	2 (18%)	15,15,17	0.80	0
5	NAG	i	1	1,5	14,14,15	2.02	3 (21%)	17,19,21	1.05	1 (5%)
5	NAG	i	2	5	14,14,15	2.04	3 (21%)	17,19,21	1.37	2 (11%)
5	BMA	i	3	5	11,11,12	1.85	2 (18%)	15,15,17	0.81	0
5	MAN	i	4	5	11,11,12	1.88	4 (36%)	15,15,17	0.82	0
5	MAN	i	5	5	11,11,12	1.83	3 (27%)	15,15,17	0.79	0
3	NAG	j	1	1,3	14,14,15	2.04	2 (14%)	17,19,21	1.16	1 (5%)
3	NAG	j	2	3	14,14,15	2.13	5 (35%)	17,19,21	1.34	2 (11%)
3	BMA	j	3	3	11,11,12	1.84	2 (18%)	15,15,17	0.76	0
3	NAG	k	1	1,3	14,14,15	2.04	2 (14%)	17,19,21	1.26	2 (11%)
3	NAG	k	2	3	14,14,15	2.04	2 (14%)	17,19,21	1.29	1 (5%)
3	BMA	k	3	3	11,11,12	1.87	2 (18%)	15,15,17	0.72	0
3	NAG	l	1	1,3	14,14,15	1.97	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	l	2	3	14,14,15	2.11	3 (21%)	17,19,21	1.40	2 (11%)
3	BMA	l	3	3	11,11,12	1.86	4 (36%)	15,15,17	0.79	0
3	NAG	m	1	1,3	14,14,15	2.00	1 (7%)	17,19,21	1.12	1 (5%)
3	NAG	m	2	3	14,14,15	2.11	3 (21%)	17,19,21	1.41	2 (11%)
3	BMA	m	3	3	11,11,12	1.87	3 (27%)	15,15,17	0.80	0
3	NAG	n	1	1,3	14,14,15	1.95	2 (14%)	17,19,21	1.33	2 (11%)
3	NAG	n	2	3	14,14,15	2.06	2 (14%)	17,19,21	1.18	1 (5%)
3	BMA	n	3	3	11,11,12	1.82	4 (36%)	15,15,17	0.79	0
2	NAG	o	1	1,2	14,14,15	1.93	1 (7%)	17,19,21	1.29	2 (11%)
2	NAG	o	2	2	14,14,15	2.00	2 (14%)	17,19,21	1.28	2 (11%)
2	BMA	o	3	2	11,11,12	1.83	1 (9%)	15,15,17	0.75	0
2	MAN	o	4	2	11,11,12	1.62	2 (18%)	15,15,17	0.72	0
2	MAN	o	5	2	11,11,12	1.86	3 (27%)	15,15,17	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	o	6	2	11,11,12	1.84	2 (18%)	15,15,17	0.82	0
4	NAG	p	1	1,4	14,14,15	2.03	3 (21%)	17,19,21	1.09	1 (5%)
4	NAG	p	2	4	14,14,15	2.05	2 (14%)	17,19,21	1.28	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	0/1/1/1
2	MAN	D	6	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
2	MAN	F	4	2	-	1/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
2	MAN	F	6	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	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	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1

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

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

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

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C2-N2	-6.38	1.35	1.46
2	d	2	NAG	C2-N2	-6.38	1.35	1.46
3	e	1	NAG	C2-N2	-6.37	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C2-N2	-6.36	1.35	1.46
3	n	2	NAG	C2-N2	-6.36	1.35	1.46
3	R	1	NAG	C2-N2	-6.35	1.35	1.46
3	a	2	NAG	C2-N2	-6.32	1.35	1.46
3	N	2	NAG	C2-N2	-6.31	1.35	1.46
2	Q	2	NAG	C2-N2	-6.30	1.35	1.46
3	U	1	NAG	C2-N2	-6.28	1.35	1.46
5	V	2	NAG	C2-N2	-6.27	1.35	1.46
2	O	1	NAG	C2-N2	-6.27	1.35	1.46
5	I	2	NAG	C2-N2	-6.24	1.35	1.46
5	i	2	NAG	C2-N2	-6.23	1.35	1.46
3	h	1	NAG	C2-N2	-6.22	1.36	1.46
2	o	1	NAG	C2-N2	-6.21	1.36	1.46
3	Z	1	NAG	C2-N2	-6.21	1.36	1.46
2	b	1	NAG	C2-N2	-6.20	1.36	1.46
3	H	1	NAG	C2-N2	-6.19	1.36	1.46
3	N	1	NAG	C2-N2	-6.18	1.36	1.46
3	R	2	NAG	C2-N2	-6.17	1.36	1.46
3	U	2	NAG	C2-N2	-6.17	1.36	1.46
3	E	2	NAG	C2-N2	-6.16	1.36	1.46
3	W	2	NAG	C2-N2	-6.16	1.36	1.46
3	j	2	NAG	C2-N2	-6.15	1.36	1.46
3	L	2	NAG	C2-N2	-6.15	1.36	1.46
2	f	2	NAG	C2-N2	-6.15	1.36	1.46
3	M	1	NAG	C2-N2	-6.14	1.36	1.46
2	O	2	NAG	C2-N2	-6.14	1.36	1.46
4	P	2	NAG	C2-N2	-6.14	1.36	1.46
3	Y	2	NAG	C2-N2	-6.14	1.36	1.46
3	m	2	NAG	C2-N2	-6.14	1.36	1.46
3	l	2	NAG	C2-N2	-6.13	1.36	1.46
3	a	1	NAG	C2-N2	-6.13	1.36	1.46
4	p	2	NAG	C2-N2	-6.13	1.36	1.46
3	n	1	NAG	C2-N2	-6.12	1.36	1.46
2	S	2	NAG	C2-N2	-6.11	1.36	1.46
3	H	2	NAG	C2-N2	-6.11	1.36	1.46
3	h	2	NAG	C2-N2	-6.11	1.36	1.46
3	e	2	NAG	C2-N2	-6.11	1.36	1.46
3	Z	2	NAG	C2-N2	-6.10	1.36	1.46
3	K	2	NAG	C2-N2	-6.10	1.36	1.46
2	o	2	NAG	C2-N2	-6.10	1.36	1.46
2	b	2	NAG	C2-N2	-6.09	1.36	1.46
4	c	2	NAG	C2-N2	-6.09	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	NAG	C2-N2	-6.08	1.36	1.46
3	J	2	NAG	C2-N2	-6.08	1.36	1.46
3	X	2	NAG	C2-N2	-6.07	1.36	1.46
4	T	2	NAG	C2-N2	-6.06	1.36	1.46
3	m	1	NAG	C2-N2	-6.06	1.36	1.46
3	j	1	NAG	C2-N2	-6.05	1.36	1.46
2	F	2	NAG	C2-N2	-6.04	1.36	1.46
3	K	1	NAG	C2-N2	-6.04	1.36	1.46
3	k	2	NAG	C2-N2	-6.03	1.36	1.46
3	W	1	NAG	C2-N2	-6.03	1.36	1.46
4	g	2	NAG	C2-N2	-6.02	1.36	1.46
3	J	1	NAG	C2-N2	-6.02	1.36	1.46
4	T	1	NAG	C2-N2	-6.00	1.36	1.46
3	k	1	NAG	C2-N2	-5.98	1.36	1.46
4	G	2	NAG	C2-N2	-5.98	1.36	1.46
5	V	1	NAG	C2-N2	-5.98	1.36	1.46
2	D	1	NAG	C2-N2	-5.97	1.36	1.46
5	i	1	NAG	C2-N2	-5.96	1.36	1.46
4	g	1	NAG	C2-N2	-5.96	1.36	1.46
3	X	1	NAG	C2-N2	-5.95	1.36	1.46
4	G	1	NAG	C2-N2	-5.94	1.36	1.46
5	I	1	NAG	C2-N2	-5.94	1.36	1.46
4	p	1	NAG	C2-N2	-5.94	1.36	1.46
3	Y	1	NAG	C2-N2	-5.92	1.36	1.46
2	d	1	NAG	C2-N2	-5.92	1.36	1.46
3	L	1	NAG	C2-N2	-5.91	1.36	1.46
4	c	1	NAG	C2-N2	-5.90	1.36	1.46
2	Q	1	NAG	C2-N2	-5.86	1.36	1.46
4	P	1	NAG	C2-N2	-5.84	1.36	1.46
3	l	1	NAG	C2-N2	-5.82	1.36	1.46
2	F	1	NAG	C2-N2	-5.77	1.36	1.46
2	f	1	NAG	C2-N2	-5.76	1.36	1.46
2	S	1	NAG	C2-N2	-5.76	1.36	1.46
2	o	3	BMA	O2-C2	-4.19	1.34	1.43
2	O	3	BMA	O2-C2	-4.18	1.34	1.43
2	b	3	BMA	O2-C2	-4.17	1.34	1.43
2	F	3	BMA	O2-C2	-4.17	1.34	1.43
2	f	3	BMA	O2-C2	-4.17	1.34	1.43
2	D	3	BMA	O2-C2	-4.17	1.34	1.43
2	S	3	BMA	O2-C2	-4.14	1.34	1.43
2	Q	3	BMA	O2-C2	-4.14	1.34	1.43
2	d	3	BMA	O2-C2	-4.10	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3	BMA	O2-C2	-4.08	1.34	1.43
5	i	3	BMA	O2-C2	-4.05	1.34	1.43
3	K	3	BMA	O2-C2	-4.05	1.34	1.43
2	D	5	MAN	O2-C2	-4.04	1.34	1.43
2	b	6	MAN	O2-C2	-4.03	1.34	1.43
3	h	3	BMA	O2-C2	-4.03	1.34	1.43
3	k	3	BMA	O2-C2	-4.03	1.34	1.43
5	I	5	MAN	O2-C2	-4.02	1.34	1.43
3	U	3	BMA	O2-C2	-4.02	1.34	1.43
3	H	3	BMA	O2-C2	-4.02	1.34	1.43
5	V	3	BMA	O2-C2	-4.01	1.34	1.43
3	X	3	BMA	O2-C2	-4.01	1.34	1.43
5	i	5	MAN	O2-C2	-4.01	1.34	1.43
2	f	6	MAN	O2-C2	-4.00	1.34	1.43
3	l	3	BMA	O2-C2	-4.00	1.34	1.43
5	V	5	MAN	O2-C2	-4.00	1.34	1.43
2	O	5	MAN	O2-C2	-4.00	1.35	1.43
2	o	6	MAN	O2-C2	-4.00	1.35	1.43
3	Y	3	BMA	O2-C2	-3.99	1.35	1.43
2	F	6	MAN	O2-C2	-3.99	1.35	1.43
2	O	6	MAN	O2-C2	-3.98	1.35	1.43
2	o	5	MAN	O2-C2	-3.98	1.35	1.43
3	e	3	BMA	O2-C2	-3.98	1.35	1.43
2	d	5	MAN	O2-C2	-3.98	1.35	1.43
3	R	3	BMA	O2-C2	-3.97	1.35	1.43
3	E	3	BMA	O2-C2	-3.97	1.35	1.43
2	D	6	MAN	O2-C2	-3.96	1.35	1.43
2	F	5	MAN	O2-C2	-3.96	1.35	1.43
2	Q	5	MAN	O2-C2	-3.96	1.35	1.43
2	d	6	MAN	O2-C2	-3.96	1.35	1.43
2	S	5	MAN	O2-C2	-3.95	1.35	1.43
3	J	3	BMA	O2-C2	-3.95	1.35	1.43
2	Q	6	MAN	O2-C2	-3.95	1.35	1.43
2	b	5	MAN	O2-C2	-3.94	1.35	1.43
2	S	6	MAN	O2-C2	-3.93	1.35	1.43
3	j	3	BMA	O2-C2	-3.93	1.35	1.43
3	Z	3	BMA	O2-C2	-3.93	1.35	1.43
2	f	5	MAN	O2-C2	-3.93	1.35	1.43
5	I	4	MAN	O2-C2	-3.92	1.35	1.43
3	W	3	BMA	O2-C2	-3.92	1.35	1.43
5	V	4	MAN	O2-C2	-3.92	1.35	1.43
3	m	3	BMA	O2-C2	-3.92	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	i	4	MAN	O2-C2	-3.92	1.35	1.43
3	L	3	BMA	O2-C2	-3.92	1.35	1.43
3	M	3	BMA	O2-C2	-3.88	1.35	1.43
3	a	3	BMA	O2-C2	-3.84	1.35	1.43
3	N	3	BMA	O2-C2	-3.81	1.35	1.43
3	n	3	BMA	O2-C2	-3.79	1.35	1.43
2	D	4	MAN	O2-C2	-3.08	1.36	1.43
2	d	4	MAN	O2-C2	-3.08	1.36	1.43
2	Q	4	MAN	O2-C2	-3.06	1.36	1.43
2	O	4	MAN	O2-C2	-2.99	1.37	1.43
2	b	4	MAN	O2-C2	-2.98	1.37	1.43
2	S	4	MAN	O2-C2	-2.97	1.37	1.43
2	o	4	MAN	O2-C2	-2.95	1.37	1.43
2	F	4	MAN	O2-C2	-2.93	1.37	1.43
2	f	4	MAN	O2-C2	-2.93	1.37	1.43
3	k	1	NAG	C4-C5	2.71	1.58	1.53
3	K	1	NAG	C4-C5	2.68	1.58	1.53
3	X	1	NAG	C4-C5	2.68	1.58	1.53
3	M	2	NAG	C4-C5	2.59	1.58	1.53
3	h	2	NAG	C4-C5	2.58	1.58	1.53
3	j	2	NAG	C4-C5	2.57	1.58	1.53
3	m	2	NAG	C4-C5	2.57	1.58	1.53
3	Z	2	NAG	C4-C5	2.56	1.58	1.53
2	D	1	NAG	C4-C5	2.56	1.58	1.53
3	J	2	NAG	C4-C5	2.56	1.58	1.53
3	Y	2	NAG	C4-C5	2.54	1.58	1.53
2	d	1	NAG	C4-C5	2.54	1.58	1.53
3	U	2	NAG	C4-C5	2.53	1.58	1.53
3	H	2	NAG	C4-C5	2.53	1.58	1.53
3	l	2	NAG	C4-C5	2.53	1.58	1.53
3	W	2	NAG	C4-C5	2.53	1.58	1.53
3	k	2	NAG	C4-C5	2.50	1.58	1.53
2	Q	1	NAG	C4-C5	2.50	1.58	1.53
3	L	2	NAG	C4-C5	2.50	1.58	1.53
3	X	2	NAG	C4-C5	2.45	1.58	1.53
3	K	2	NAG	C4-C5	2.45	1.58	1.53
2	f	2	NAG	C4-C5	2.41	1.58	1.53
5	i	4	MAN	O5-C1	2.41	1.47	1.43
2	F	2	NAG	C4-C5	2.38	1.58	1.53
2	o	5	MAN	O5-C1	2.37	1.47	1.43
5	V	1	NAG	C1-C2	2.35	1.55	1.52
4	G	1	NAG	C4-C5	2.35	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	i	1	NAG	C1-C2	2.34	1.55	1.52
3	m	3	BMA	O5-C1	2.33	1.47	1.43
5	i	2	NAG	C4-C5	2.33	1.58	1.53
2	S	2	NAG	C4-C5	2.33	1.58	1.53
3	K	3	BMA	O5-C1	2.33	1.47	1.43
5	I	2	NAG	C4-C5	2.33	1.58	1.53
2	b	5	MAN	O5-C1	2.32	1.47	1.43
5	I	4	MAN	O5-C1	2.32	1.47	1.43
5	V	4	MAN	O5-C1	2.32	1.47	1.43
2	O	5	MAN	O5-C1	2.32	1.47	1.43
5	V	2	NAG	C4-C5	2.31	1.57	1.53
2	F	5	MAN	O5-C1	2.31	1.47	1.43
3	W	3	BMA	O5-C1	2.31	1.47	1.43
4	g	1	NAG	C4-C5	2.30	1.57	1.53
3	l	3	BMA	O5-C1	2.30	1.47	1.43
3	R	3	BMA	O5-C1	2.30	1.47	1.43
5	I	1	NAG	C1-C2	2.30	1.55	1.52
3	M	3	BMA	O5-C1	2.30	1.47	1.43
2	D	5	MAN	O5-C1	2.29	1.47	1.43
3	k	3	BMA	O5-C1	2.29	1.47	1.43
3	l	1	NAG	C4-C5	2.29	1.57	1.53
3	Z	3	BMA	O5-C1	2.29	1.47	1.43
4	T	1	NAG	C4-C5	2.29	1.57	1.53
2	S	5	MAN	O5-C1	2.29	1.47	1.43
3	W	1	NAG	C4-C5	2.29	1.57	1.53
3	j	1	NAG	C4-C5	2.29	1.57	1.53
2	d	5	MAN	O5-C1	2.28	1.47	1.43
2	f	5	MAN	O5-C1	2.28	1.47	1.43
3	Y	1	NAG	C4-C5	2.28	1.57	1.53
3	Y	3	BMA	O5-C1	2.27	1.47	1.43
3	E	3	BMA	O5-C1	2.27	1.47	1.43
3	e	3	BMA	O5-C1	2.27	1.47	1.43
3	J	1	NAG	C4-C5	2.26	1.57	1.53
2	Q	5	MAN	O5-C1	2.26	1.47	1.43
3	X	3	BMA	O5-C1	2.26	1.47	1.43
3	N	3	BMA	O5-C1	2.26	1.47	1.43
3	n	3	BMA	O5-C1	2.26	1.47	1.43
2	f	6	MAN	O5-C1	2.25	1.47	1.43
3	L	3	BMA	O5-C1	2.25	1.47	1.43
3	a	3	BMA	O5-C1	2.25	1.47	1.43
3	J	3	BMA	O5-C1	2.24	1.47	1.43
3	j	3	BMA	O5-C1	2.24	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	6	MAN	O5-C1	2.24	1.47	1.43
3	L	1	NAG	C4-C5	2.24	1.57	1.53
2	F	4	MAN	O5-C1	2.23	1.47	1.43
3	H	3	BMA	O5-C1	2.23	1.47	1.43
3	h	3	BMA	O5-C1	2.23	1.47	1.43
2	S	6	MAN	O5-C1	2.22	1.47	1.43
2	b	6	MAN	O5-C1	2.22	1.47	1.43
2	Q	4	MAN	O5-C1	2.22	1.47	1.43
3	j	2	NAG	O5-C1	2.22	1.47	1.43
3	J	2	NAG	O5-C1	2.21	1.47	1.43
3	U	3	BMA	O5-C1	2.21	1.47	1.43
2	Q	2	NAG	C4-C5	2.21	1.57	1.53
2	D	2	NAG	C4-C5	2.21	1.57	1.53
3	W	2	NAG	O5-C1	2.21	1.47	1.43
2	o	6	MAN	O5-C1	2.21	1.47	1.43
2	b	2	NAG	C4-C5	2.21	1.57	1.53
3	U	2	NAG	O5-C1	2.21	1.47	1.43
2	D	4	MAN	O5-C1	2.21	1.47	1.43
2	o	2	NAG	C4-C5	2.21	1.57	1.53
2	F	6	MAN	O5-C1	2.20	1.47	1.43
3	U	1	NAG	C4-C5	2.20	1.57	1.53
4	p	1	NAG	C1-C2	2.20	1.55	1.52
2	D	6	MAN	O5-C1	2.20	1.47	1.43
2	O	6	MAN	O5-C1	2.19	1.47	1.43
3	H	2	NAG	O5-C1	2.19	1.47	1.43
2	d	2	NAG	C4-C5	2.19	1.57	1.53
2	S	4	MAN	O5-C1	2.19	1.47	1.43
3	l	2	NAG	O5-C1	2.19	1.47	1.43
3	Y	2	NAG	O5-C1	2.19	1.47	1.43
2	O	2	NAG	C4-C5	2.19	1.57	1.53
3	M	2	NAG	O5-C1	2.18	1.47	1.43
3	h	1	NAG	C4-C5	2.18	1.57	1.53
3	H	1	NAG	C4-C5	2.18	1.57	1.53
2	f	4	MAN	O5-C1	2.17	1.47	1.43
3	E	2	NAG	C4-C5	2.16	1.57	1.53
2	d	4	MAN	O5-C1	2.16	1.47	1.43
5	V	5	MAN	O5-C1	2.16	1.47	1.43
3	L	2	NAG	O5-C1	2.16	1.47	1.43
3	R	2	NAG	C4-C5	2.15	1.57	1.53
5	I	4	MAN	C4-C5	2.15	1.57	1.53
3	a	3	BMA	C4-C5	2.14	1.57	1.53
3	n	3	BMA	C4-C5	2.14	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	1	NAG	C1-C2	2.14	1.55	1.52
3	h	2	NAG	O5-C1	2.14	1.47	1.43
2	d	2	NAG	O5-C1	2.14	1.47	1.43
2	d	6	MAN	O5-C1	2.14	1.47	1.43
3	m	2	NAG	O5-C1	2.14	1.47	1.43
2	D	2	NAG	O5-C1	2.13	1.47	1.43
3	Z	2	NAG	O5-C1	2.12	1.47	1.43
2	Q	2	NAG	O5-C1	2.11	1.47	1.43
5	I	5	MAN	O5-C1	2.11	1.47	1.43
5	V	4	MAN	C6-C5	2.10	1.58	1.51
4	P	1	NAG	C1-C2	2.10	1.55	1.52
2	O	4	MAN	O5-C1	2.09	1.47	1.43
3	N	1	NAG	C4-C5	2.09	1.57	1.53
2	o	4	MAN	O5-C1	2.09	1.47	1.43
5	i	5	MAN	O5-C1	2.09	1.47	1.43
3	R	1	NAG	C4-C5	2.09	1.57	1.53
3	N	3	BMA	C4-C5	2.09	1.57	1.53
5	I	4	MAN	C6-C5	2.09	1.58	1.51
5	i	4	MAN	C6-C5	2.09	1.58	1.51
3	N	2	NAG	C4-C5	2.09	1.57	1.53
2	f	1	NAG	C1-C2	2.08	1.55	1.52
2	b	4	MAN	O5-C1	2.08	1.47	1.43
2	F	1	NAG	C1-C2	2.07	1.55	1.52
3	e	2	NAG	C4-C5	2.07	1.57	1.53
3	e	1	NAG	C4-C5	2.07	1.57	1.53
2	S	1	NAG	C1-C2	2.06	1.55	1.52
3	E	1	NAG	C4-C5	2.06	1.57	1.53
3	N	3	BMA	C6-C5	2.06	1.58	1.51
3	j	2	NAG	C1-C2	2.06	1.55	1.52
5	i	3	BMA	C6-C5	2.06	1.58	1.51
3	n	2	NAG	C4-C5	2.06	1.57	1.53
3	a	1	NAG	C4-C5	2.05	1.57	1.53
3	a	3	BMA	C6-C5	2.05	1.58	1.51
3	a	2	NAG	C4-C5	2.05	1.57	1.53
5	i	2	NAG	C6-C5	2.05	1.58	1.51
3	n	1	NAG	C4-C5	2.05	1.57	1.53
5	V	4	MAN	C4-C5	2.05	1.57	1.53
5	i	4	MAN	C4-C5	2.05	1.57	1.53
2	F	6	MAN	C4-C5	2.04	1.57	1.53
3	J	3	BMA	C4-C5	2.04	1.57	1.53
5	I	2	NAG	C6-C5	2.04	1.58	1.51
5	I	3	BMA	C6-C5	2.04	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	5	MAN	C6-C5	2.04	1.58	1.51
2	f	6	MAN	C4-C5	2.04	1.57	1.53
5	i	5	MAN	C4-C5	2.03	1.57	1.53
3	H	2	NAG	C6-C5	2.03	1.58	1.51
3	E	1	NAG	C6-C5	2.03	1.58	1.51
3	X	2	NAG	C6-C5	2.03	1.58	1.51
5	V	1	NAG	O5-C1	2.03	1.47	1.43
3	L	3	BMA	C4-C5	2.03	1.57	1.53
4	P	2	NAG	C4-C5	2.03	1.57	1.53
4	p	2	NAG	C4-C5	2.03	1.57	1.53
3	M	2	NAG	C6-C5	2.03	1.58	1.51
3	W	2	NAG	C1-C2	2.03	1.55	1.52
5	V	2	NAG	C6-C5	2.02	1.58	1.51
5	V	5	MAN	C4-C5	2.02	1.57	1.53
3	n	3	BMA	C6-C5	2.02	1.58	1.51
4	p	1	NAG	C6-C5	2.02	1.58	1.51
5	V	3	BMA	C6-C5	2.02	1.58	1.51
3	K	1	NAG	C6-C5	2.02	1.58	1.51
2	D	2	NAG	C1-C2	2.02	1.55	1.52
3	W	3	BMA	C4-C5	2.01	1.57	1.53
3	K	3	BMA	C4-C5	2.01	1.57	1.53
4	c	2	NAG	C4-C5	2.01	1.57	1.53
2	o	5	MAN	C6-C5	2.01	1.58	1.51
2	b	5	MAN	C6-C5	2.01	1.58	1.51
3	Z	3	BMA	C4-C5	2.01	1.57	1.53
4	g	2	NAG	O5-C1	2.01	1.47	1.43
5	I	5	MAN	C4-C5	2.01	1.57	1.53
3	U	2	NAG	C6-C5	2.01	1.58	1.51
3	m	3	BMA	C4-C5	2.01	1.57	1.53
3	W	2	NAG	C6-C5	2.01	1.58	1.51
3	J	2	NAG	C6-C5	2.01	1.58	1.51
2	F	5	MAN	C4-C5	2.01	1.57	1.53
3	j	2	NAG	C6-C5	2.01	1.58	1.51
2	D	2	NAG	C6-C5	2.01	1.58	1.51
3	X	1	NAG	C6-C5	2.01	1.58	1.51
3	E	2	NAG	C6-C5	2.00	1.58	1.51
3	U	3	BMA	C4-C5	2.00	1.57	1.53
2	d	2	NAG	C6-C5	2.00	1.58	1.51
3	X	3	BMA	C4-C5	2.00	1.57	1.53
5	i	1	NAG	O5-C1	2.00	1.47	1.43
3	l	3	BMA	C6-C5	2.00	1.58	1.51
3	l	3	BMA	C4-C5	2.00	1.57	1.53

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C4-C3-C2	-3.16	106.39	111.02
3	U	2	NAG	C4-C3-C2	-3.15	106.40	111.02
3	h	2	NAG	C4-C3-C2	-3.15	106.41	111.02
3	Z	2	NAG	C4-C3-C2	-2.90	106.76	111.02
3	M	2	NAG	C4-C3-C2	-2.87	106.81	111.02
3	m	2	NAG	C4-C3-C2	-2.86	106.83	111.02
3	L	2	NAG	C4-C3-C2	-2.82	106.88	111.02
3	l	2	NAG	C4-C3-C2	-2.81	106.91	111.02
3	Y	2	NAG	C4-C3-C2	-2.79	106.94	111.02
3	J	2	NAG	C4-C3-C2	-2.64	107.15	111.02
2	D	2	NAG	C8-C7-N2	2.64	120.49	116.12
3	W	2	NAG	C4-C3-C2	-2.61	107.19	111.02
2	Q	2	NAG	C8-C7-N2	2.61	120.45	116.12
3	j	2	NAG	C4-C3-C2	-2.61	107.20	111.02
2	d	2	NAG	C8-C7-N2	2.58	120.41	116.12
5	I	2	NAG	C4-C3-C2	-2.52	107.33	111.02
5	V	2	NAG	C4-C3-C2	-2.50	107.36	111.02
5	i	2	NAG	C4-C3-C2	-2.47	107.39	111.02
2	O	1	NAG	C8-C7-N2	2.47	120.21	116.12
4	T	2	NAG	C8-C7-N2	2.46	120.20	116.12
4	g	2	NAG	C8-C7-N2	2.46	120.20	116.12
3	n	1	NAG	C4-C3-C2	-2.46	107.42	111.02
2	o	1	NAG	C8-C7-N2	2.45	120.19	116.12
2	f	1	NAG	C8-C7-N2	2.45	120.18	116.12
2	F	1	NAG	C8-C7-N2	2.44	120.16	116.12
5	i	2	NAG	C8-C7-N2	2.43	120.16	116.12
3	N	1	NAG	C8-C7-N2	2.43	120.15	116.12
5	I	2	NAG	C8-C7-N2	2.43	120.14	116.12
3	n	1	NAG	C8-C7-N2	2.42	120.14	116.12
3	a	1	NAG	C8-C7-N2	2.42	120.14	116.12
2	b	1	NAG	C8-C7-N2	2.42	120.13	116.12
2	S	1	NAG	C8-C7-N2	2.42	120.13	116.12
3	a	1	NAG	C4-C3-C2	-2.42	107.48	111.02
3	R	2	NAG	C8-C7-N2	2.42	120.13	116.12
3	E	2	NAG	C8-C7-N2	2.41	120.12	116.12
4	G	2	NAG	C8-C7-N2	2.41	120.12	116.12
3	Y	1	NAG	C8-C7-N2	2.40	120.11	116.12
5	V	2	NAG	C8-C7-N2	2.40	120.10	116.12
3	N	1	NAG	C4-C3-C2	-2.38	107.53	111.02
3	X	2	NAG	C8-C7-N2	2.38	120.06	116.12
4	P	2	NAG	C8-C7-N2	2.38	120.06	116.12
3	e	2	NAG	C8-C7-N2	2.38	120.06	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	2	NAG	C8-C7-N2	2.38	120.06	116.12
3	U	2	NAG	C8-C7-N2	2.37	120.06	116.12
3	h	2	NAG	C8-C7-N2	2.37	120.05	116.12
3	K	2	NAG	C8-C7-N2	2.37	120.04	116.12
3	L	1	NAG	C8-C7-N2	2.36	120.04	116.12
3	k	2	NAG	C8-C7-N2	2.36	120.04	116.12
3	H	2	NAG	C8-C7-N2	2.36	120.04	116.12
4	c	2	NAG	C8-C7-N2	2.36	120.03	116.12
3	X	1	NAG	C8-C7-N2	2.35	120.02	116.12
4	p	2	NAG	C8-C7-N2	2.35	120.01	116.12
3	Z	2	NAG	C8-C7-N2	2.35	120.01	116.12
3	M	2	NAG	C8-C7-N2	2.35	120.01	116.12
2	O	2	NAG	C8-C7-N2	2.34	120.00	116.12
3	l	2	NAG	C8-C7-N2	2.34	120.00	116.12
3	l	1	NAG	C8-C7-N2	2.33	119.98	116.12
2	o	2	NAG	C8-C7-N2	2.33	119.98	116.12
3	Y	2	NAG	C8-C7-N2	2.31	119.95	116.12
3	K	1	NAG	C8-C7-N2	2.31	119.95	116.12
2	b	2	NAG	C8-C7-N2	2.31	119.94	116.12
3	L	2	NAG	C8-C7-N2	2.30	119.94	116.12
3	J	2	NAG	C8-C7-N2	2.30	119.93	116.12
2	f	2	NAG	C8-C7-N2	2.30	119.93	116.12
3	W	2	NAG	C8-C7-N2	2.29	119.92	116.12
3	k	1	NAG	C8-C7-N2	2.29	119.92	116.12
4	c	1	NAG	C8-C7-N2	2.29	119.91	116.12
4	p	1	NAG	C8-C7-N2	2.28	119.90	116.12
4	P	1	NAG	C8-C7-N2	2.28	119.89	116.12
3	j	2	NAG	C8-C7-N2	2.27	119.89	116.12
2	S	2	NAG	C8-C7-N2	2.27	119.88	116.12
3	Z	1	NAG	C8-C7-N2	2.27	119.88	116.12
3	N	2	NAG	C8-C7-N2	2.26	119.87	116.12
4	P	2	NAG	C4-C3-C2	-2.26	107.70	111.02
4	p	2	NAG	C4-C3-C2	-2.26	107.71	111.02
2	F	2	NAG	C8-C7-N2	2.25	119.86	116.12
4	c	2	NAG	C4-C3-C2	-2.25	107.72	111.02
3	M	1	NAG	C8-C7-N2	2.24	119.84	116.12
3	m	1	NAG	C8-C7-N2	2.24	119.84	116.12
5	I	1	NAG	C8-C7-N2	2.23	119.82	116.12
3	n	2	NAG	C8-C7-N2	2.23	119.82	116.12
3	W	1	NAG	C8-C7-N2	2.21	119.79	116.12
5	i	1	NAG	C8-C7-N2	2.21	119.79	116.12
3	E	2	NAG	C4-C3-C2	-2.21	107.79	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	2	NAG	C8-C7-N2	2.20	119.77	116.12
3	j	1	NAG	C8-C7-N2	2.20	119.76	116.12
5	V	1	NAG	C8-C7-N2	2.19	119.74	116.12
3	J	1	NAG	C8-C7-N2	2.17	119.72	116.12
4	T	1	NAG	C8-C7-N2	2.17	119.72	116.12
3	e	2	NAG	C4-C3-C2	-2.17	107.84	111.02
3	U	1	NAG	C8-C7-N2	2.16	119.71	116.12
4	T	2	NAG	C4-C3-C2	-2.16	107.86	111.02
4	G	2	NAG	C4-C3-C2	-2.16	107.86	111.02
4	g	1	NAG	C8-C7-N2	2.15	119.69	116.12
3	R	2	NAG	C4-C3-C2	-2.15	107.87	111.02
2	b	2	NAG	O4-C4-C3	-2.15	105.31	110.38
2	O	2	NAG	O4-C4-C3	-2.15	105.31	110.38
3	k	1	NAG	O4-C4-C3	-2.15	105.31	110.38
4	G	1	NAG	C8-C7-N2	2.15	119.68	116.12
3	h	1	NAG	C8-C7-N2	2.14	119.67	116.12
3	X	1	NAG	O4-C4-C3	-2.14	105.33	110.38
2	d	1	NAG	C8-C7-N2	2.14	119.66	116.12
2	f	2	NAG	C1-C2-N2	-2.13	107.08	110.43
2	D	1	NAG	C8-C7-N2	2.13	119.65	116.12
2	D	2	NAG	O4-C4-C3	-2.13	105.36	110.38
2	o	2	NAG	O4-C4-C3	-2.12	105.38	110.38
2	Q	2	NAG	O4-C4-C3	-2.12	105.38	110.38
3	H	1	NAG	C8-C7-N2	2.12	119.63	116.12
3	K	1	NAG	O4-C4-C3	-2.11	105.39	110.38
2	d	2	NAG	O4-C4-C3	-2.11	105.40	110.38
2	F	2	NAG	C1-C2-N2	-2.11	107.11	110.43
3	e	1	NAG	C8-C7-N2	2.10	119.61	116.12
4	g	2	NAG	C4-C3-C2	-2.10	107.94	111.02
3	E	1	NAG	C8-C7-N2	2.08	119.57	116.12
2	Q	1	NAG	C8-C7-N2	2.08	119.56	116.12
2	S	2	NAG	C1-C2-N2	-2.07	107.17	110.43
2	o	1	NAG	C4-C3-C2	-2.06	108.00	111.02
2	d	1	NAG	C3-C4-C5	-2.06	106.50	110.23
3	R	1	NAG	C8-C7-N2	2.05	119.52	116.12
2	D	1	NAG	C3-C4-C5	-2.04	106.54	110.23
5	I	2	NAG	O5-C1-C2	-2.03	108.15	111.29
2	b	1	NAG	C4-C3-C2	-2.03	108.04	111.02
2	Q	1	NAG	C3-C4-C5	-2.03	106.56	110.23
5	V	2	NAG	O5-C1-C2	-2.02	108.16	111.29
3	a	2	NAG	O5-C1-C2	-2.02	108.17	111.29
2	O	1	NAG	C4-C3-C2	-2.01	108.07	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	NAG	C2-N2-C7	-2.01	120.20	122.90
3	h	2	NAG	C2-N2-C7	-2.01	120.21	122.90
4	G	2	NAG	C2-N2-C7	-2.01	120.21	122.90
2	Q	1	NAG	C1-C2-N2	-2.01	107.27	110.43
2	d	1	NAG	C1-C2-N2	-2.01	107.27	110.43
3	H	2	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	3	BMA	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
5	i	3	BMA	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	n	1	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	S	3	BMA	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	f	3	BMA	O5-C5-C6-O6
2	o	3	BMA	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	n	1	NAG	C4-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
5	V	3	BMA	C4-C5-C6-O6
5	V	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	i	3	BMA	C4-C5-C6-O6
5	i	4	MAN	C4-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
5	V	4	MAN	O5-C5-C6-O6
5	i	4	MAN	O5-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
2	b	5	MAN	O5-C5-C6-O6
2	o	5	MAN	O5-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	S	3	BMA	C4-C5-C6-O6
2	f	3	BMA	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
2	b	3	BMA	C4-C5-C6-O6
2	d	3	BMA	C4-C5-C6-O6
2	o	3	BMA	C4-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
3	Z	3	BMA	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	Q	4	MAN	O5-C5-C6-O6
2	Q	5	MAN	O5-C5-C6-O6
2	S	4	MAN	O5-C5-C6-O6
2	d	4	MAN	O5-C5-C6-O6
2	d	5	MAN	O5-C5-C6-O6
2	f	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	M	3	BMA	O5-C5-C6-O6
3	m	3	BMA	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	Q	6	MAN	O5-C5-C6-O6
2	d	6	MAN	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
3	a	3	BMA	O5-C5-C6-O6
3	n	3	BMA	O5-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	R	3	BMA	O5-C5-C6-O6
3	e	3	BMA	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	i	1	NAG	C4-C5-C6-O6
2	O	4	MAN	O5-C5-C6-O6
2	b	4	MAN	O5-C5-C6-O6
2	o	4	MAN	O5-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	S	5	MAN	O5-C5-C6-O6
2	f	5	MAN	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	W	3	BMA	O5-C5-C6-O6
3	j	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6
5	V	5	MAN	O5-C5-C6-O6
5	i	5	MAN	O5-C5-C6-O6
2	b	6	MAN	O5-C5-C6-O6
2	O	6	MAN	O5-C5-C6-O6
2	o	6	MAN	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
3	X	3	BMA	O5-C5-C6-O6
3	k	3	BMA	O5-C5-C6-O6
2	F	6	MAN	O5-C5-C6-O6
2	S	6	MAN	O5-C5-C6-O6
2	f	6	MAN	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
3	Y	3	BMA	O5-C5-C6-O6

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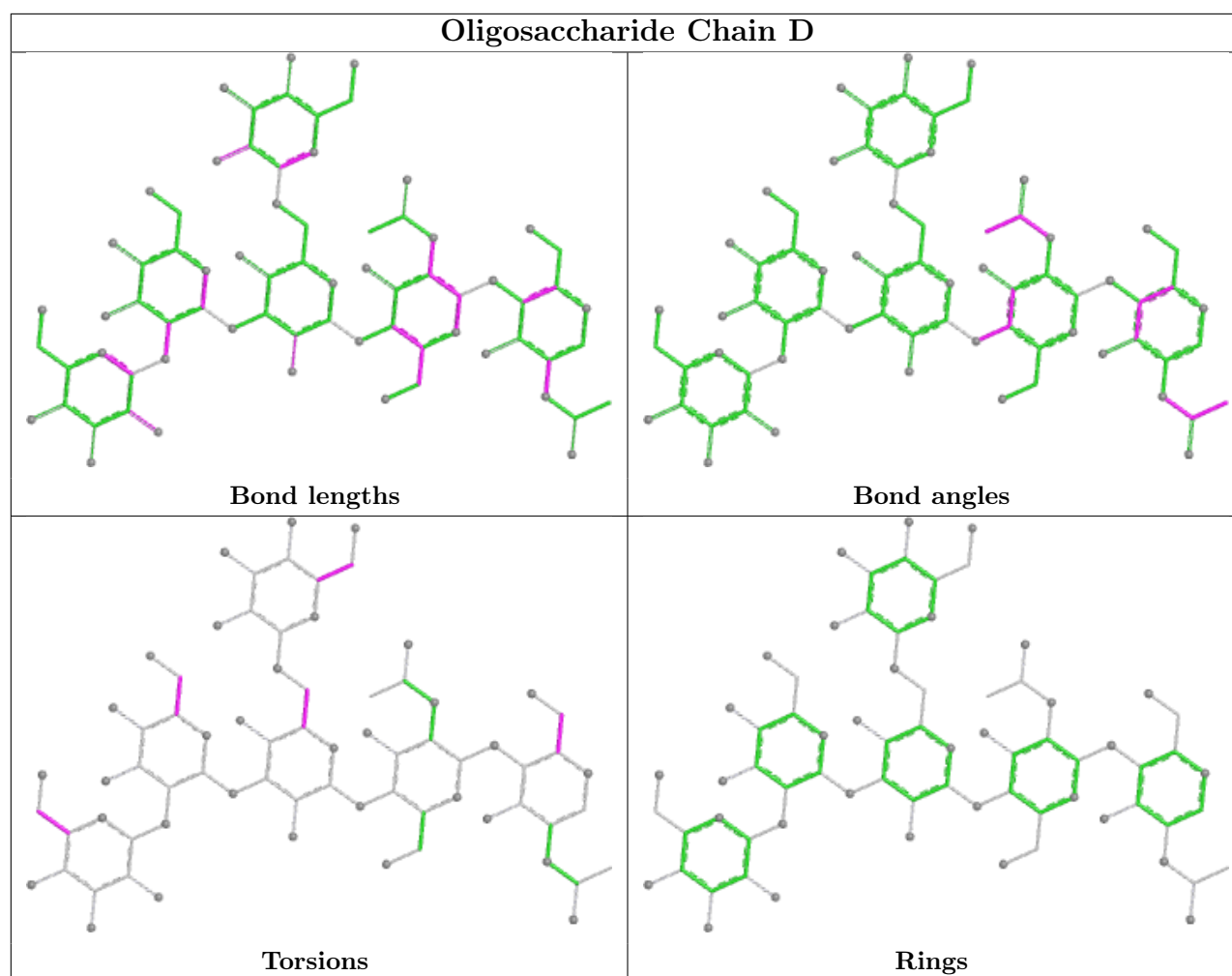
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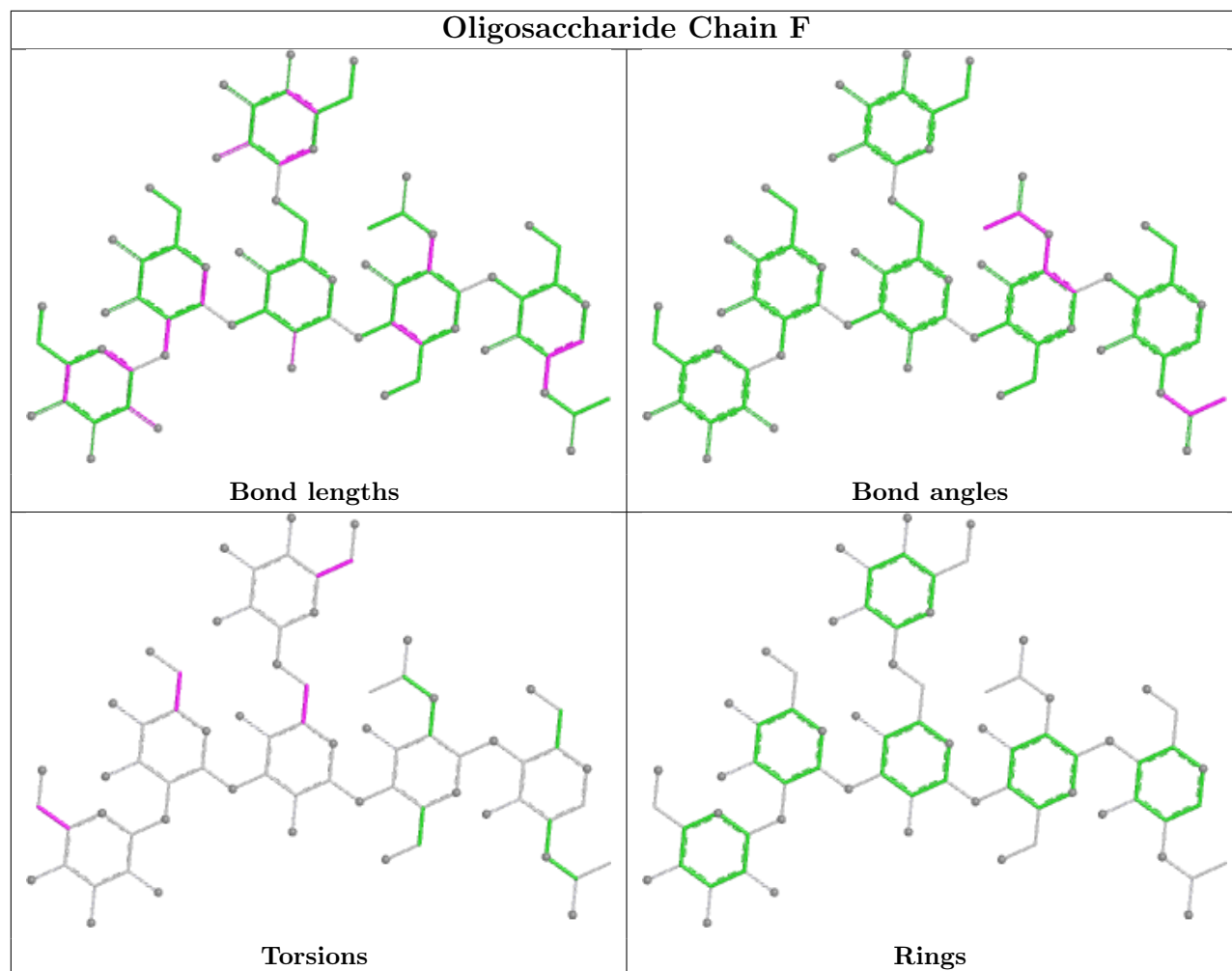
Mol	Chain	Res	Type	Atoms
3	h	3	BMA	O5-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C1-C2-N2-C7
3	Y	2	NAG	C1-C2-N2-C7
3	l	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
3	n	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6

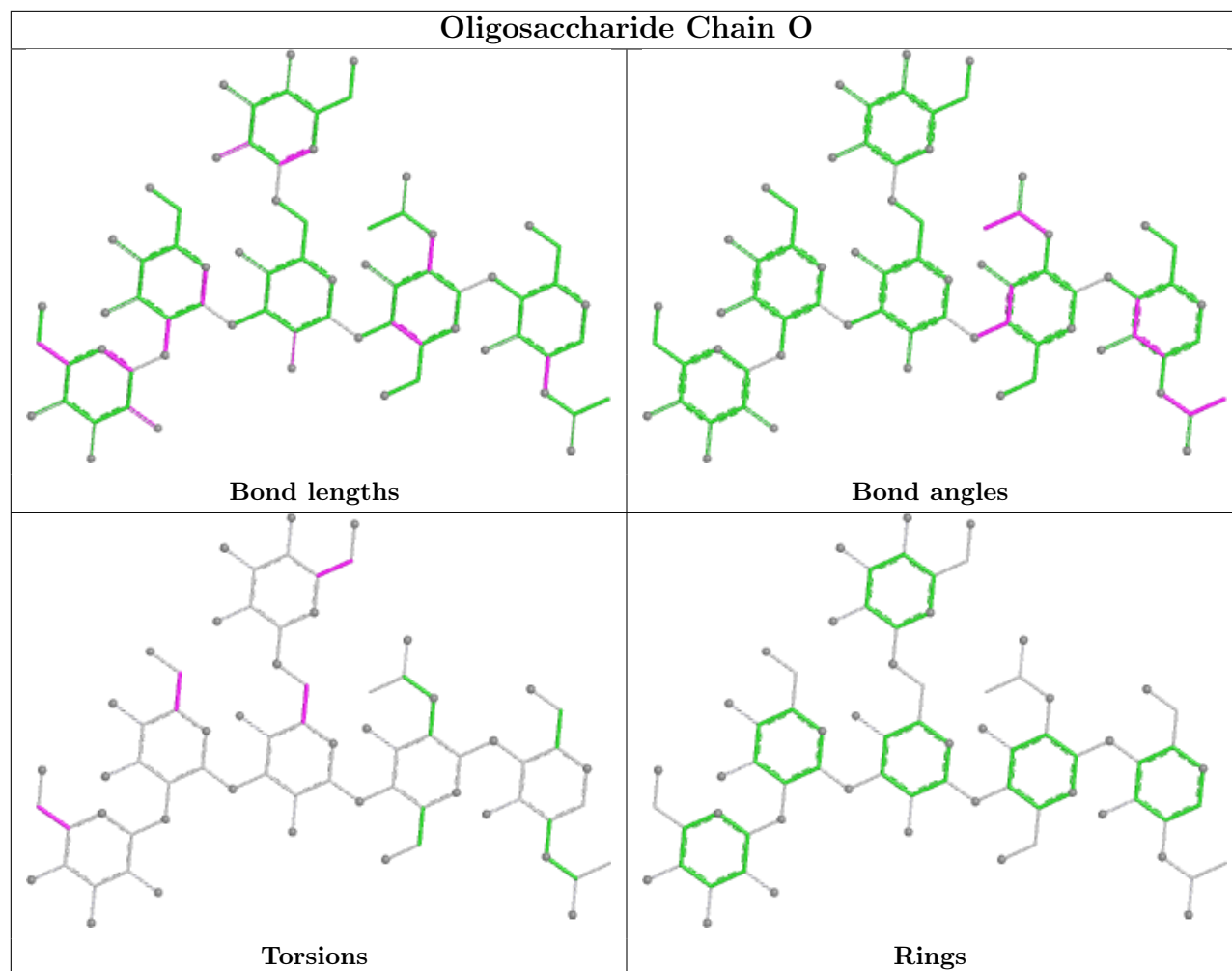
There are no ring outliers.

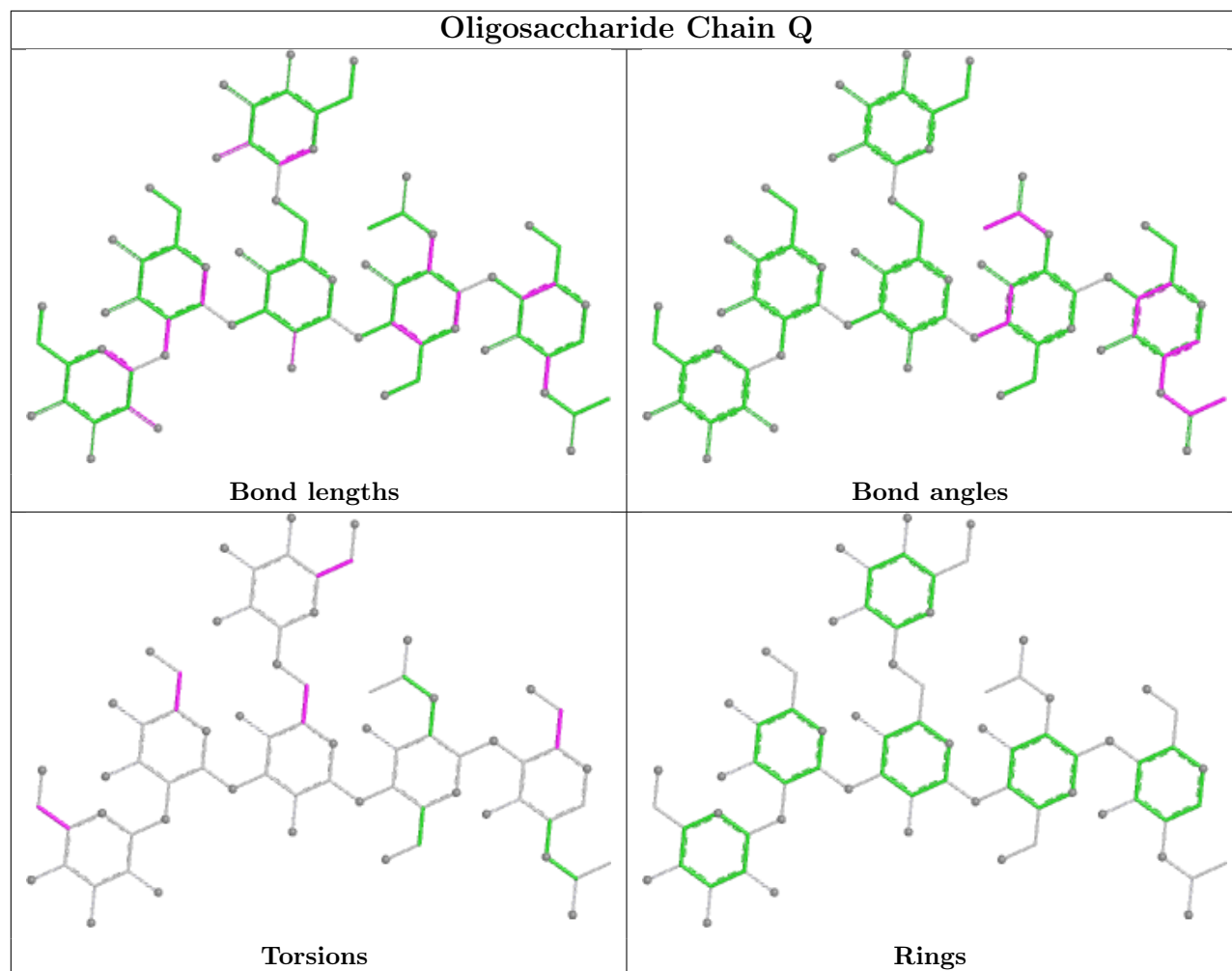
No monomer is involved in short contacts.

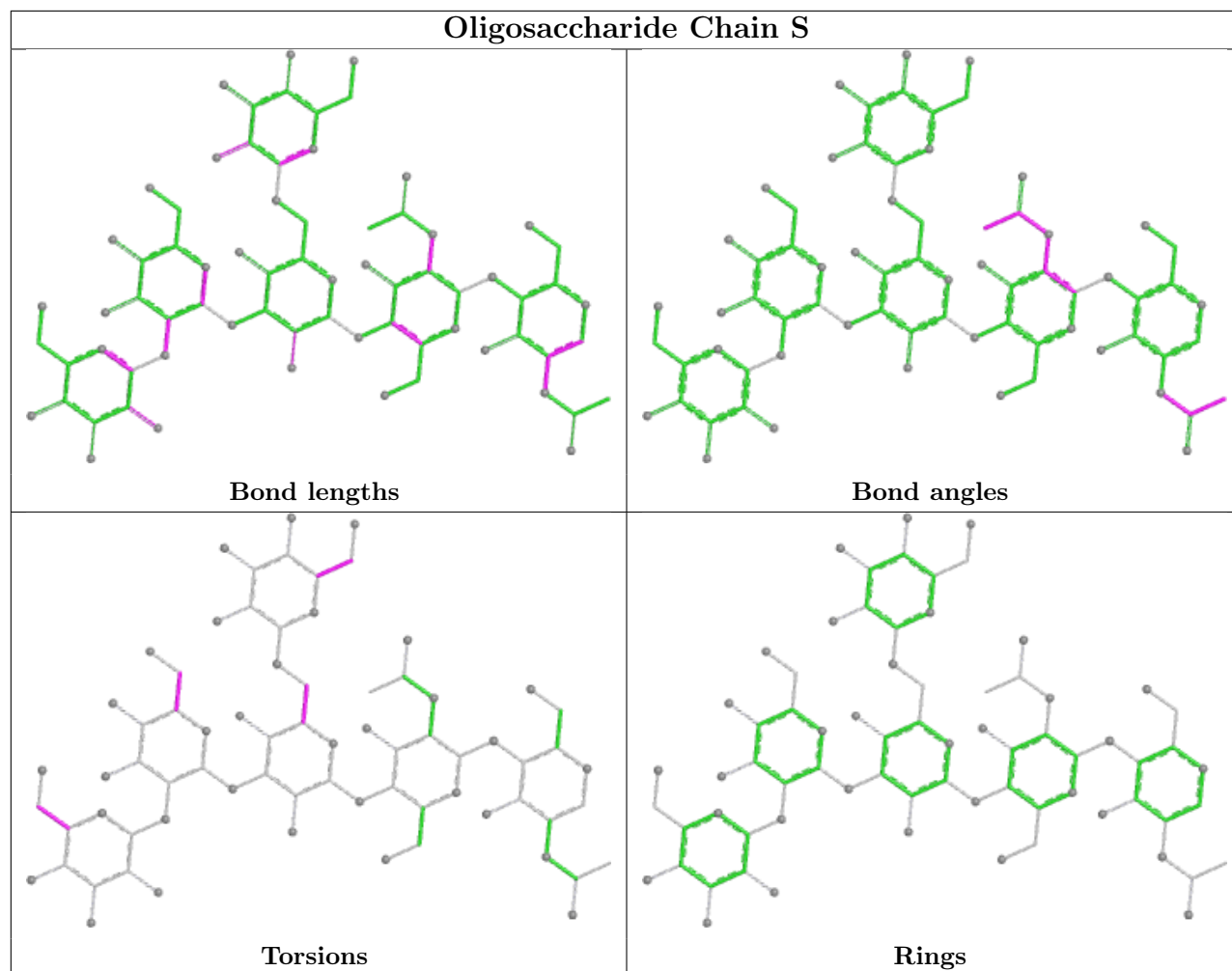
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

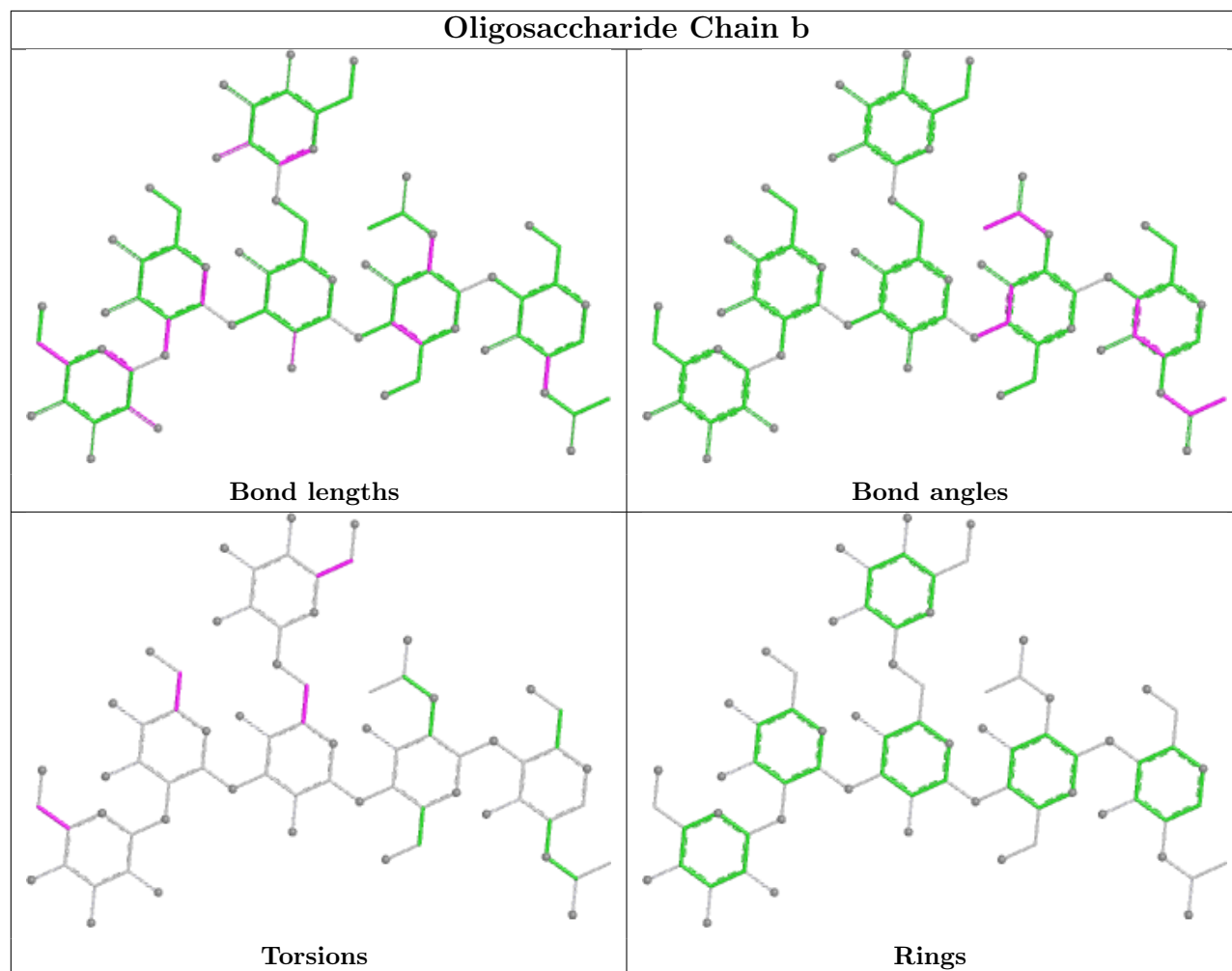


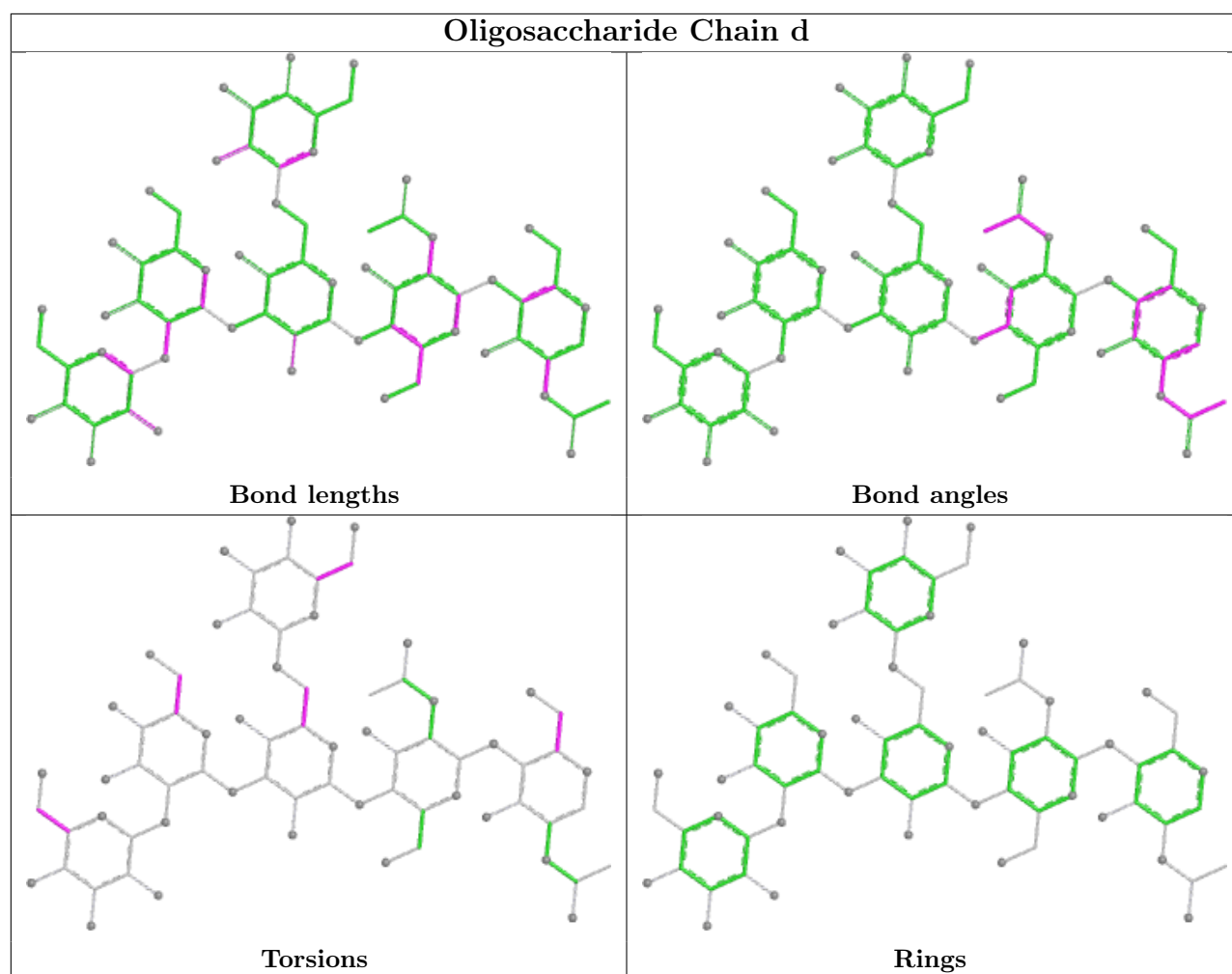


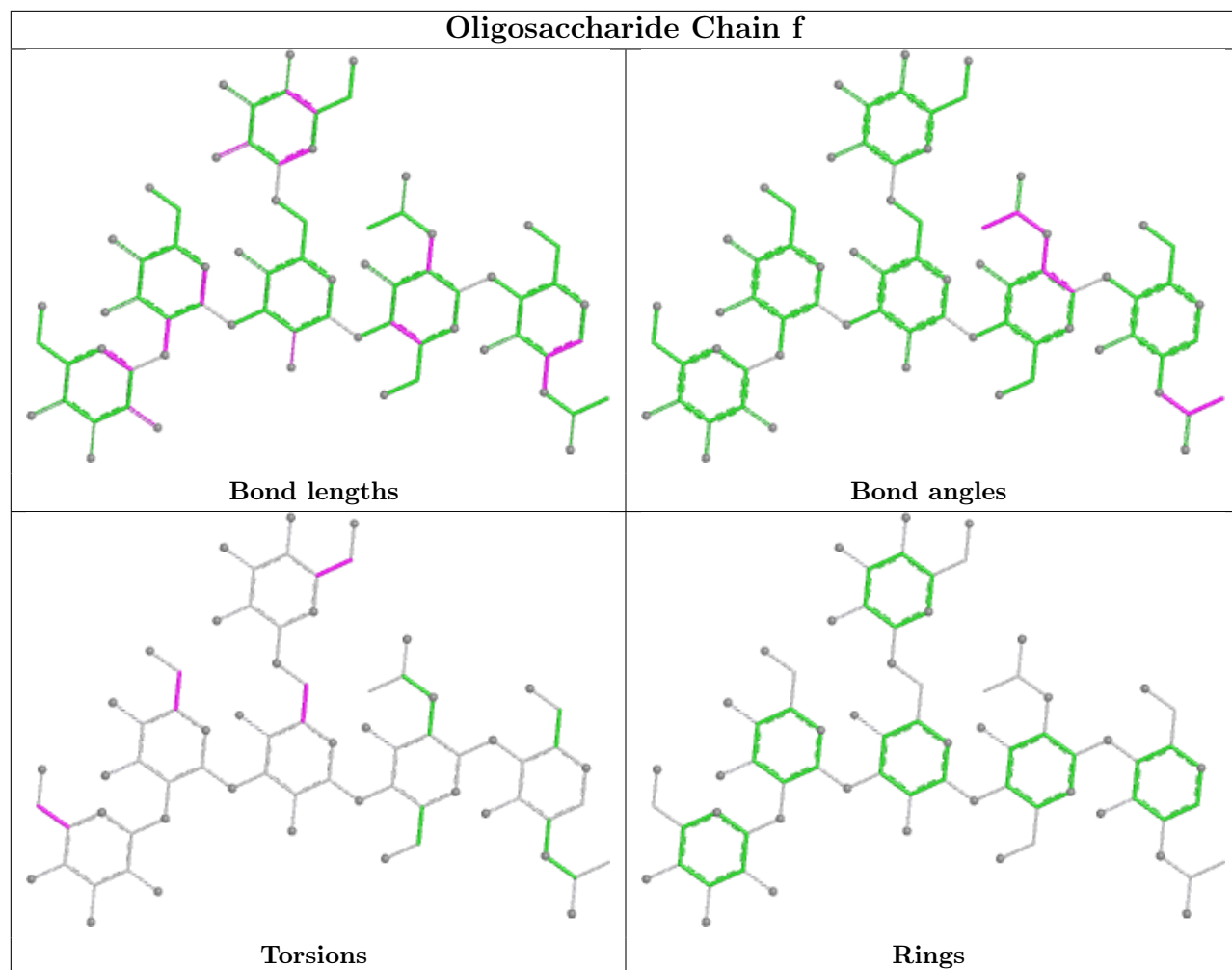


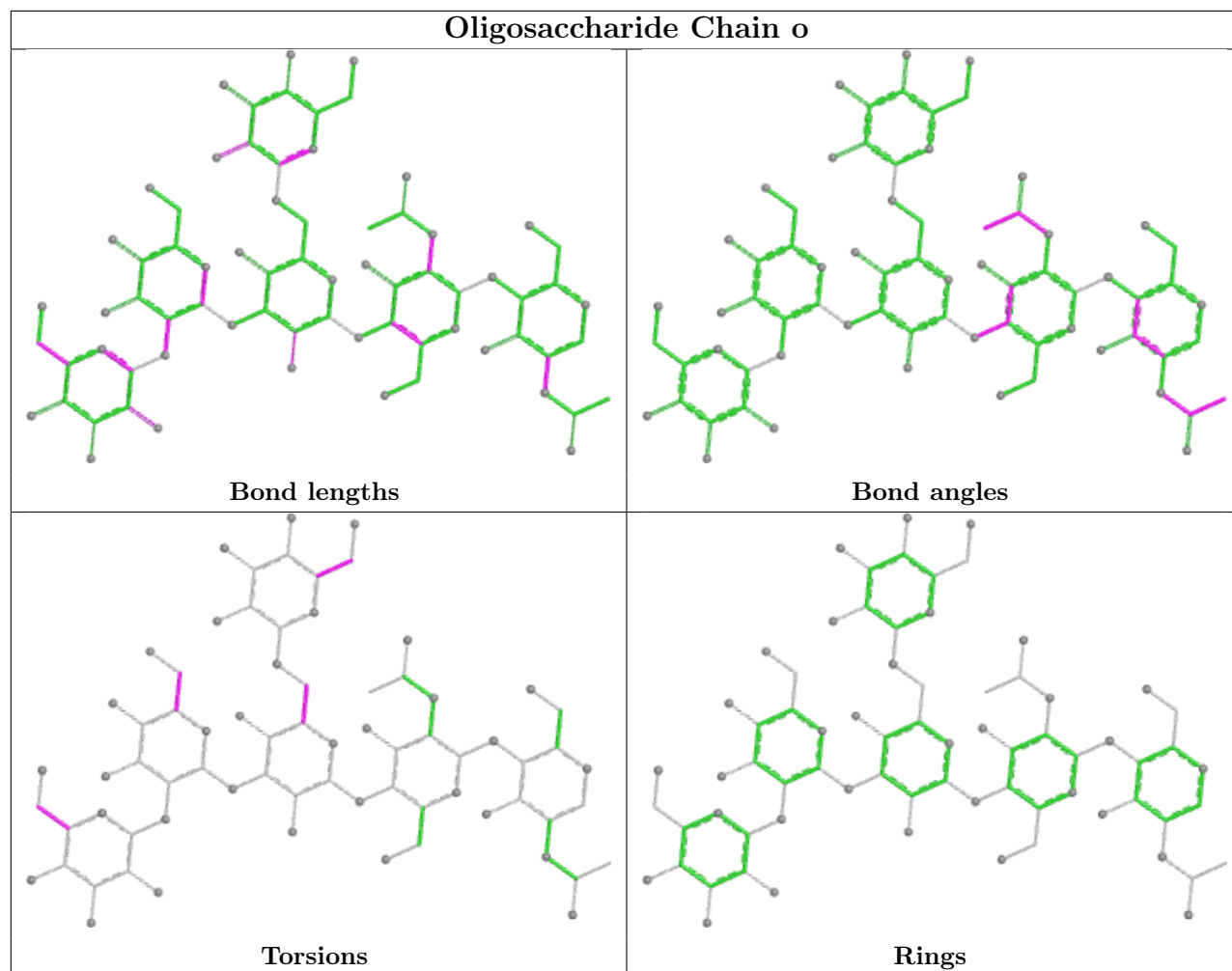


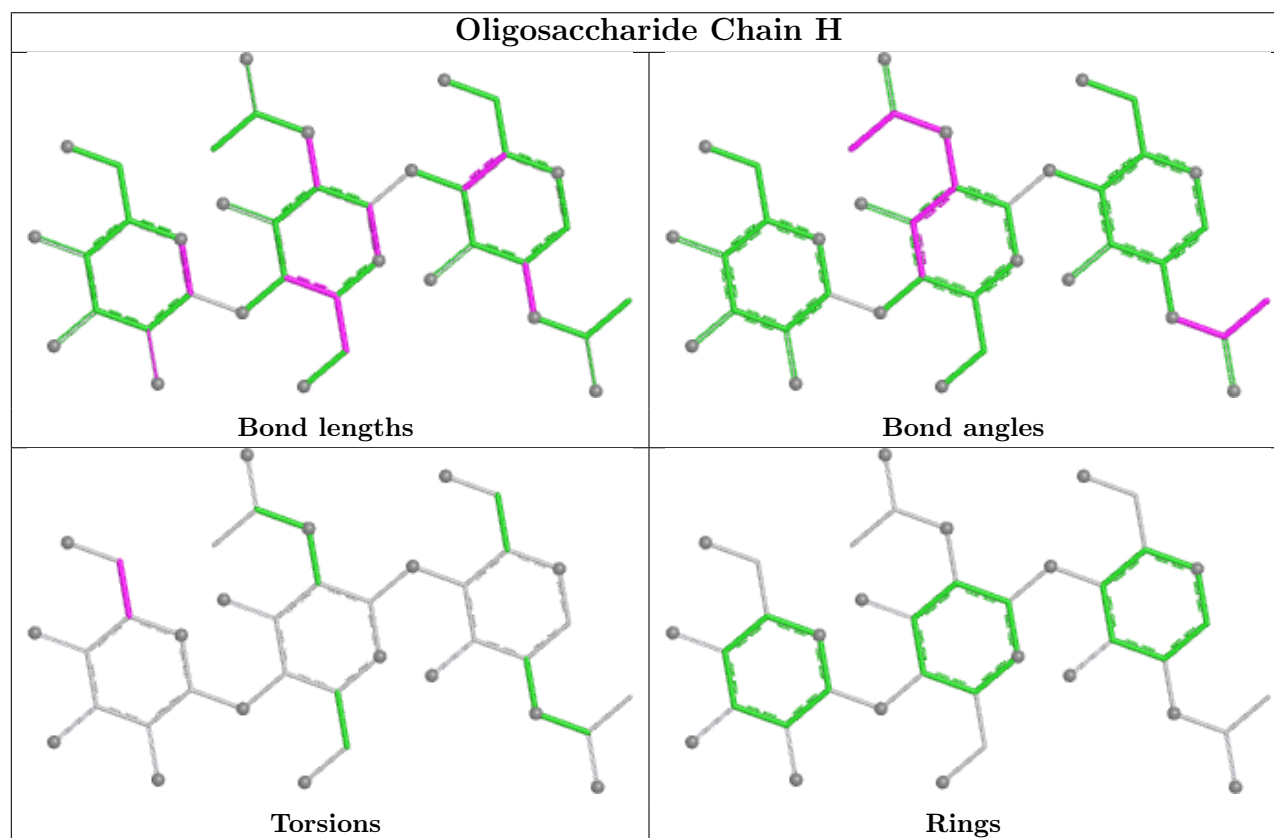
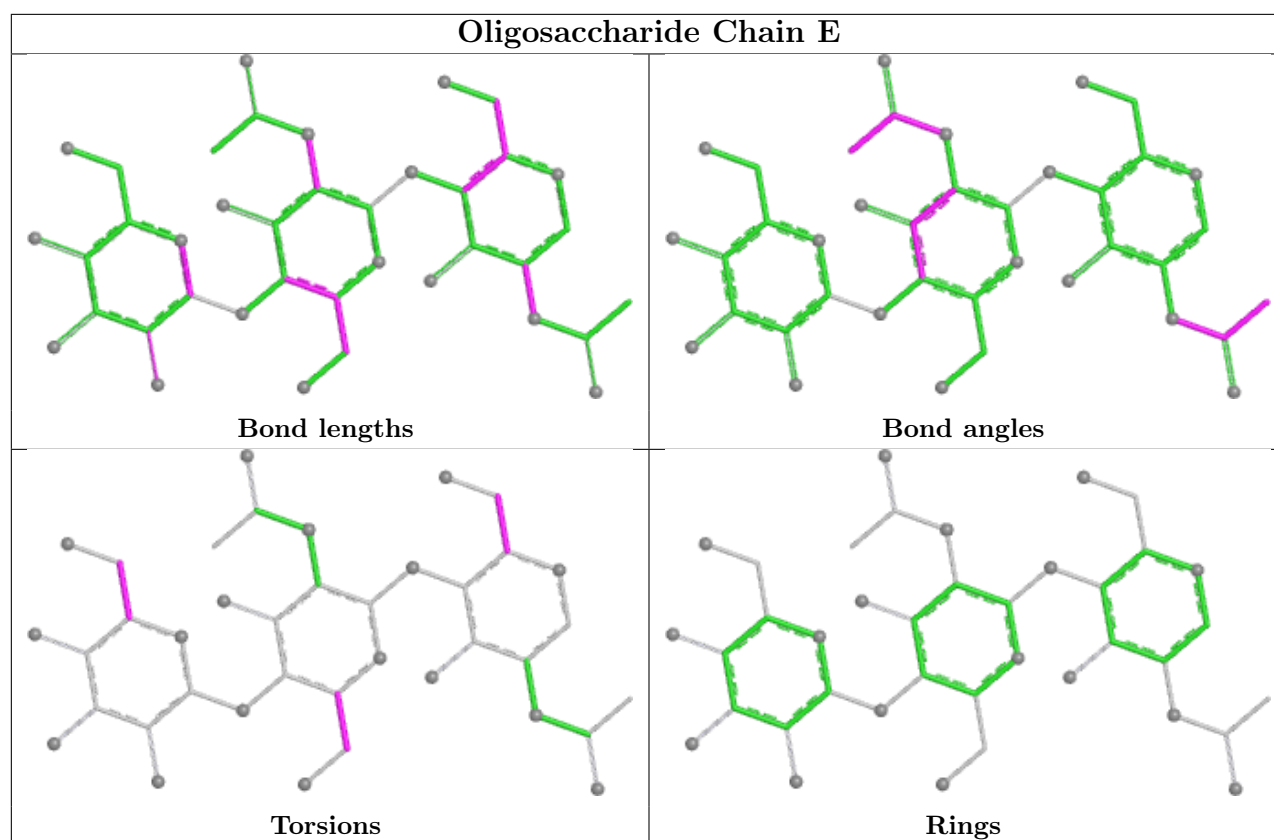


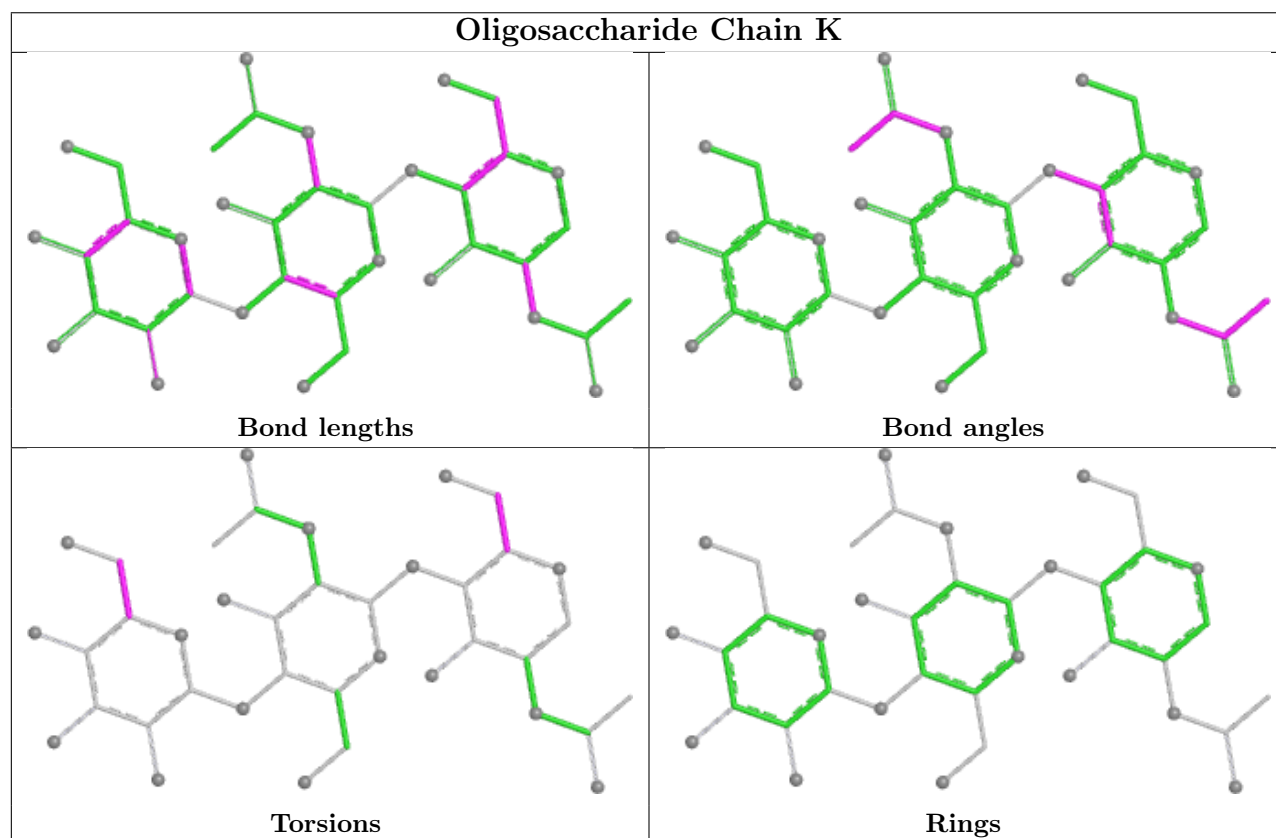
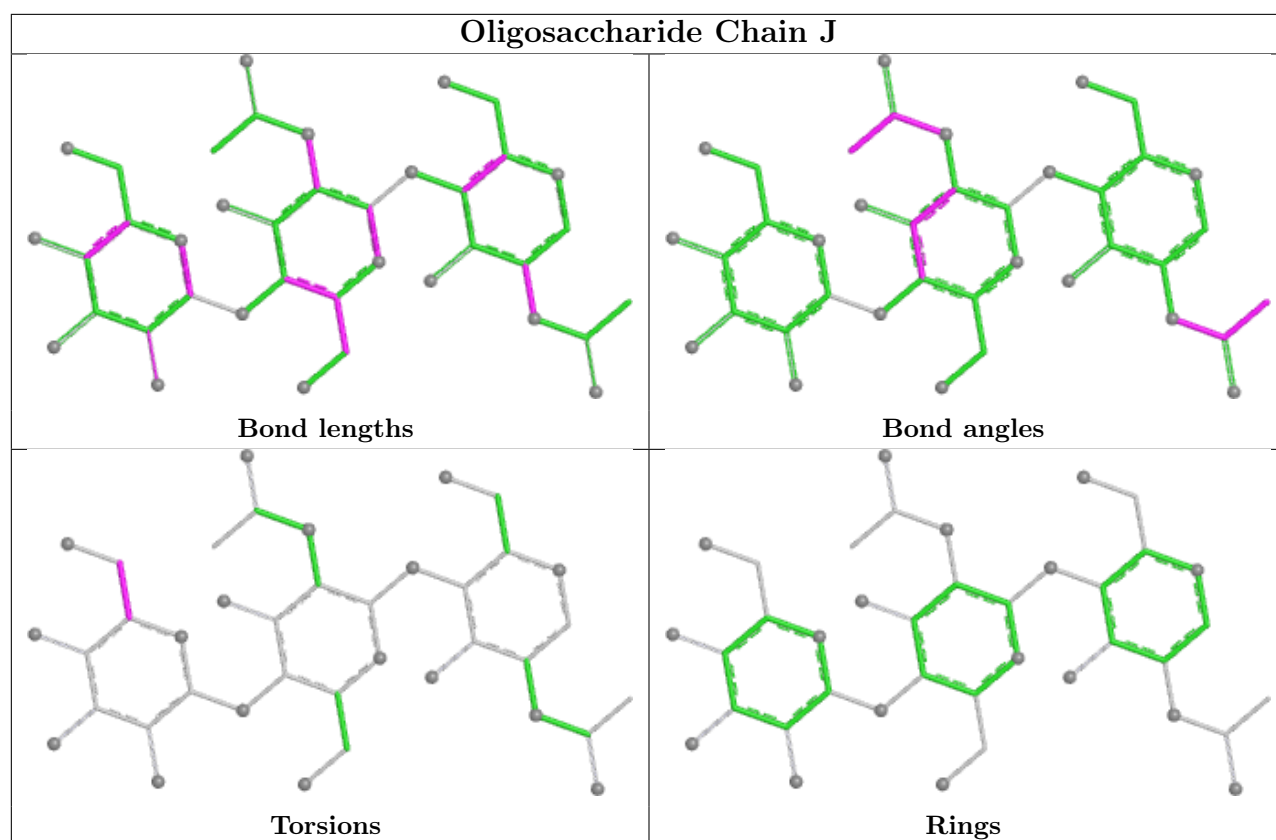


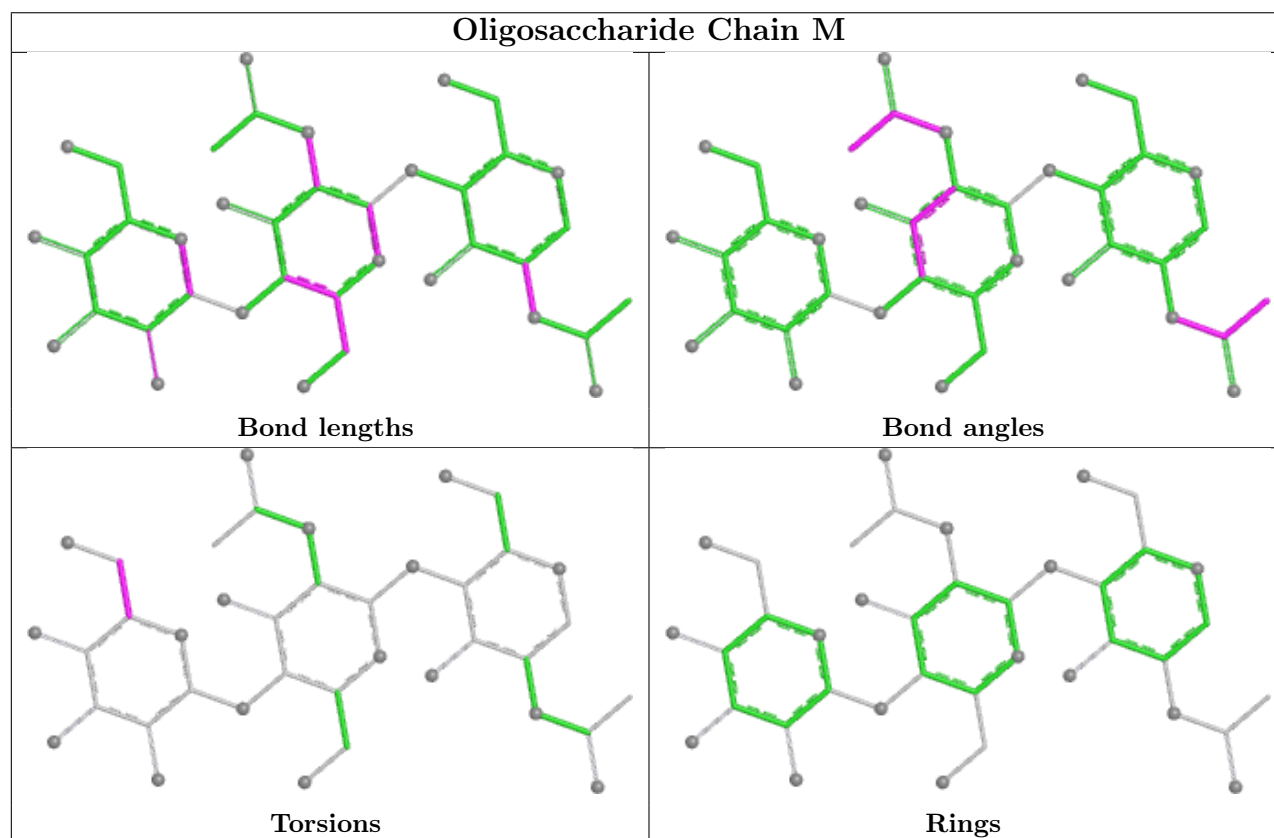
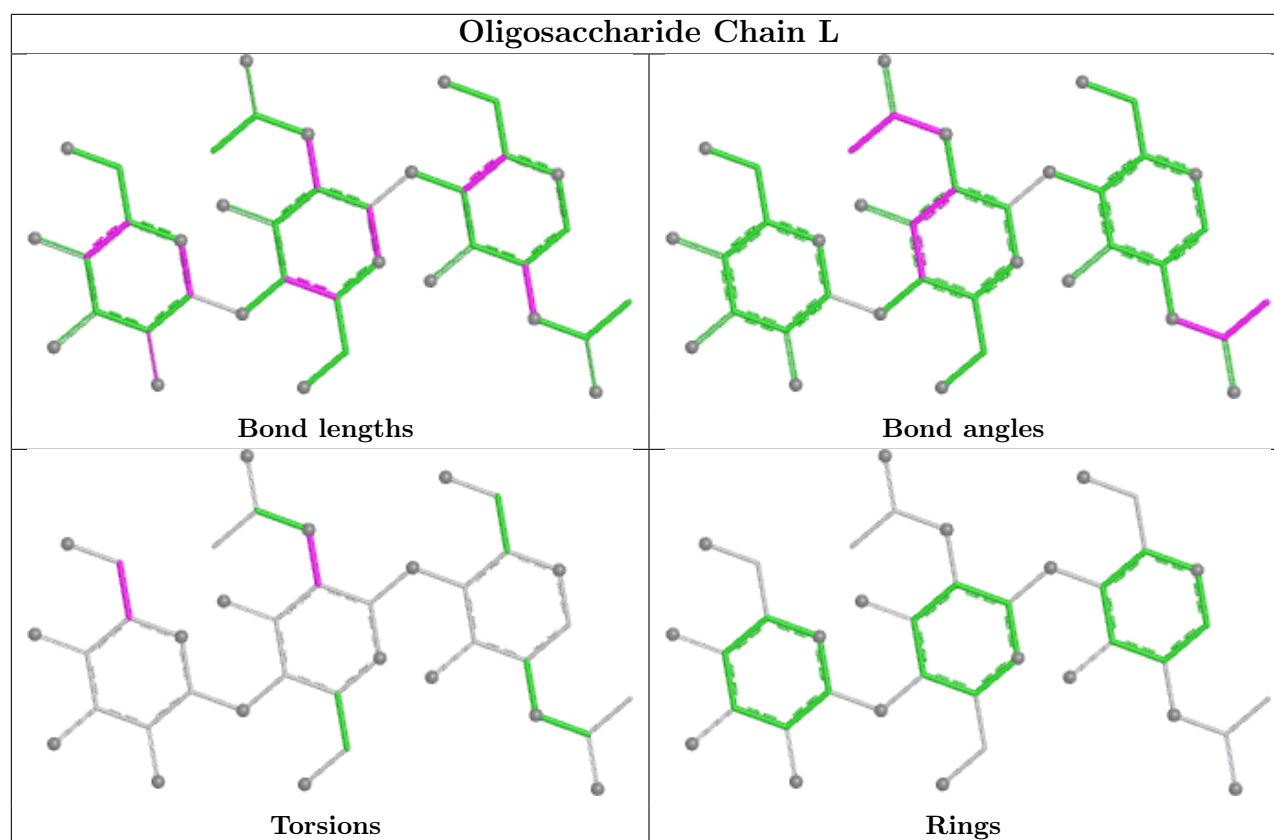


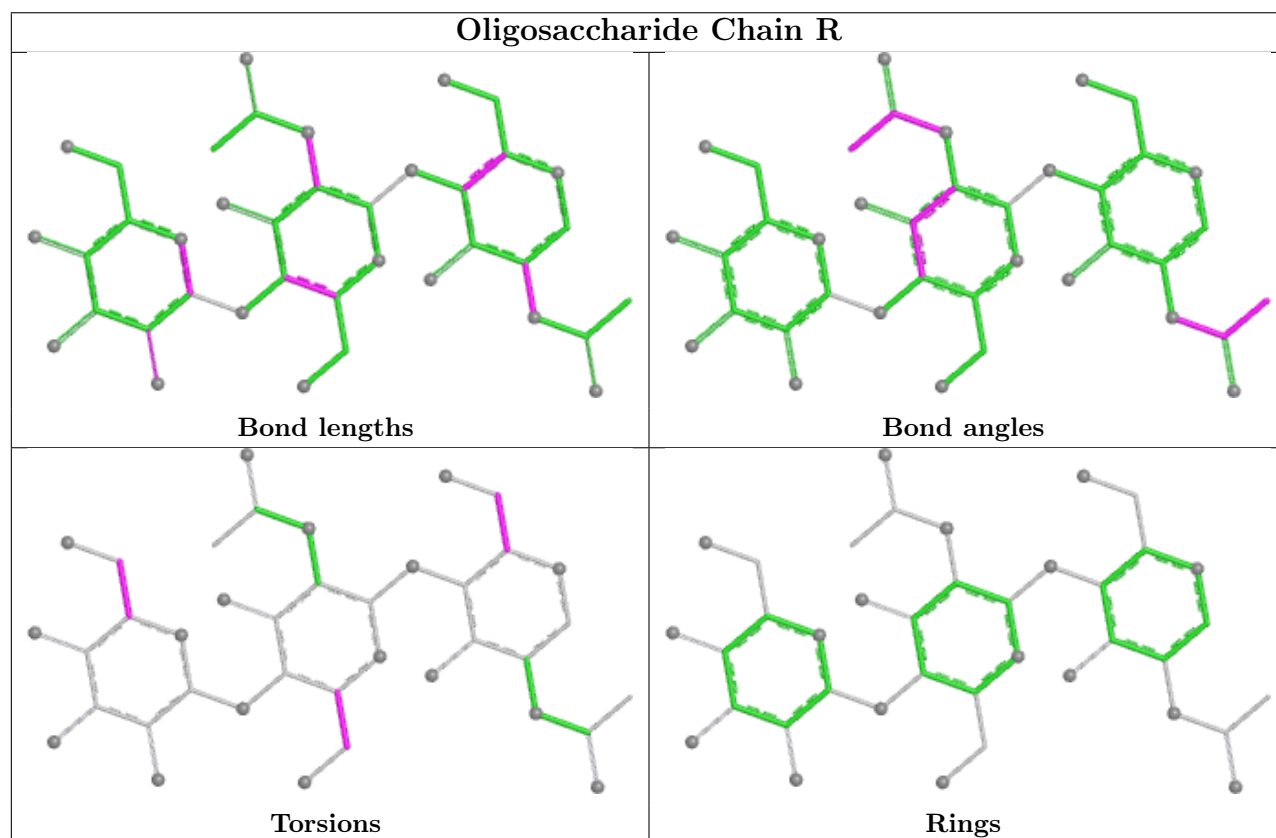
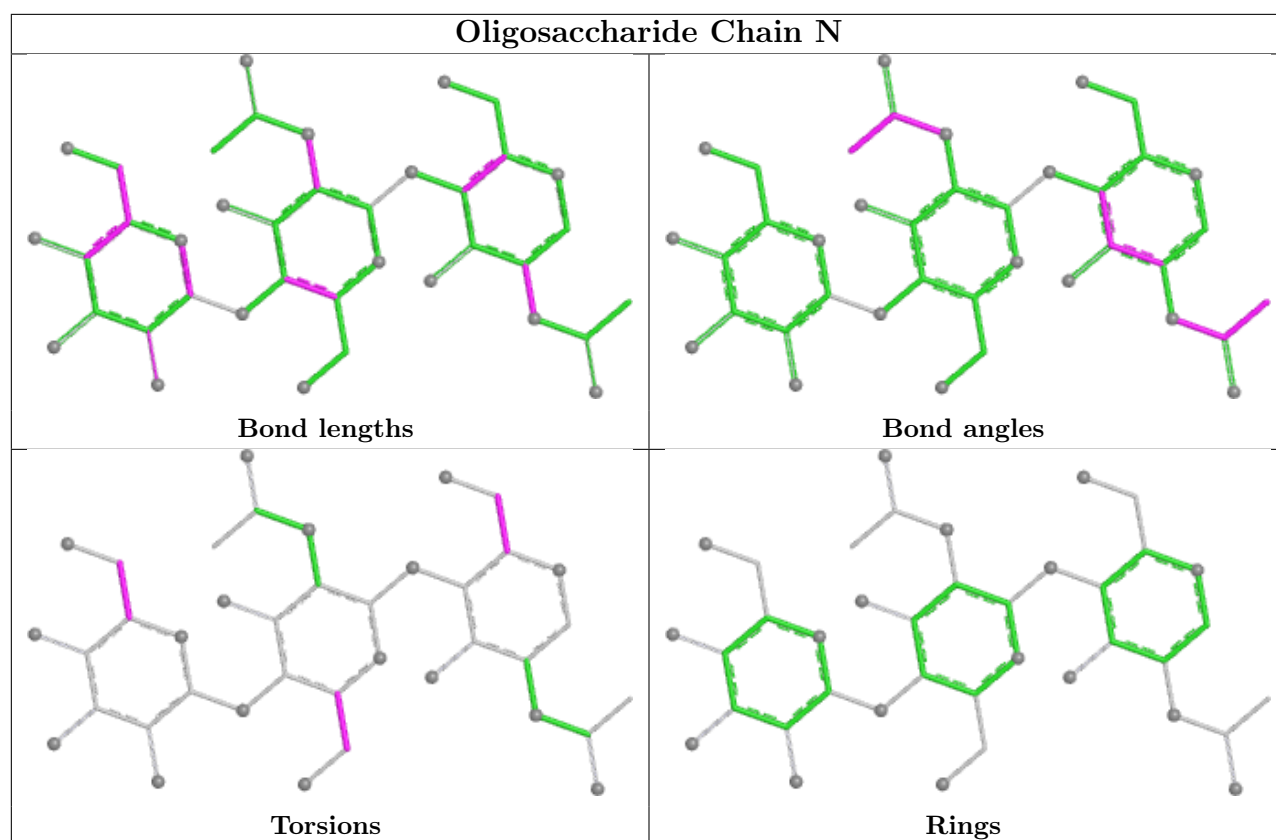


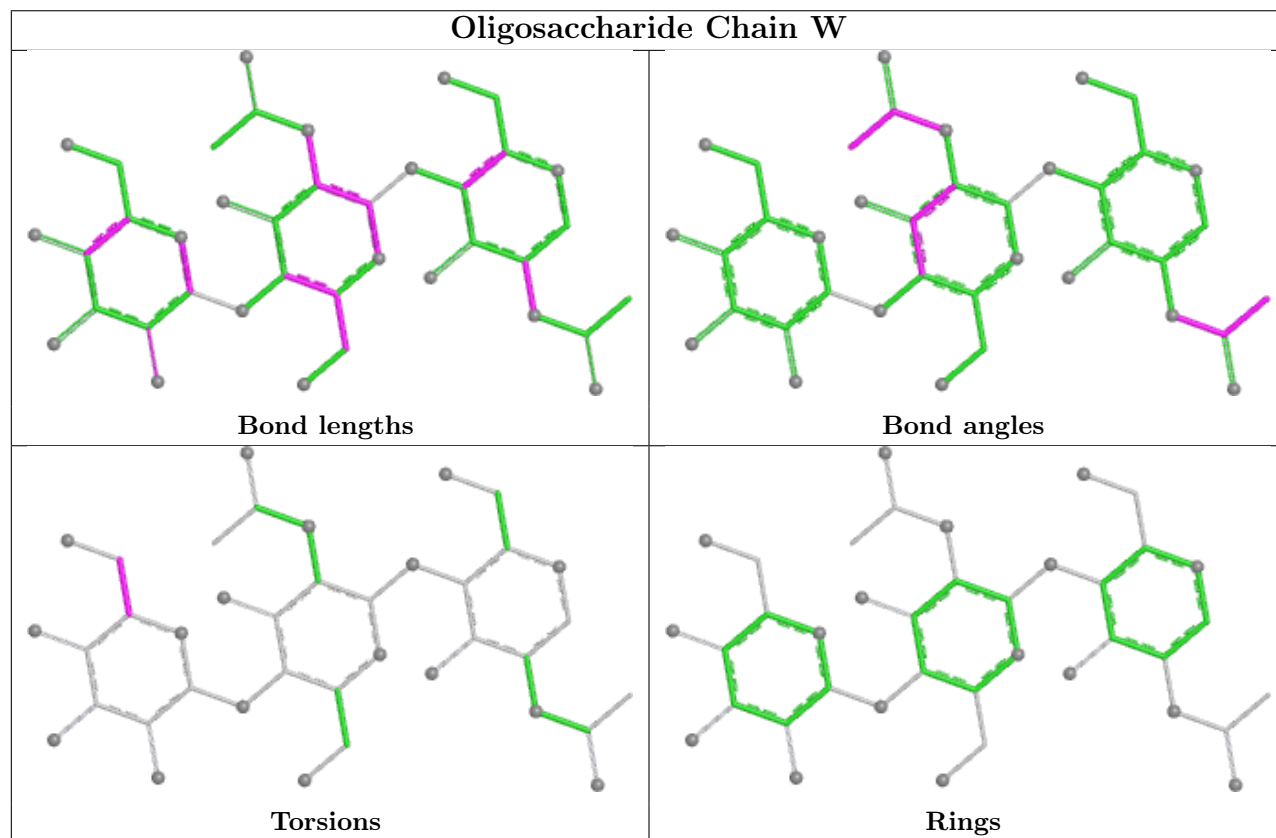
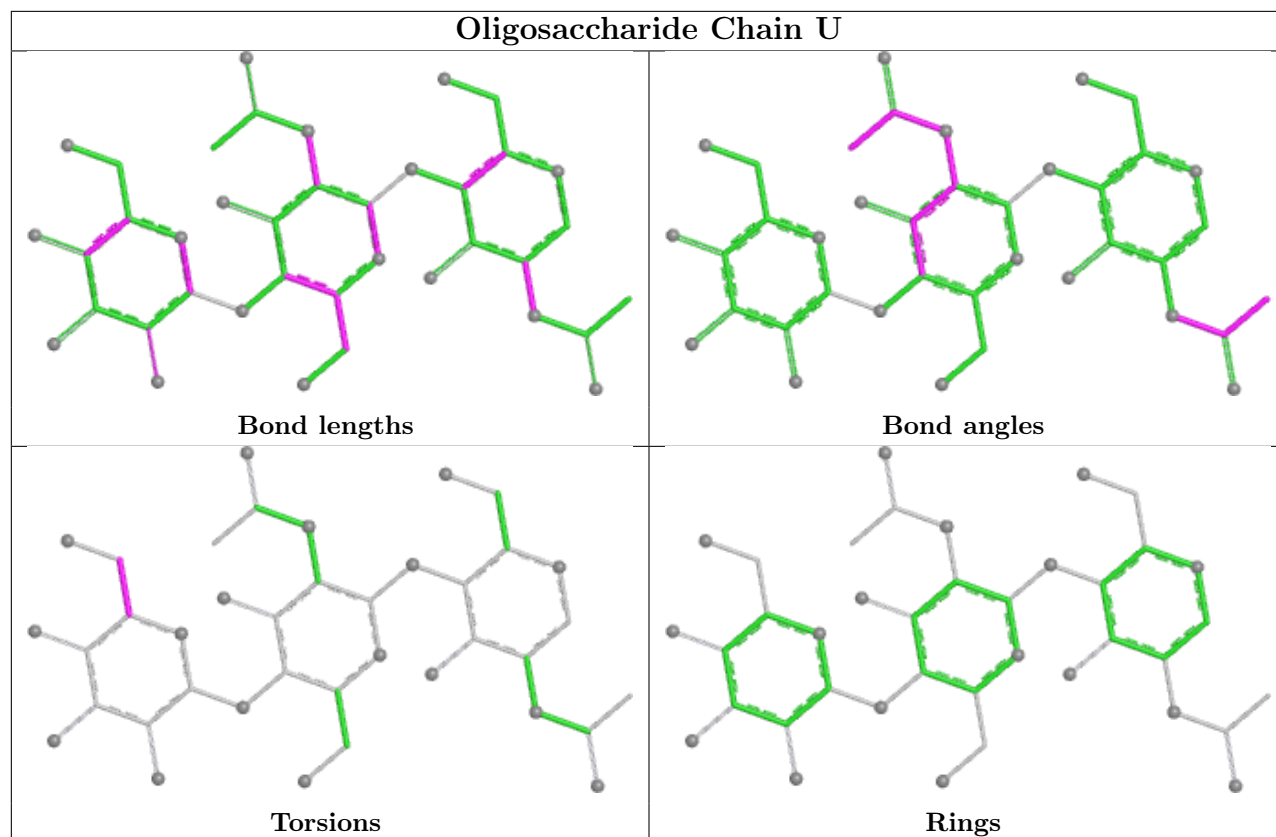


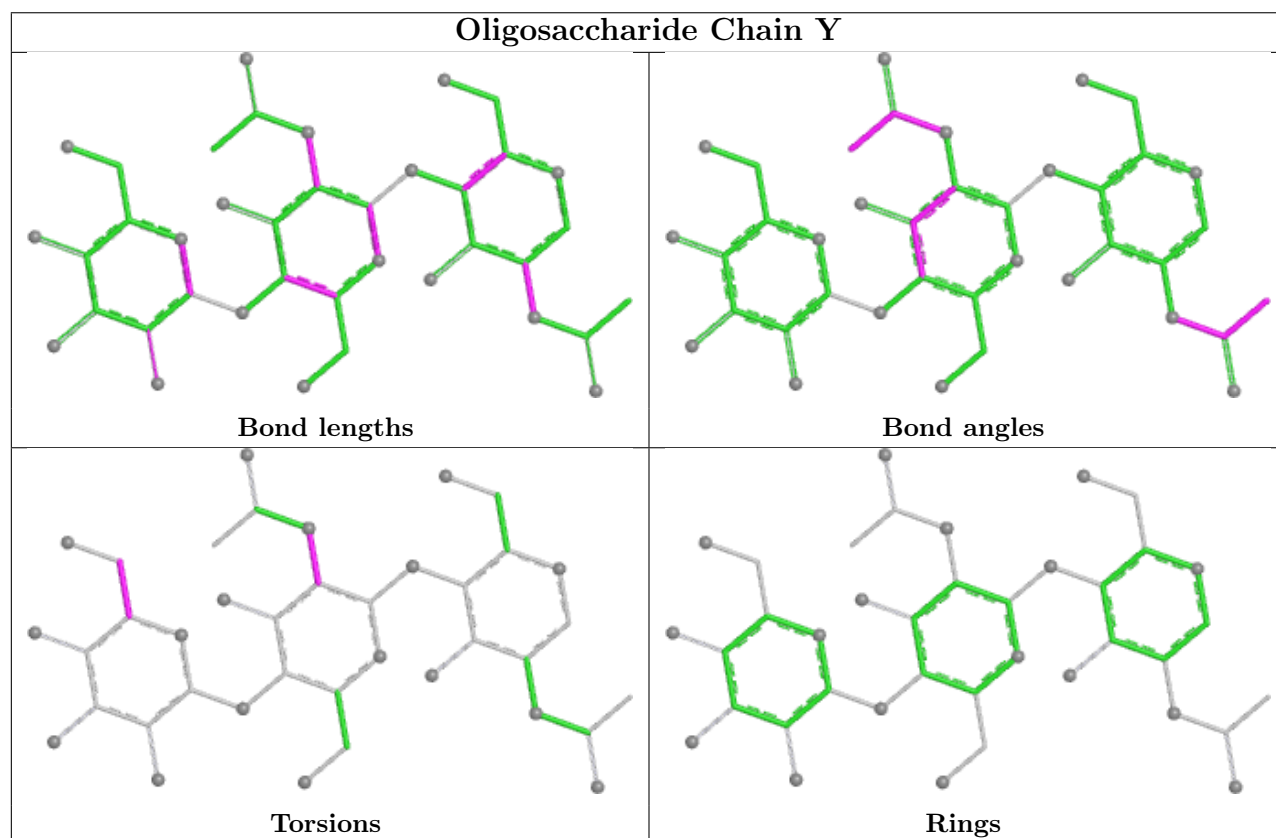
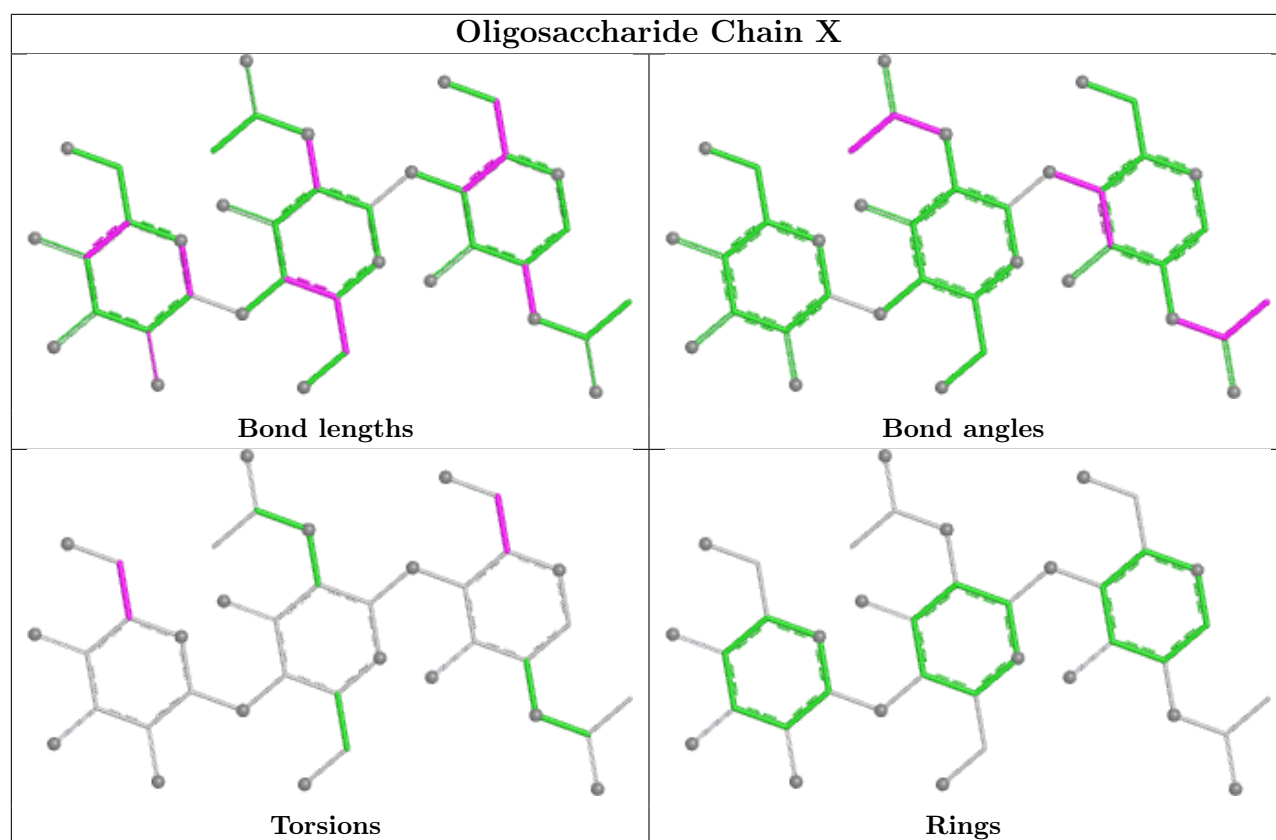


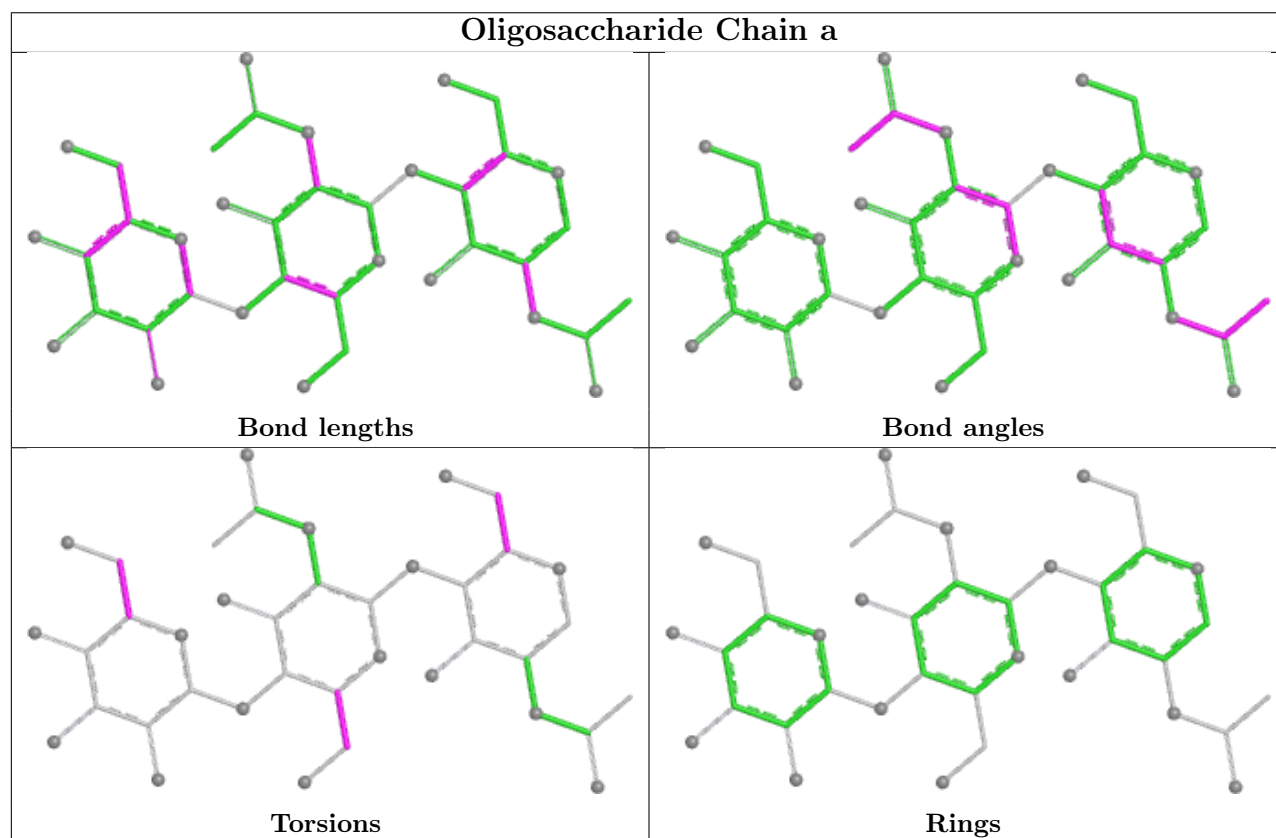
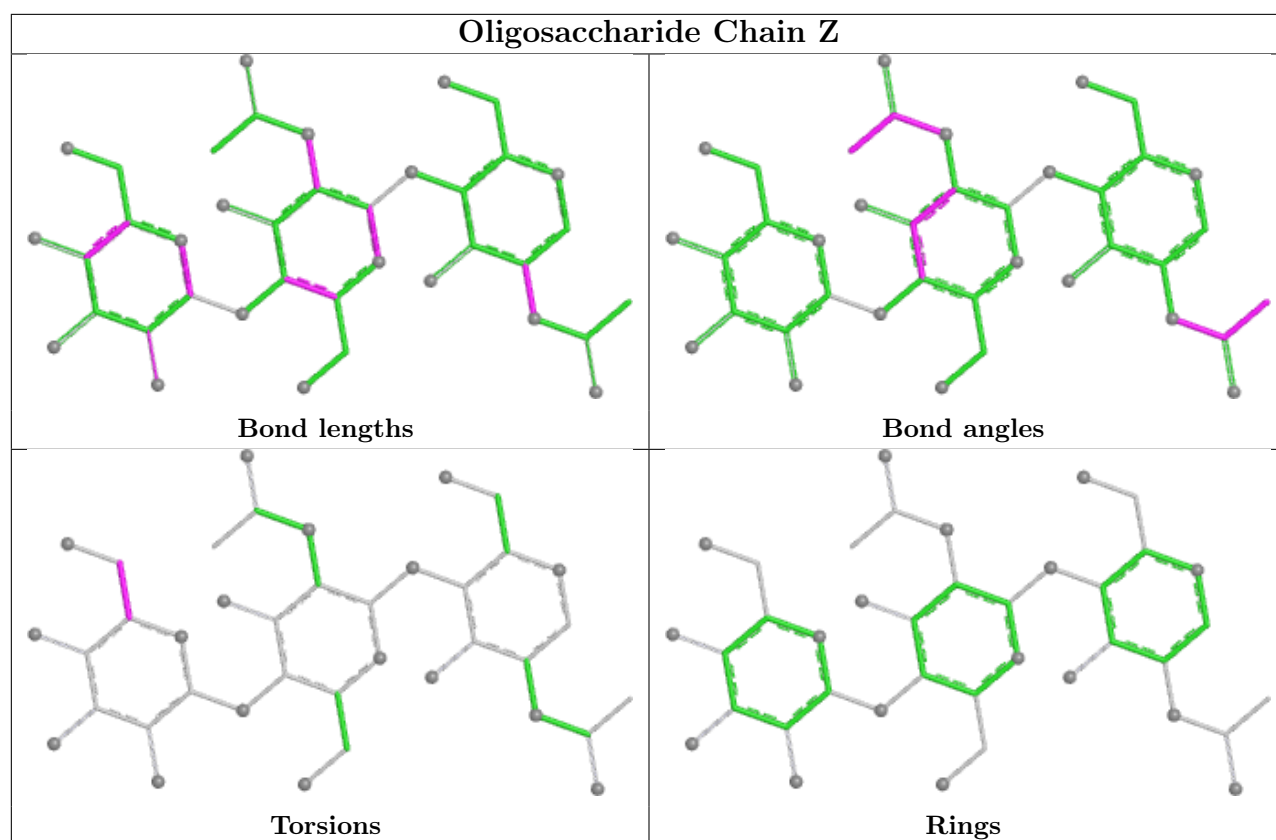


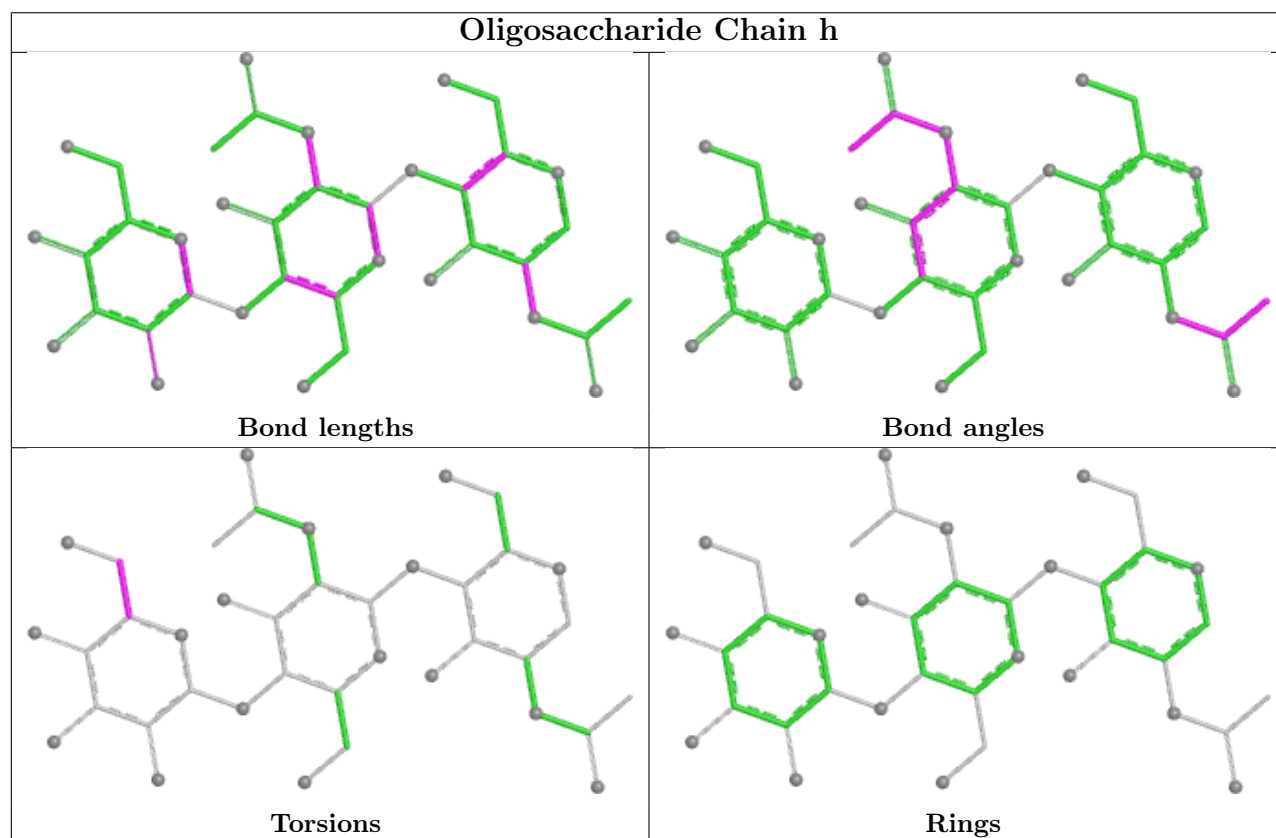
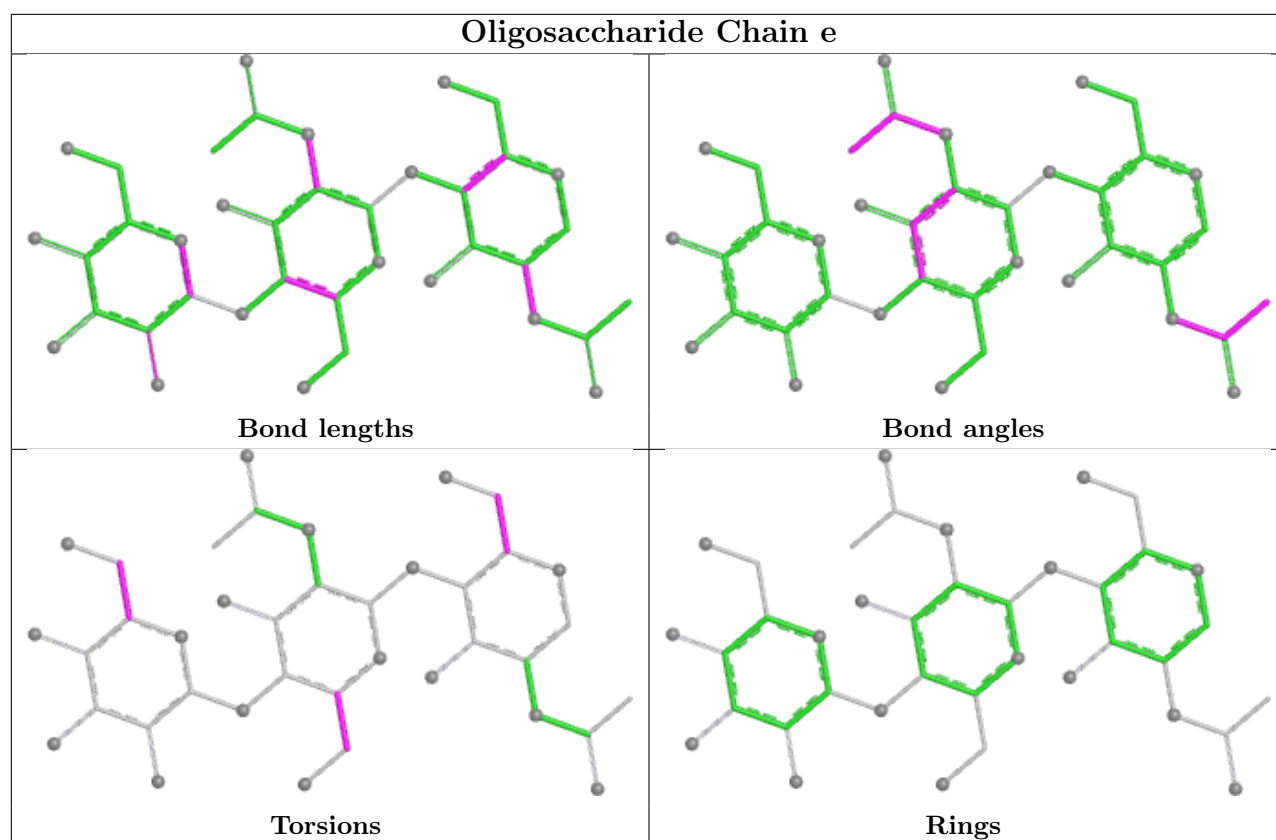


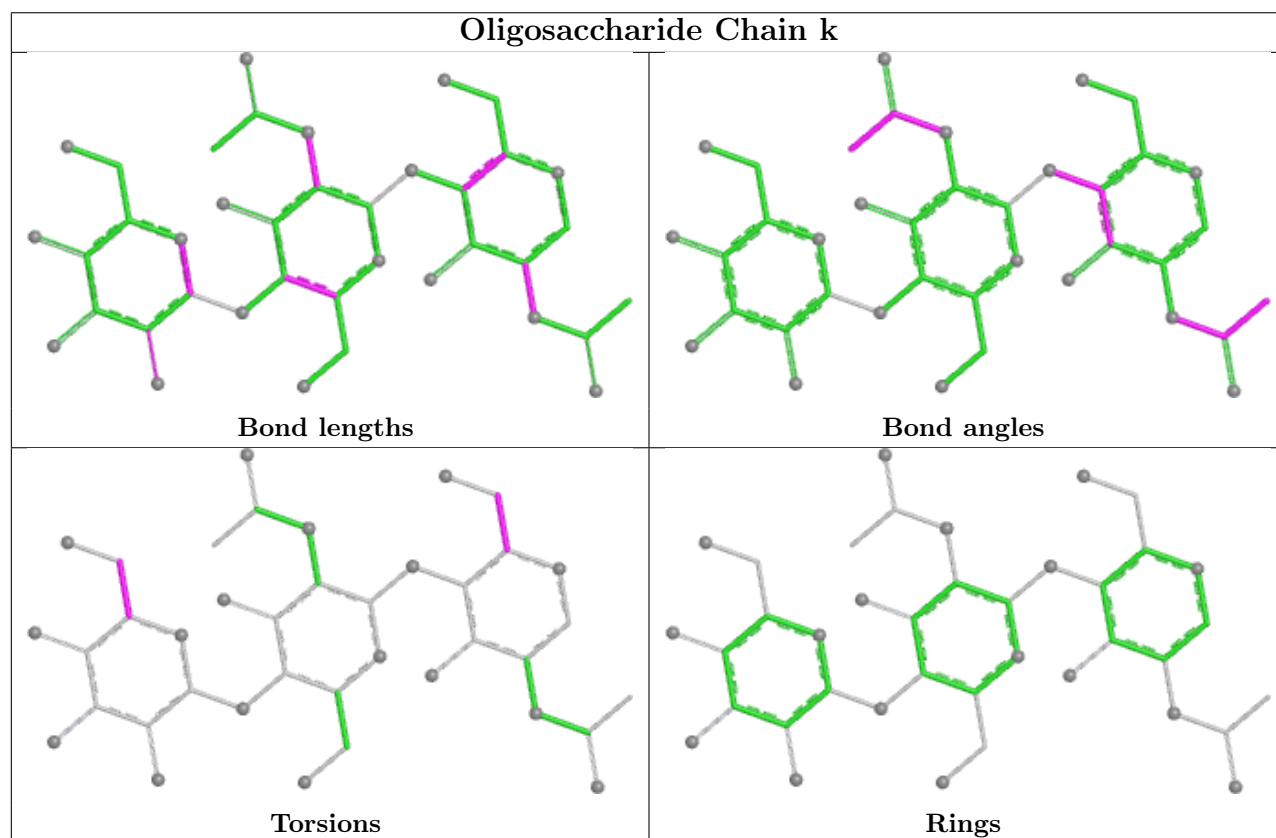
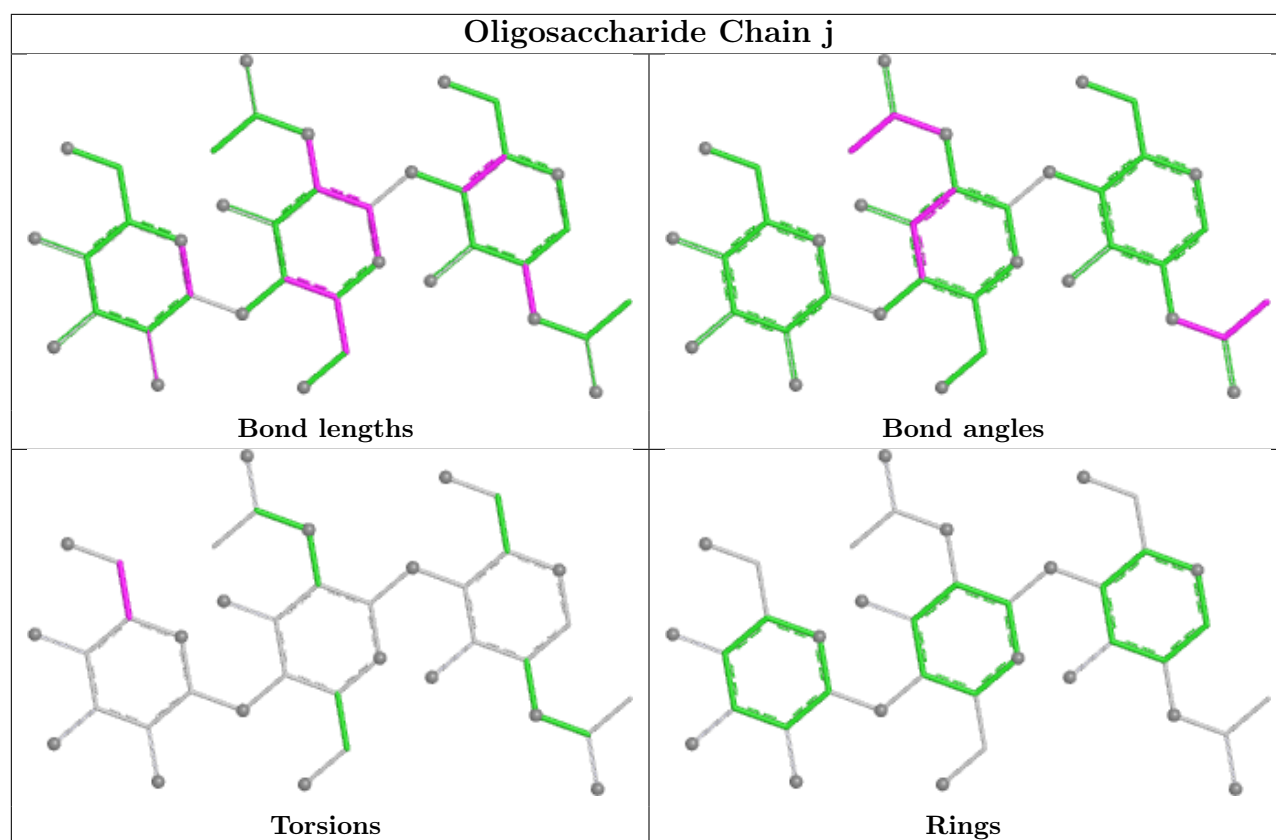


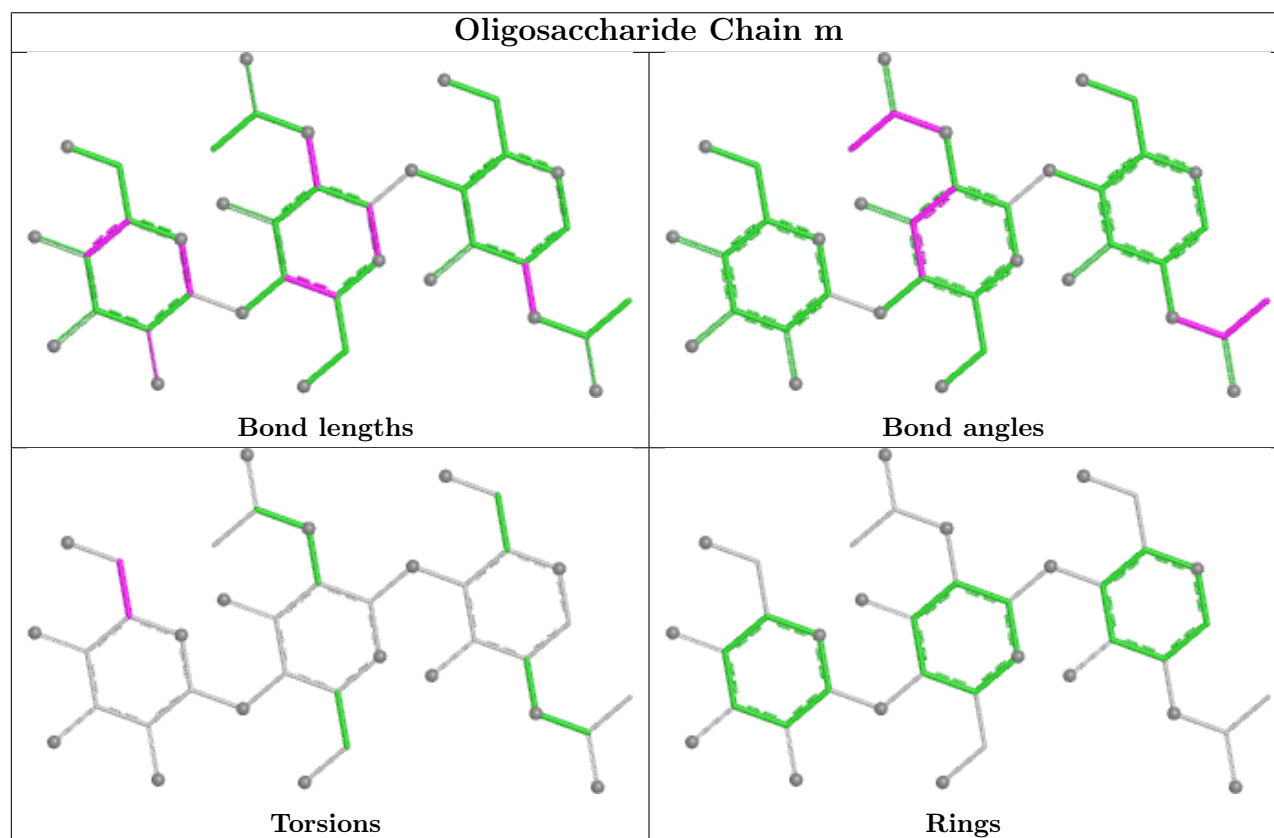
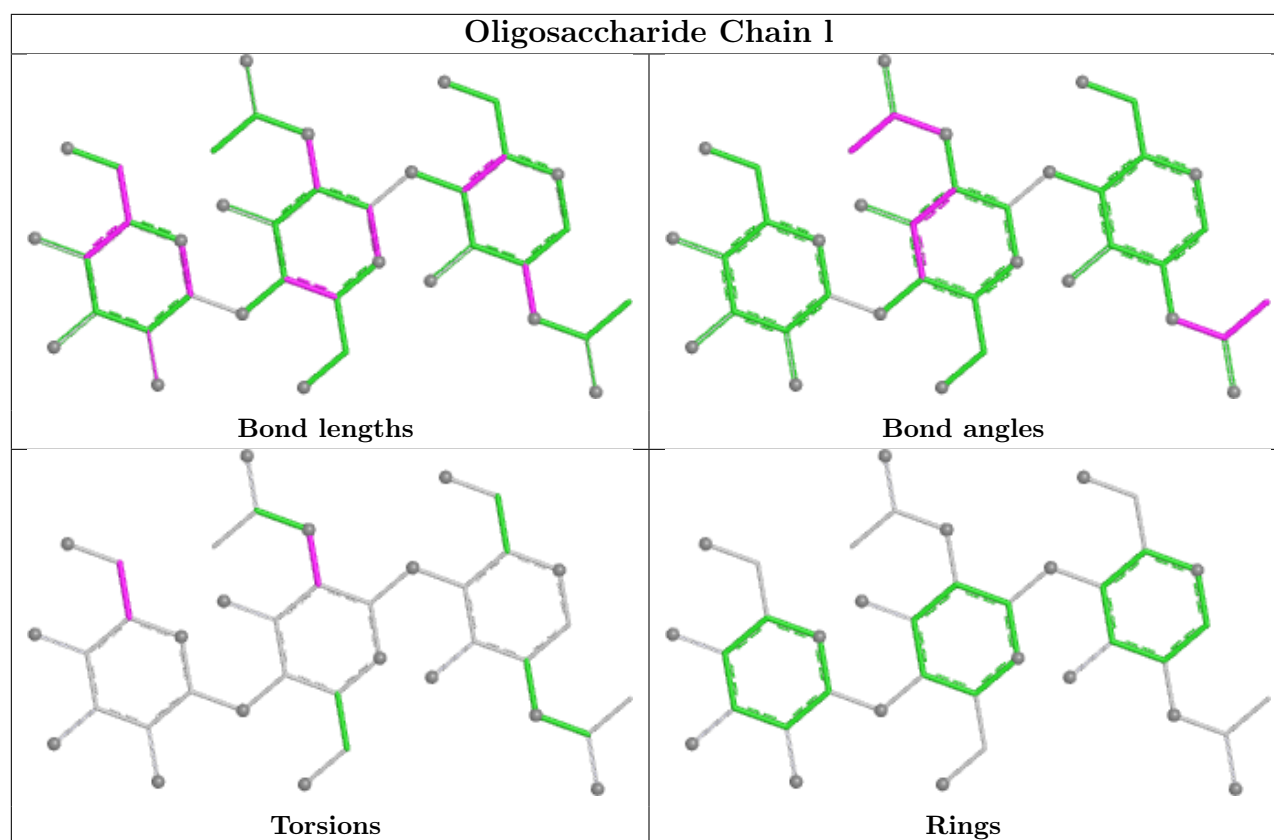


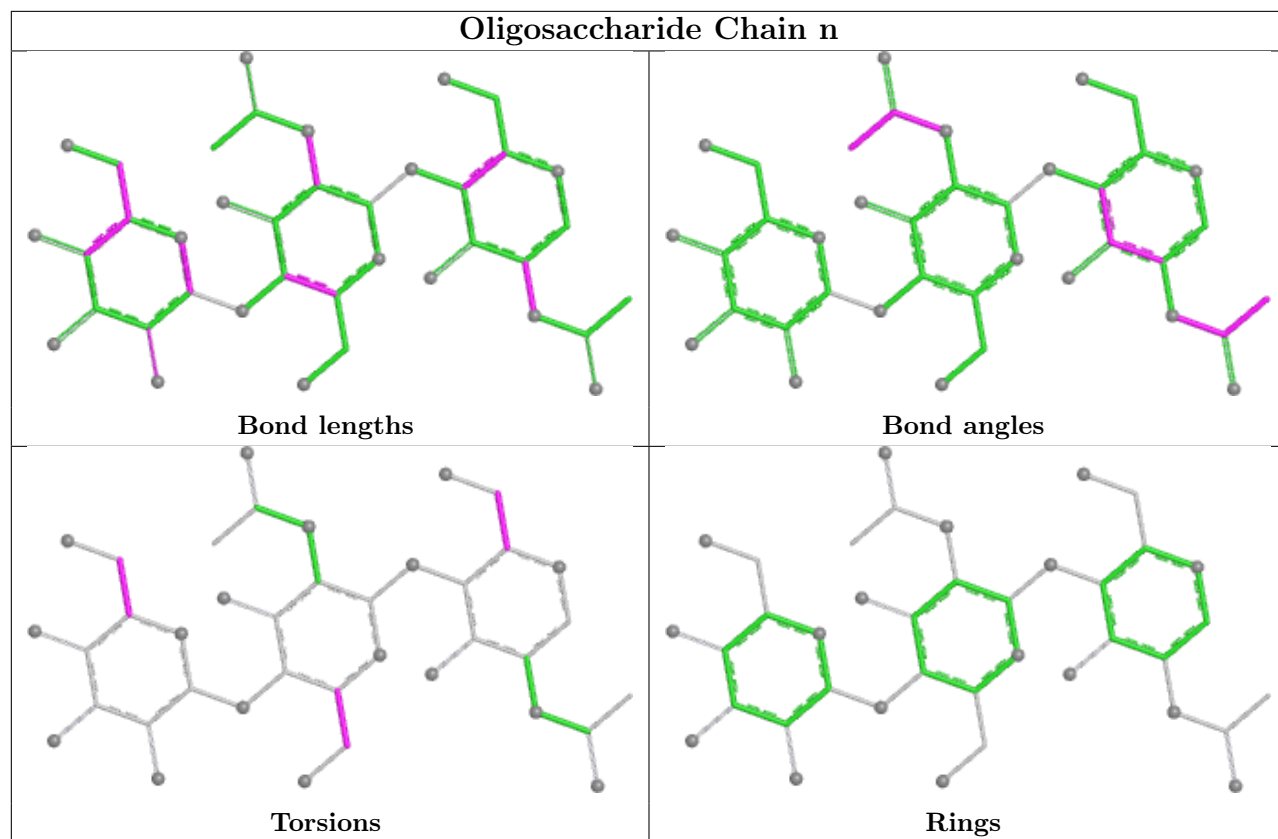


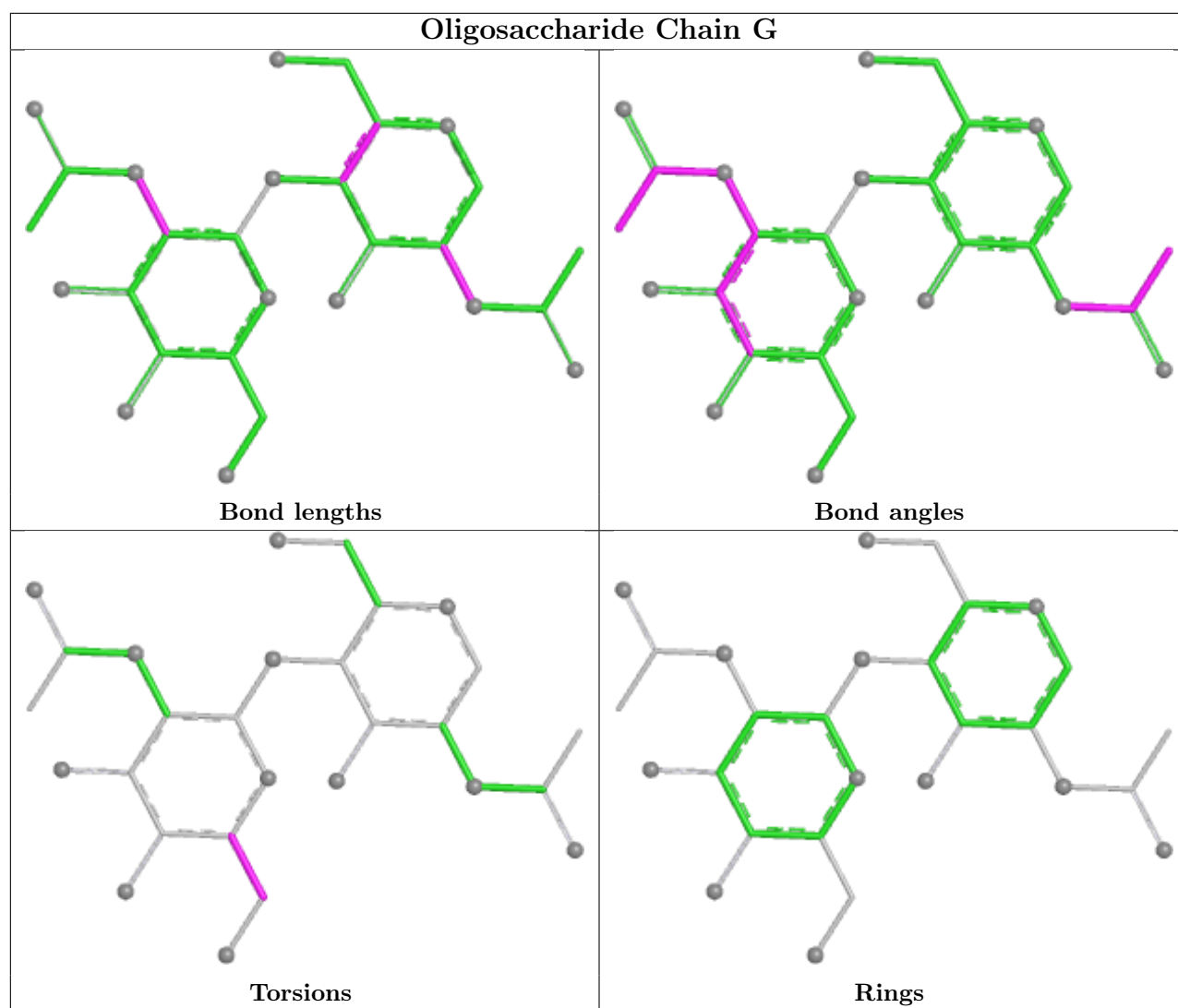


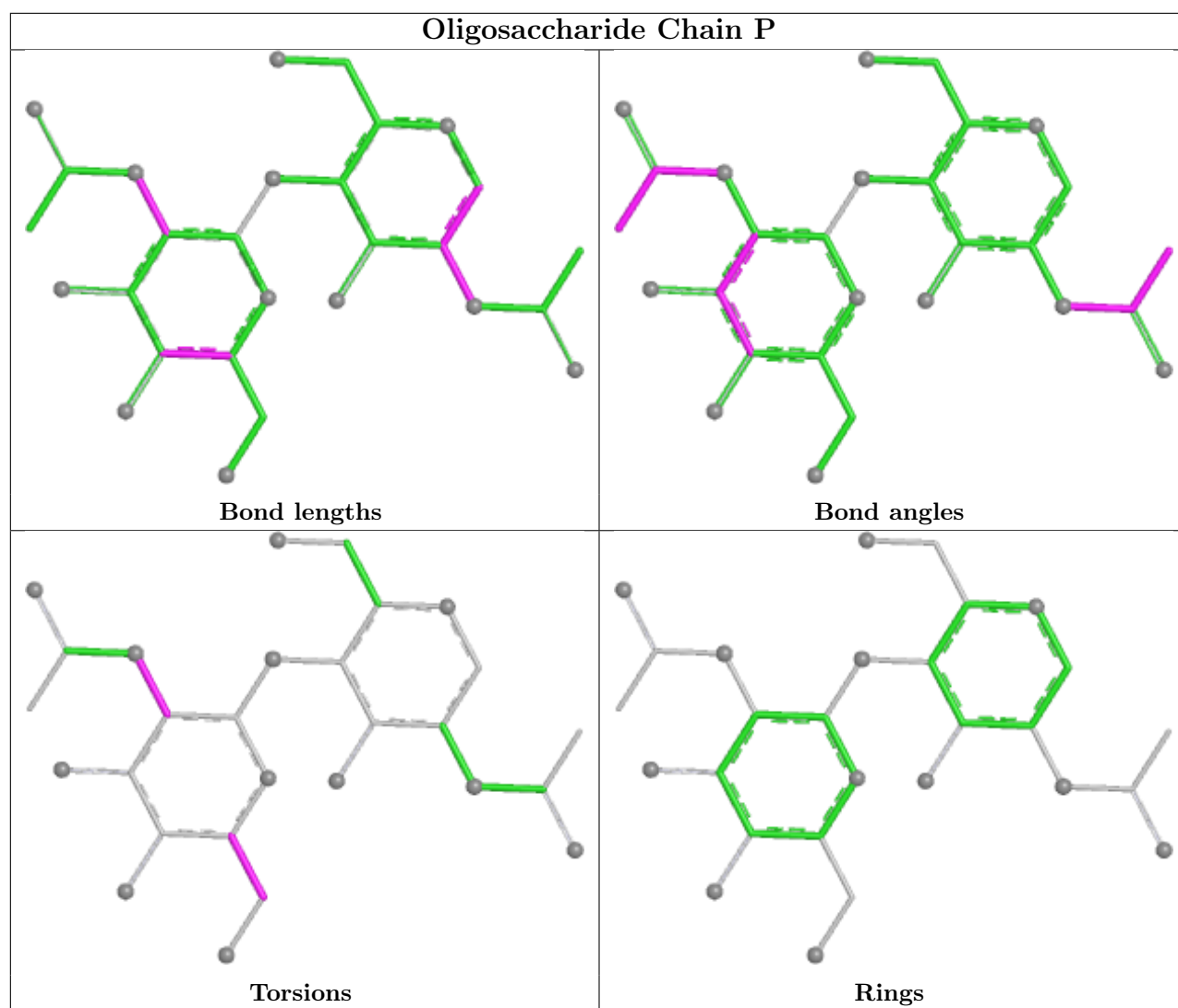


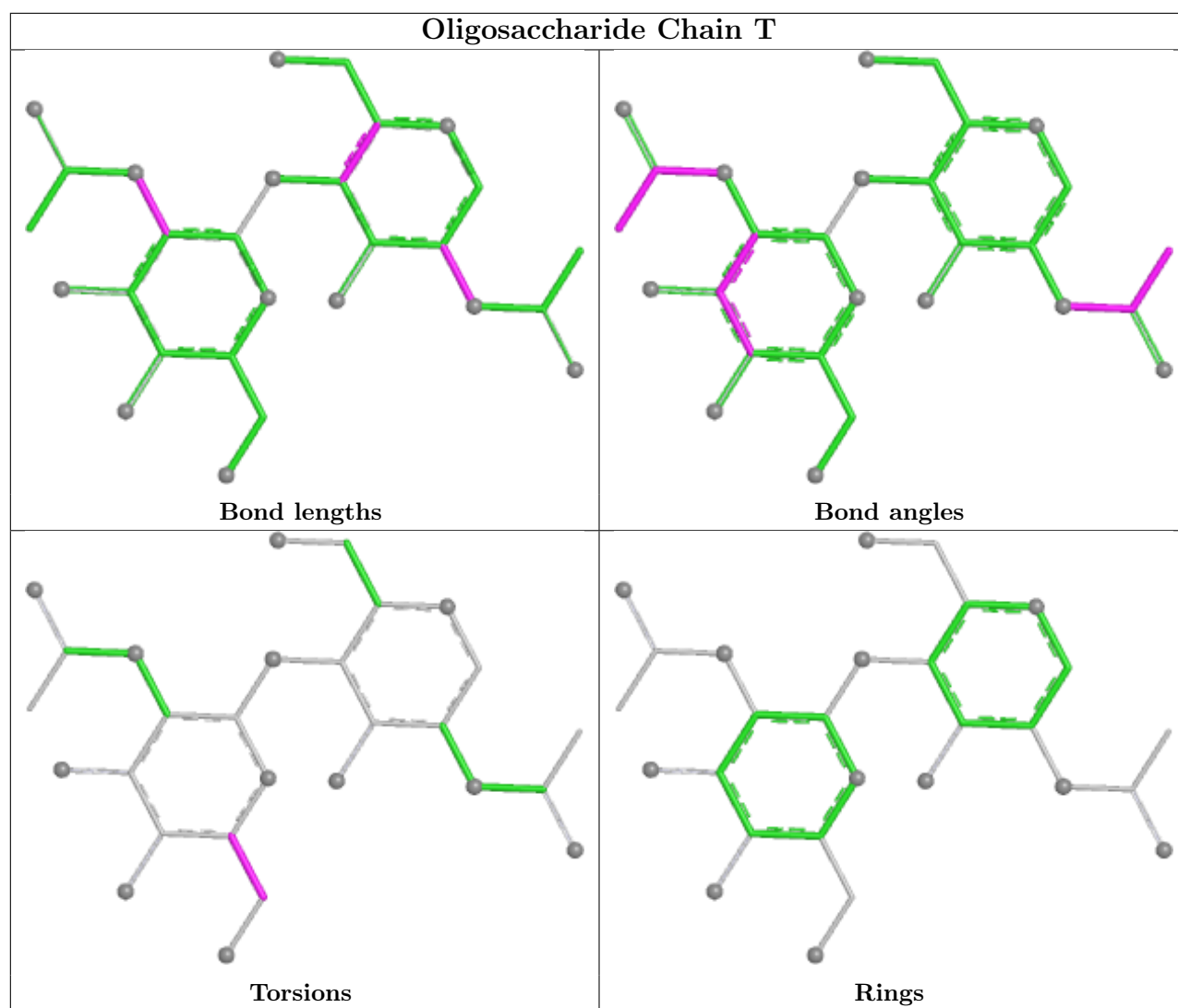


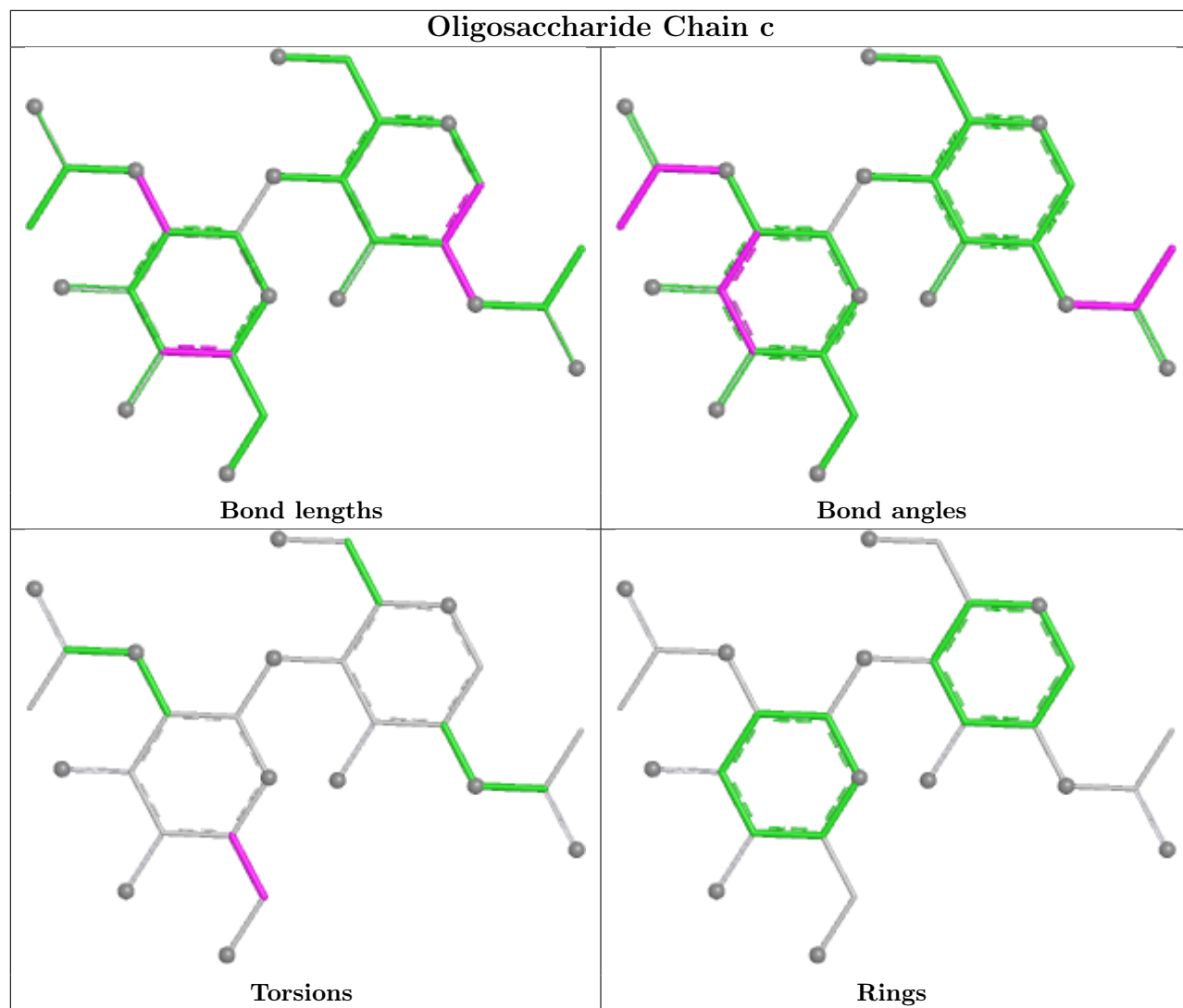


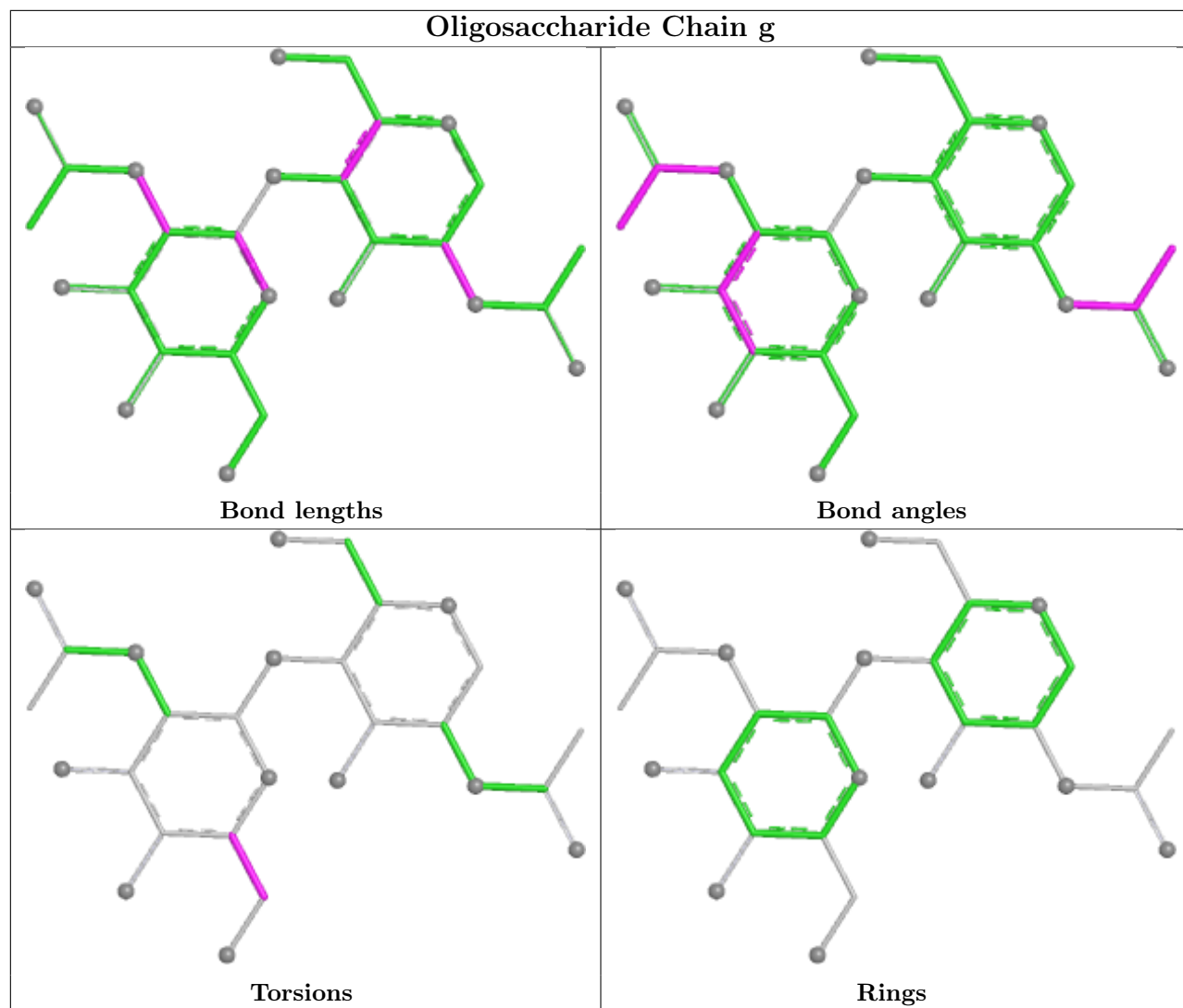


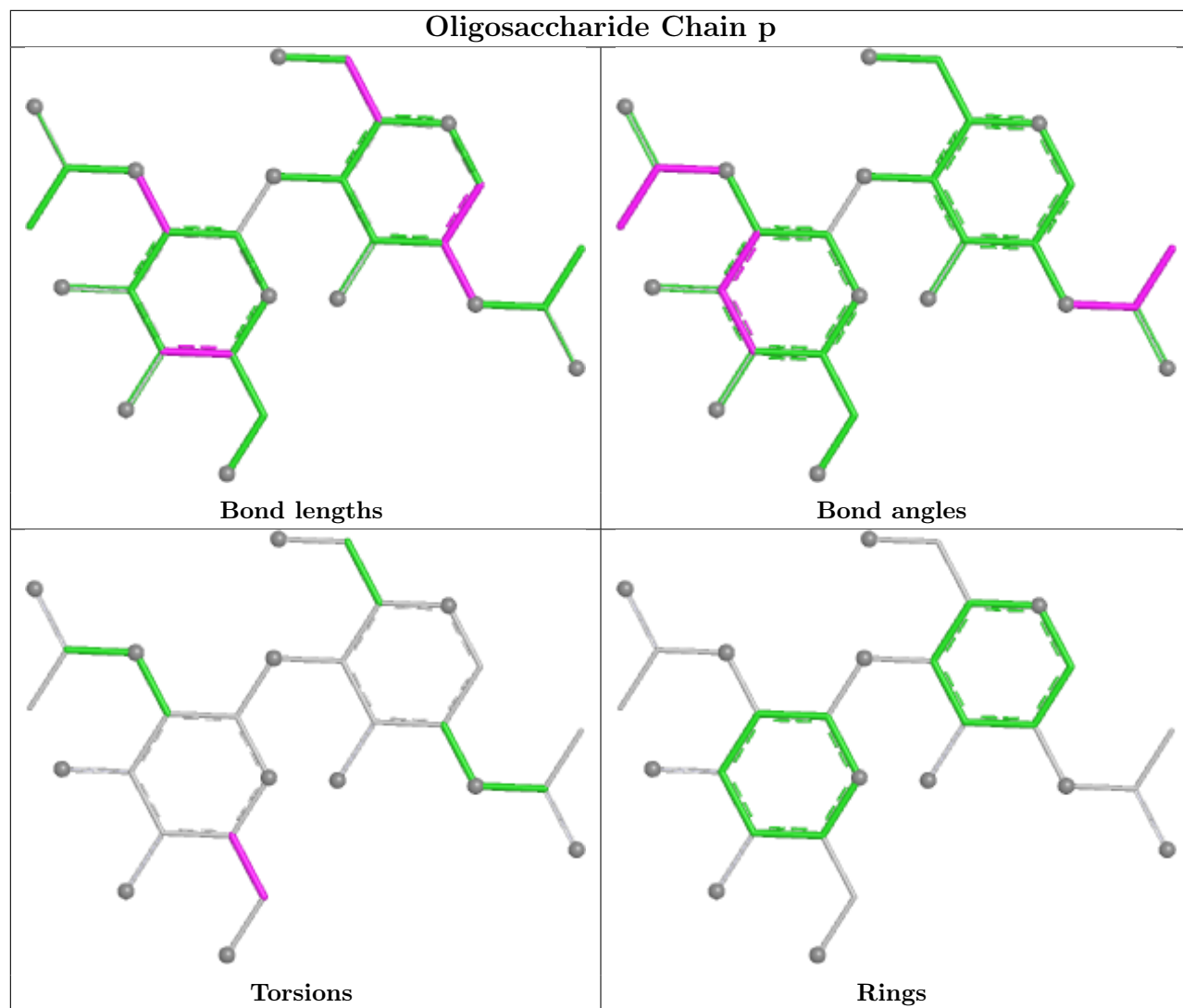


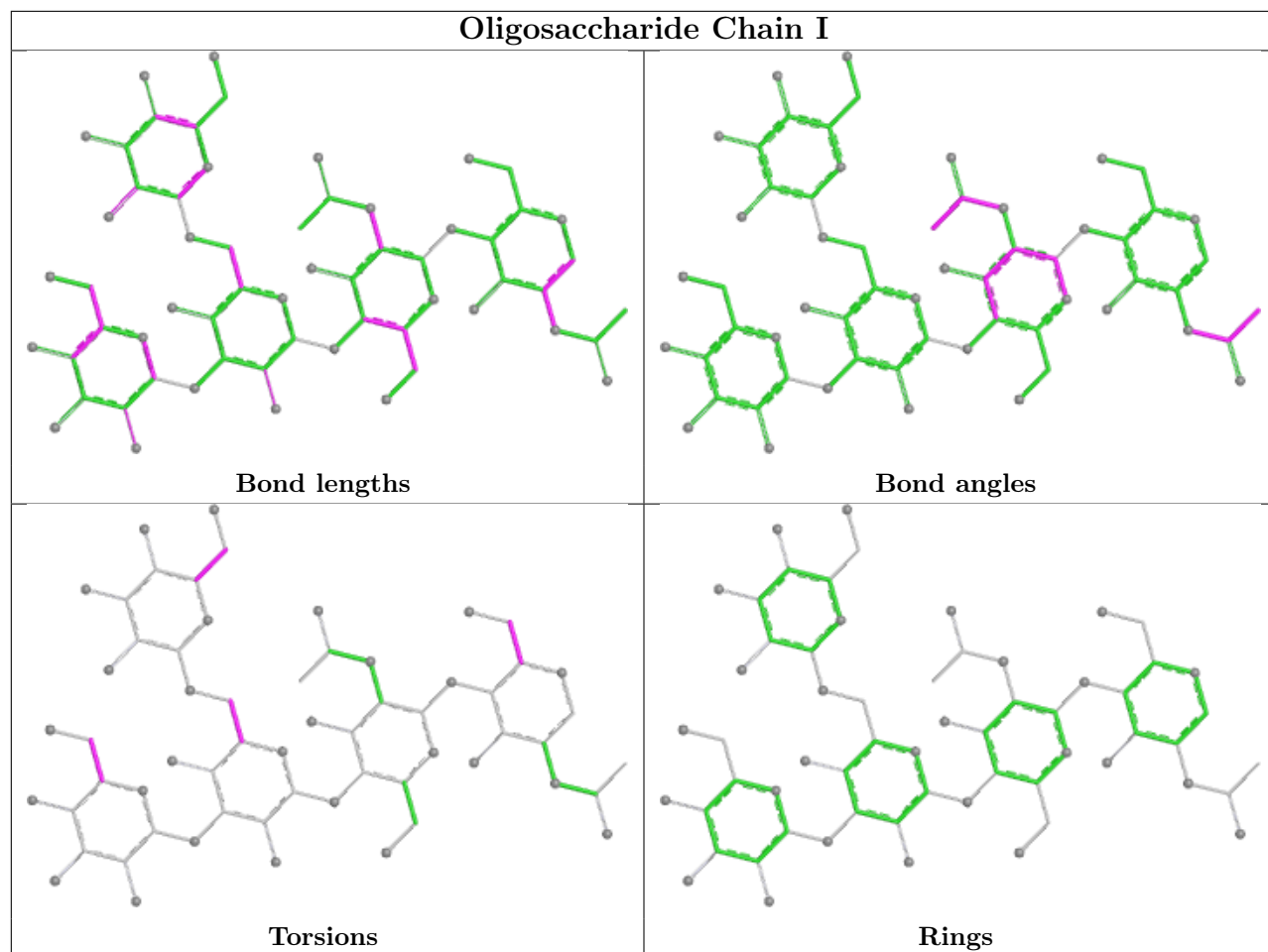


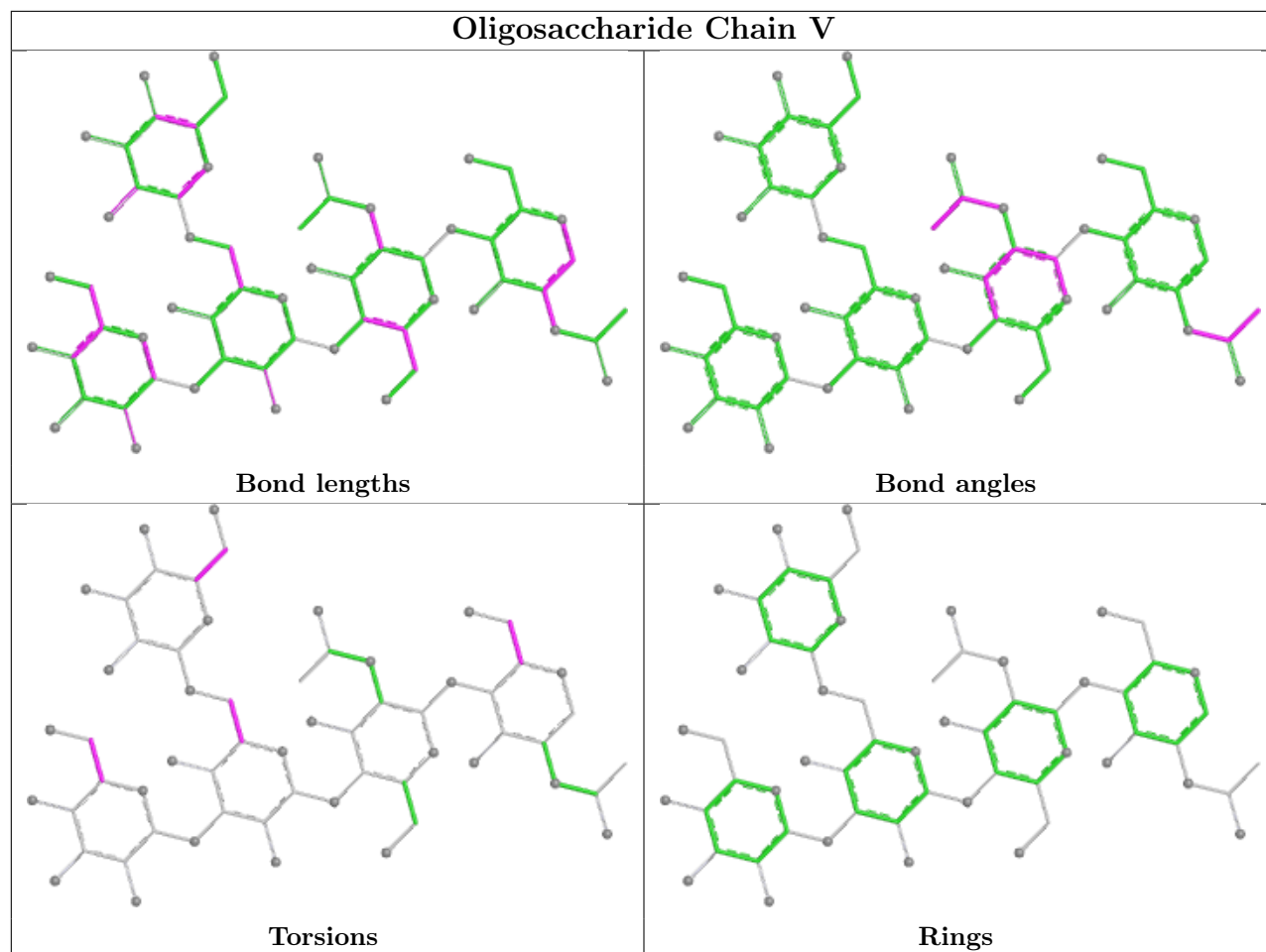


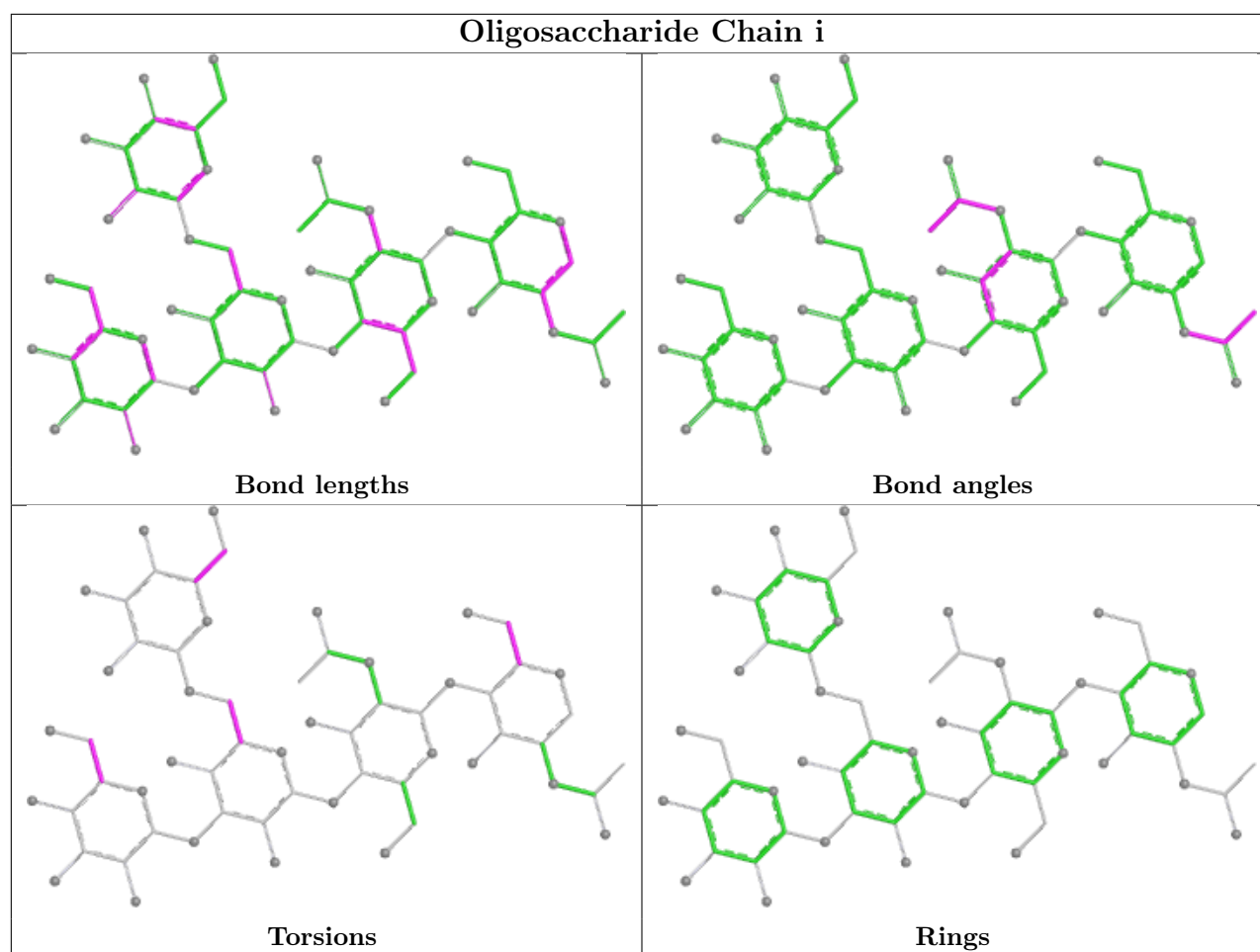












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
6	NAG	A	1970	1	14,14,15	2.02	3 (21%)	17,19,21	1.22	2 (11%)
6	NAG	B	1505	1	14,14,15	1.96	2 (14%)	17,19,21	1.20	2 (11%)
6	NAG	A	1331	1	14,14,15	2.03	2 (14%)	17,19,21	1.22	2 (11%)
6	NAG	B	1531	1	14,14,15	2.01	3 (21%)	17,19,21	1.30	2 (11%)
6	NAG	C	1531	1	14,14,15	2.00	2 (14%)	17,19,21	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1945	1	14,14,15	1.99	1 (7%)	17,19,21	1.28	2 (11%)
6	NAG	C	1505	1	14,14,15	1.95	2 (14%)	17,19,21	1.20	2 (11%)
6	NAG	B	1945	1	14,14,15	1.99	1 (7%)	17,19,21	1.29	2 (11%)
6	NAG	A	1531	1	14,14,15	2.01	3 (21%)	17,19,21	1.30	2 (11%)
6	NAG	B	1970	1	14,14,15	2.03	3 (21%)	17,19,21	1.22	2 (11%)
6	NAG	A	1945	1	14,14,15	1.99	1 (7%)	17,19,21	1.29	2 (11%)
6	NAG	B	1099	1	14,14,15	1.95	1 (7%)	17,19,21	1.31	2 (11%)
6	NAG	C	1099	1	14,14,15	1.93	1 (7%)	17,19,21	1.31	3 (17%)
6	NAG	A	1162	1	14,14,15	2.02	1 (7%)	17,19,21	1.24	2 (11%)
6	NAG	A	1505	1	14,14,15	1.97	1 (7%)	17,19,21	1.20	2 (11%)
6	NAG	A	1169	1	14,14,15	1.99	1 (7%)	17,19,21	1.23	2 (11%)
6	NAG	A	1099	1	14,14,15	1.93	1 (7%)	17,19,21	1.32	2 (11%)
6	NAG	C	1331	1	14,14,15	2.03	3 (21%)	17,19,21	1.22	2 (11%)
6	NAG	B	1162	1	14,14,15	2.02	1 (7%)	17,19,21	1.24	2 (11%)
6	NAG	C	1162	1	14,14,15	2.02	1 (7%)	17,19,21	1.25	2 (11%)
6	NAG	C	1169	1	14,14,15	2.00	1 (7%)	17,19,21	1.22	2 (11%)
6	NAG	C	1970	1	14,14,15	2.04	3 (21%)	17,19,21	1.22	2 (11%)
6	NAG	B	1169	1	14,14,15	1.97	1 (7%)	17,19,21	1.22	2 (11%)
6	NAG	B	1331	1	14,14,15	2.05	2 (14%)	17,19,21	1.22	3 (17%)

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
6	NAG	A	1970	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1505	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1331	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1531	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1531	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1945	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1505	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1945	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1531	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1970	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1945	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1099	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1099	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1162	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1505	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1169	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1099	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1331	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1162	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1162	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1169	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1970	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1169	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1331	1	-	1/6/23/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1162	NAG	C2-N2	-6.04	1.36	1.46
6	A	1162	NAG	C2-N2	-6.04	1.36	1.46
6	B	1162	NAG	C2-N2	-6.02	1.36	1.46
6	B	1945	NAG	C2-N2	-5.98	1.36	1.46
6	C	1945	NAG	C2-N2	-5.96	1.36	1.46
6	A	1945	NAG	C2-N2	-5.95	1.36	1.46
6	B	1331	NAG	C2-N2	-5.95	1.36	1.46
6	B	1531	NAG	C2-N2	-5.94	1.36	1.46
6	A	1531	NAG	C2-N2	-5.93	1.36	1.46
6	C	1331	NAG	C2-N2	-5.91	1.36	1.46
6	C	1169	NAG	C2-N2	-5.90	1.36	1.46
6	A	1331	NAG	C2-N2	-5.88	1.36	1.46
6	C	1970	NAG	C2-N2	-5.87	1.36	1.46
6	C	1531	NAG	C2-N2	-5.87	1.36	1.46
6	B	1970	NAG	C2-N2	-5.84	1.36	1.46
6	A	1169	NAG	C2-N2	-5.84	1.36	1.46
6	B	1169	NAG	C2-N2	-5.82	1.36	1.46
6	A	1970	NAG	C2-N2	-5.82	1.36	1.46
6	A	1505	NAG	C2-N2	-5.74	1.36	1.46
6	B	1099	NAG	C2-N2	-5.73	1.36	1.46
6	C	1505	NAG	C2-N2	-5.72	1.36	1.46
6	B	1505	NAG	C2-N2	-5.72	1.36	1.46
6	A	1099	NAG	C2-N2	-5.67	1.36	1.46
6	C	1099	NAG	C2-N2	-5.67	1.36	1.46
6	B	1331	NAG	C1-C2	2.21	1.55	1.52
6	B	1970	NAG	C1-C2	2.13	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1331	NAG	C1-C2	2.12	1.55	1.52
6	C	1331	NAG	C1-C2	2.11	1.55	1.52
6	C	1531	NAG	C1-C2	2.11	1.55	1.52
6	A	1531	NAG	C1-C2	2.11	1.55	1.52
6	C	1970	NAG	C1-C2	2.11	1.55	1.52
6	B	1531	NAG	C1-C2	2.08	1.55	1.52
6	C	1970	NAG	O5-C1	2.06	1.47	1.43
6	A	1970	NAG	O5-C1	2.03	1.47	1.43
6	A	1531	NAG	O5-C1	2.03	1.47	1.43
6	B	1531	NAG	O5-C1	2.01	1.47	1.43
6	A	1970	NAG	C1-C2	2.01	1.55	1.52
6	B	1970	NAG	O5-C1	2.01	1.47	1.43
6	C	1505	NAG	C4-C5	2.01	1.57	1.53
6	C	1331	NAG	O5-C1	2.01	1.47	1.43
6	B	1505	NAG	C4-C5	2.00	1.57	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1099	NAG	C8-C7-N2	2.70	120.60	116.12
6	A	1099	NAG	C8-C7-N2	2.68	120.56	116.12
6	C	1099	NAG	C8-C7-N2	2.63	120.47	116.12
6	A	1531	NAG	C8-C7-N2	2.55	120.34	116.12
6	B	1531	NAG	C8-C7-N2	2.50	120.27	116.12
6	C	1531	NAG	C8-C7-N2	2.49	120.25	116.12
6	C	1945	NAG	C4-C3-C2	-2.43	107.46	111.02
6	B	1945	NAG	C4-C3-C2	-2.41	107.48	111.02
6	A	1169	NAG	C8-C7-N2	2.41	120.11	116.12
6	A	1945	NAG	C4-C3-C2	-2.41	107.49	111.02
6	C	1505	NAG	C8-C7-N2	2.38	120.06	116.12
6	A	1505	NAG	C8-C7-N2	2.38	120.06	116.12
6	C	1531	NAG	C4-C3-C2	-2.38	107.54	111.02
6	B	1505	NAG	C8-C7-N2	2.37	120.05	116.12
6	A	1531	NAG	C4-C3-C2	-2.37	107.55	111.02
6	B	1531	NAG	C4-C3-C2	-2.36	107.55	111.02
6	C	1169	NAG	C8-C7-N2	2.36	120.03	116.12
6	B	1169	NAG	C8-C7-N2	2.36	120.03	116.12
6	A	1945	NAG	C8-C7-N2	2.31	119.96	116.12
6	A	1162	NAG	C8-C7-N2	2.31	119.94	116.12
6	C	1162	NAG	C8-C7-N2	2.29	119.91	116.12
6	B	1945	NAG	C8-C7-N2	2.28	119.90	116.12
6	B	1162	NAG	C8-C7-N2	2.27	119.88	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1970	NAG	C8-C7-N2	2.26	119.87	116.12
6	C	1945	NAG	C8-C7-N2	2.26	119.86	116.12
6	A	1970	NAG	C8-C7-N2	2.24	119.84	116.12
6	B	1970	NAG	C8-C7-N2	2.24	119.83	116.12
6	C	1162	NAG	C4-C3-C2	-2.23	107.76	111.02
6	B	1169	NAG	C4-C3-C2	-2.22	107.77	111.02
6	A	1162	NAG	C4-C3-C2	-2.20	107.80	111.02
6	B	1970	NAG	C4-C3-C2	-2.20	107.80	111.02
6	B	1331	NAG	C8-C7-N2	2.20	119.76	116.12
6	C	1970	NAG	C4-C3-C2	-2.19	107.81	111.02
6	B	1162	NAG	C4-C3-C2	-2.19	107.81	111.02
6	A	1970	NAG	C4-C3-C2	-2.19	107.81	111.02
6	C	1331	NAG	C4-C3-C2	-2.18	107.82	111.02
6	A	1169	NAG	C4-C3-C2	-2.18	107.83	111.02
6	C	1169	NAG	C4-C3-C2	-2.17	107.84	111.02
6	C	1331	NAG	C8-C7-N2	2.16	119.70	116.12
6	A	1331	NAG	C4-C3-C2	-2.16	107.86	111.02
6	A	1331	NAG	C8-C7-N2	2.16	119.69	116.12
6	B	1331	NAG	C4-C3-C2	-2.14	107.88	111.02
6	C	1505	NAG	C4-C3-C2	-2.10	107.94	111.02
6	B	1505	NAG	C4-C3-C2	-2.07	107.98	111.02
6	A	1505	NAG	C4-C3-C2	-2.06	108.00	111.02
6	A	1099	NAG	C4-C3-C2	-2.04	108.03	111.02
6	C	1099	NAG	C4-C3-C2	-2.02	108.06	111.02
6	B	1331	NAG	O5-C1-C2	-2.02	108.17	111.29
6	B	1099	NAG	C4-C3-C2	-2.01	108.07	111.02
6	C	1099	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1945	NAG	O5-C5-C6-O6
6	B	1945	NAG	O5-C5-C6-O6
6	C	1945	NAG	O5-C5-C6-O6
6	A	1162	NAG	O5-C5-C6-O6
6	A	1331	NAG	O5-C5-C6-O6
6	B	1162	NAG	O5-C5-C6-O6
6	C	1162	NAG	O5-C5-C6-O6
6	B	1331	NAG	O5-C5-C6-O6
6	C	1331	NAG	O5-C5-C6-O6
6	A	1531	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1531	NAG	O5-C5-C6-O6
6	C	1531	NAG	O5-C5-C6-O6
6	A	1505	NAG	O5-C5-C6-O6
6	B	1505	NAG	O5-C5-C6-O6
6	C	1505	NAG	O5-C5-C6-O6
6	A	1099	NAG	O5-C5-C6-O6
6	A	1169	NAG	O5-C5-C6-O6
6	B	1099	NAG	O5-C5-C6-O6
6	B	1169	NAG	O5-C5-C6-O6
6	C	1099	NAG	O5-C5-C6-O6
6	C	1169	NAG	O5-C5-C6-O6
6	A	1970	NAG	O5-C5-C6-O6
6	B	1970	NAG	O5-C5-C6-O6
6	C	1970	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1099	NAG	1	0

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.

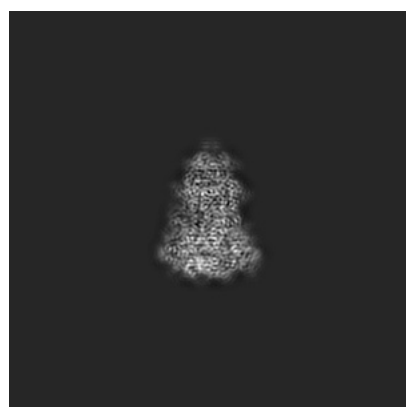
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7094. These allow visual inspection of the internal detail of the map and identification of artifacts.

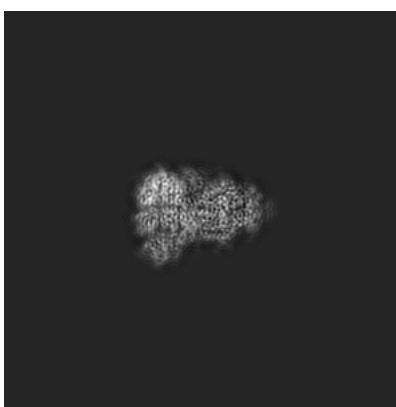
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

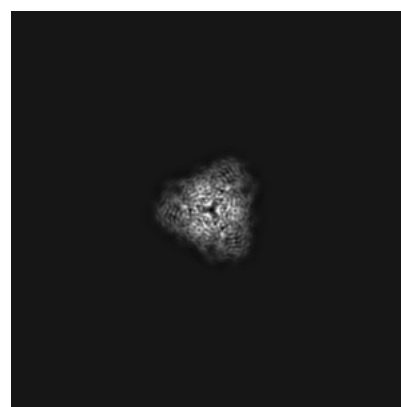
6.1.1 Primary map



X



Y

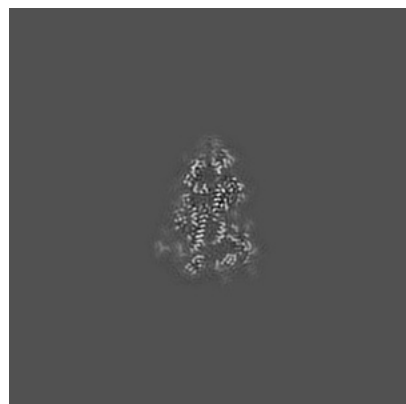


Z

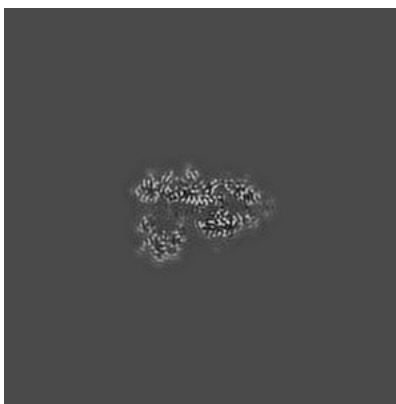
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

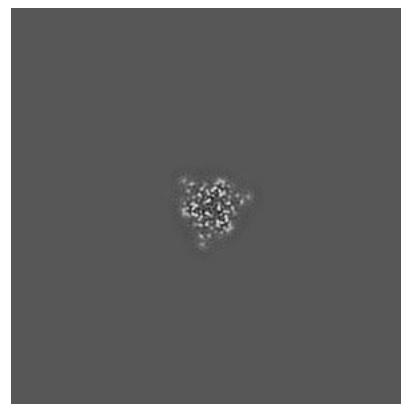
6.2.1 Primary map



X Index: 160



Y Index: 160

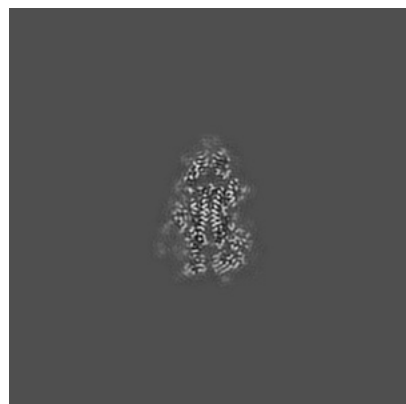


Z Index: 160

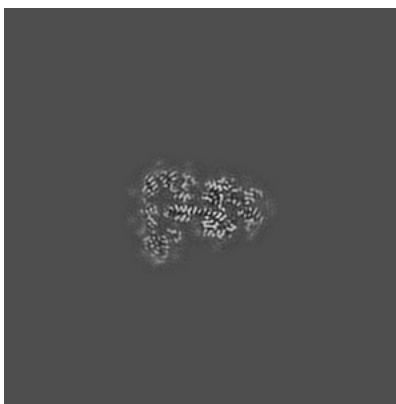
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

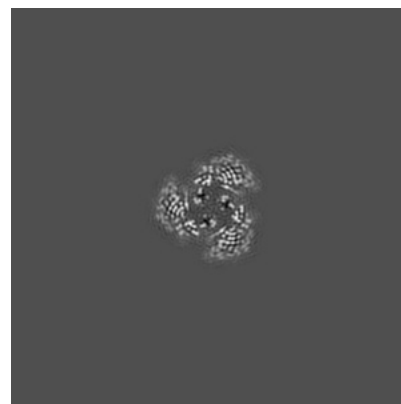
6.3.1 Primary map



X Index: 157



Y Index: 154

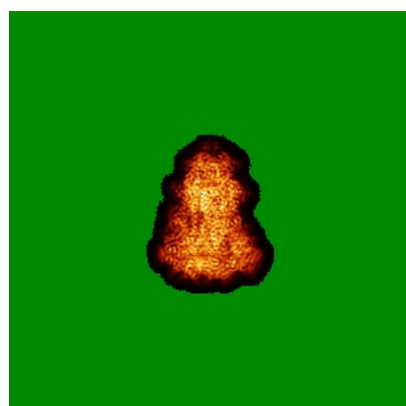


Z Index: 127

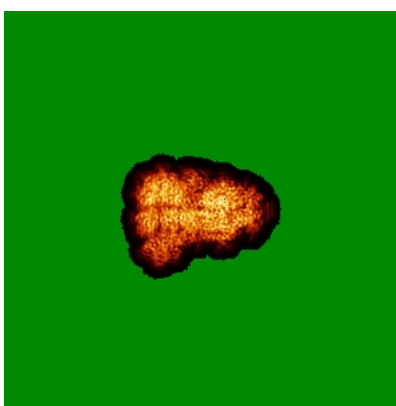
The images above show the largest variance slices of the map in three orthogonal directions.

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

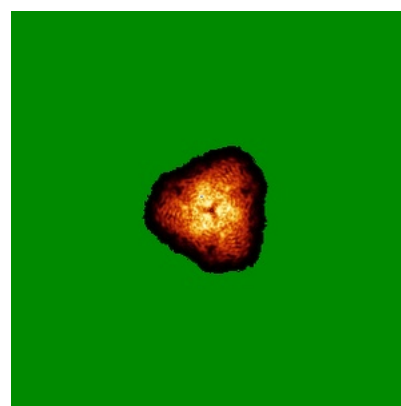
6.4.1 Primary map



X



Y

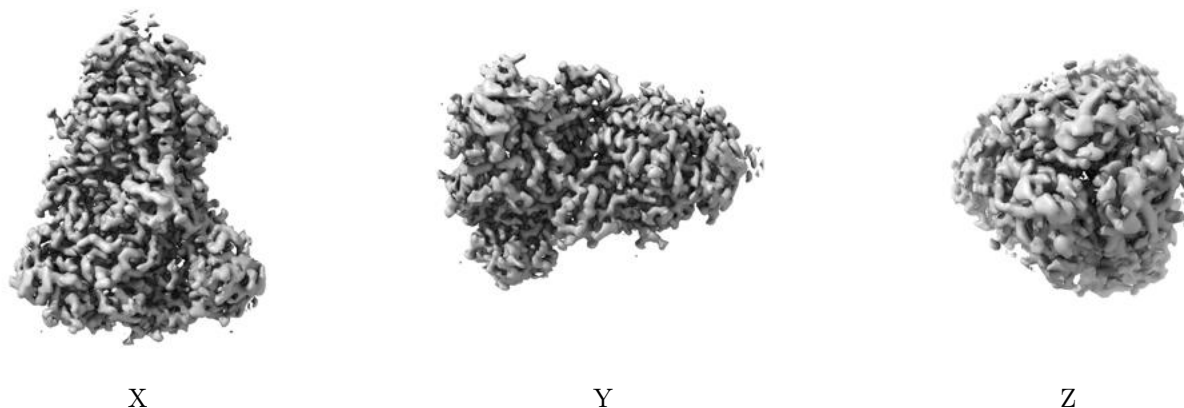


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

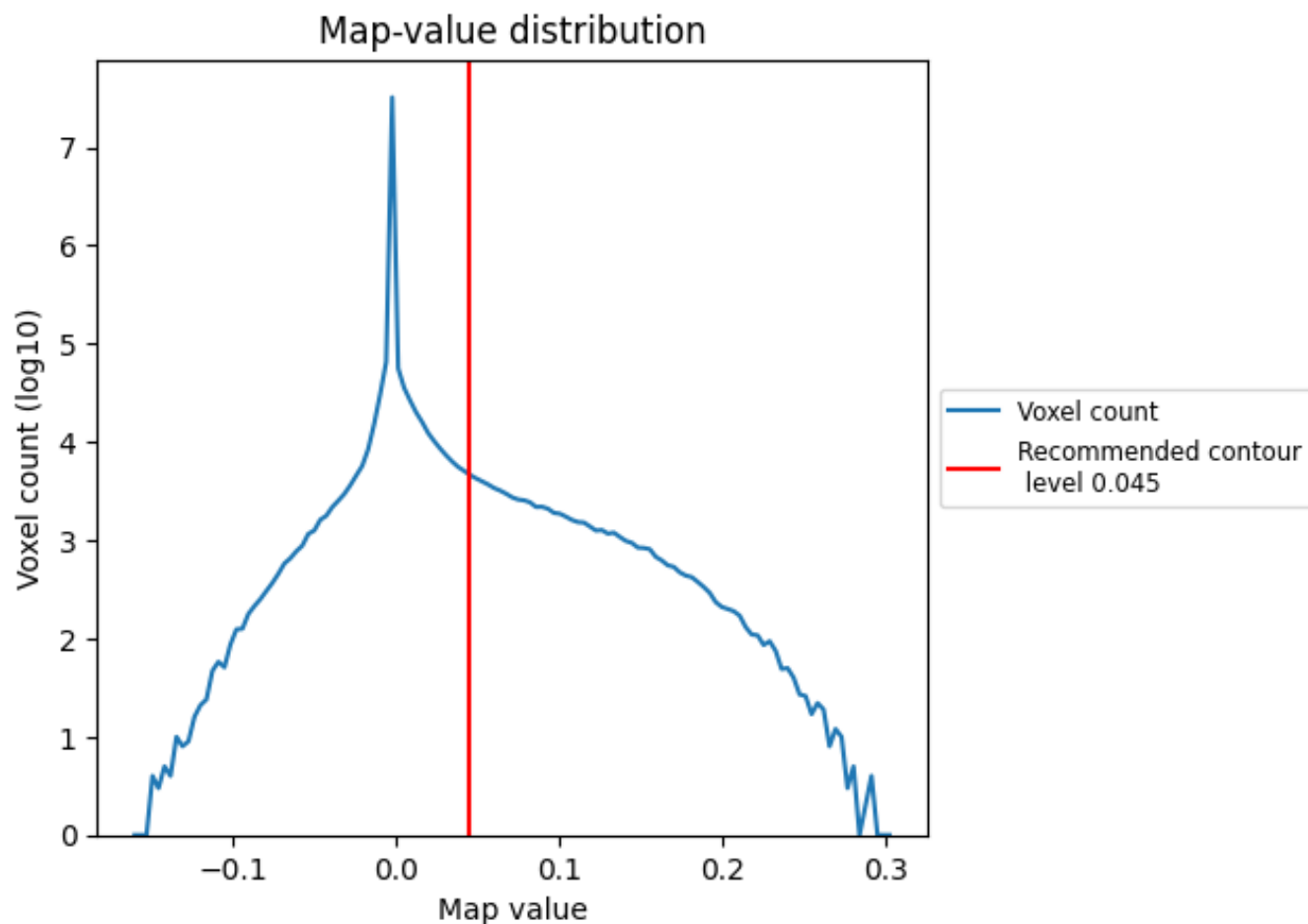
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

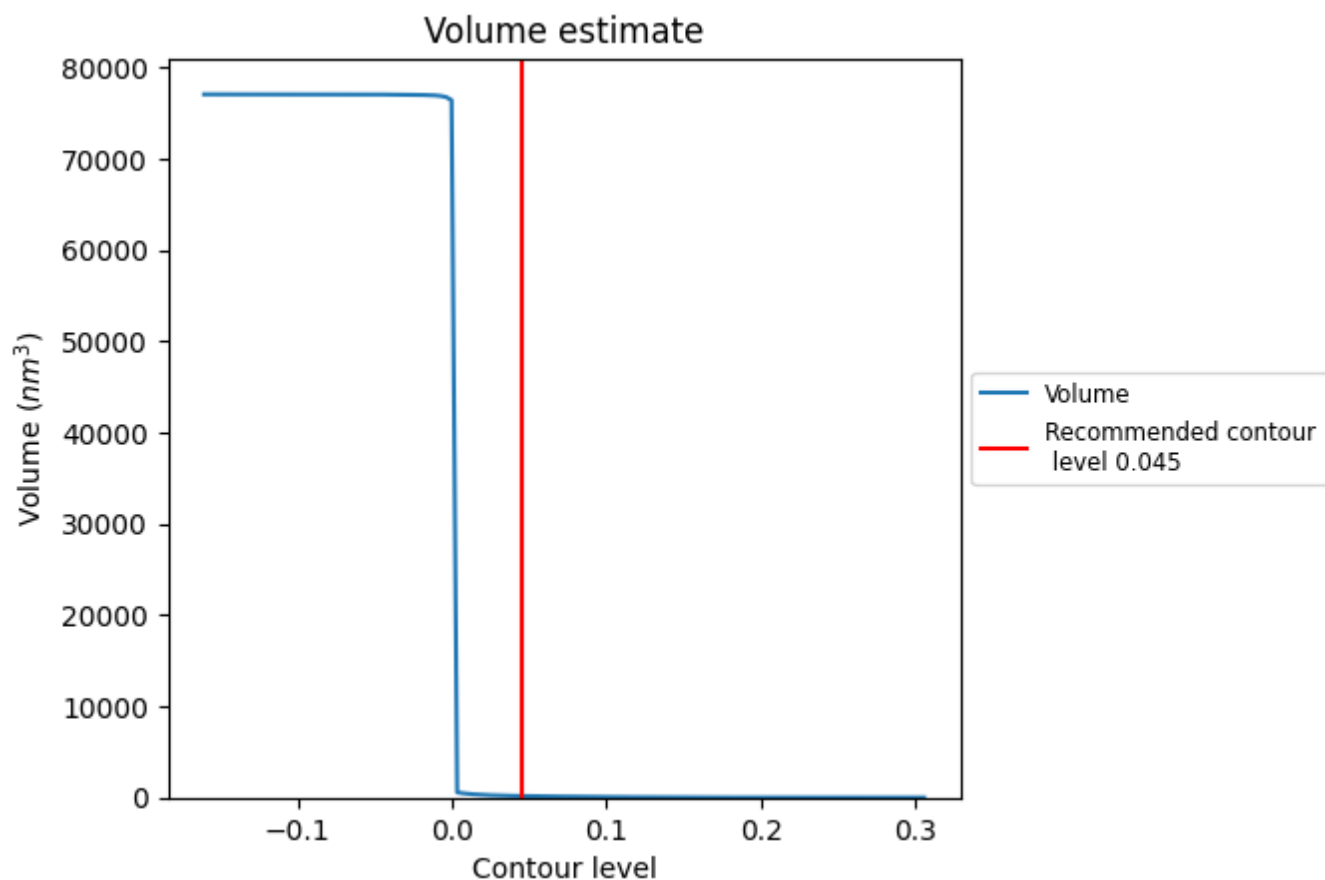
This section contains the results of statistical analysis of the map.

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.

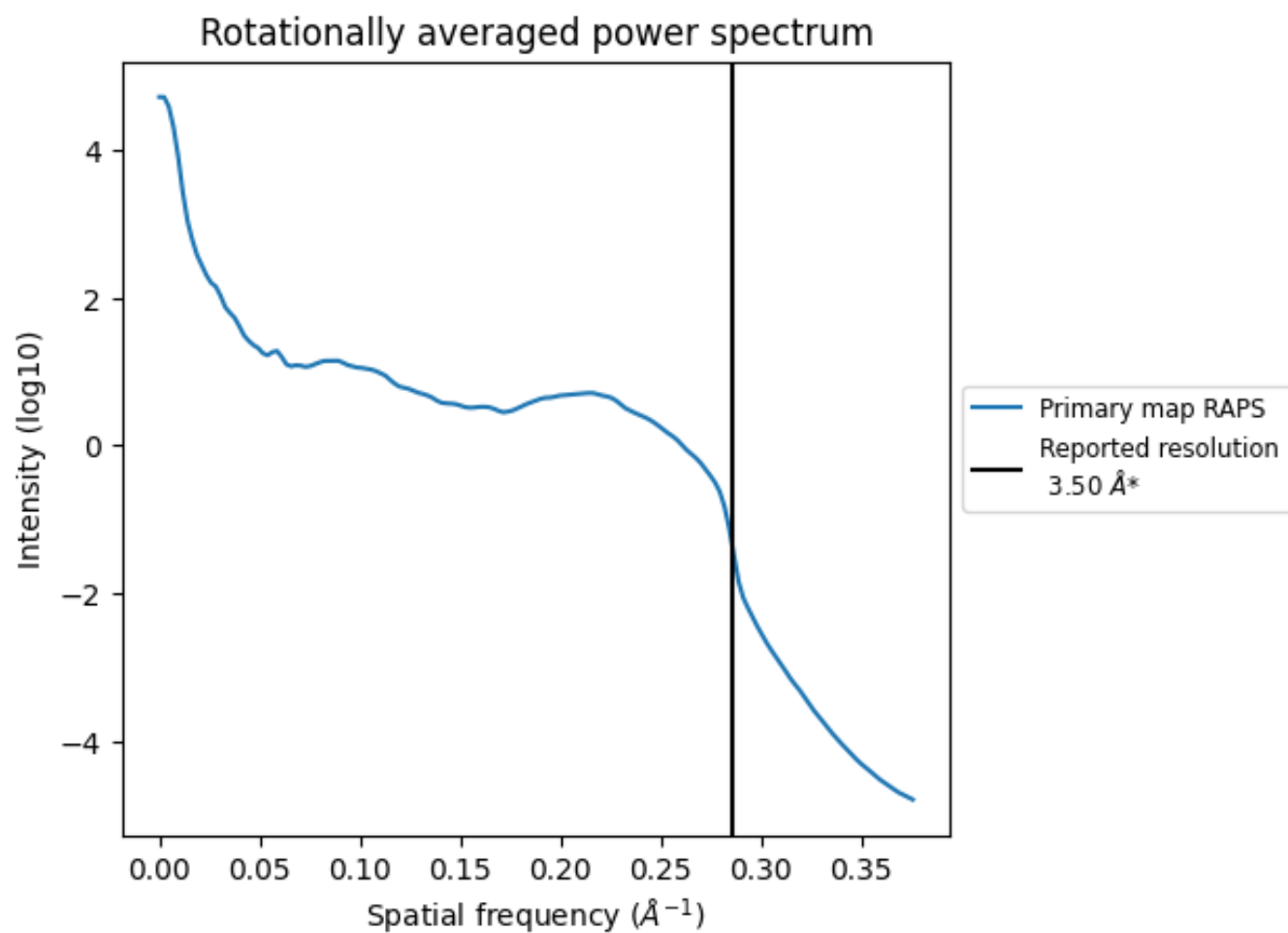
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 152 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 0.286 Å⁻¹

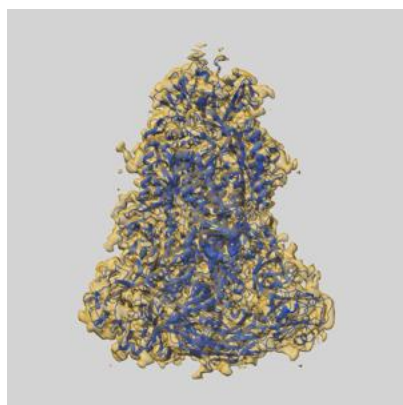
8 Fourier-Shell correlation ⓘ

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

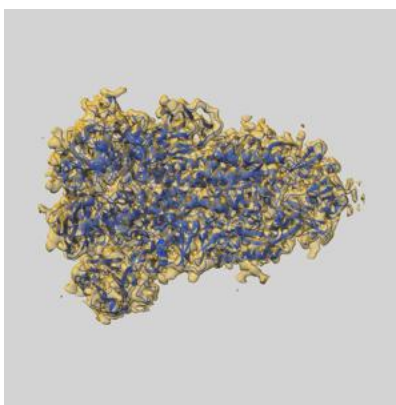
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7094 and PDB model 6BFU. Per-residue inclusion information can be found in section 3 on page 12.

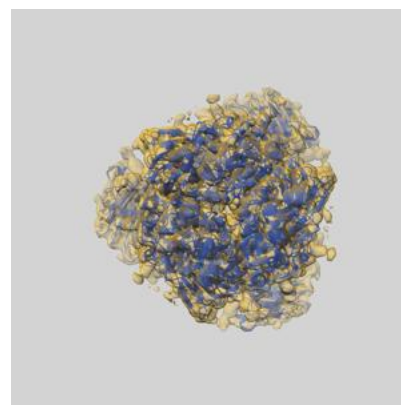
9.1 Map-model overlay [i](#)



X



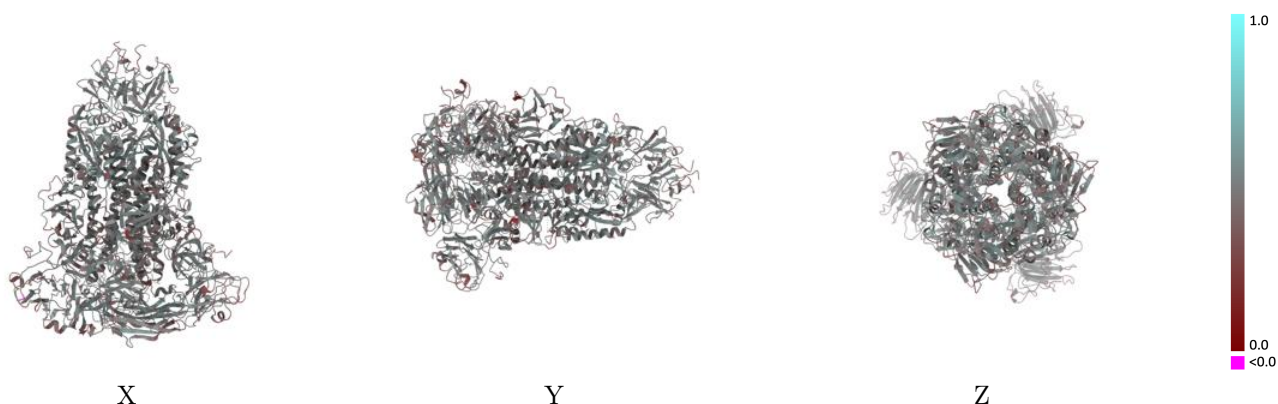
Y



Z

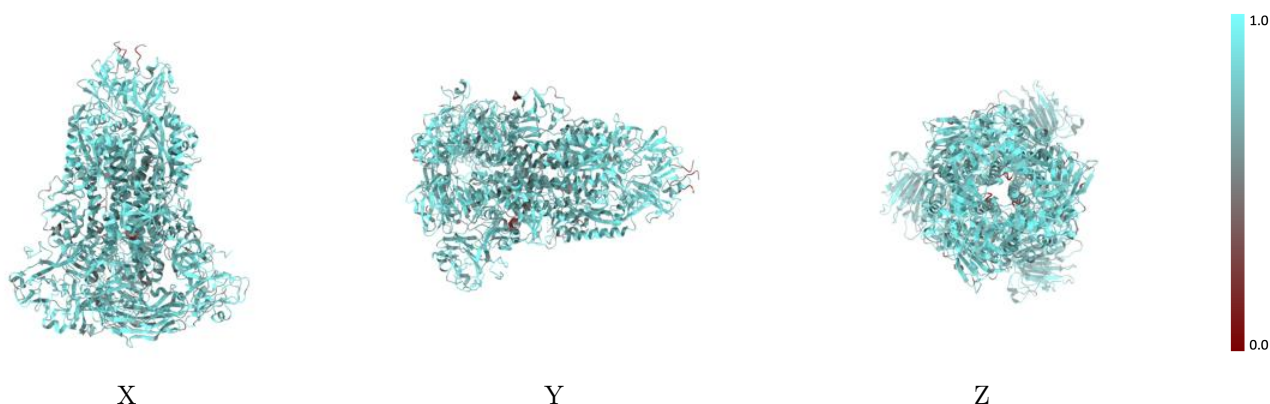
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



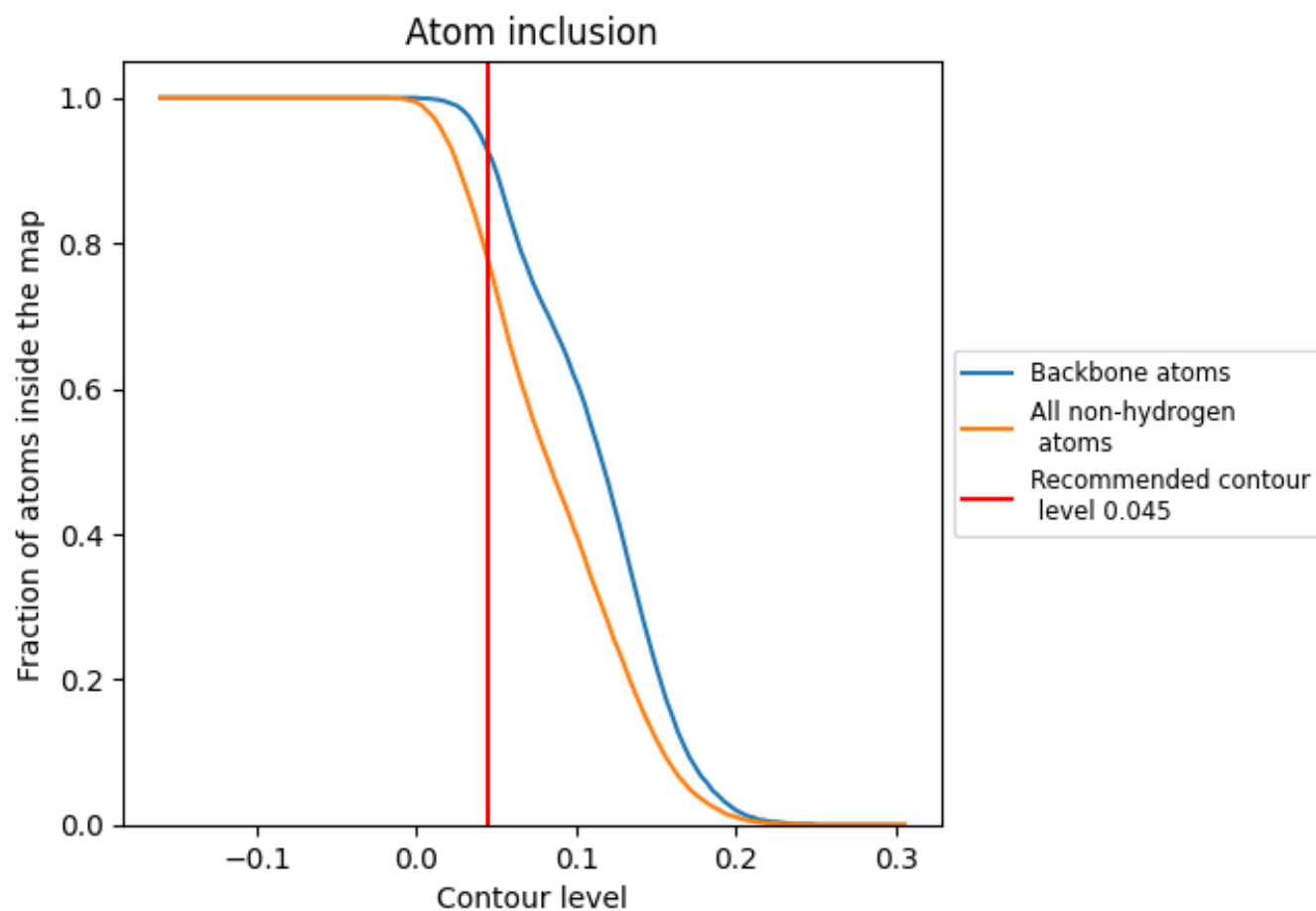
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 77% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.4490
A	 0.7940	 0.4570
B	 0.7960	 0.4580
C	 0.7950	 0.4560
D	 0.5970	 0.3700
E	 0.5380	 0.3940
F	 0.5280	 0.3680
G	 0.4640	 0.3320
H	 0.4360	 0.3190
I	 0.3280	 0.2360
J	 0.2310	 0.1850
K	 0.4870	 0.3390
L	 0.4100	 0.3220
M	 0.5130	 0.3500
N	 0.8210	 0.4670
O	 0.6940	 0.4070
P	 0.5360	 0.3790
Q	 0.6250	 0.3920
R	 0.5380	 0.3900
S	 0.5140	 0.3740
T	 0.4640	 0.3310
U	 0.4360	 0.3290
V	 0.3280	 0.2610
W	 0.2050	 0.1920
X	 0.4360	 0.3440
Y	 0.4100	 0.3200
Z	 0.5130	 0.3500
a	 0.8210	 0.4700
b	 0.6940	 0.4080
c	 0.5360	 0.3810
d	 0.6250	 0.3800
e	 0.5380	 0.3850
f	 0.5140	 0.3770
g	 0.4640	 0.3250
h	 0.4360	 0.3370



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Chain	Atom inclusion	Q-score
i	 0.3110	 0.2470
j	 0.2050	 0.1800
k	 0.4360	 0.3560
l	 0.4100	 0.3330
m	 0.4620	 0.3350
n	 0.7950	 0.4580
o	 0.6810	 0.4070
p	 0.5360	 0.3560