



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 02:08 PM EST

PDB ID : 4F7B  
Title : Structure of the lysosomal domain of limp-2  
Authors : Neculai, D.; Ravichandran, M.; Seitova, A.; Neculai, M.; Pizzaro, J.C.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Dhe-Paganon, D.; Structural Genomics Consortium (SGC)  
Deposited on : 2012-05-15  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

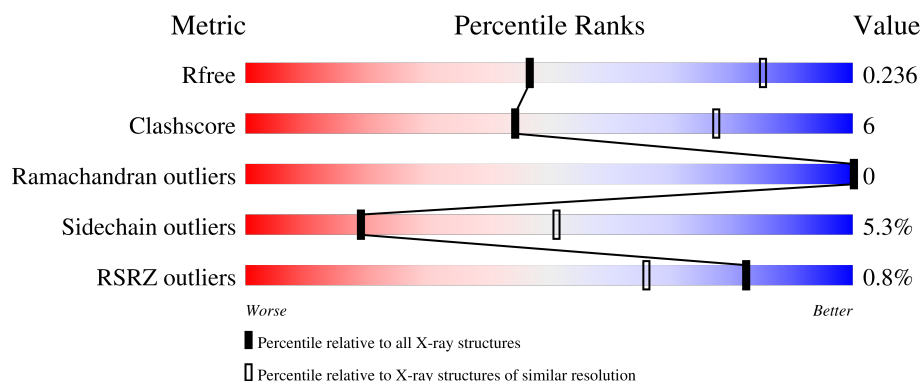
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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







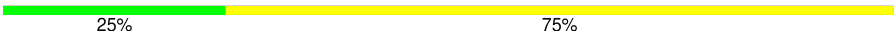
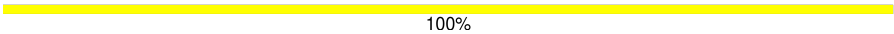
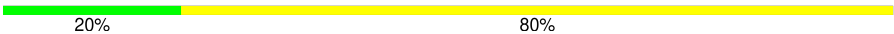
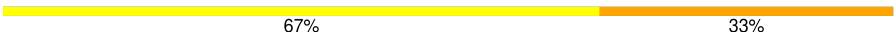
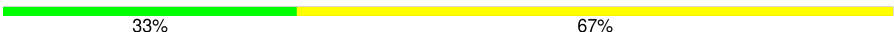
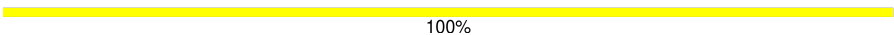
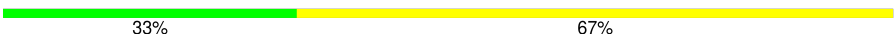
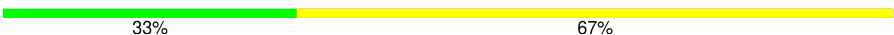
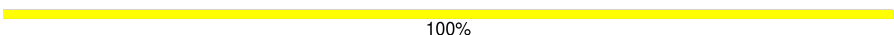
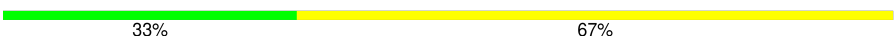


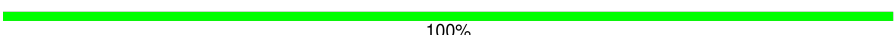



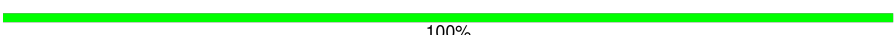

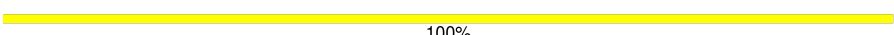


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	423	<div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
1	B	423	<div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
1	C	423	<div> <div>2%</div> <div>78%</div> <div>10%</div> <div>11%</div> </div>
1	D	423	<div> <div>76%</div> <div>14%</div> <div>8%</div> </div>
1	E	423	<div> <div>75%</div> <div>16%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	423	
2	G	4	
2	X	4	
2	b	4	
2	c	4	
3	H	5	
3	T	5	
4	I	3	
4	K	3	
4	N	3	
4	P	3	
4	U	3	
4	a	3	
4	e	3	
4	f	3	
5	J	2	
5	L	2	
5	O	2	
5	Q	2	
5	R	2	
5	S	2	
5	V	2	
5	W	2	
5	Z	2	
5	g	2	

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Mol	Chain	Length	Quality of chain
6	M	6	<div><div></div><div>17%67%17%</div></div>
6	Y	6	<div><div></div><div>83%17%</div></div>
7	d	5	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19810 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3093	1995	503	584	11			
1	B	393	Total	C	N	O	S	0	0	0
			3073	1981	493	588	11			
1	C	378	Total	C	N	O	S	0	0	0
			2969	1919	475	564	11			
1	D	389	Total	C	N	O	S	0	0	0
			3090	1989	501	589	11			
1	E	390	Total	C	N	O	S	0	0	0
			3100	1999	503	587	11			
1	F	390	Total	C	N	O	S	0	0	0
			3100	1997	501	591	11			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	expression tag	UNP Q14108
A	9	ALA	-	expression tag	UNP Q14108
A	10	PRO	-	expression tag	UNP Q14108
A	11	GLU	-	expression tag	UNP Q14108
A	12	HIS	-	expression tag	UNP Q14108
A	13	HIS	-	expression tag	UNP Q14108
A	14	HIS	-	expression tag	UNP Q14108
A	15	HIS	-	expression tag	UNP Q14108
A	16	HIS	-	expression tag	UNP Q14108
A	17	HIS	-	expression tag	UNP Q14108
A	18	ASP	-	expression tag	UNP Q14108
A	19	TYR	-	expression tag	UNP Q14108
A	20	ASP	-	expression tag	UNP Q14108
A	21	ILE	-	expression tag	UNP Q14108
A	22	PRO	-	expression tag	UNP Q14108
A	23	THR	-	expression tag	UNP Q14108
A	24	THR	-	expression tag	UNP Q14108

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	expression tag	UNP Q14108
A	26	ASN	-	expression tag	UNP Q14108
A	27	LEU	-	expression tag	UNP Q14108
A	28	TYR	-	expression tag	UNP Q14108
A	29	PHE	-	expression tag	UNP Q14108
A	30	GLN	-	expression tag	UNP Q14108
A	31	GLY	-	expression tag	UNP Q14108
A	32	ALA	-	expression tag	UNP Q14108
A	33	MET	-	expression tag	UNP Q14108
A	34	ASP	-	expression tag	UNP Q14108
B	8	ALA	-	expression tag	UNP Q14108
B	9	ALA	-	expression tag	UNP Q14108
B	10	PRO	-	expression tag	UNP Q14108
B	11	GLU	-	expression tag	UNP Q14108
B	12	HIS	-	expression tag	UNP Q14108
B	13	HIS	-	expression tag	UNP Q14108
B	14	HIS	-	expression tag	UNP Q14108
B	15	HIS	-	expression tag	UNP Q14108
B	16	HIS	-	expression tag	UNP Q14108
B	17	HIS	-	expression tag	UNP Q14108
B	18	ASP	-	expression tag	UNP Q14108
B	19	TYR	-	expression tag	UNP Q14108
B	20	ASP	-	expression tag	UNP Q14108
B	21	ILE	-	expression tag	UNP Q14108
B	22	PRO	-	expression tag	UNP Q14108
B	23	THR	-	expression tag	UNP Q14108
B	24	THR	-	expression tag	UNP Q14108
B	25	GLU	-	expression tag	UNP Q14108
B	26	ASN	-	expression tag	UNP Q14108
B	27	LEU	-	expression tag	UNP Q14108
B	28	TYR	-	expression tag	UNP Q14108
B	29	PHE	-	expression tag	UNP Q14108
B	30	GLN	-	expression tag	UNP Q14108
B	31	GLY	-	expression tag	UNP Q14108
B	32	ALA	-	expression tag	UNP Q14108
B	33	MET	-	expression tag	UNP Q14108
B	34	ASP	-	expression tag	UNP Q14108
C	8	ALA	-	expression tag	UNP Q14108
C	9	ALA	-	expression tag	UNP Q14108
C	10	PRO	-	expression tag	UNP Q14108
C	11	GLU	-	expression tag	UNP Q14108
C	12	HIS	-	expression tag	UNP Q14108

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	HIS	-	expression tag	UNP Q14108
C	14	HIS	-	expression tag	UNP Q14108
C	15	HIS	-	expression tag	UNP Q14108
C	16	HIS	-	expression tag	UNP Q14108
C	17	HIS	-	expression tag	UNP Q14108
C	18	ASP	-	expression tag	UNP Q14108
C	19	TYR	-	expression tag	UNP Q14108
C	20	ASP	-	expression tag	UNP Q14108
C	21	ILE	-	expression tag	UNP Q14108
C	22	PRO	-	expression tag	UNP Q14108
C	23	THR	-	expression tag	UNP Q14108
C	24	THR	-	expression tag	UNP Q14108
C	25	GLU	-	expression tag	UNP Q14108
C	26	ASN	-	expression tag	UNP Q14108
C	27	LEU	-	expression tag	UNP Q14108
C	28	TYR	-	expression tag	UNP Q14108
C	29	PHE	-	expression tag	UNP Q14108
C	30	GLN	-	expression tag	UNP Q14108
C	31	GLY	-	expression tag	UNP Q14108
C	32	ALA	-	expression tag	UNP Q14108
C	33	MET	-	expression tag	UNP Q14108
C	34	ASP	-	expression tag	UNP Q14108
D	8	ALA	-	expression tag	UNP Q14108
D	9	ALA	-	expression tag	UNP Q14108
D	10	PRO	-	expression tag	UNP Q14108
D	11	GLU	-	expression tag	UNP Q14108
D	12	HIS	-	expression tag	UNP Q14108
D	13	HIS	-	expression tag	UNP Q14108
D	14	HIS	-	expression tag	UNP Q14108
D	15	HIS	-	expression tag	UNP Q14108
D	16	HIS	-	expression tag	UNP Q14108
D	17	HIS	-	expression tag	UNP Q14108
D	18	ASP	-	expression tag	UNP Q14108
D	19	TYR	-	expression tag	UNP Q14108
D	20	ASP	-	expression tag	UNP Q14108
D	21	ILE	-	expression tag	UNP Q14108
D	22	PRO	-	expression tag	UNP Q14108
D	23	THR	-	expression tag	UNP Q14108
D	24	THR	-	expression tag	UNP Q14108
D	25	GLU	-	expression tag	UNP Q14108
D	26	ASN	-	expression tag	UNP Q14108
D	27	LEU	-	expression tag	UNP Q14108

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	TYR	-	expression tag	UNP Q14108
D	29	PHE	-	expression tag	UNP Q14108
D	30	GLN	-	expression tag	UNP Q14108
D	31	GLY	-	expression tag	UNP Q14108
D	32	ALA	-	expression tag	UNP Q14108
D	33	MET	-	expression tag	UNP Q14108
D	34	ASP	-	expression tag	UNP Q14108
E	8	ALA	-	expression tag	UNP Q14108
E	9	ALA	-	expression tag	UNP Q14108
E	10	PRO	-	expression tag	UNP Q14108
E	11	GLU	-	expression tag	UNP Q14108
E	12	HIS	-	expression tag	UNP Q14108
E	13	HIS	-	expression tag	UNP Q14108
E	14	HIS	-	expression tag	UNP Q14108
E	15	HIS	-	expression tag	UNP Q14108
E	16	HIS	-	expression tag	UNP Q14108
E	17	HIS	-	expression tag	UNP Q14108
E	18	ASP	-	expression tag	UNP Q14108
E	19	TYR	-	expression tag	UNP Q14108
E	20	ASP	-	expression tag	UNP Q14108
E	21	ILE	-	expression tag	UNP Q14108
E	22	PRO	-	expression tag	UNP Q14108
E	23	THR	-	expression tag	UNP Q14108
E	24	THR	-	expression tag	UNP Q14108
E	25	GLU	-	expression tag	UNP Q14108
E	26	ASN	-	expression tag	UNP Q14108
E	27	LEU	-	expression tag	UNP Q14108
E	28	TYR	-	expression tag	UNP Q14108
E	29	PHE	-	expression tag	UNP Q14108
E	30	GLN	-	expression tag	UNP Q14108
E	31	GLY	-	expression tag	UNP Q14108
E	32	ALA	-	expression tag	UNP Q14108
E	33	MET	-	expression tag	UNP Q14108
E	34	ASP	-	expression tag	UNP Q14108
F	8	ALA	-	expression tag	UNP Q14108
F	9	ALA	-	expression tag	UNP Q14108
F	10	PRO	-	expression tag	UNP Q14108
F	11	GLU	-	expression tag	UNP Q14108
F	12	HIS	-	expression tag	UNP Q14108
F	13	HIS	-	expression tag	UNP Q14108
F	14	HIS	-	expression tag	UNP Q14108
F	15	HIS	-	expression tag	UNP Q14108

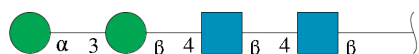
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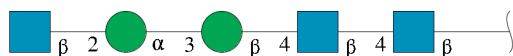
Chain	Residue	Modelled	Actual	Comment	Reference
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F	17	HIS	-	expression tag	UNP Q14108
F	18	ASP	-	expression tag	UNP Q14108
F	19	TYR	-	expression tag	UNP Q14108
F	20	ASP	-	expression tag	UNP Q14108
F	21	ILE	-	expression tag	UNP Q14108
F	22	PRO	-	expression tag	UNP Q14108
F	23	THR	-	expression tag	UNP Q14108
F	24	THR	-	expression tag	UNP Q14108
F	25	GLU	-	expression tag	UNP Q14108
F	26	ASN	-	expression tag	UNP Q14108
F	27	LEU	-	expression tag	UNP Q14108
F	28	TYR	-	expression tag	UNP Q14108
F	29	PHE	-	expression tag	UNP Q14108
F	30	GLN	-	expression tag	UNP Q14108
F	31	GLY	-	expression tag	UNP Q14108
F	32	ALA	-	expression tag	UNP Q14108
F	33	MET	-	expression tag	UNP Q14108
F	34	ASP	-	expression tag	UNP Q14108

- Molecule 2 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.



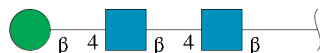
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	X	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	b	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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				ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	0	0	0
			64	36	3	25			
3	T	5	Total	C	N	O	0	0	0
			64	36	3	25			

- Molecule 4 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.



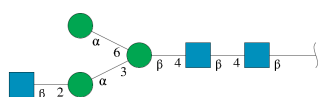
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	e	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	f	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



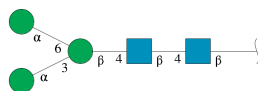
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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.



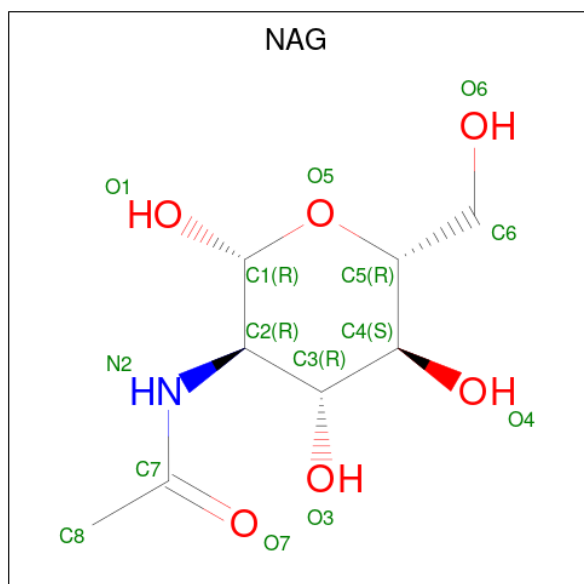
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	6	Total	C	N	O	0	0	0
			75	42	3	30			
6	Y	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 7 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				ZeroOcc	AltConf	Trace
7	d	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



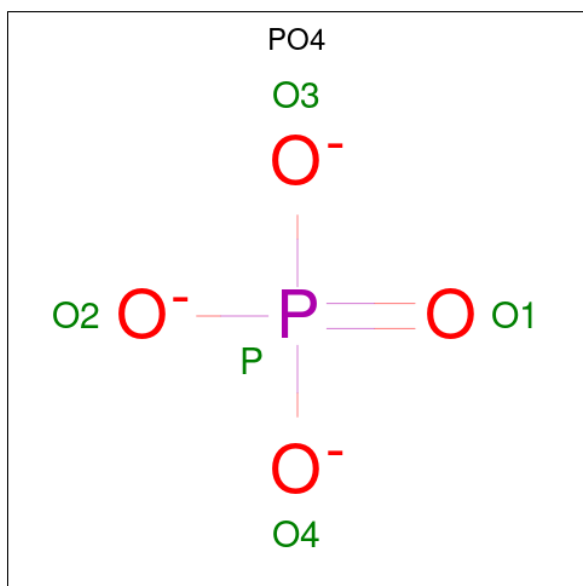
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1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

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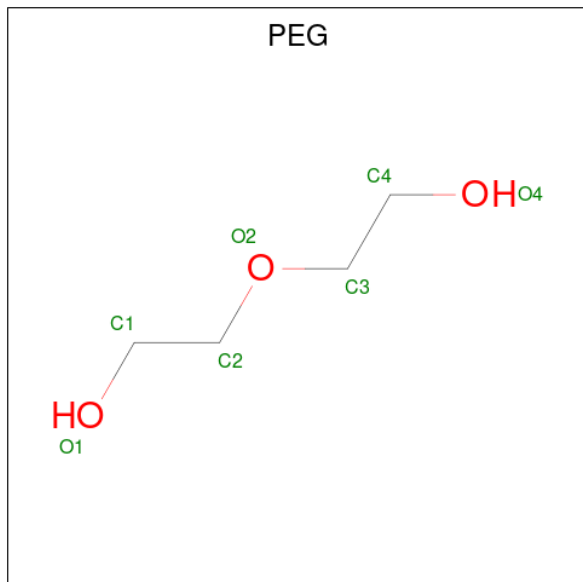
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O P	0	0
			5 4 1			
9	B	1	Total	O P	0	0
			5 4 1			
9	C	1	Total	O P	0	0
			5 4 1			
9	D	1	Total	O P	0	0
			5 4 1			
9	E	1	Total	O P	0	0
			5 4 1			
9	F	1	Total	O P	0	0
			5 4 1			

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).

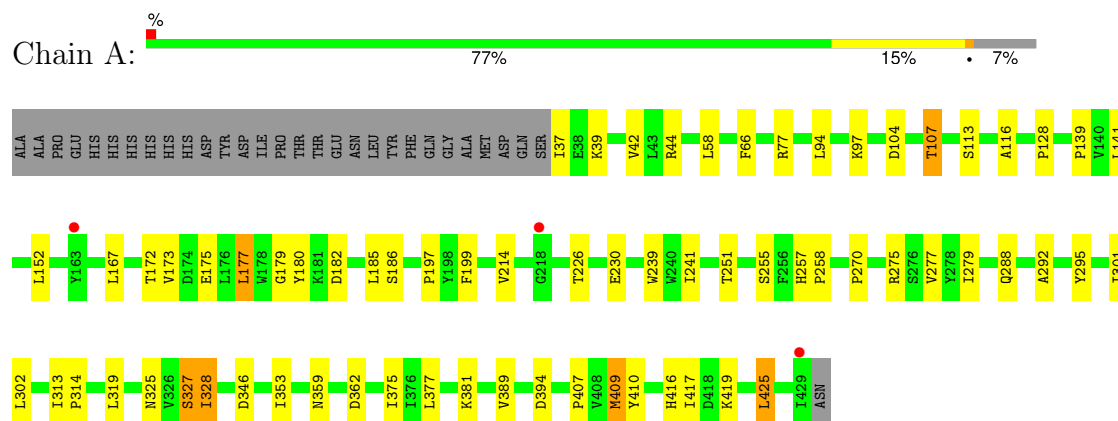


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	F	1	Total	C	O	0	0
			7	4	3		

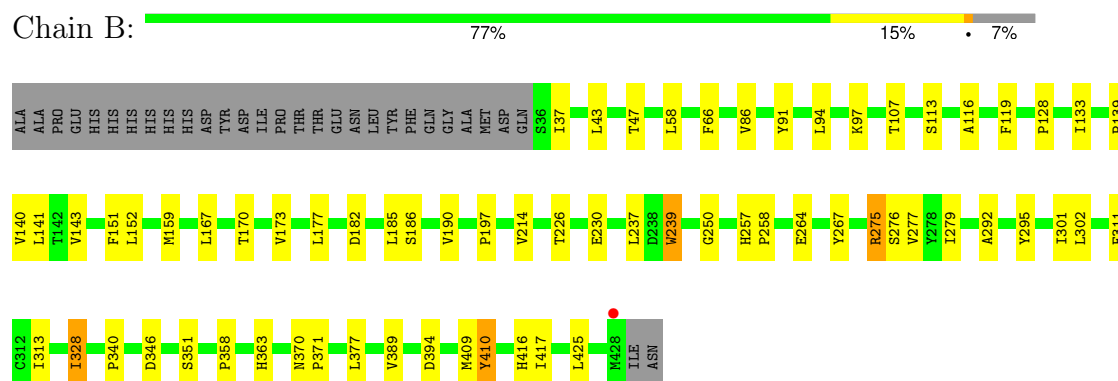
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

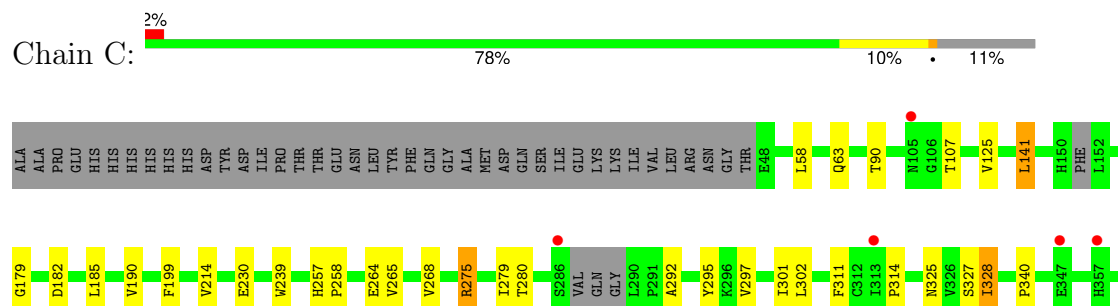
#### • Molecule 1: Lysosome membrane protein 2



#### • Molecule 1: Lysosome membrane protein 2

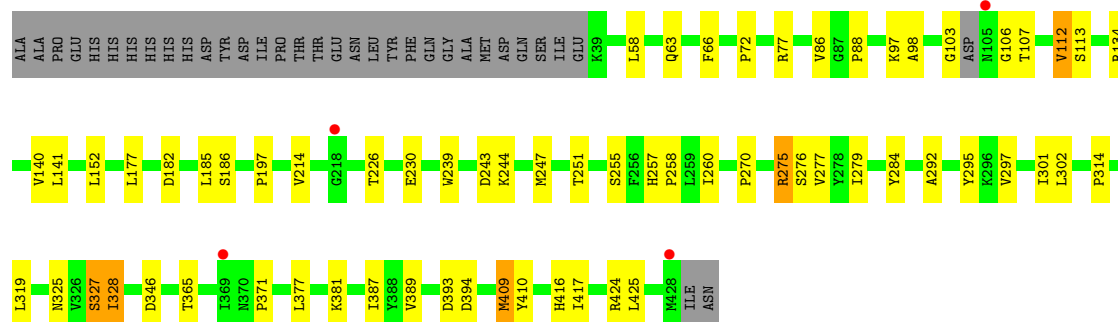
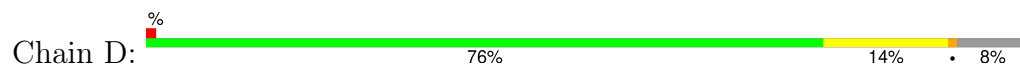


#### • Molecule 1: Lysosome membrane protein 2

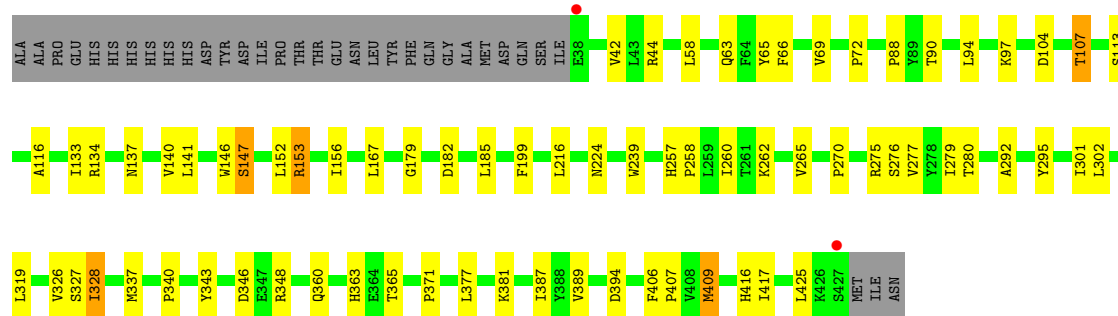




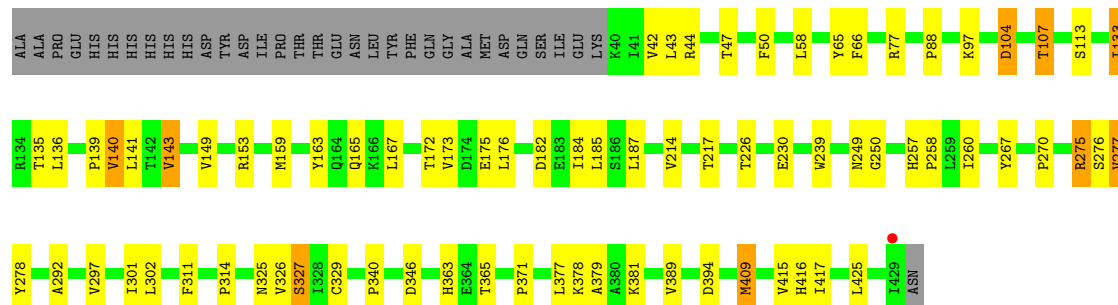
- Molecule 1: Lysosome membrane protein 2



- Molecule 1: Lysosome membrane protein 2



- Molecule 1: Lysosome membrane protein 2



- Molecule 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







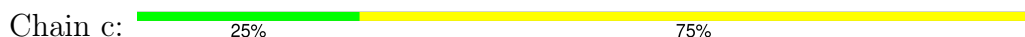
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

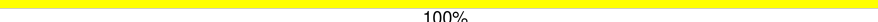


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67%



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

Chain N:  100%




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

Chain P:  33% 67%



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

Chain U:  33% 67%



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

Chain a:  100%



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

Chain e:  33% 67%



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

Chain f:  67% 33%



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

Chain J:  50%  50%



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

Chain L:  100%



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

Chain O:  50%  50%



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

Chain Q:  50%  50%



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

Chain R:  50%  50%



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

Chain S:  100%

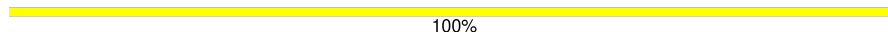


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%

NAG1  
NAG2

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

Chain W:  100%

NAG1  
NAG2

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

Chain Z:  50% 50%

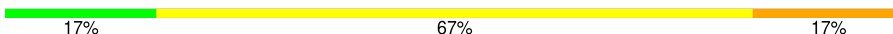
NAG1  
NAG2

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

Chain g:  50% 50%


NAG1  
NAG2

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

Chain M:  17% 67% 17%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
MAN6

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

Chain Y:  83% 17%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
MAN6

- Molecule 7:  $\alpha$ -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 d:

100%

MAG1  
MAG2  
EMJ3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.77Å 115.98Å 145.08Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	34.64 – 3.00 34.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.64-3.00) 99.9 (34.64-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.198 , 0.232 0.234 , 0.236	Depositor DCC
$R_{free}$ test set	3358 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 68.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PO4, MAN, BMA, PEG

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	0.57	0/3174	0.77	0/4328
1	B	0.56	0/3155	0.77	2/4307 (0.0%)
1	C	0.53	0/3049	0.74	0/4158
1	D	0.52	0/3171	0.73	0/4322
1	E	0.59	0/3183	0.77	0/4338
1	F	0.54	0/3182	0.75	0/4338
All	All	0.55	0/18914	0.76	2/25791 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	LEU	CB-CA-C	-9.37	92.40	110.20
1	B	151	PHE	CB-CA-C	-6.11	98.18	110.40

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	3093	0	2912	39	0
1	B	3073	0	2854	41	0
1	C	2969	0	2760	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3090	0	2918	36	0
1	E	3100	0	2938	36	0
1	F	3100	0	2926	46	0
2	G	50	0	43	0	0
2	X	50	0	43	0	0
2	b	50	0	43	0	0
2	c	50	0	43	0	0
3	H	64	0	55	0	0
3	T	64	0	55	0	0
4	I	39	0	34	1	0
4	K	39	0	34	2	0
4	N	39	0	34	2	0
4	P	39	0	34	0	0
4	U	39	0	34	0	0
4	a	39	0	34	0	0
4	e	39	0	34	0	0
4	f	39	0	34	0	0
5	J	28	0	25	0	0
5	L	28	0	25	0	0
5	O	28	0	25	0	0
5	Q	28	0	25	3	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	Z	28	0	25	0	0
5	g	28	0	25	0	0
6	M	75	0	64	2	0
6	Y	75	0	64	1	0
7	d	61	0	52	0	0
8	A	42	0	39	0	0
8	B	56	0	52	1	0
8	C	28	0	26	0	0
8	D	14	0	13	0	0
8	E	14	0	13	0	0
8	F	56	0	52	0	0
9	A	5	0	0	0	0
9	B	5	0	0	0	0
9	C	5	0	0	0	0
9	D	5	0	0	0	0
9	E	5	0	0	0	0
9	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	7	0	10	1	0
10	F	7	0	10	2	0
All	All	19810	0	18507	221	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 6.

The worst 5 of 221 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)
5:Q:2:NAG:HN2	5:Q:2:NAG:H5	1.43	0.83
1:A:313:ILE:HG21	4:K:1:NAG:H61	1.61	0.82
1:B:313:ILE:HG21	4:N:1:NAG:H61	1.62	0.81
1:F:326:VAL:HG22	1:F:329:CYS:SG	2.21	0.81
1:D:297:VAL:HG12	1:D:365:THR:HB	1.67	0.77

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 X-ray entries followed by that with respect to entries of similar resolution.

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	391/423 (92%)	372 (95%)	19 (5%)	0	100	100
1	B	391/423 (92%)	369 (94%)	22 (6%)	0	100	100
1	C	372/423 (88%)	358 (96%)	14 (4%)	0	100	100
1	D	385/423 (91%)	366 (95%)	19 (5%)	0	100	100
1	E	388/423 (92%)	369 (95%)	19 (5%)	0	100	100
1	F	388/423 (92%)	371 (96%)	17 (4%)	0	100	100
All	All	2315/2538 (91%)	2205 (95%)	110 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	328/380 (86%)	312 (95%)	16 (5%)	21	54
1	B	324/380 (85%)	309 (95%)	15 (5%)	23	56
1	C	313/380 (82%)	298 (95%)	15 (5%)	21	55
1	D	334/380 (88%)	313 (94%)	21 (6%)	15	45
1	E	335/380 (88%)	319 (95%)	16 (5%)	21	55
1	F	335/380 (88%)	313 (93%)	22 (7%)	14	43
All	All	1969/2280 (86%)	1864 (95%)	105 (5%)	19	51

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	327	SER
1	E	239	TRP
1	F	378	LYS
1	D	346	ASP
1	D	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	257	HIS
1	F	257	HIS
1	C	257	HIS
1	C	384	GLN
1	C	386	ASN

### 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 ⓘ

87 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	G	1	1,2	14,14,15	0.31	0	17,19,21	0.69	0
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	0.85	0
2	BMA	G	3	2	11,11,12	0.30	0	15,15,17	0.75	1 (6%)
2	MAN	G	4	2	11,11,12	0.41	0	15,15,17	1.26	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	2.89	5 (29%)
3	NAG	H	2	3	14,14,15	0.47	0	17,19,21	1.24	2 (11%)
3	BMA	H	3	3	11,11,12	0.25	0	15,15,17	0.76	1 (6%)
3	MAN	H	4	3	11,11,12	0.41	0	15,15,17	0.88	1 (6%)
3	NAG	H	5	3	14,14,15	0.44	0	17,19,21	1.66	3 (17%)
4	NAG	I	1	1,4	14,14,15	0.33	0	17,19,21	1.10	1 (5%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	1.09	1 (5%)
4	BMA	I	3	4	11,11,12	0.36	0	15,15,17	0.57	0
5	NAG	J	1	1,5	14,14,15	0.35	0	17,19,21	0.70	0
5	NAG	J	2	5	14,14,15	0.39	0	17,19,21	2.19	2 (11%)
4	NAG	K	1	1,4	14,14,15	0.29	0	17,19,21	0.75	0
4	NAG	K	2	4	14,14,15	0.37	0	17,19,21	0.78	0
4	BMA	K	3	4	11,11,12	0.42	0	15,15,17	0.80	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.28	0	17,19,21	0.73	0
5	NAG	L	2	5	14,14,15	0.31	0	17,19,21	0.58	0
6	NAG	M	1	1,6	14,14,15	0.31	0	17,19,21	1.30	3 (17%)
6	NAG	M	2	6	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
6	BMA	M	3	6	11,11,12	0.24	0	15,15,17	0.49	0
6	MAN	M	4	6	11,11,12	0.31	0	15,15,17	0.82	1 (6%)
6	NAG	M	5	6	14,14,15	0.42	0	17,19,21	1.87	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	M	6	6	11,11,12	0.45	0	15,15,17	0.97	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.35	0	17,19,21	0.77	0
4	NAG	N	2	4	14,14,15	0.43	0	17,19,21	0.88	1 (5%)
4	BMA	N	3	4	11,11,12	0.46	0	15,15,17	0.99	1 (6%)
5	NAG	O	1	1,5	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
5	NAG	O	2	5	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	P	1	1,4	14,14,15	0.32	0	17,19,21	1.29	2 (11%)
4	NAG	P	2	4	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
4	BMA	P	3	4	11,11,12	0.20	0	15,15,17	0.41	0
5	NAG	Q	1	1,5	14,14,15	0.36	0	17,19,21	0.66	0
5	NAG	Q	2	5	14,14,15	0.35	0	17,19,21	0.63	0
5	NAG	R	1	1,5	14,14,15	0.32	0	17,19,21	0.98	1 (5%)
5	NAG	R	2	5	14,14,15	0.32	0	17,19,21	0.60	0
5	NAG	S	1	1,5	14,14,15	0.32	0	17,19,21	0.62	0
5	NAG	S	2	5	14,14,15	0.27	0	17,19,21	0.62	0
3	NAG	T	1	1,3	14,14,15	0.32	0	17,19,21	1.25	3 (17%)
3	NAG	T	2	3	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	BMA	T	3	3	11,11,12	0.24	0	15,15,17	0.53	0
3	MAN	T	4	3	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
3	NAG	T	5	3	14,14,15	0.40	0	17,19,21	1.59	2 (11%)
4	NAG	U	1	1,4	14,14,15	0.30	0	17,19,21	1.36	2 (11%)
4	NAG	U	2	4	14,14,15	0.31	0	17,19,21	1.65	1 (5%)
4	BMA	U	3	4	11,11,12	0.36	0	15,15,17	0.63	0
5	NAG	V	1	1,5	14,14,15	0.33	0	17,19,21	0.61	0
5	NAG	V	2	5	14,14,15	0.36	0	17,19,21	1.41	1 (5%)
5	NAG	W	1	1,5	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
5	NAG	W	2	5	14,14,15	0.37	0	17,19,21	1.07	1 (5%)
2	NAG	X	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	X	2	2	14,14,15	0.32	0	17,19,21	1.19	2 (11%)
2	BMA	X	3	2	11,11,12	0.37	0	15,15,17	0.98	2 (13%)
2	MAN	X	4	2	11,11,12	0.51	0	15,15,17	1.57	2 (13%)
6	NAG	Y	1	1,6	14,14,15	0.32	0	17,19,21	1.06	2 (11%)
6	NAG	Y	2	6	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
6	BMA	Y	3	6	11,11,12	0.26	0	15,15,17	0.73	1 (6%)
6	MAN	Y	4	6	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
6	NAG	Y	5	6	14,14,15	0.38	0	17,19,21	1.56	2 (11%)
6	MAN	Y	6	6	11,11,12	0.45	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	Z	1	1,5	14,14,15	0.32	0	17,19,21	1.30	2 (11%)
5	NAG	Z	2	5	14,14,15	0.44	0	17,19,21	0.80	0
4	NAG	a	1	1,4	14,14,15	0.35	0	17,19,21	1.05	1 (5%)
4	NAG	a	2	4	14,14,15	0.35	0	17,19,21	1.16	1 (5%)
4	BMA	a	3	4	11,11,12	0.45	0	15,15,17	1.52	2 (13%)
2	NAG	b	1	1,2	14,14,15	0.29	0	17,19,21	0.78	0
2	NAG	b	2	2	14,14,15	0.34	0	17,19,21	0.67	0
2	BMA	b	3	2	11,11,12	0.30	0	15,15,17	1.08	1 (6%)
2	MAN	b	4	2	11,11,12	0.46	0	15,15,17	1.18	1 (6%)
2	NAG	c	1	1,2	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
2	NAG	c	2	2	14,14,15	0.33	0	17,19,21	0.61	0
2	BMA	c	3	2	11,11,12	0.37	0	15,15,17	1.08	1 (6%)
2	MAN	c	4	2	11,11,12	0.56	0	15,15,17	1.60	1 (6%)
7	NAG	d	1	1,7	14,14,15	0.28	0	17,19,21	1.04	2 (11%)
7	NAG	d	2	7	14,14,15	0.48	0	17,19,21	0.97	1 (5%)
7	BMA	d	3	7	11,11,12	1.30	1 (9%)	15,15,17	1.07	2 (13%)
7	MAN	d	4	7	11,11,12	0.42	0	15,15,17	0.89	1 (6%)
7	MAN	d	5	7	11,11,12	0.73	0	15,15,17	1.64	2 (13%)
4	NAG	e	1	1,4	14,14,15	0.28	0	17,19,21	1.08	1 (5%)
4	NAG	e	2	4	14,14,15	0.39	0	17,19,21	1.25	2 (11%)
4	BMA	e	3	4	11,11,12	0.37	0	15,15,17	0.51	0
4	NAG	f	1	1,4	14,14,15	0.33	0	17,19,21	0.87	0
4	NAG	f	2	4	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
4	BMA	f	3	4	11,11,12	0.36	0	15,15,17	0.58	0
5	NAG	g	1	1,5	14,14,15	0.39	0	17,19,21	0.61	0
5	NAG	g	2	5	14,14,15	0.40	0	17,19,21	0.94	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	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	1/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	BMA	f	3	4	-	0/2/19/22	0/1/1/1
5	NAG	g	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	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)
7	d	3	BMA	O6-C6	-4.23	1.24	1.42

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O5-C1-C2	-7.26	100.06	111.29
3	H	1	NAG	C1-C2-N2	7.17	121.72	110.43
5	J	2	NAG	C1-O5-C5	6.35	120.69	112.19
4	U	2	NAG	O5-C1-C2	-6.02	101.98	111.29
6	M	5	NAG	C1-C2-N2	5.84	119.64	110.43

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
2	X	4	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
2	X	4	MAN	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	MAN	C1-C2-C3-C4-C5-O5
2	c	4	MAN	C1-C2-C3-C4-C5-O5
2	G	4	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	5	NAG	2	0
5	Q	2	NAG	3	0

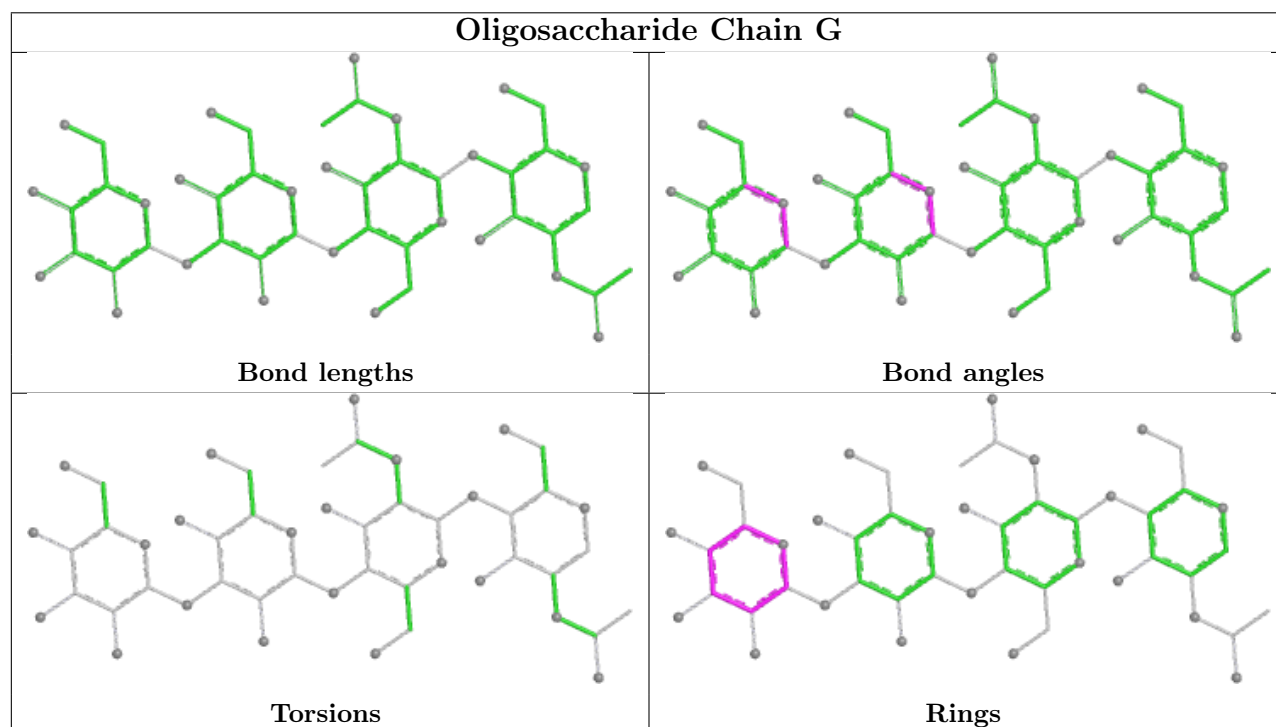
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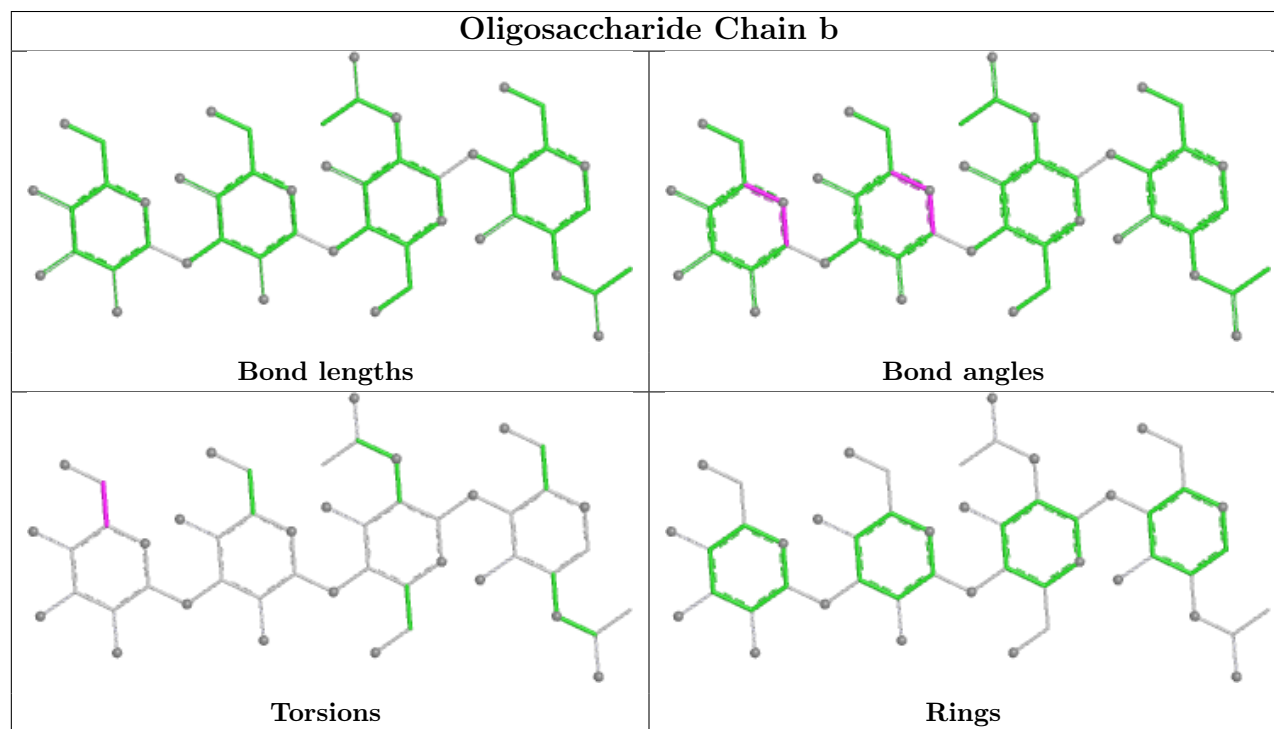
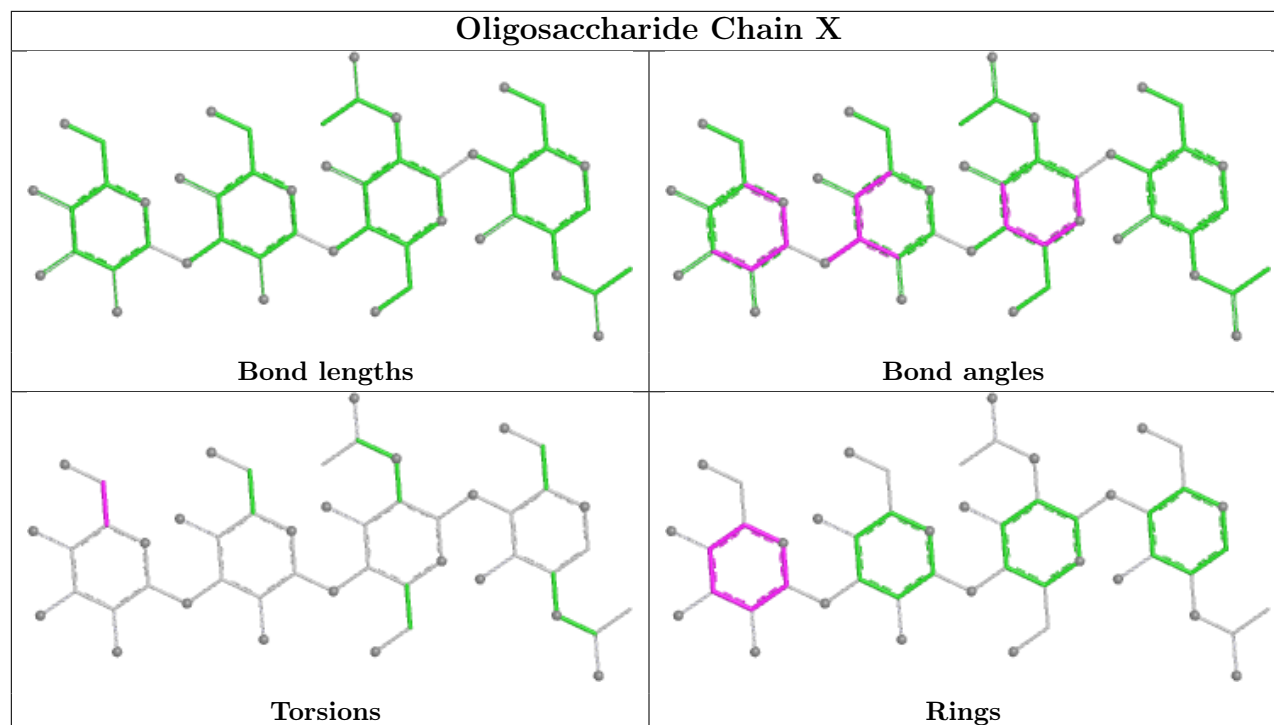


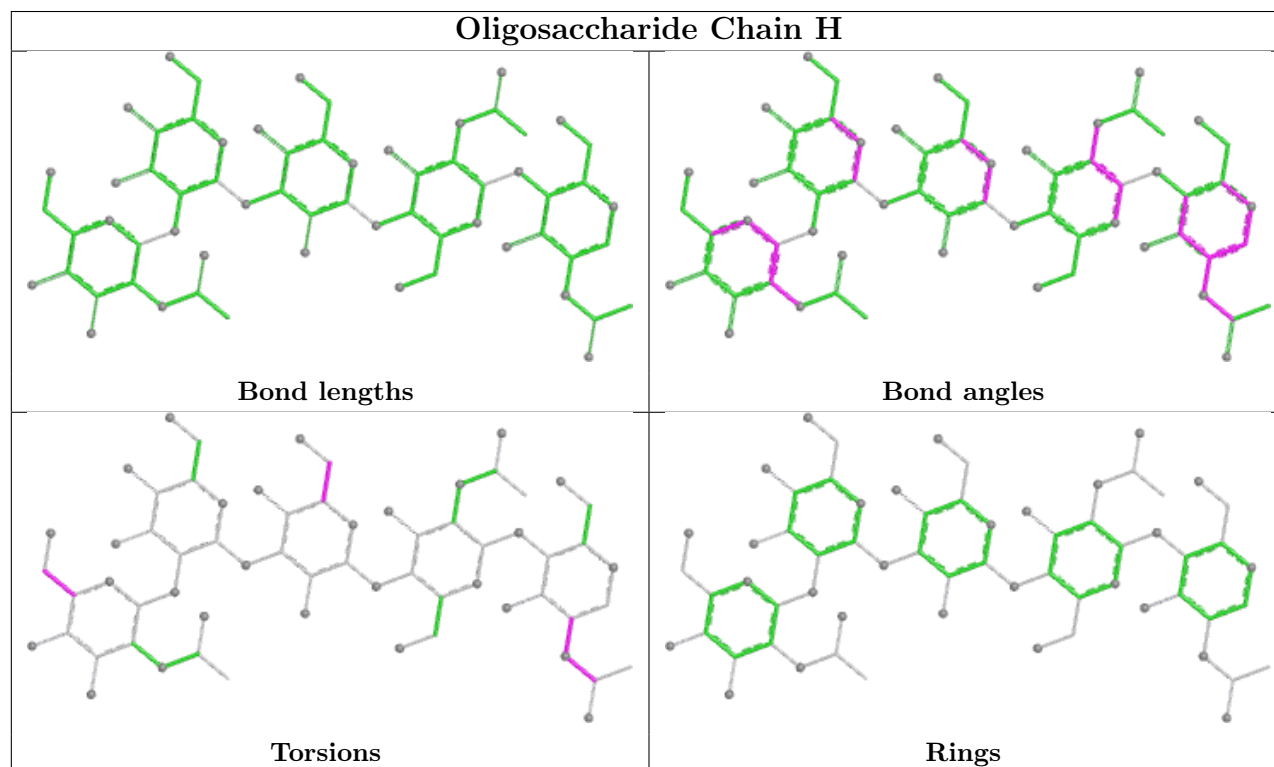
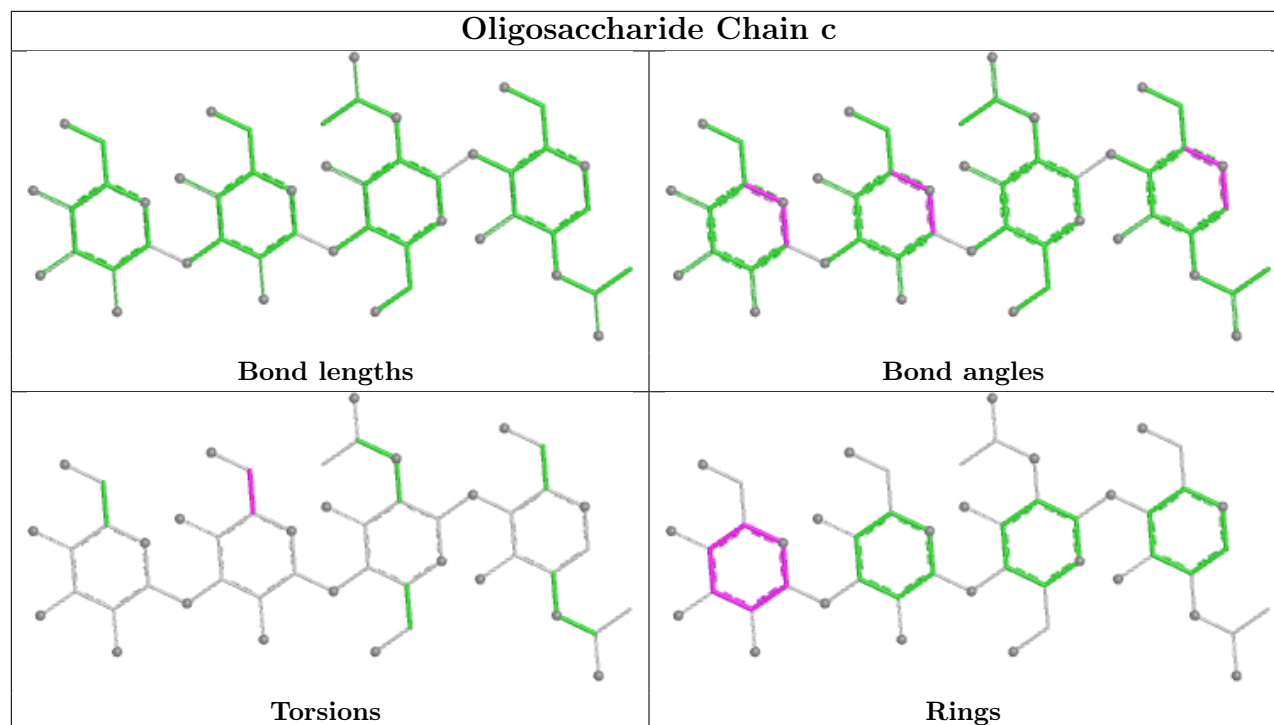
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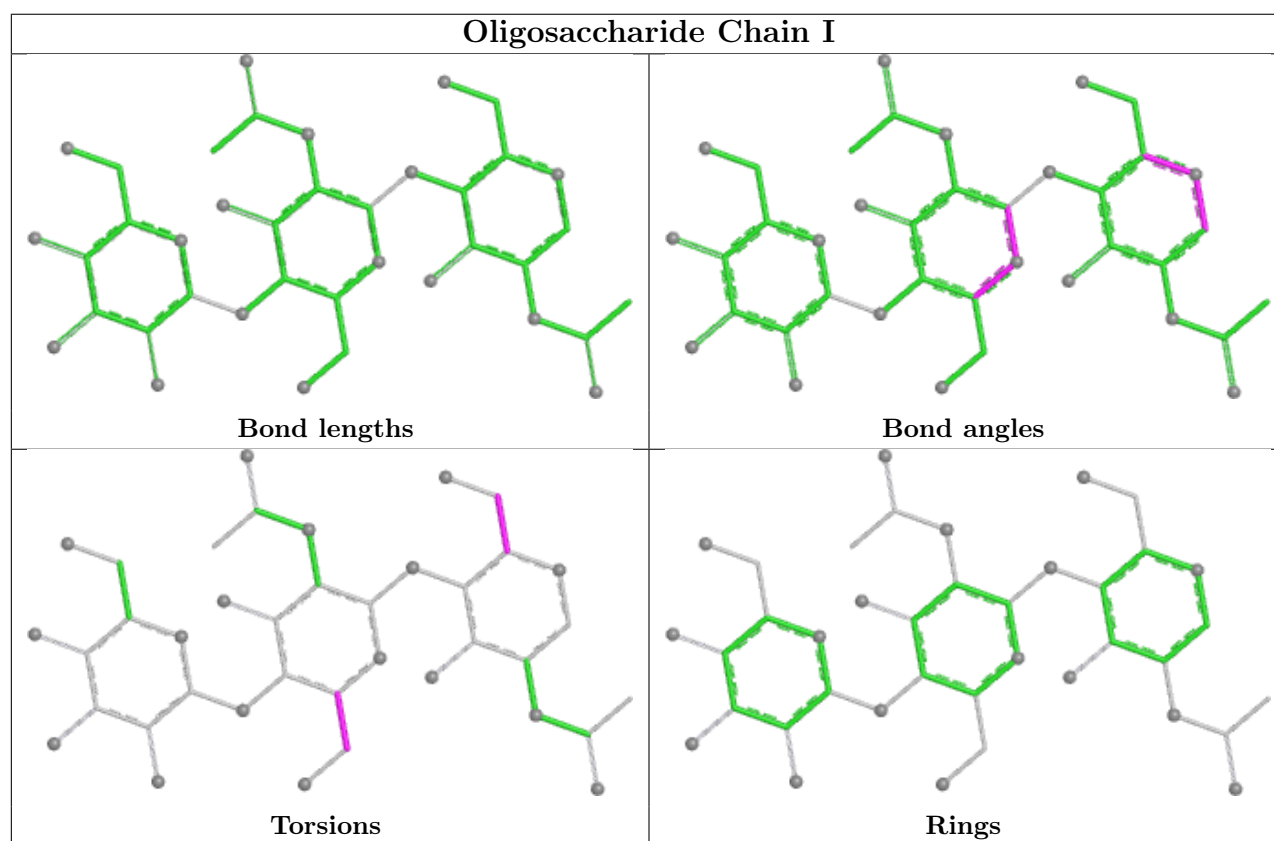
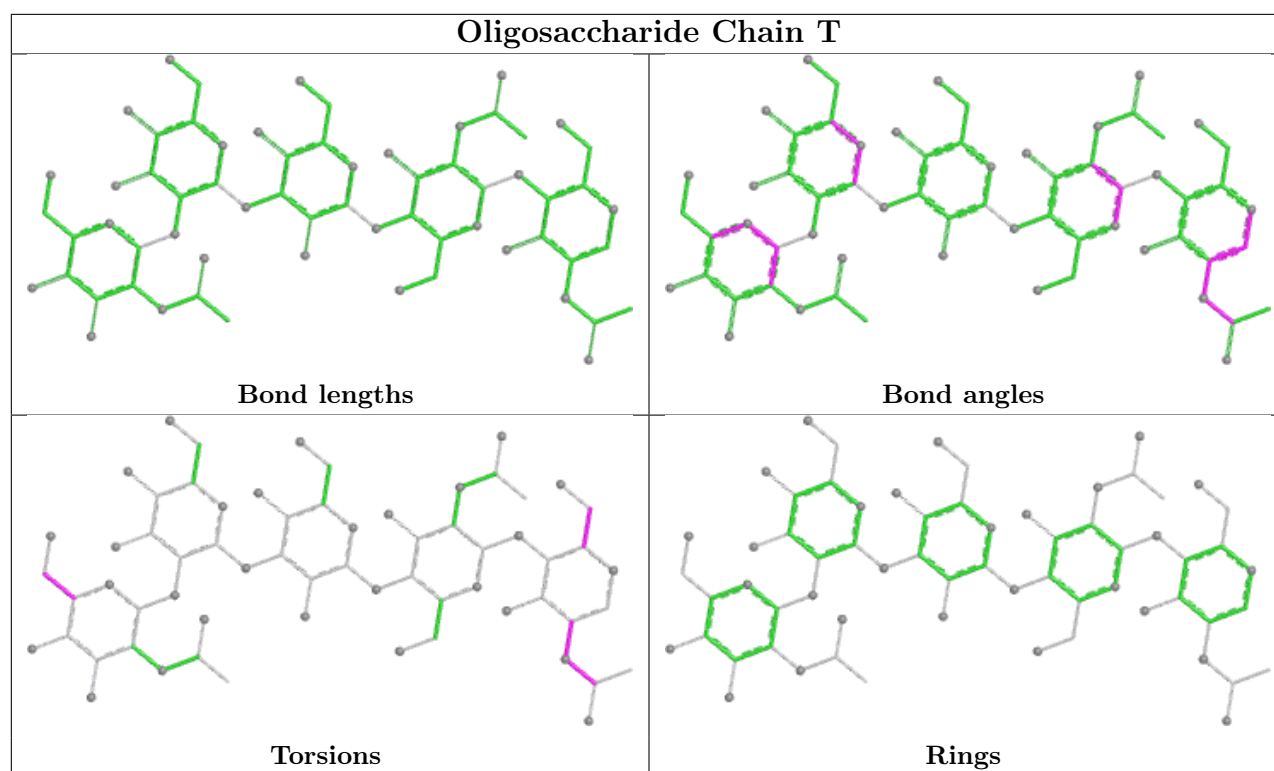
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	3	BMA	1	0
4	N	1	NAG	2	0
6	Y	1	NAG	1	0
4	I	2	NAG	1	0
4	K	1	NAG	2	0

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

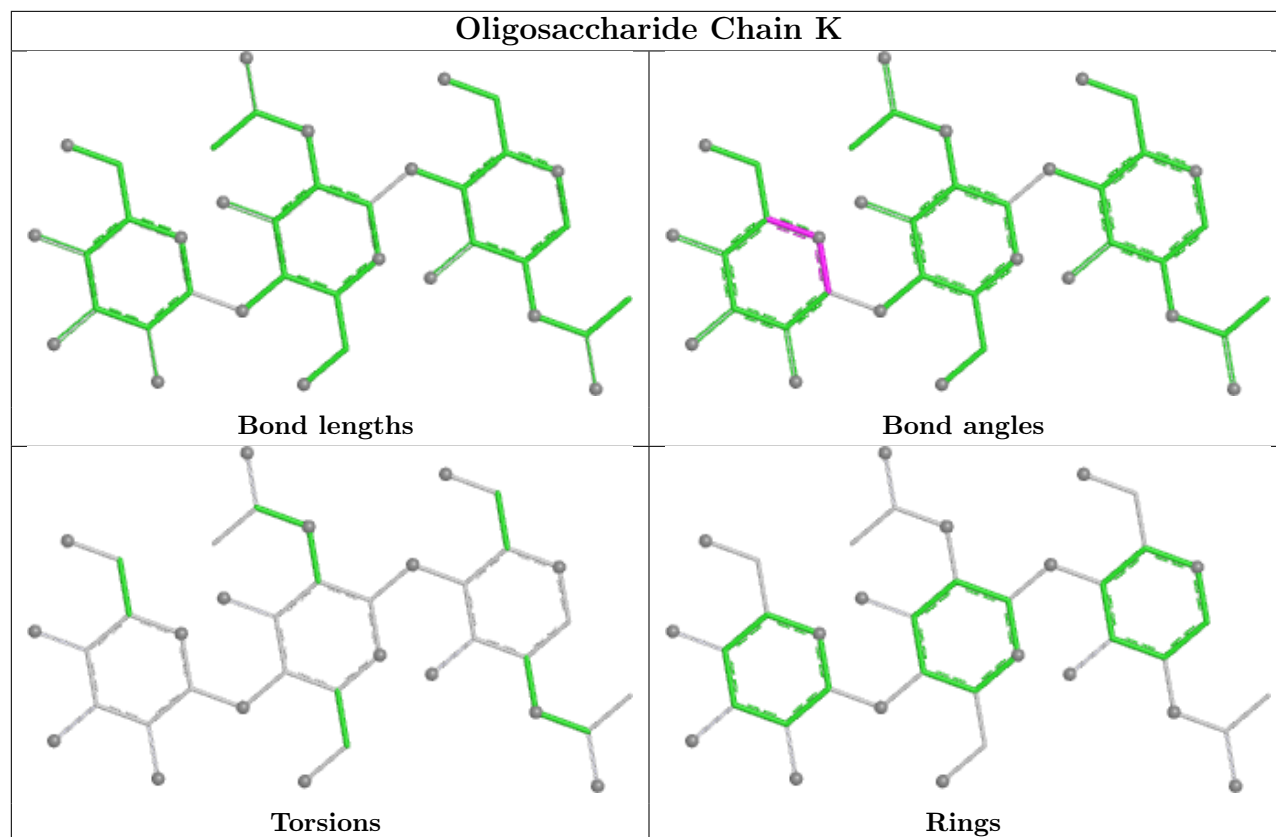




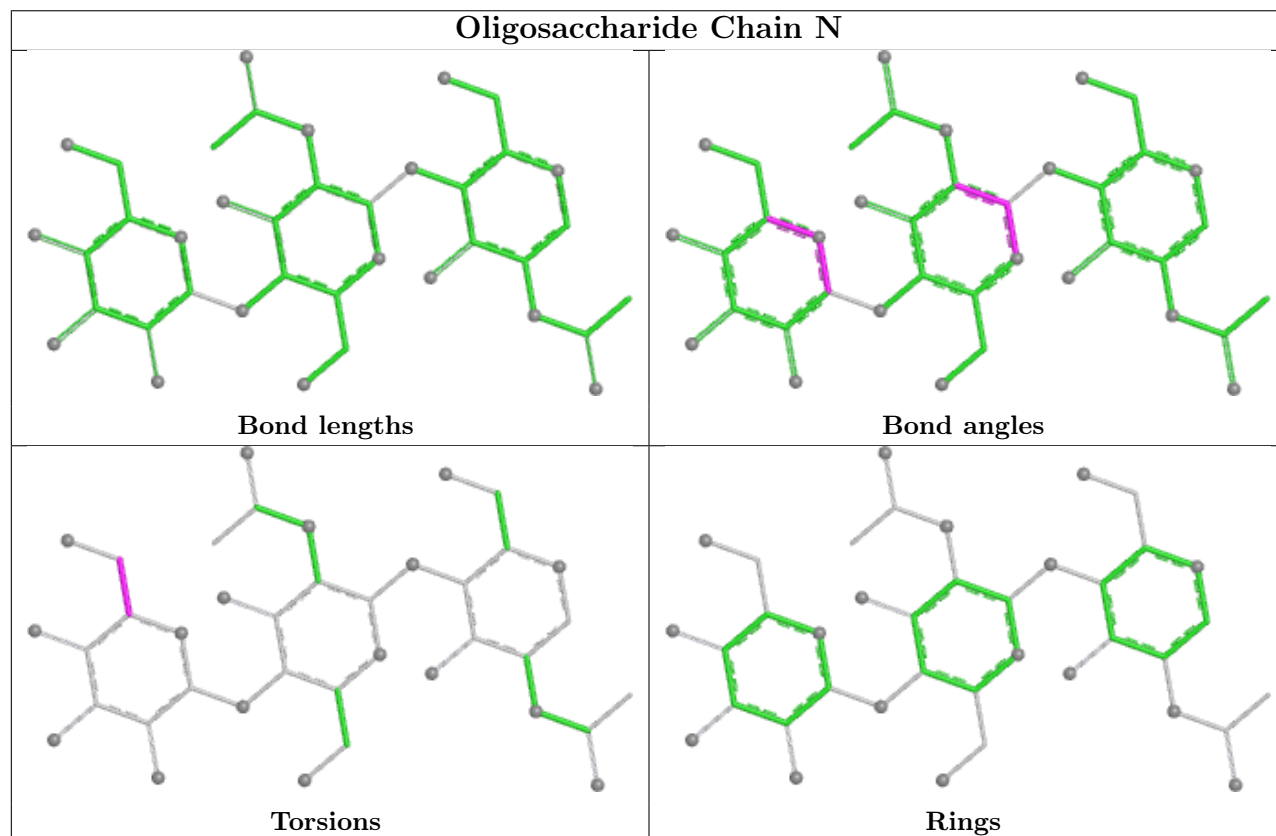


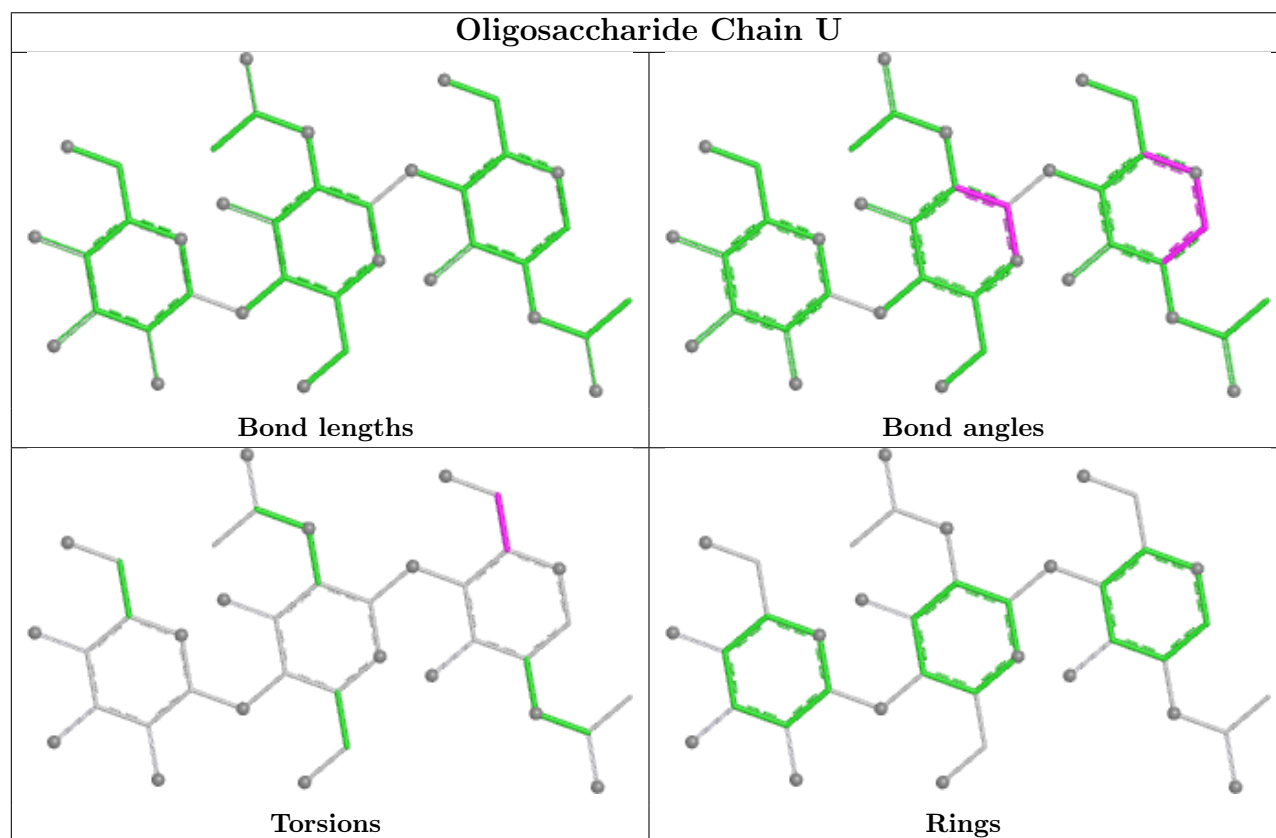
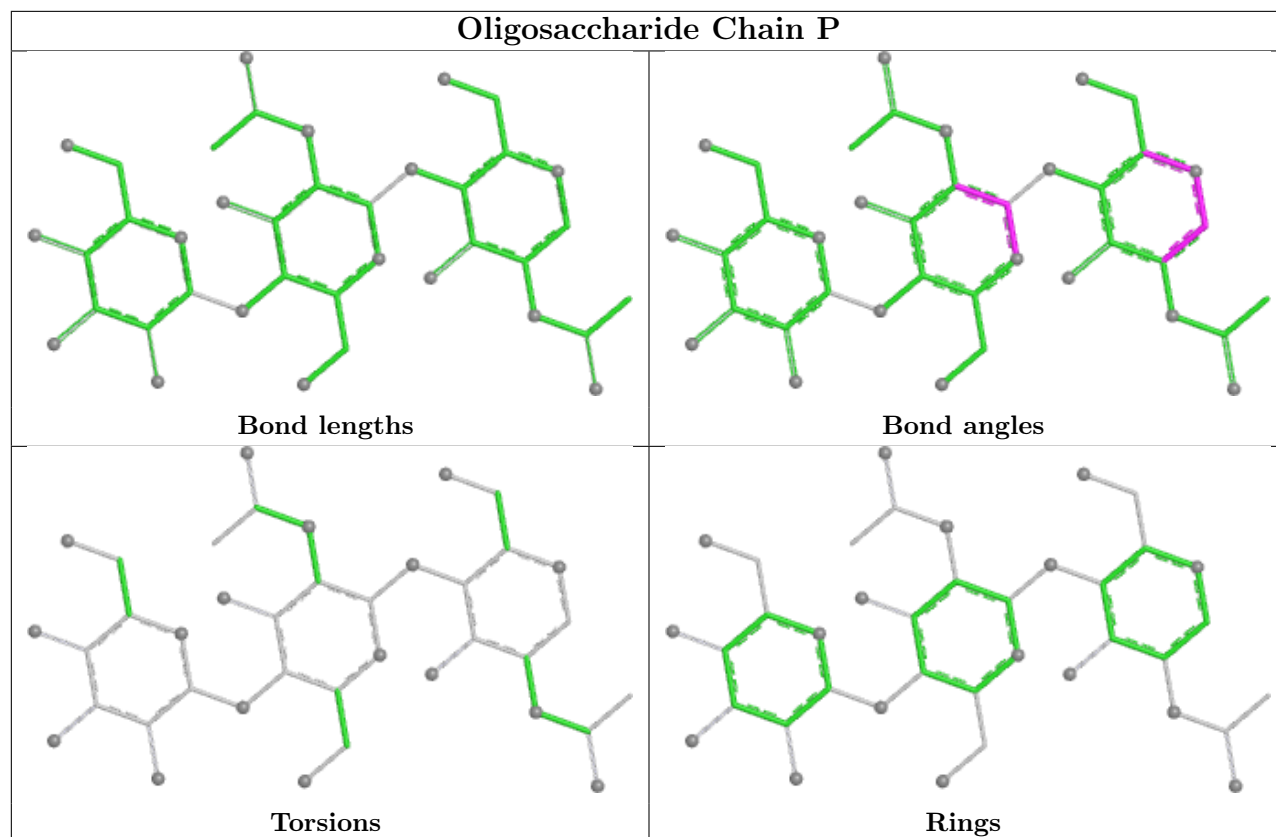


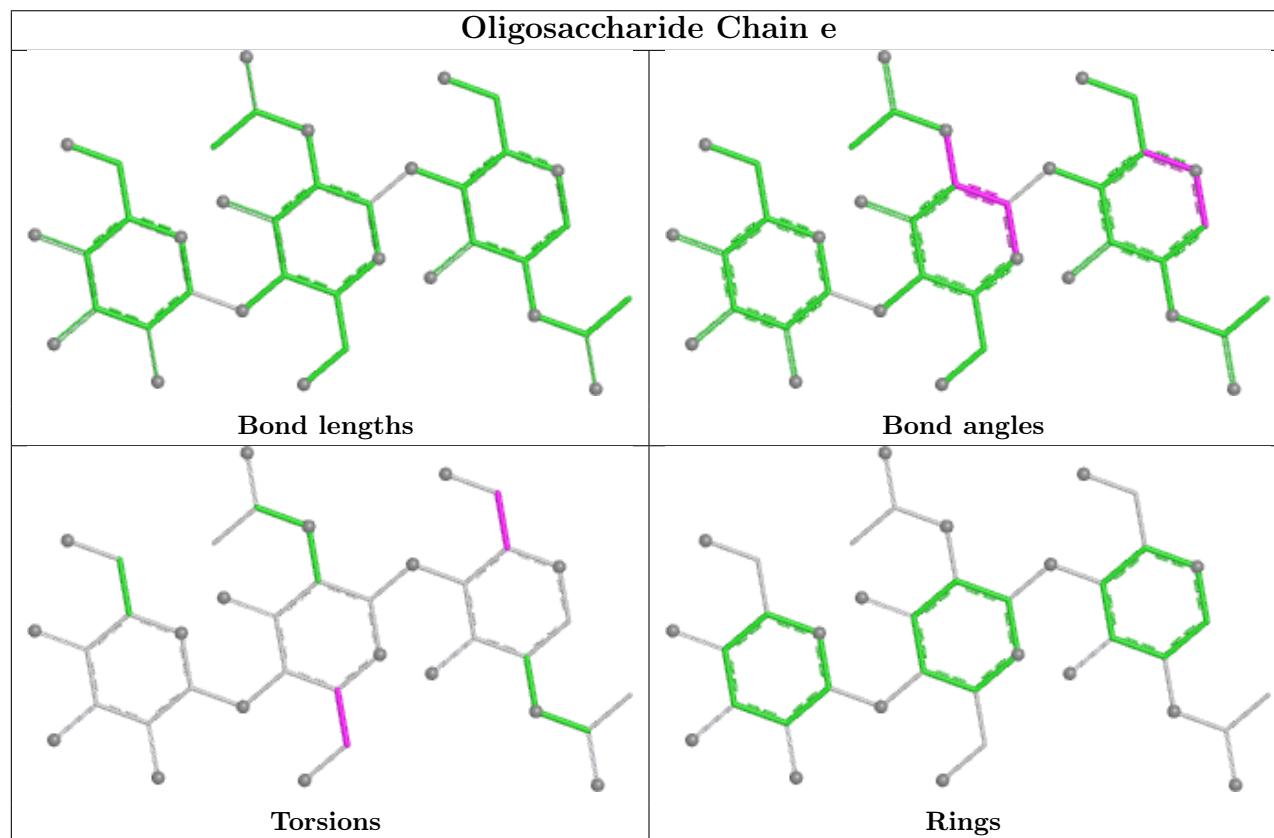
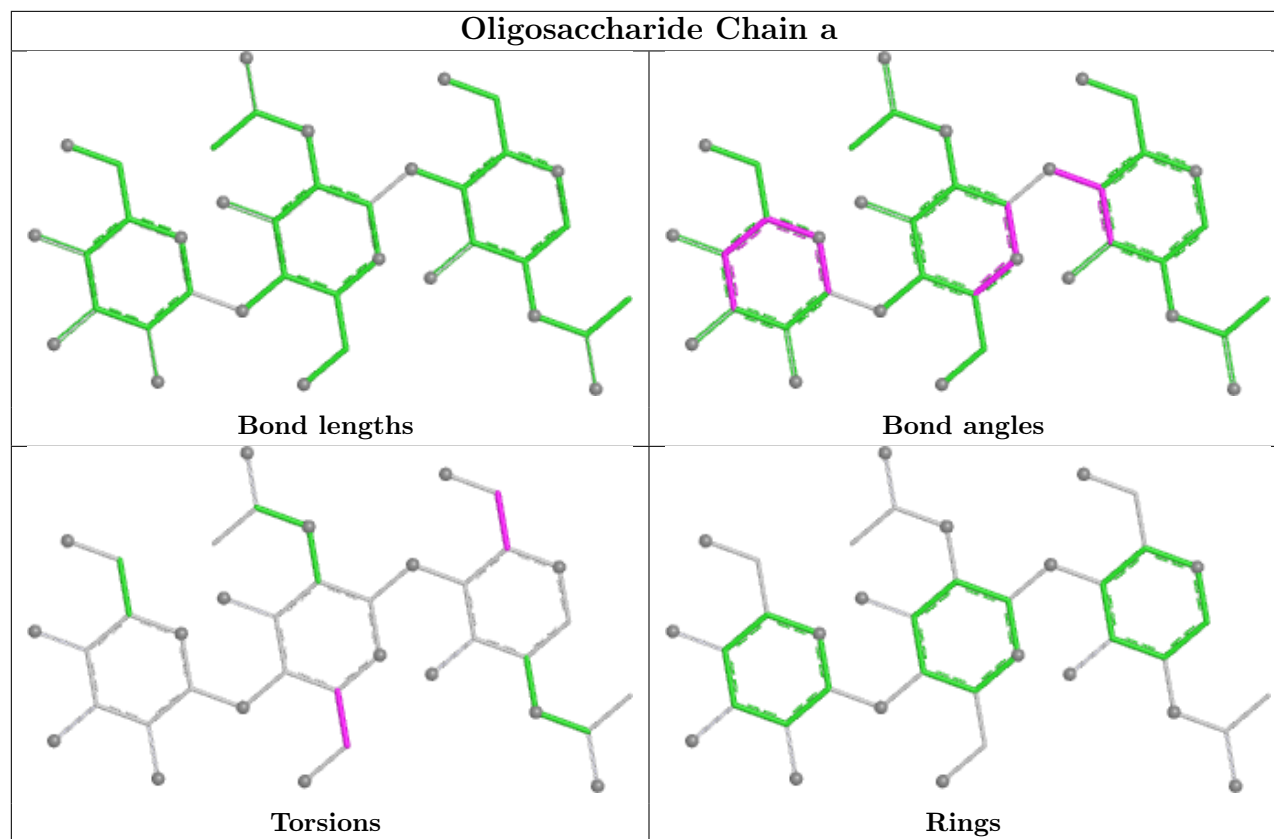
## Oligosaccharide Chain K

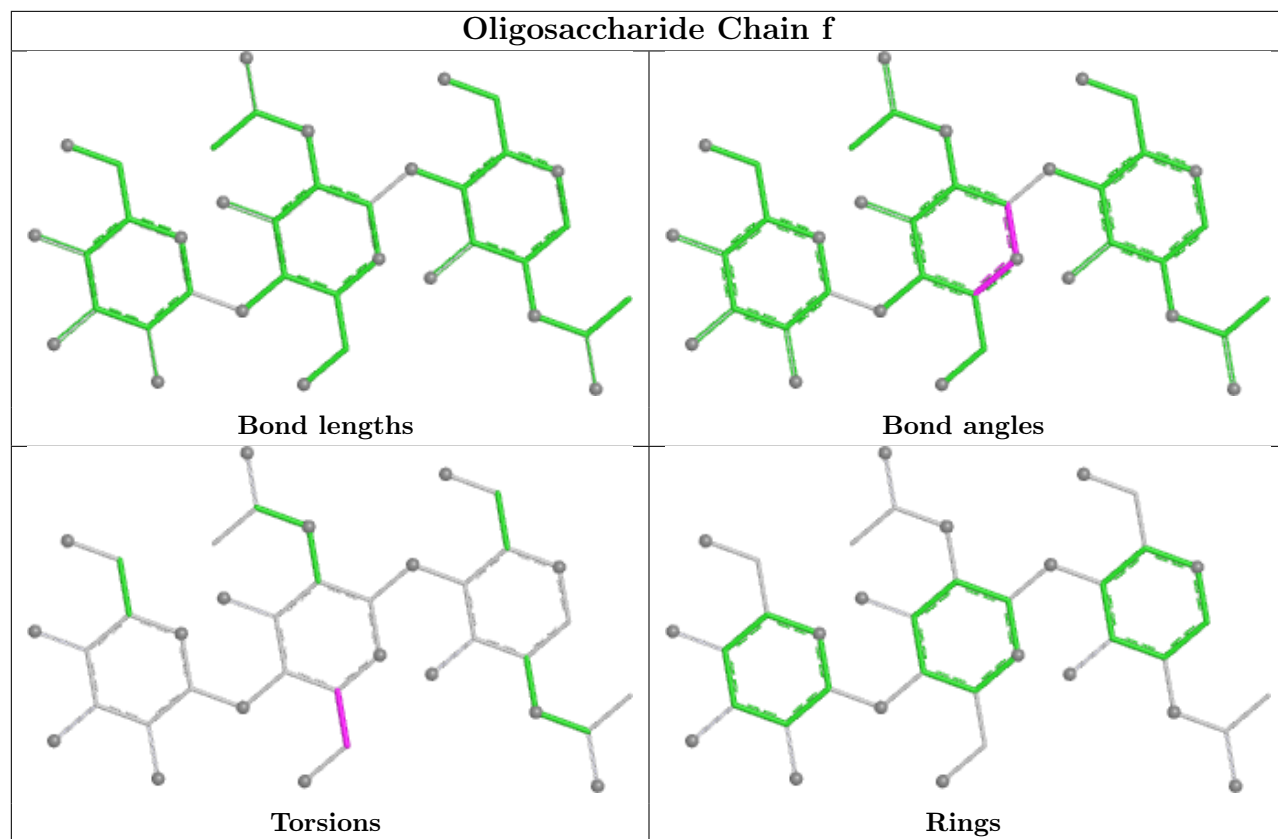


## Oligosaccharide Chain N

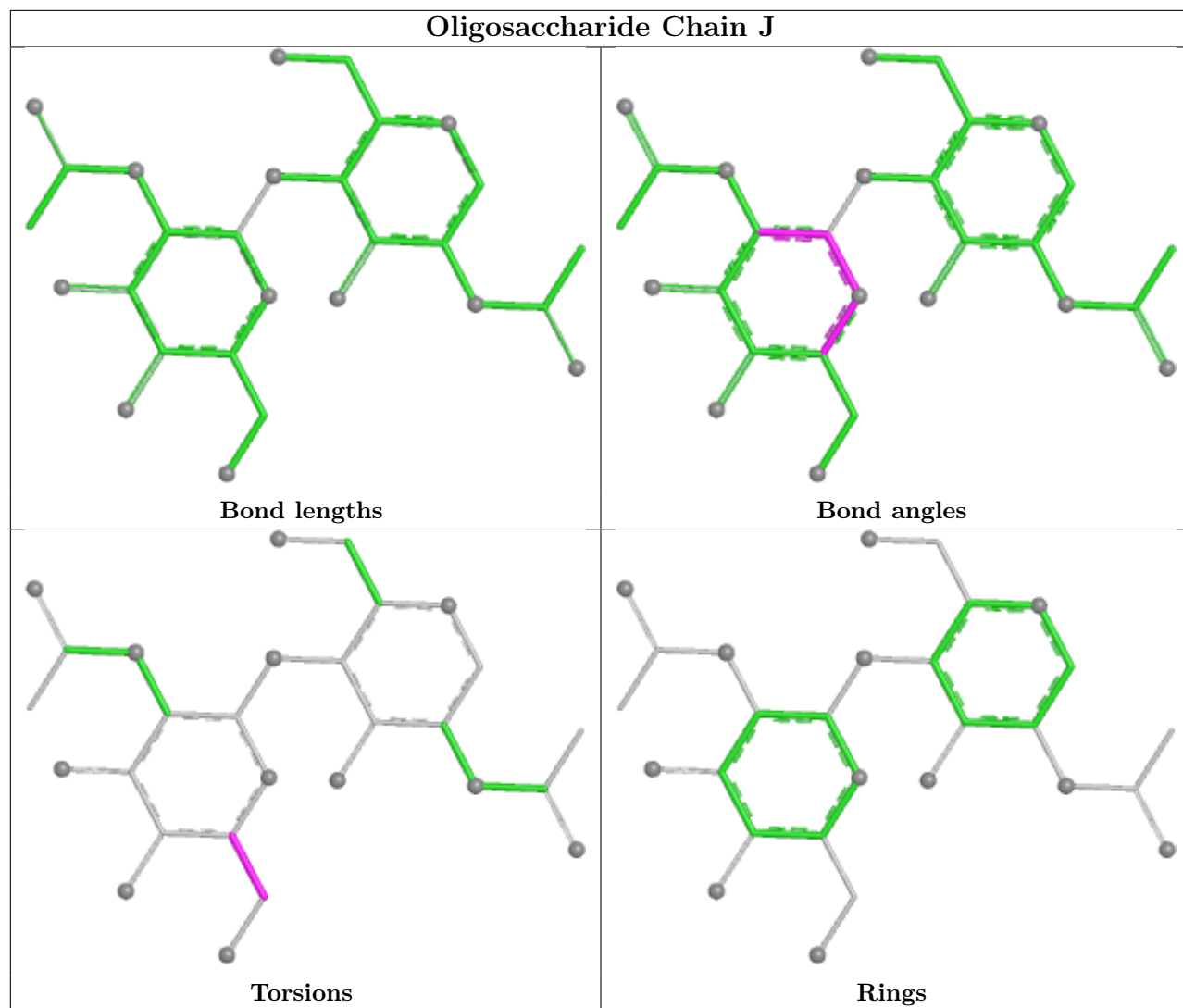


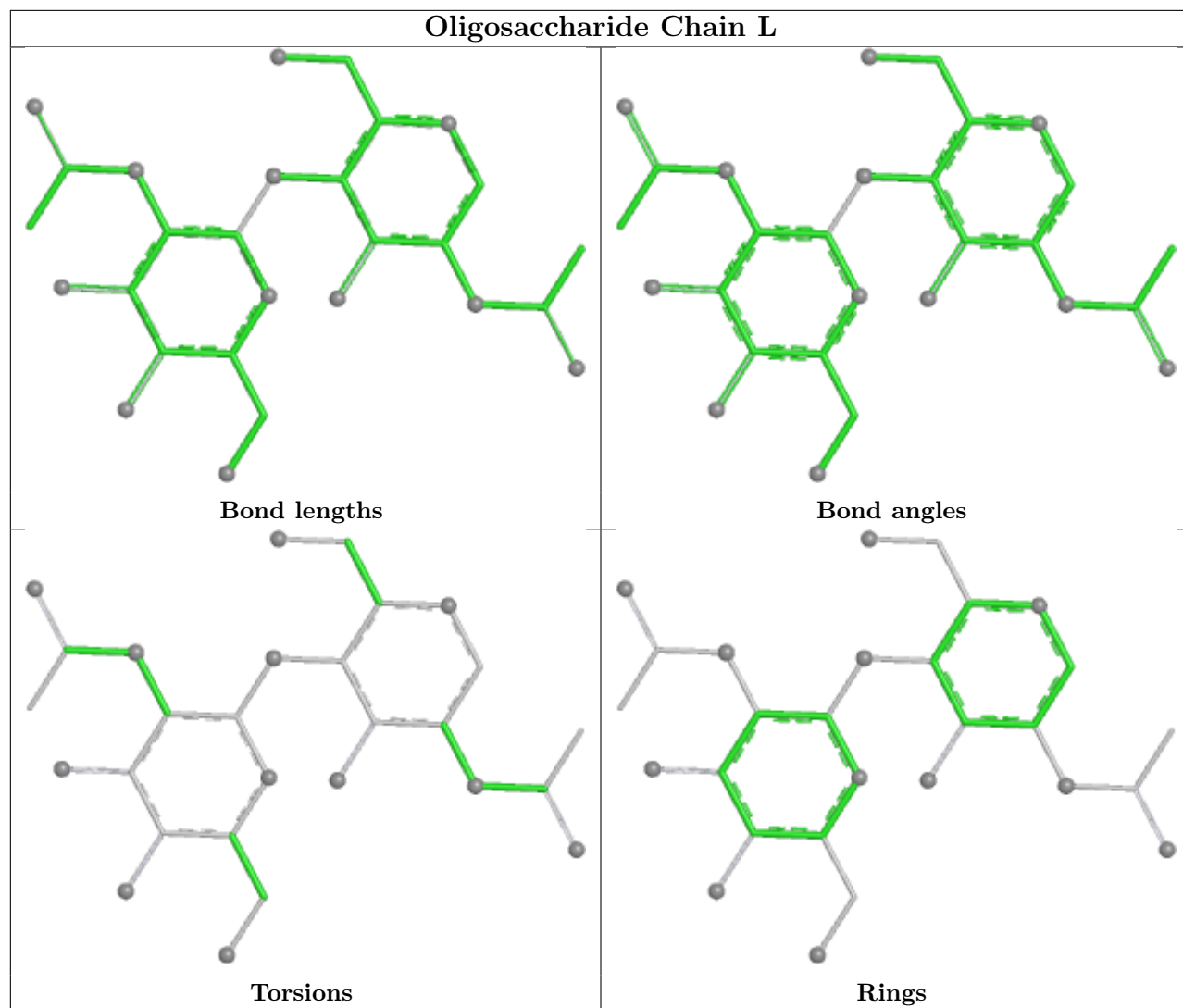


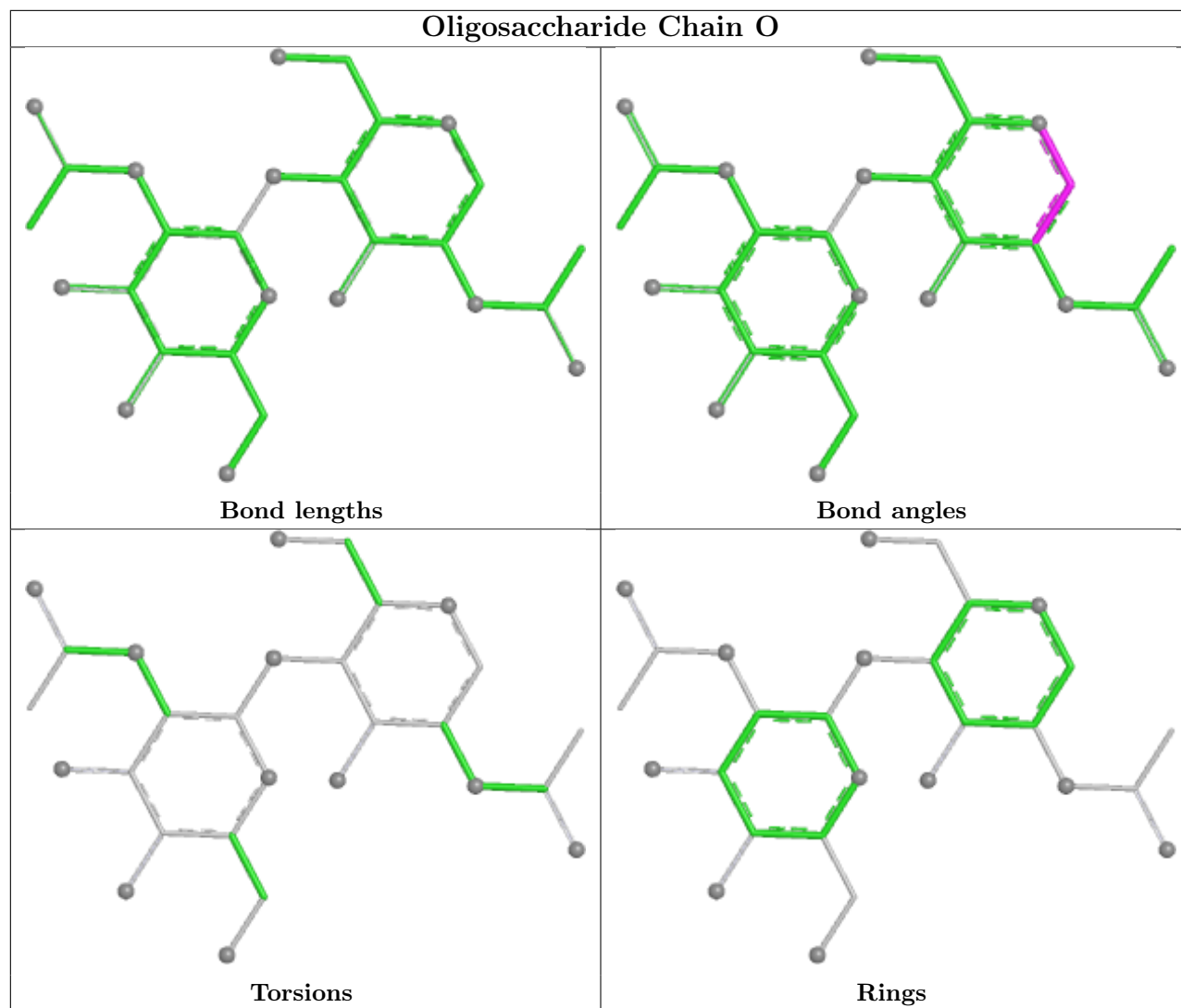


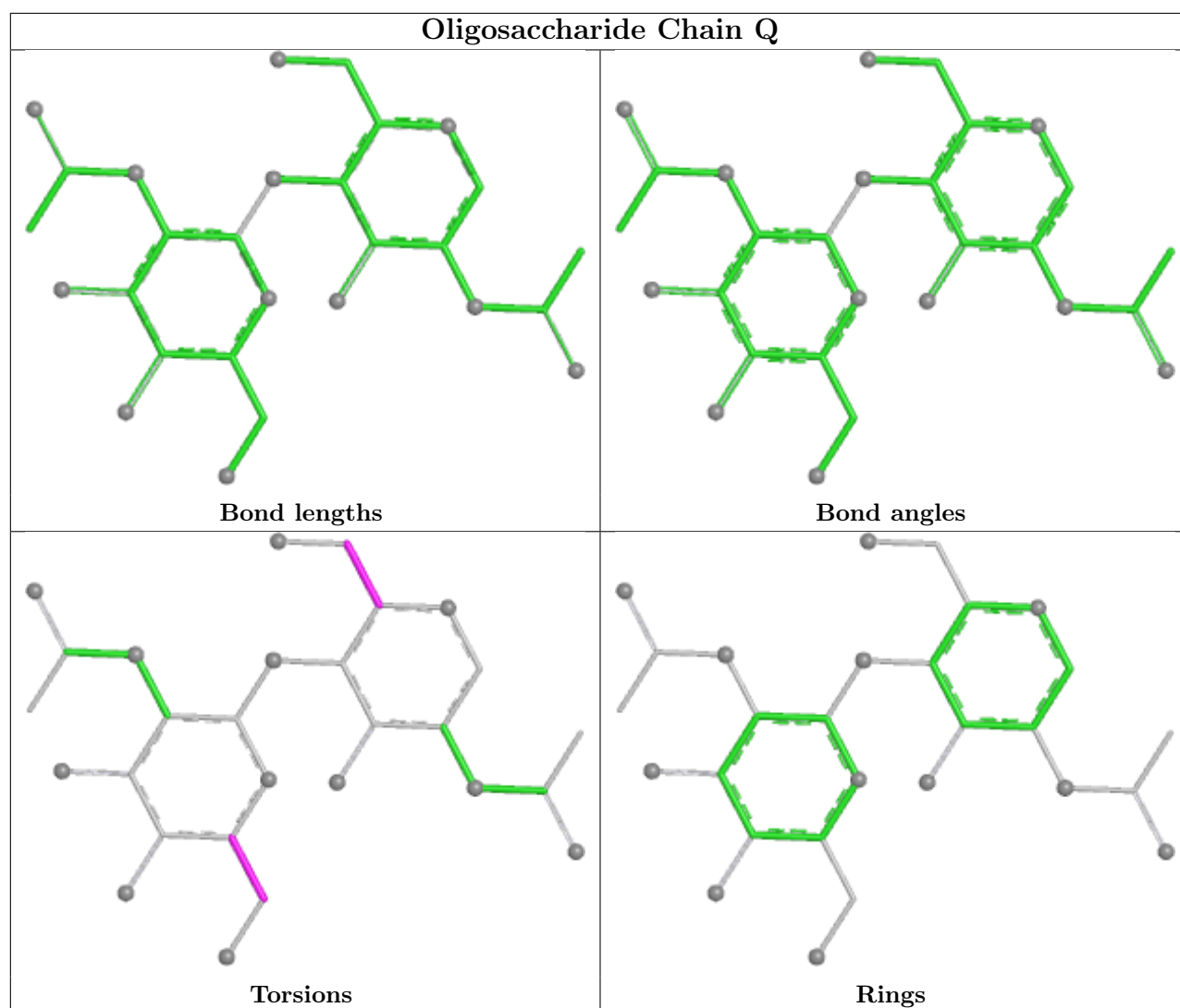


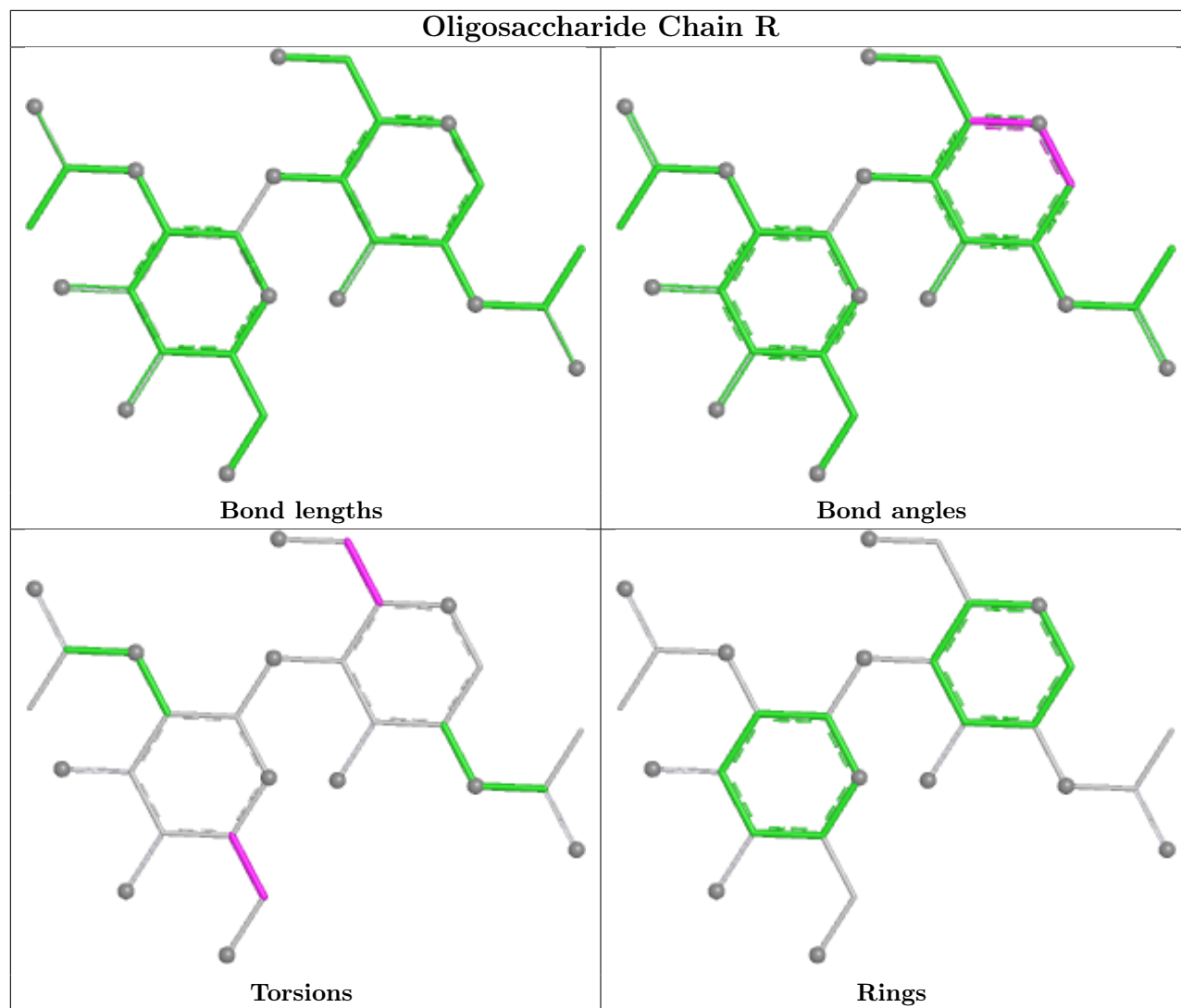


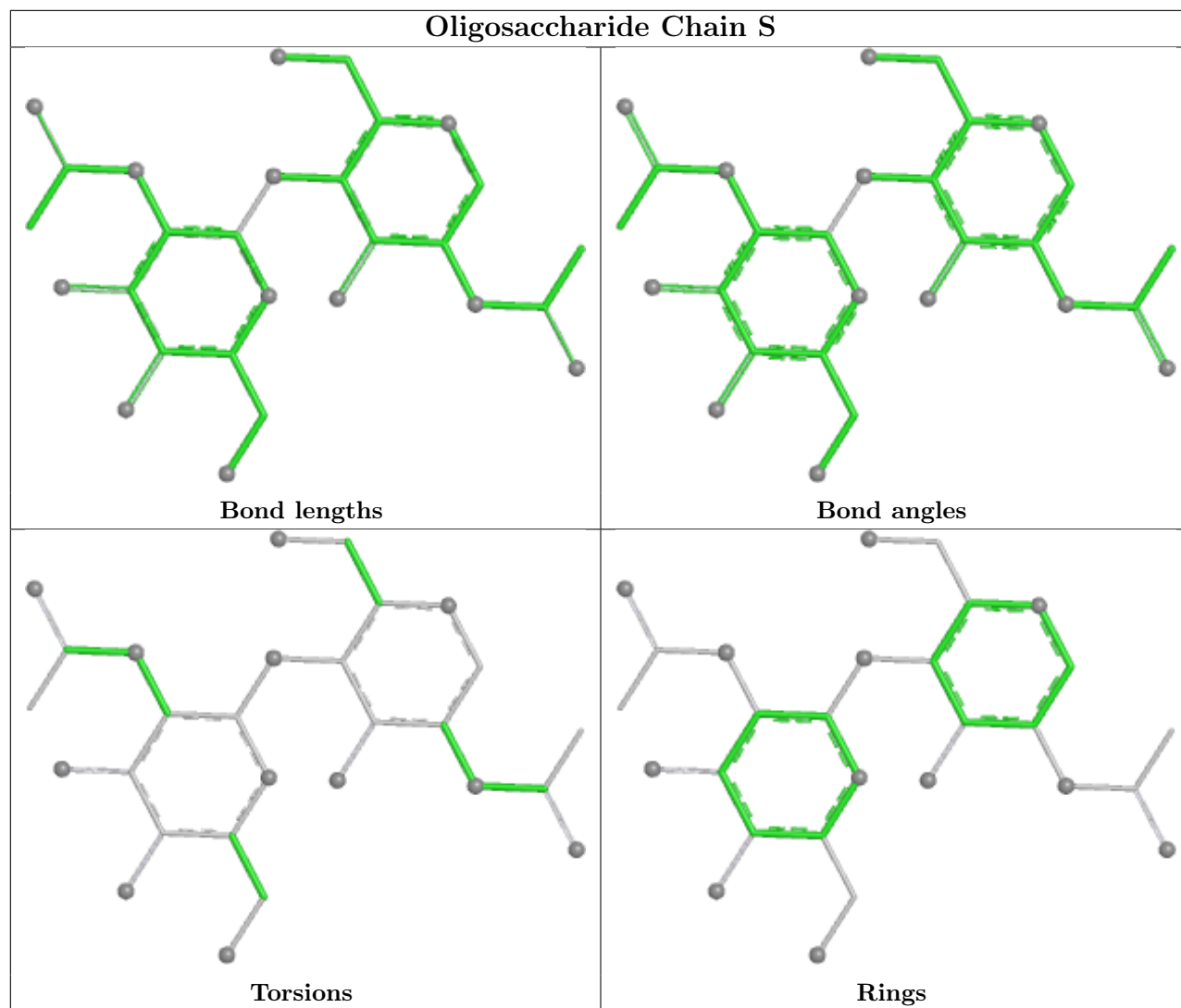


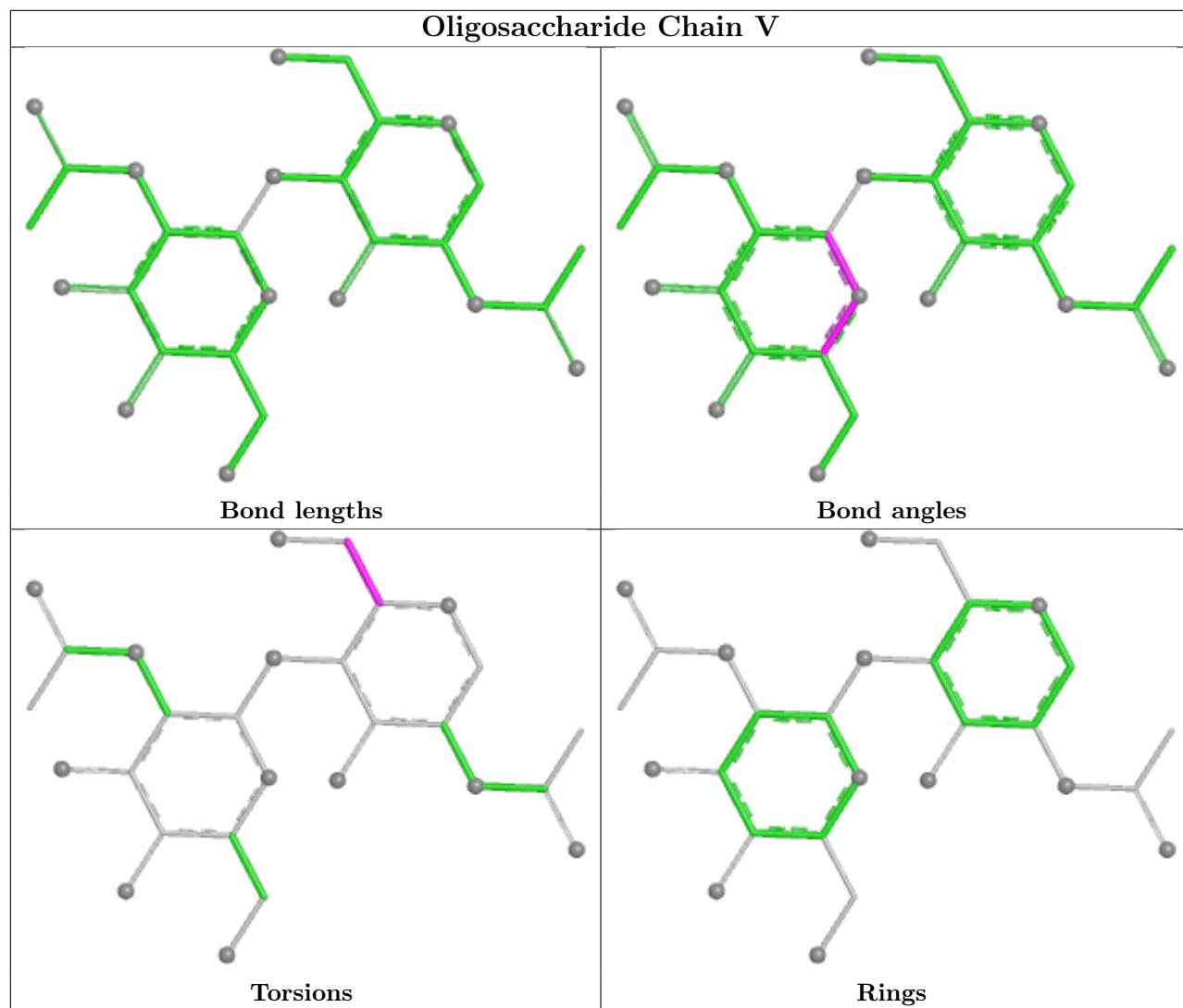


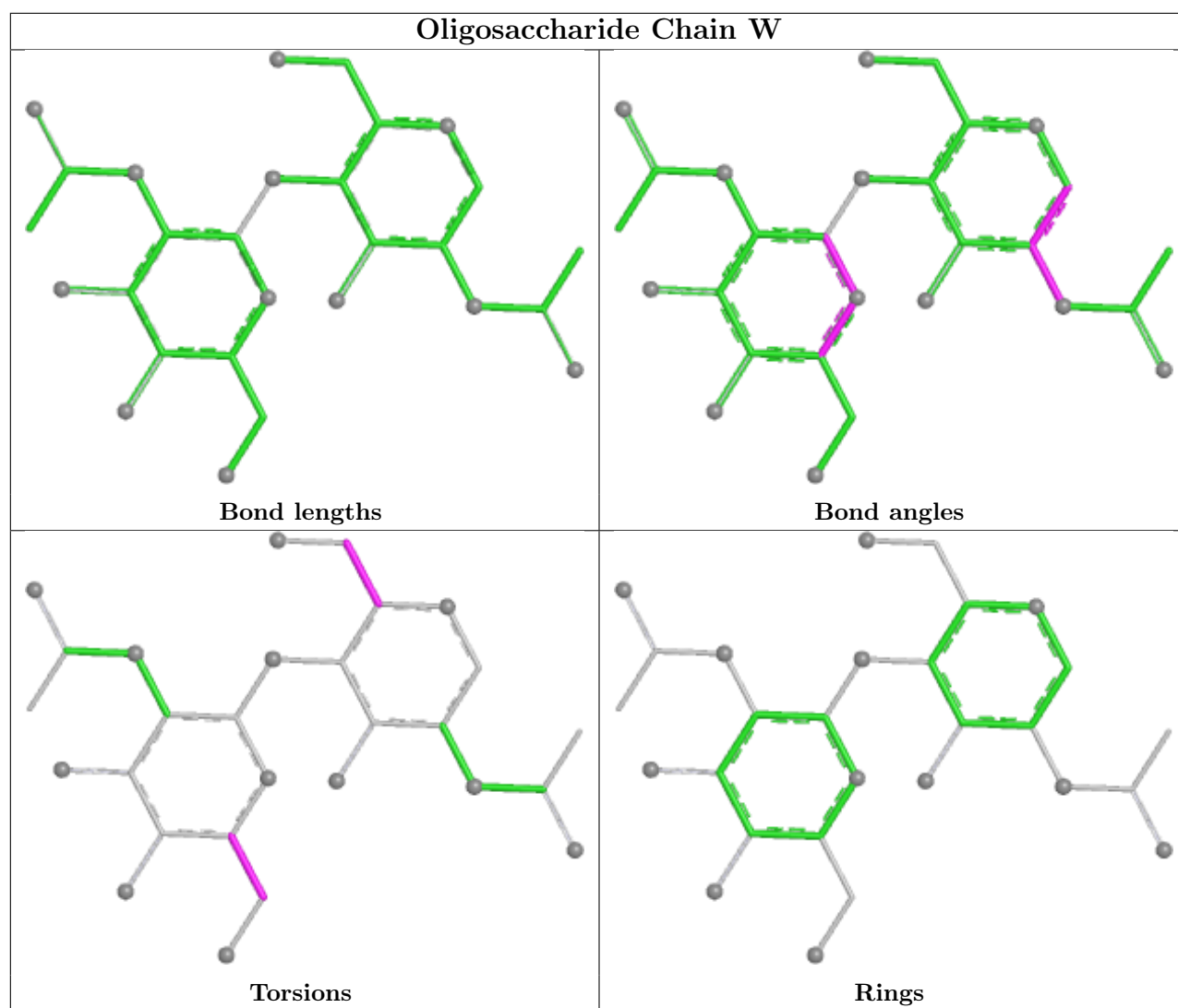




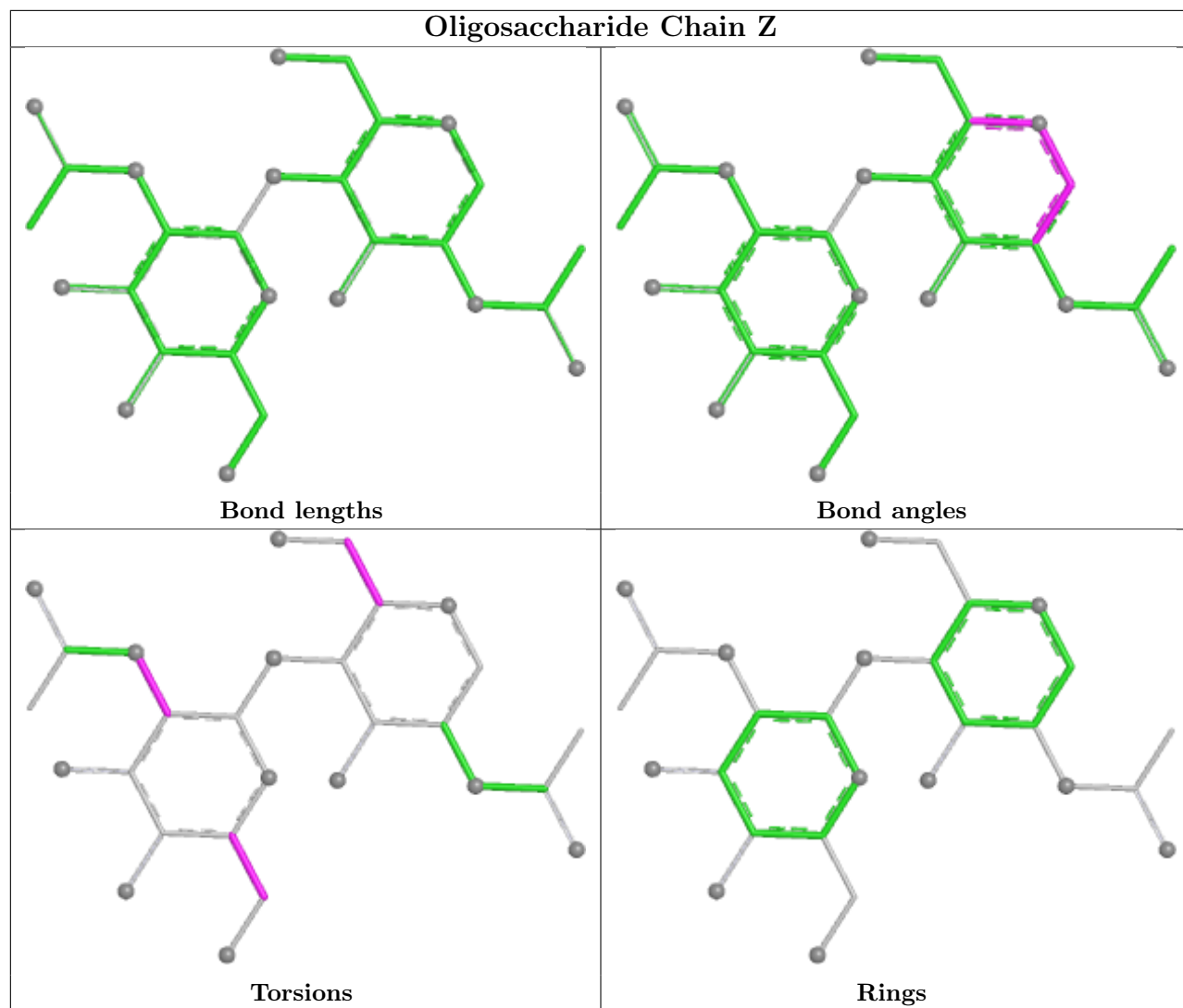


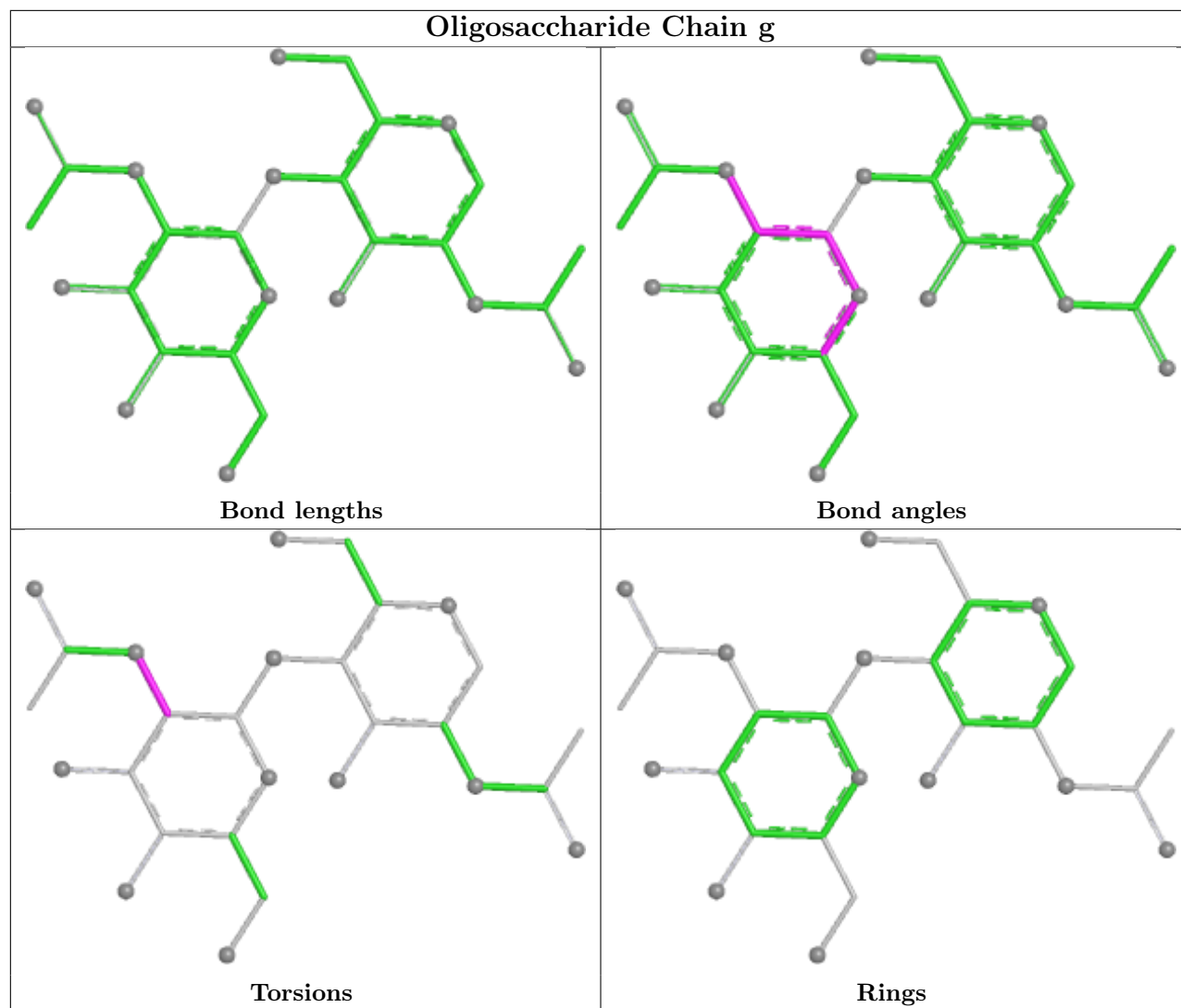


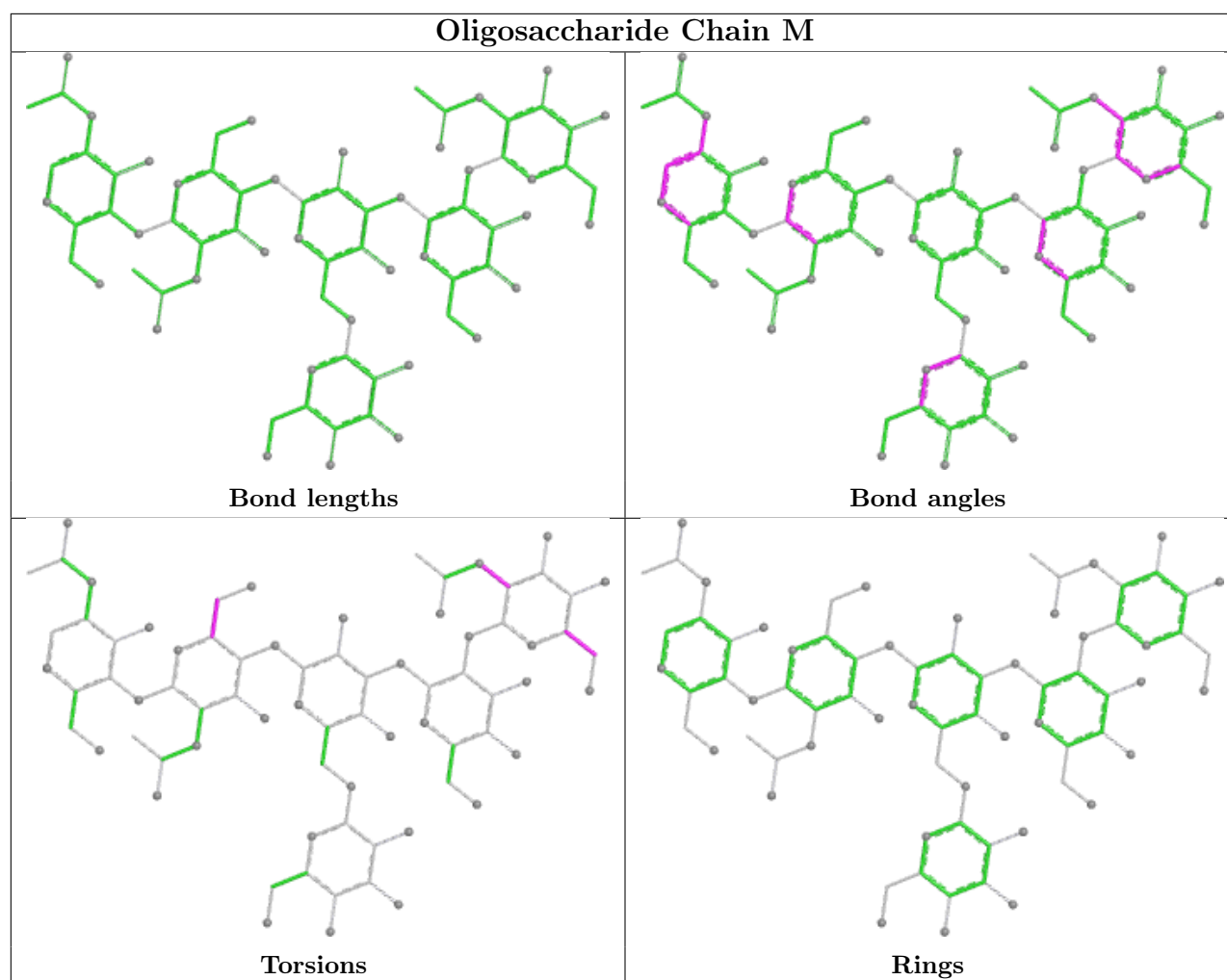


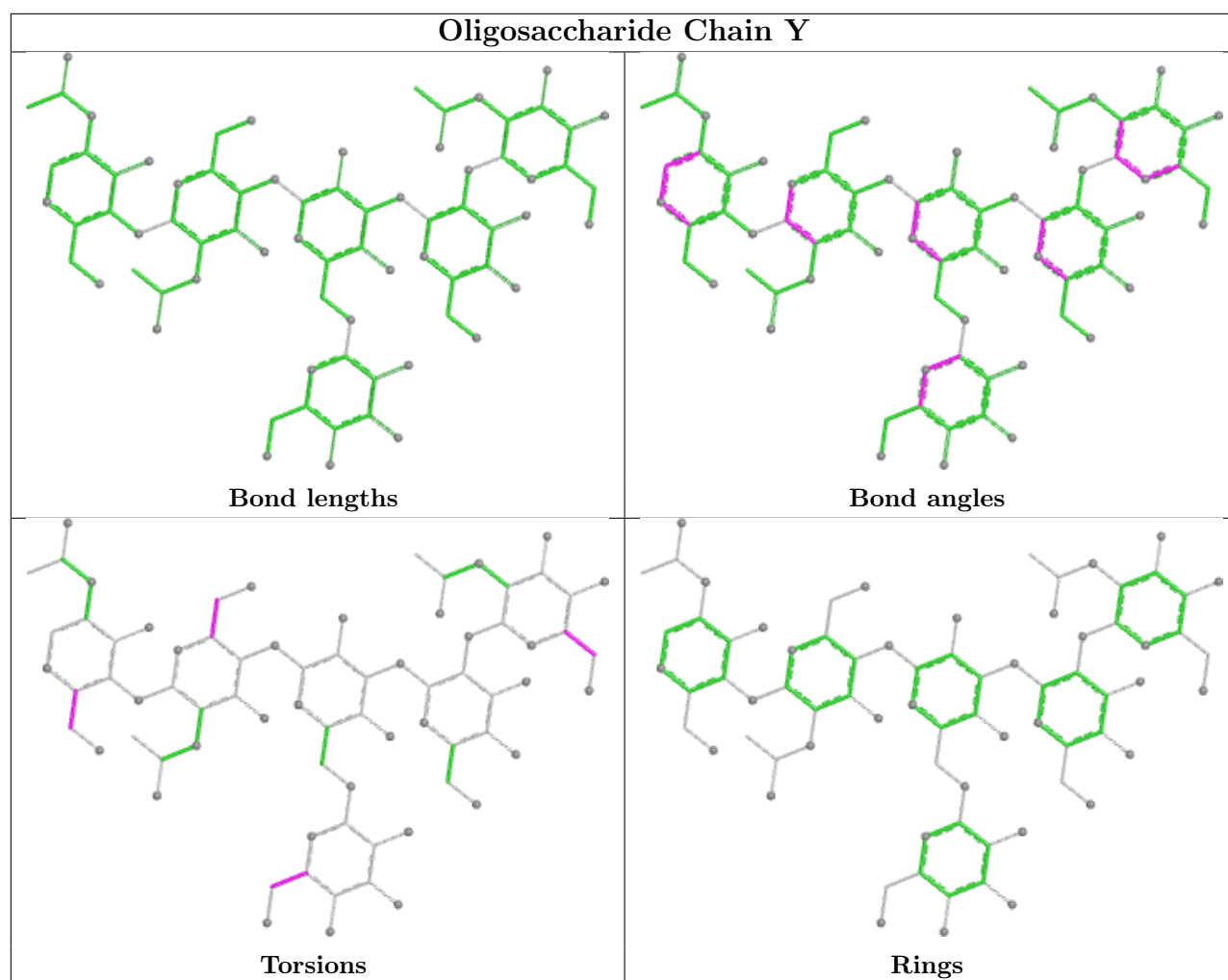


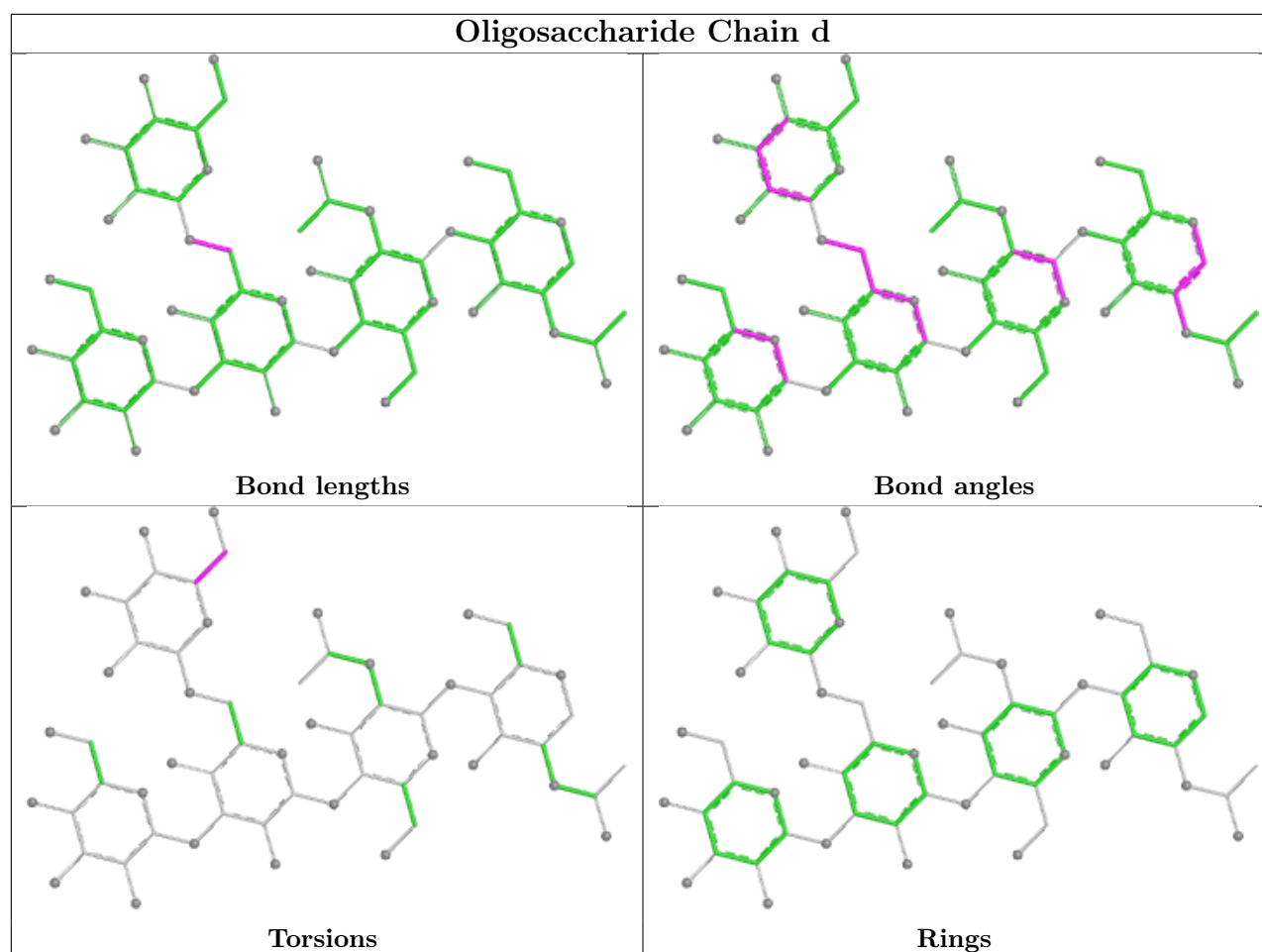












## 5.6 Ligand geometry [i](#)

23 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	$\# Z  > 2$
8	NAG	C	711	1	14,14,15	0.36	0	17,19,21	0.76	0
10	PEG	F	723	-	6,6,6	0.23	0	5,5,5	0.23	0
8	NAG	B	715	1	14,14,15	0.37	0	17,19,21	0.59	0
9	PO4	A	721	-	4,4,4	1.09	0	6,6,6	0.47	0
8	NAG	F	715	1	14,14,15	0.41	0	17,19,21	1.75	4 (23%)
8	NAG	B	709	1	14,14,15	0.37	0	17,19,21	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	PEG	A	722	-	6,6,6	0.35	0	5,5,5	0.20	0
8	NAG	C	708	1	14,14,15	0.31	0	17,19,21	1.32	1 (5%)
8	NAG	A	719	1	14,14,15	0.32	0	17,19,21	0.59	0
8	NAG	A	720	1	14,14,15	0.34	0	17,19,21	2.76	3 (17%)
9	PO4	B	716	-	4,4,4	1.31	1 (25%)	6,6,6	1.06	0
8	NAG	D	715	1	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
9	PO4	F	722	-	4,4,4	1.89	1 (25%)	6,6,6	0.47	0
8	NAG	A	715	1	14,14,15	0.40	0	17,19,21	2.34	2 (11%)
8	NAG	B	711	1	14,14,15	0.38	0	17,19,21	1.50	2 (11%)
8	NAG	F	720	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
9	PO4	C	712	-	4,4,4	1.45	1 (25%)	6,6,6	0.62	0
8	NAG	E	720	1	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
8	NAG	B	710	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
8	NAG	F	721	1	14,14,15	0.35	0	17,19,21	1.62	2 (11%)
8	NAG	F	719	1	14,14,15	0.28	0	17,19,21	0.63	0
9	PO4	D	716	-	4,4,4	1.51	1 (25%)	6,6,6	0.80	0
9	PO4	E	721	-	4,4,4	1.80	1 (25%)	6,6,6	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	709	1	-	0/6/23/26	0/1/1/1
8	NAG	A	720	1	-	2/6/23/26	0/1/1/1
8	NAG	C	711	1	-	0/6/23/26	0/1/1/1
10	PEG	A	722	-	-	3/4/4/4	-
8	NAG	D	715	1	-	0/6/23/26	0/1/1/1
10	PEG	F	723	-	-	2/4/4/4	-
8	NAG	B	715	1	-	1/6/23/26	0/1/1/1
8	NAG	C	708	1	-	1/6/23/26	0/1/1/1
8	NAG	A	719	1	-	1/6/23/26	0/1/1/1
8	NAG	E	720	1	-	1/6/23/26	0/1/1/1
8	NAG	B	710	1	-	2/6/23/26	0/1/1/1
8	NAG	F	721	1	-	1/6/23/26	0/1/1/1
8	NAG	A	715	1	-	2/6/23/26	0/1/1/1
8	NAG	B	711	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	719	1	-	0/6/23/26	0/1/1/1
8	NAG	F	715	1	-	1/6/23/26	0/1/1/1
8	NAG	F	720	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	721	PO4	P-O1	3.31	1.58	1.50
9	F	722	PO4	P-O1	3.22	1.58	1.50
9	D	716	PO4	P-O1	2.45	1.56	1.50
9	C	712	PO4	P-O1	2.35	1.56	1.50
9	B	716	PO4	P-O1	2.11	1.55	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	715	NAG	C1-O5-C5	7.82	122.67	112.19
8	A	720	NAG	C1-C2-N2	7.68	122.53	110.43
8	A	720	NAG	C1-O5-C5	6.57	121.00	112.19
8	A	715	NAG	O5-C1-C2	5.22	119.37	111.29
8	F	715	NAG	C1-C2-N2	5.09	118.46	110.43

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	720	NAG	O5-C5-C6-O6
8	A	715	NAG	O5-C5-C6-O6
8	A	720	NAG	C4-C5-C6-O6
8	F	720	NAG	O5-C5-C6-O6
8	F	720	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	723	PEG	2	0
8	B	709	NAG	1	0
10	A	722	PEG	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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	393/423 (92%)	-0.46	3 (0%) 82 66	41, 69, 107, 127	0
1	B	393/423 (92%)	-0.48	1 (0%) 90 81	46, 75, 107, 146	0
1	C	378/423 (89%)	0.01	8 (2%) 63 41	60, 116, 161, 195	0
1	D	389/423 (91%)	-0.28	4 (1%) 79 60	43, 81, 128, 149	0
1	E	390/423 (92%)	-0.40	2 (0%) 87 75	37, 68, 115, 140	0
1	F	390/423 (92%)	-0.46	1 (0%) 90 81	48, 78, 118, 139	0
All	All	2333/2538 (91%)	-0.35	19 (0%) 82 66	37, 78, 134, 195	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	38	GLU	3.7
1	D	105	ASN	2.9
1	D	218	GLY	2.8
1	C	425	LEU	2.7
1	F	429	ILE	2.7

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

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

### 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	F	719	14/15	0.55	0.13	152,161,166,167	0
8	NAG	D	715	14/15	0.67	0.18	149,156,161,162	0
8	NAG	B	715	14/15	0.67	0.17	120,130,144,146	0
8	NAG	A	715	14/15	0.71	0.14	126,136,143,146	0
8	NAG	F	715	14/15	0.72	0.13	139,155,159,161	0
8	NAG	A	719	14/15	0.74	0.11	100,106,113,113	0
8	NAG	F	721	14/15	0.74	0.12	109,114,118,118	0
8	NAG	C	708	14/15	0.76	0.14	162,164,167,168	0
8	NAG	B	711	14/15	0.77	0.14	97,111,121,125	0
8	NAG	C	711	14/15	0.77	0.14	131,141,147,149	0
8	NAG	F	720	14/15	0.81	0.12	157,164,167,167	0
8	NAG	A	720	14/15	0.84	0.11	89,104,113,114	0
10	PEG	F	723	7/7	0.84	0.50	40,43,45,45	7
10	PEG	A	722	7/7	0.88	0.33	30,33,37,38	7
8	NAG	E	720	14/15	0.88	0.10	123,129,136,139	0
9	PO4	D	716	5/5	0.91	0.19	55,58,60,60	5
8	NAG	B	710	14/15	0.91	0.09	76,93,98,100	0
8	NAG	B	709	14/15	0.91	0.10	83,89,91,93	0
9	PO4	E	721	5/5	0.92	0.14	92,95,99,100	0
9	PO4	B	716	5/5	0.95	0.12	93,93,95,95	0
9	PO4	C	712	5/5	0.95	0.09	92,95,99,101	0
9	PO4	A	721	5/5	0.96	0.17	37,38,39,41	5
9	PO4	F	722	5/5	0.97	0.07	82,84,86,88	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.