



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:51 AM UTC

PDB ID : 5D9Q / pdb_00005d9q
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122 and scFv NIH45-46
Authors : Julien, J.-P.; Stanfield, R.L.; Ward, A.B.; Wilson, I.A.
Deposited on : 2015-08-18
Resolution : 4.40 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

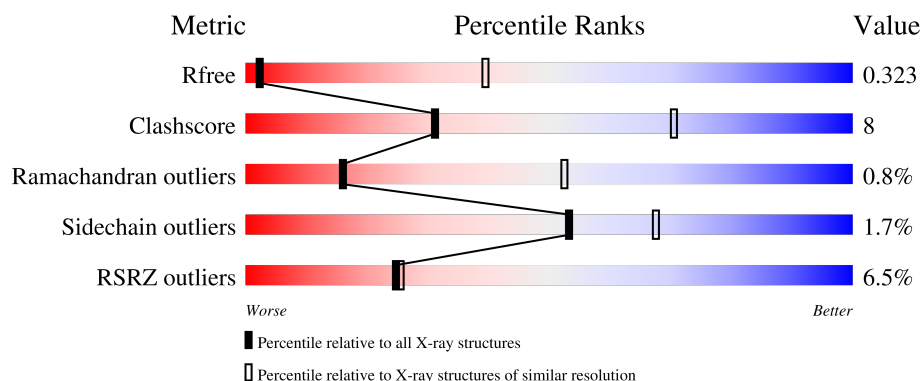
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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 ≥ 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	472	7% 67% 26% • 5%
1	G	472	7% 69% 25% • 5%
1	J	472	4% 66% 28% • 5%
2	B	152	7% 59% 18% • 20%
2	C	152	9% 55% 22% • 20%

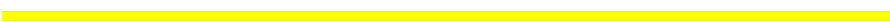
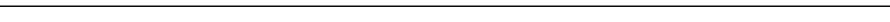
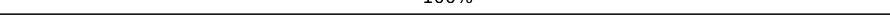
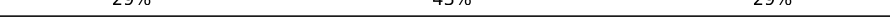
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Mol	Chain	Length	Quality of chain
2	K	152	
3	E	211	
3	L	211	
3	M	211	
4	F	235	
4	H	235	
4	N	235	
5	D	241	
5	I	241	
5	O	241	
6	P	5	
6	R	5	
6	V	5	
6	d	5	
6	f	5	
6	j	5	
6	r	5	
6	t	5	
6	x	5	
7	Q	4	
7	e	4	
7	s	4	
8	1	2	
8	2	2	
8	3	2	

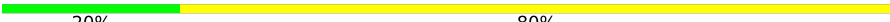
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Mol	Chain	Length	Quality of chain
8	4	2	 50% 50%
8	S	2	 50% 50%
8	W	2	 100%
8	Z	2	 100%
8	a	2	 100%
8	b	2	 50% 50%
8	c	2	 50% 50%
8	g	2	 50% 50%
8	k	2	 100%
8	n	2	 100%
8	o	2	 100%
8	p	2	 100%
8	q	2	 50% 50%
8	u	2	 50% 50%
8	y	2	 100%
9	T	7	 29% 43% 29%
9	X	7	 29% 71%
9	h	7	 29% 71%
9	l	7	 29% 71%
9	v	7	 29% 57% 14%
9	z	7	 29% 71%
10	U	11	 18% 82%
10	i	11	 9% 91%
10	w	11	 18% 82%
11	0	10	 20% 80%

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Mol	Chain	Length	Quality of chain
11	Y	10	 20%80%
11	m	10	 10%90%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31374 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	A	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	J	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	460	ALA	SER	conflict	UNP Q2N0S6
G	461	ASN	THR	conflict	UNP Q2N0S6
G	463	THR	SER	conflict	UNP Q2N0S6
G	464	SER	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	460	ALA	SER	conflict	UNP Q2N0S6
A	461	ASN	THR	conflict	UNP Q2N0S6
A	463	THR	SER	conflict	UNP Q2N0S6
A	464	SER	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
J	332	ASN	THR	conflict	UNP Q2N0S6
J	460	ALA	SER	conflict	UNP Q2N0S6
J	461	ASN	THR	conflict	UNP Q2N0S6
J	463	THR	SER	conflict	UNP Q2N0S6
J	464	SER	THR	conflict	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	C	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	K	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
C	559	PRO	ILE	conflict	UNP Q2N0S9
C	605	CYS	THR	conflict	UNP Q2N0S9
K	559	PRO	ILE	conflict	UNP Q2N0S9
K	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called PGT122 light chain,Ig lambda-3 chain C regions.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	E	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	M	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	156	VAL	ALA	conflict	UNP P0CG06
E	156	VAL	ALA	conflict	UNP P0CG06
M	156	VAL	ALA	conflict	UNP P0CG06

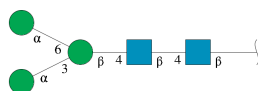
- Molecule 4 is a protein called PGT122 heavy chain,IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	F	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	N	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			

- Molecule 5 is a protein called NIH45-46 single chain Fv.

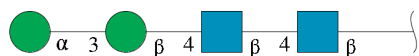
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	I	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	O	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			

- Molecule 6 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
6	P	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	R	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	V	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	j	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	r	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	t	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	x	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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
7	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	e	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	s	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



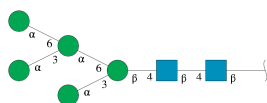
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	k	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	n	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	o	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	p	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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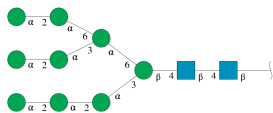
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	u	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	y	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	1	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	2	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	3	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	4	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



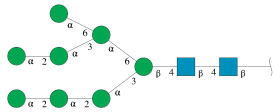
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	X	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	h	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	l	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	v	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	z	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



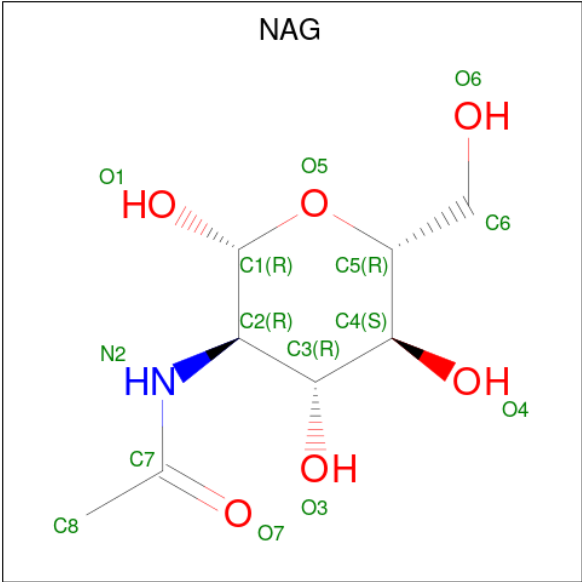
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	U	11	Total	C	N	O	0	0	0
			127	70	2	55			
10	i	11	Total	C	N	O	0	0	0
			127	70	2	55			
10	w	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Y	10	Total	C	N	O	0	0	0
			116	64	2	50			
11	m	10	Total	C	N	O	0	0	0
			116	64	2	50			
11	0	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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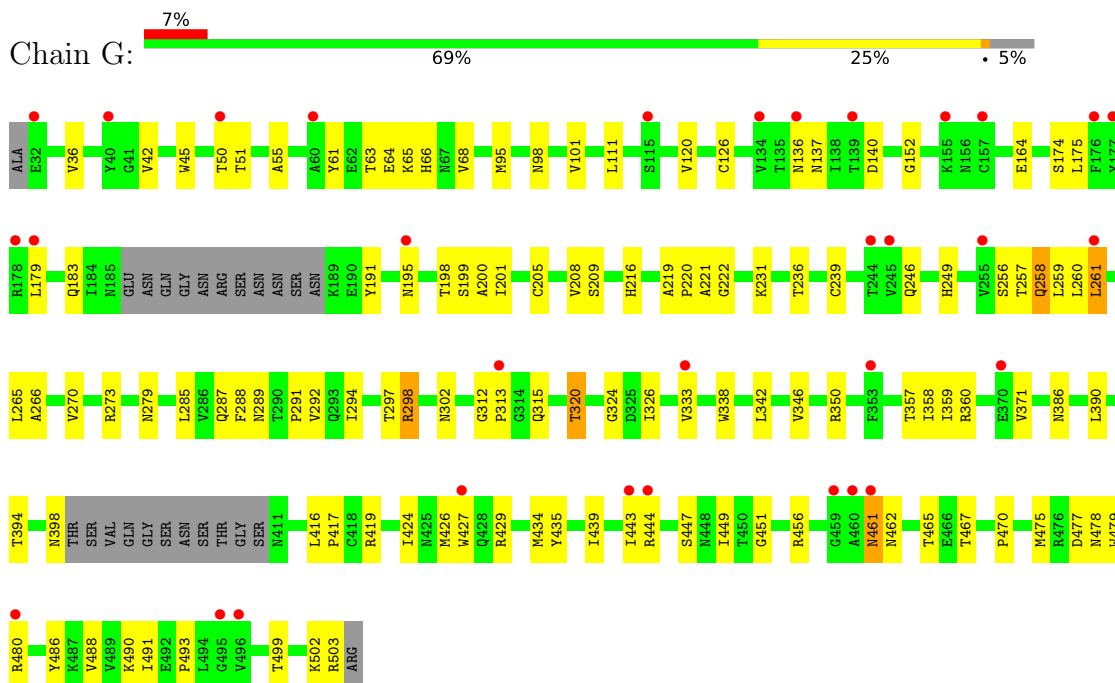
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	J	1	Total	C	N	O	0	0
			14	8	1	5		
12	J	1	Total	C	N	O	0	0
			14	8	1	5		
12	K	1	Total	C	N	O	0	0
			14	8	1	5		
12	K	1	Total	C	N	O	0	0
			14	8	1	5		

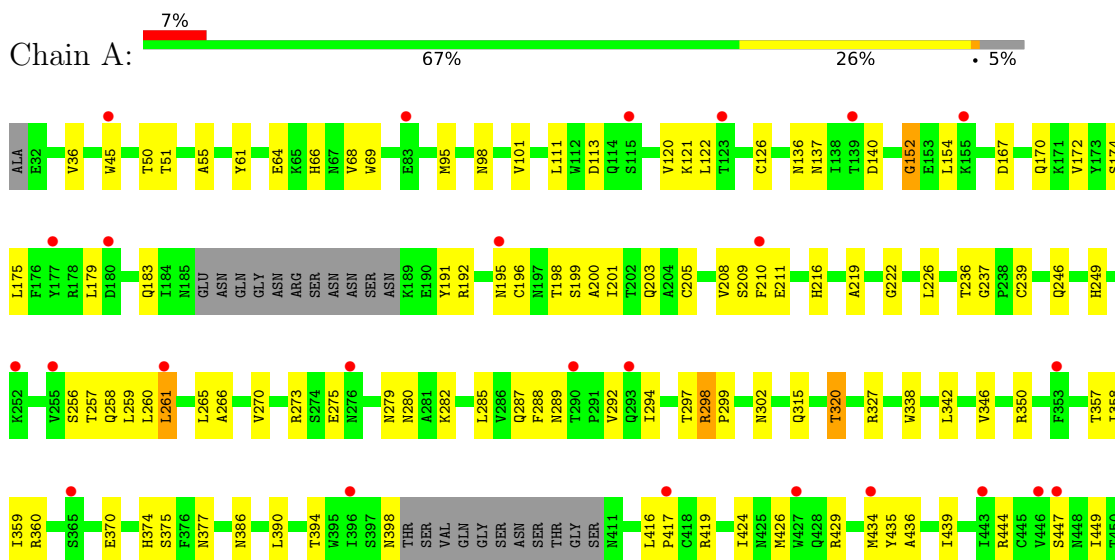
3 Residue-property plots [i](#)

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 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: Envelope glycoprotein gp120

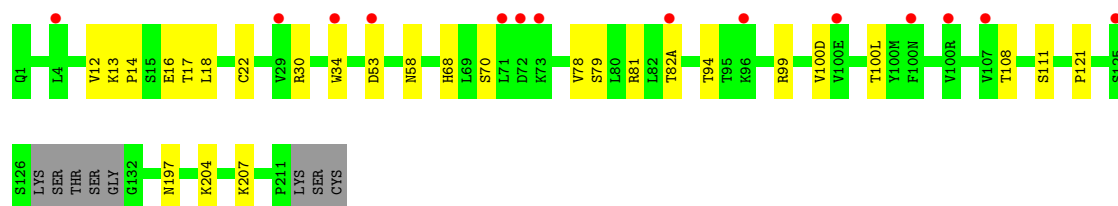


- Molecule 1: Envelope glycoprotein gp120

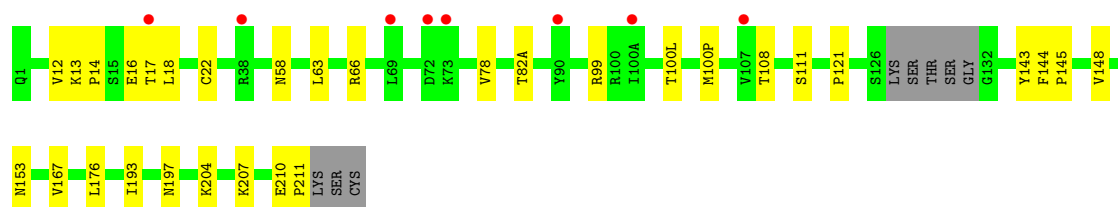




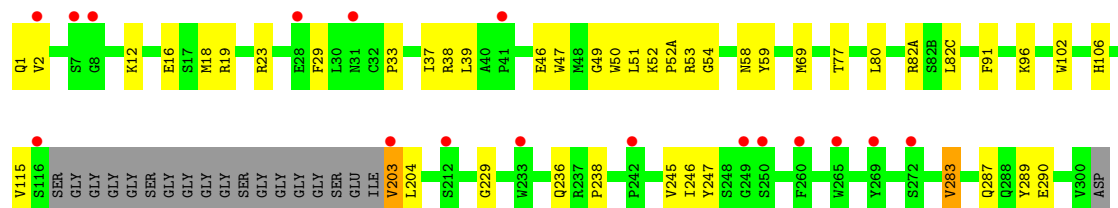
Chain F: 6% 85% 11%



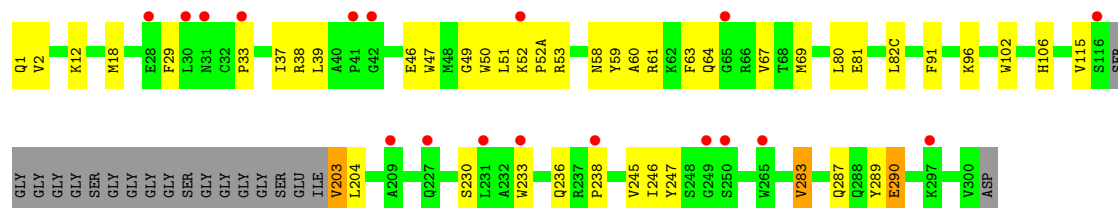
Chain N: 3% 83% 13%



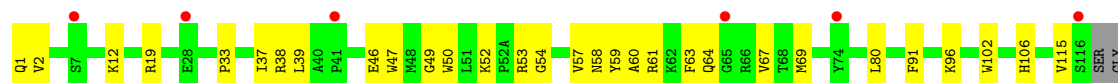
Chain D: 7% 73% 18% 2%



Chain I: 7% 73% 18% 2%



Chain O: 6% 74% 17% 8%





- Molecule 6: 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 P: 20% 60% 20%



- Molecule 6: 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 R: 60% 40%



- Molecule 6: 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 V: 20% 80%



- Molecule 6: 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: 40% 40% 20%

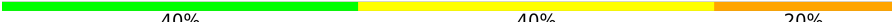


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 80% 20%

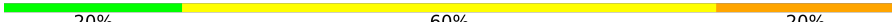


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  40% 40% 20%



- Molecule 6: 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 r:  20% 60% 20%

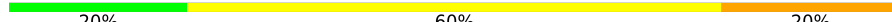


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  60% 40%

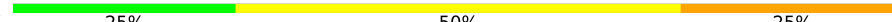


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  20% 60% 20%



- Molecule 7: 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

Chain Q:  25% 50% 25%



- Molecule 7: 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

Chain e:  50% 50%



- Molecule 7: 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

Chain s:  50% 25% 25%



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

Chain S:  50% 50%

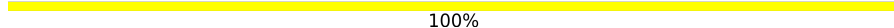


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

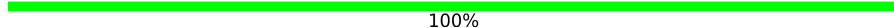


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  50% 50%



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

Chain c:  50% 50%



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

Chain g:  50% 50%

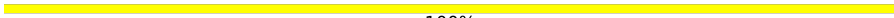
MAG1
MAG2

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

Chain k:  100%

MAG1
MAG2

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

Chain n:  100%

MAG1
MAG2

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

Chain o:  100%

MAG1
MAG2

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

Chain p:  100%

MAG1
MAG2

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

Chain q:  50% 50%

MAG1
MAG2

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

Chain u:  50% 50%

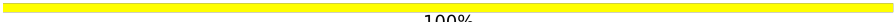


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  100%



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

Chain 1:  100%



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

Chain 2:  100%



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

Chain 3:  100%

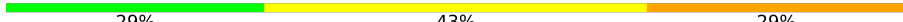


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  50% 50%



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

Chain T:  29% 43% 29%



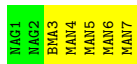
- Molecule 9: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X: 29% 71%



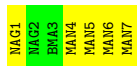
- Molecule 9: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain h: 29% 71%



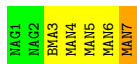
- Molecule 9: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain l: 29% 71%



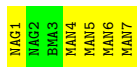
- Molecule 9: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain v: 29% 57% 14%



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

Chain z: 29% 71%



- Molecule 10: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1

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

Chain U:  18% 82%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10	MAN11
------	------	------	------	------	------	------	------	------	-------	-------

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

Chain i:  9% 91%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10	MAN11
------	------	------	------	------	------	------	------	------	-------	-------

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

Chain w:  18% 82%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10	MAN11
------	------	------	------	------	------	------	------	------	-------	-------

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  20% 80%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
------	------	------	------	------	------	------	------	------	-------

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  10% 90%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
------	------	------	------	------	------	------	------	------	-------

- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain 0:  20% 80%

MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.76Å 254.35Å 283.55Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	39.89 – 4.40 39.89 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.89-4.40) 99.8 (39.89-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.290 , 0.320 0.300 , 0.323	Depositor DCC
R_{free} test set	1008 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	144.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 199.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	31374	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PCA, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/3602	0.84	10/4891 (0.2%)
1	G	0.36	0/3602	0.83	6/4891 (0.1%)
1	J	0.37	0/3602	0.83	8/4891 (0.2%)
2	B	0.35	0/986	0.70	0/1337
2	C	0.36	0/986	0.72	0/1337
2	K	0.35	0/986	0.69	0/1337
3	E	0.33	0/1619	0.74	0/2217
3	L	0.32	0/1619	0.74	0/2217
3	M	0.34	0/1619	0.75	0/2217
4	F	0.34	0/1785	0.75	0/2437
4	H	0.33	0/1785	0.73	0/2437
4	N	0.34	0/1785	0.74	0/2437
5	D	0.31	0/1792	0.72	0/2428
5	I	0.31	0/1792	0.73	0/2428
5	O	0.32	0/1792	0.73	0/2428
All	All	0.35	0/29352	0.77	24/39930 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	298	ARG	CA-C-N	6.92	126.89	119.28
1	G	298	ARG	C-N-CA	6.92	126.89	119.28
1	G	462	ASN	N-CA-C	6.05	117.67	111.14
1	A	298	ARG	CA-C-N	6.04	125.93	119.28
1	A	298	ARG	C-N-CA	6.04	125.93	119.28

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	3528	0	3456	88	0
1	G	3528	0	3456	80	0
1	J	3528	0	3456	89	0
2	B	968	0	944	23	0
2	C	968	0	944	30	0
2	K	968	0	944	30	0
3	E	1577	0	1518	24	0
3	L	1577	0	1518	26	0
3	M	1577	0	1518	25	0
4	F	1738	0	1711	18	0
4	H	1738	0	1711	22	0
4	N	1738	0	1711	21	0
5	D	1753	0	1678	28	0
5	I	1753	0	1678	31	0
5	O	1753	0	1678	27	0
6	P	61	0	52	2	0
6	R	61	0	52	0	0
6	V	61	0	52	0	0
6	d	61	0	52	1	0
6	f	61	0	52	0	0
6	j	61	0	52	1	0
6	r	61	0	52	2	0
6	t	61	0	52	0	0
6	x	61	0	52	1	0
7	Q	50	0	43	3	0
7	e	50	0	43	1	0
7	s	50	0	43	2	0
8	1	28	0	25	1	0
8	2	28	0	25	0	0
8	3	28	0	25	0	0
8	4	28	0	25	0	0
8	S	28	0	25	1	0
8	W	28	0	25	0	0
8	Z	28	0	25	1	0
8	a	28	0	25	0	0
8	b	28	0	25	1	0
8	c	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	g	28	0	25	2	0
8	k	28	0	25	0	0
8	n	28	0	25	1	0
8	o	28	0	25	0	0
8	p	28	0	25	0	0
8	q	28	0	25	0	0
8	u	28	0	25	1	0
8	y	28	0	25	0	0
9	T	83	0	70	2	0
9	X	83	0	70	0	0
9	h	83	0	70	0	0
9	l	83	0	70	0	0
9	v	83	0	70	1	0
9	z	83	0	70	0	0
10	U	127	0	106	0	0
10	i	127	0	106	0	0
10	w	127	0	106	0	0
11	0	116	0	97	0	0
11	Y	116	0	97	0	0
11	m	116	0	97	1	0
12	A	56	0	52	0	0
12	B	28	0	26	0	0
12	C	28	0	26	0	0
12	G	56	0	52	1	0
12	J	56	0	52	1	0
12	K	28	0	26	0	0
All	All	31374	0	30231	506	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 8.

The worst 5 of 506 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)
4:N:197:ASN:HD22	4:N:204:LYS:HG2	1.48	0.78
4:H:14:PRO:HG3	4:H:111:SER:HB3	1.67	0.77
1:J:68:VAL:HG22	1:J:209:SER:HB3	1.67	0.76
3:E:39:ARG:HD3	3:E:40:PRO:HD2	1.68	0.76
1:J:279:ASN:OD1	5:O:102:TRP:NE1	2.15	0.76

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 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	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	14	49
1	G	442/472 (94%)	410 (93%)	28 (6%)	4 (1%)	14	49
1	J	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	14	49
2	B	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	7	35
2	C	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	7	35
2	K	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	7	35
3	E	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	24	62
3	L	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	24	62
3	M	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	24	62
4	F	223/235 (95%)	214 (96%)	9 (4%)	0	100	100
4	H	223/235 (95%)	213 (96%)	10 (4%)	0	100	100
4	N	223/235 (95%)	212 (95%)	11 (5%)	0	100	100
5	D	218/241 (90%)	205 (94%)	11 (5%)	2 (1%)	14	49
5	I	218/241 (90%)	206 (94%)	9 (4%)	3 (1%)	9	39
5	O	218/241 (90%)	205 (94%)	10 (5%)	3 (1%)	9	39
All	All	3618/3933 (92%)	3371 (93%)	218 (6%)	29 (1%)	16	52

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	140	ASP
5	D	53	ARG
1	A	140	ASP
5	I	53	ARG
1	J	140	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 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	399/419 (95%)	394 (99%)	5 (1%)	61	72
1	G	399/419 (95%)	394 (99%)	5 (1%)	61	72
1	J	399/419 (95%)	394 (99%)	5 (1%)	61	72
2	B	104/128 (81%)	97 (93%)	7 (7%)	15	37
2	C	104/128 (81%)	99 (95%)	5 (5%)	23	45
2	K	104/128 (81%)	98 (94%)	6 (6%)	18	40
3	E	177/180 (98%)	175 (99%)	2 (1%)	65	74
3	L	177/180 (98%)	175 (99%)	2 (1%)	65	74
3	M	177/180 (98%)	175 (99%)	2 (1%)	65	74
4	F	197/205 (96%)	196 (100%)	1 (0%)	81	81
4	H	197/205 (96%)	196 (100%)	1 (0%)	81	81
4	N	197/205 (96%)	196 (100%)	1 (0%)	81	81
5	D	183/190 (96%)	179 (98%)	4 (2%)	45	64
5	I	183/190 (96%)	179 (98%)	4 (2%)	45	64
5	O	183/190 (96%)	179 (98%)	4 (2%)	45	64
All	All	3180/3366 (94%)	3126 (98%)	54 (2%)	53	67

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	606	THR
5	I	290	GLU
4	N	108	THR
3	E	54	ARG
5	I	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
4	N	32	ASN
4	F	32	ASN
3	M	189	HIS
5	O	106	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PCA	O	1	5	7,8,9	1.92	1 (14%)	9,10,12	2.25	5 (55%)
5	PCA	D	1	5	7,8,9	1.91	1 (14%)	9,10,12	2.21	5 (55%)
5	PCA	I	1	5	7,8,9	1.93	1 (14%)	9,10,12	2.27	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PCA	O	1	5	-	0/0/11/13	0/1/1/1
5	PCA	D	1	5	-	0/0/11/13	0/1/1/1
5	PCA	I	1	5	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	PCA	CD-N	5.02	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1	PCA	CD-N	4.97	1.46	1.34
5	D	1	PCA	CD-N	4.95	1.46	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	PCA	CB-CA-C	-3.18	108.29	112.66
5	O	1	PCA	CB-CA-C	-3.09	108.42	112.66
5	O	1	PCA	OE-CD-CG	-3.04	121.30	126.72
5	I	1	PCA	OE-CD-CG	-3.00	121.36	126.72
5	D	1	PCA	OE-CD-CG	-2.98	121.40	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

198 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
11	NAG	0	1	11,1	14,14,15	0.23	0	17,19,21	0.42	0
11	MAN	0	10	11	11,11,12	0.74	0	15,15,17	0.99	1 (6%)
11	NAG	0	2	11	14,14,15	0.32	0	17,19,21	0.56	0
11	BMA	0	3	11	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
11	MAN	0	4	11	11,11,12	0.70	0	15,15,17	1.23	2 (13%)
11	MAN	0	5	11	11,11,12	0.71	1 (9%)	15,15,17	0.87	1 (6%)
11	MAN	0	6	11	11,11,12	0.55	0	15,15,17	1.18	2 (13%)
11	MAN	0	7	11	11,11,12	0.83	1 (9%)	15,15,17	0.98	2 (13%)
11	MAN	0	8	11	11,11,12	0.71	0	15,15,17	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	0	9	11	11,11,12	0.79	0	15,15,17	1.11	2 (13%)
8	NAG	1	1	8,1	14,14,15	0.27	0	17,19,21	0.63	0
8	NAG	1	2	8	14,14,15	0.25	0	17,19,21	0.42	0
8	NAG	2	1	8,1	14,14,15	0.25	0	17,19,21	0.43	0
8	NAG	2	2	8	14,14,15	0.41	0	17,19,21	0.50	0
8	NAG	3	1	8,1	14,14,15	0.21	0	17,19,21	0.58	0
8	NAG	3	2	8	14,14,15	0.29	0	17,19,21	0.42	0
8	NAG	4	1	8,1	14,14,15	0.67	1 (7%)	17,19,21	0.66	0
8	NAG	4	2	8	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	P	1	6,1	14,14,15	0.33	0	17,19,21	0.48	0
6	NAG	P	2	6	14,14,15	0.61	1 (7%)	17,19,21	1.36	2 (11%)
6	BMA	P	3	6	11,11,12	0.60	0	15,15,17	0.63	0
6	MAN	P	4	6	11,11,12	0.80	0	15,15,17	1.21	2 (13%)
6	MAN	P	5	6	11,11,12	0.91	0	15,15,17	0.99	1 (6%)
7	NAG	Q	1	7,1	14,14,15	0.51	0	17,19,21	0.43	0
7	NAG	Q	2	7	14,14,15	0.28	0	17,19,21	0.38	0
7	BMA	Q	3	7	11,11,12	0.62	0	15,15,17	0.60	0
7	MAN	Q	4	7	11,11,12	0.88	1 (9%)	15,15,17	0.89	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	R	2	6	14,14,15	0.24	0	17,19,21	0.38	0
6	BMA	R	3	6	11,11,12	0.61	0	15,15,17	0.49	0
6	MAN	R	4	6	11,11,12	0.70	0	15,15,17	1.01	2 (13%)
6	MAN	R	5	6	11,11,12	0.66	0	15,15,17	0.97	2 (13%)
8	NAG	S	1	8,1	14,14,15	0.27	0	17,19,21	0.51	0
8	NAG	S	2	8	14,14,15	0.54	0	17,19,21	1.31	2 (11%)
9	NAG	T	1	9,1	14,14,15	0.46	0	17,19,21	0.64	0
9	NAG	T	2	9	14,14,15	0.34	0	17,19,21	0.43	0
9	BMA	T	3	9	11,11,12	0.64	0	15,15,17	1.35	2 (13%)
9	MAN	T	4	9	11,11,12	1.19	2 (18%)	15,15,17	1.23	1 (6%)
9	MAN	T	5	9	11,11,12	0.79	0	15,15,17	1.30	2 (13%)
9	MAN	T	6	9	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
9	MAN	T	7	9	11,11,12	0.68	0	15,15,17	1.20	1 (6%)
10	NAG	U	1	10,1	14,14,15	0.62	0	17,19,21	0.68	0
10	MAN	U	10	10	11,11,12	0.66	0	15,15,17	1.37	2 (13%)
10	MAN	U	11	10	11,11,12	0.77	0	15,15,17	1.21	2 (13%)
10	NAG	U	2	10	14,14,15	0.37	0	17,19,21	0.42	0
10	BMA	U	3	10	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
10	MAN	U	4	10	11,11,12	0.66	0	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	U	5	10	11,11,12	0.89	0	15,15,17	1.03	2 (13%)
10	MAN	U	6	10	11,11,12	0.90	0	15,15,17	1.05	1 (6%)
10	MAN	U	7	10	11,11,12	1.16	2 (18%)	15,15,17	1.28	2 (13%)
10	MAN	U	8	10	11,11,12	1.02	0	15,15,17	1.15	1 (6%)
10	MAN	U	9	10	11,11,12	0.78	0	15,15,17	1.13	1 (6%)
6	NAG	V	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	0.67	0
6	NAG	V	2	6	14,14,15	0.32	0	17,19,21	0.48	0
6	BMA	V	3	6	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
6	MAN	V	4	6	11,11,12	0.73	0	15,15,17	1.19	2 (13%)
6	MAN	V	5	6	11,11,12	0.86	0	15,15,17	0.98	1 (6%)
8	NAG	W	1	8,1	14,14,15	0.41	0	17,19,21	0.50	0
8	NAG	W	2	8	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	X	1	9,1	14,14,15	0.65	1 (7%)	17,19,21	0.79	1 (5%)
9	NAG	X	2	9	14,14,15	0.41	0	17,19,21	0.36	0
9	BMA	X	3	9	11,11,12	0.63	0	15,15,17	0.75	0
9	MAN	X	4	9	11,11,12	1.01	0	15,15,17	1.13	1 (6%)
9	MAN	X	5	9	11,11,12	0.68	0	15,15,17	1.12	2 (13%)
9	MAN	X	6	9	11,11,12	0.73	0	15,15,17	1.33	1 (6%)
9	MAN	X	7	9	11,11,12	0.74	0	15,15,17	1.21	1 (6%)
11	NAG	Y	1	11,1	14,14,15	0.29	0	17,19,21	0.43	0
11	MAN	Y	10	11	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
11	NAG	Y	2	11	14,14,15	0.28	0	17,19,21	0.56	0
11	BMA	Y	3	11	11,11,12	0.71	0	15,15,17	1.13	2 (13%)
11	MAN	Y	4	11	11,11,12	0.66	0	15,15,17	1.23	2 (13%)
11	MAN	Y	5	11	11,11,12	0.69	1 (9%)	15,15,17	0.87	1 (6%)
11	MAN	Y	6	11	11,11,12	0.54	0	15,15,17	1.22	2 (13%)
11	MAN	Y	7	11	11,11,12	0.82	1 (9%)	15,15,17	1.05	2 (13%)
11	MAN	Y	8	11	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
11	MAN	Y	9	11	11,11,12	0.75	0	15,15,17	1.11	2 (13%)
8	NAG	Z	1	8,1	14,14,15	0.26	0	17,19,21	0.67	0
8	NAG	Z	2	8	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	a	1	8,1	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	a	2	8	14,14,15	0.46	0	17,19,21	0.49	0
8	NAG	b	1	8,1	14,14,15	0.18	0	17,19,21	0.54	0
8	NAG	b	2	8	14,14,15	0.28	0	17,19,21	0.38	0
8	NAG	c	1	8,1	14,14,15	0.78	1 (7%)	17,19,21	0.68	0
8	NAG	c	2	8	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	d	1	6,1	14,14,15	0.29	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	d	2	6	14,14,15	0.57	0	17,19,21	1.35	2 (11%)
6	BMA	d	3	6	11,11,12	0.64	0	15,15,17	0.63	0
6	MAN	d	4	6	11,11,12	0.89	1 (9%)	15,15,17	1.28	2 (13%)
6	MAN	d	5	6	11,11,12	0.89	0	15,15,17	0.96	1 (6%)
7	NAG	e	1	7,1	14,14,15	0.45	0	17,19,21	0.47	0
7	NAG	e	2	7	14,14,15	0.27	0	17,19,21	0.37	0
7	BMA	e	3	7	11,11,12	0.64	0	15,15,17	0.61	0
7	MAN	e	4	7	11,11,12	0.74	0	15,15,17	0.95	1 (6%)
6	NAG	f	1	6,1	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	f	2	6	14,14,15	0.24	0	17,19,21	0.36	0
6	BMA	f	3	6	11,11,12	0.61	0	15,15,17	0.46	0
6	MAN	f	4	6	11,11,12	0.79	0	15,15,17	0.94	0
6	MAN	f	5	6	11,11,12	0.65	0	15,15,17	0.95	2 (13%)
8	NAG	g	1	8,1	14,14,15	0.28	0	17,19,21	0.52	0
8	NAG	g	2	8	14,14,15	0.50	0	17,19,21	1.31	2 (11%)
9	NAG	h	1	9,1	14,14,15	0.51	0	17,19,21	0.62	0
9	NAG	h	2	9	14,14,15	0.28	0	17,19,21	0.43	0
9	BMA	h	3	9	11,11,12	0.66	0	15,15,17	1.48	2 (13%)
9	MAN	h	4	9	11,11,12	1.13	1 (9%)	15,15,17	1.27	1 (6%)
9	MAN	h	5	9	11,11,12	0.83	0	15,15,17	1.29	2 (13%)
9	MAN	h	6	9	11,11,12	0.73	0	15,15,17	1.40	2 (13%)
9	MAN	h	7	9	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
10	NAG	i	1	10,1	14,14,15	0.77	1 (7%)	17,19,21	0.72	0
10	MAN	i	10	10	11,11,12	0.64	0	15,15,17	1.31	2 (13%)
10	MAN	i	11	10	11,11,12	0.69	0	15,15,17	1.16	2 (13%)
10	NAG	i	2	10	14,14,15	0.41	0	17,19,21	0.44	0
10	BMA	i	3	10	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
10	MAN	i	4	10	11,11,12	0.66	0	15,15,17	1.34	2 (13%)
10	MAN	i	5	10	11,11,12	0.86	0	15,15,17	1.10	1 (6%)
10	MAN	i	6	10	11,11,12	0.92	0	15,15,17	1.00	1 (6%)
10	MAN	i	7	10	11,11,12	1.09	2 (18%)	15,15,17	1.23	2 (13%)
10	MAN	i	8	10	11,11,12	0.96	0	15,15,17	1.20	1 (6%)
10	MAN	i	9	10	11,11,12	0.82	0	15,15,17	1.11	2 (13%)
6	NAG	j	1	6,1	14,14,15	0.67	1 (7%)	17,19,21	0.68	0
6	NAG	j	2	6	14,14,15	0.29	0	17,19,21	0.45	0
6	BMA	j	3	6	11,11,12	0.65	0	15,15,17	0.90	0
6	MAN	j	4	6	11,11,12	0.73	0	15,15,17	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	j	5	6	11,11,12	0.78	0	15,15,17	1.01	1 (6%)
8	NAG	k	1	8,1	14,14,15	0.33	0	17,19,21	0.53	0
8	NAG	k	2	8	14,14,15	0.27	0	17,19,21	0.41	0
9	NAG	l	1	9,1	14,14,15	0.58	1 (7%)	17,19,21	0.78	1 (5%)
9	NAG	l	2	9	14,14,15	0.46	0	17,19,21	0.37	0
9	BMA	l	3	9	11,11,12	0.63	0	15,15,17	0.79	0
9	MAN	l	4	9	11,11,12	0.97	0	15,15,17	1.21	2 (13%)
9	MAN	l	5	9	11,11,12	0.66	0	15,15,17	1.17	1 (6%)
9	MAN	l	6	9	11,11,12	0.76	0	15,15,17	1.31	1 (6%)
9	MAN	l	7	9	11,11,12	0.71	0	15,15,17	1.17	1 (6%)
11	NAG	m	1	11,1	14,14,15	0.38	0	17,19,21	0.40	0
11	MAN	m	10	11	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
11	NAG	m	2	11	14,14,15	0.33	0	17,19,21	0.53	0
11	BMA	m	3	11	11,11,12	0.75	0	15,15,17	1.05	2 (13%)
11	MAN	m	4	11	11,11,12	0.74	0	15,15,17	1.27	2 (13%)
11	MAN	m	5	11	11,11,12	0.80	1 (9%)	15,15,17	0.83	0
11	MAN	m	6	11	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
11	MAN	m	7	11	11,11,12	0.79	0	15,15,17	0.95	2 (13%)
11	MAN	m	8	11	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
11	MAN	m	9	11	11,11,12	0.76	0	15,15,17	1.11	2 (13%)
8	NAG	n	1	8,1	14,14,15	0.29	0	17,19,21	0.67	0
8	NAG	n	2	8	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	o	1	8,1	14,14,15	0.26	0	17,19,21	0.40	0
8	NAG	o	2	8	14,14,15	0.38	0	17,19,21	0.48	0
8	NAG	p	1	8,1	14,14,15	0.21	0	17,19,21	0.56	0
8	NAG	p	2	8	14,14,15	0.29	0	17,19,21	0.41	0
8	NAG	q	1	8,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
8	NAG	q	2	8	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	r	1	6,1	14,14,15	0.36	0	17,19,21	0.49	0
6	NAG	r	2	6	14,14,15	0.59	0	17,19,21	1.37	2 (11%)
6	BMA	r	3	6	11,11,12	0.59	0	15,15,17	0.55	0
6	MAN	r	4	6	11,11,12	0.84	0	15,15,17	1.18	2 (13%)
6	MAN	r	5	6	11,11,12	0.90	0	15,15,17	0.94	1 (6%)
7	NAG	s	1	7,1	14,14,15	0.44	0	17,19,21	0.50	0
7	NAG	s	2	7	14,14,15	0.28	0	17,19,21	0.38	0
7	BMA	s	3	7	11,11,12	0.65	0	15,15,17	0.58	0
7	MAN	s	4	7	11,11,12	0.75	1 (9%)	15,15,17	0.93	1 (6%)
6	NAG	t	1	6,1	14,14,15	0.15	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	t	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	BMA	t	3	6	11,11,12	0.61	0	15,15,17	0.47	0
6	MAN	t	4	6	11,11,12	0.78	0	15,15,17	0.98	1 (6%)
6	MAN	t	5	6	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
8	NAG	u	1	8,1	14,14,15	0.27	0	17,19,21	0.51	0
8	NAG	u	2	8	14,14,15	0.56	0	17,19,21	1.35	2 (11%)
9	NAG	v	1	9,1	14,14,15	0.49	0	17,19,21	0.62	0
9	NAG	v	2	9	14,14,15	0.35	0	17,19,21	0.42	0
9	BMA	v	3	9	11,11,12	0.63	0	15,15,17	1.24	1 (6%)
9	MAN	v	4	9	11,11,12	1.22	1 (9%)	15,15,17	1.20	1 (6%)
9	MAN	v	5	9	11,11,12	0.81	0	15,15,17	1.21	2 (13%)
9	MAN	v	6	9	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
9	MAN	v	7	9	11,11,12	0.67	0	15,15,17	1.22	1 (6%)
10	NAG	w	1	10,1	14,14,15	0.66	0	17,19,21	0.72	0
10	MAN	w	10	10	11,11,12	0.64	0	15,15,17	1.39	2 (13%)
10	MAN	w	11	10	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
10	NAG	w	2	10	14,14,15	0.37	0	17,19,21	0.40	0
10	BMA	w	3	10	11,11,12	0.68	0	15,15,17	1.22	3 (20%)
10	MAN	w	4	10	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
10	MAN	w	5	10	11,11,12	0.90	0	15,15,17	1.11	1 (6%)
10	MAN	w	6	10	11,11,12	0.93	0	15,15,17	1.03	1 (6%)
10	MAN	w	7	10	11,11,12	1.10	2 (18%)	15,15,17	1.18	1 (6%)
10	MAN	w	8	10	11,11,12	0.91	0	15,15,17	1.22	1 (6%)
10	MAN	w	9	10	11,11,12	0.76	0	15,15,17	1.07	1 (6%)
6	NAG	x	1	6,1	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
6	NAG	x	2	6	14,14,15	0.34	0	17,19,21	0.49	0
6	BMA	x	3	6	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
6	MAN	x	4	6	11,11,12	0.79	0	15,15,17	1.20	2 (13%)
6	MAN	x	5	6	11,11,12	0.83	0	15,15,17	0.96	1 (6%)
8	NAG	y	1	8,1	14,14,15	0.37	0	17,19,21	0.52	0
8	NAG	y	2	8	14,14,15	0.25	0	17,19,21	0.38	0
9	NAG	z	1	9,1	14,14,15	0.66	1 (7%)	17,19,21	0.81	1 (5%)
9	NAG	z	2	9	14,14,15	0.41	0	17,19,21	0.38	0
9	BMA	z	3	9	11,11,12	0.63	0	15,15,17	0.82	0
9	MAN	z	4	9	11,11,12	1.02	0	15,15,17	1.17	1 (6%)
9	MAN	z	5	9	11,11,12	0.70	0	15,15,17	1.13	2 (13%)
9	MAN	z	6	9	11,11,12	0.73	0	15,15,17	1.32	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	z	7	9	11,11,12	0.69	0	15,15,17	1.16	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	0	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	0	10	11	-	0/2/19/22	0/1/1/1
11	NAG	0	2	11	-	4/6/23/26	0/1/1/1
11	BMA	0	3	11	-	0/2/19/22	0/1/1/1
11	MAN	0	4	11	-	0/2/19/22	0/1/1/1
11	MAN	0	5	11	-	0/2/19/22	0/1/1/1
11	MAN	0	6	11	-	1/2/19/22	0/1/1/1
11	MAN	0	7	11	-	2/2/19/22	0/1/1/1
11	MAN	0	8	11	-	0/2/19/22	0/1/1/1
11	MAN	0	9	11	-	0/2/19/22	1/1/1/1
8	NAG	1	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	NAG	2	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	2	2	8	-	2/6/23/26	0/1/1/1
8	NAG	3	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	3	2	8	-	0/6/23/26	0/1/1/1
8	NAG	4	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	4	2	8	-	2/6/23/26	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	5/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	0/2/19/22	0/1/1/1
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1
8	NAG	S	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	S	2	8	-	4/6/23/26	0/1/1/1
9	NAG	T	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	2/2/19/22	0/1/1/1
9	MAN	T	5	9	-	0/2/19/22	0/1/1/1
9	MAN	T	6	9	-	0/2/19/22	0/1/1/1
9	MAN	T	7	9	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	U	10	10	-	1/2/19/22	0/1/1/1
10	MAN	U	11	10	-	0/2/19/22	0/1/1/1
10	NAG	U	2	10	-	0/6/23/26	0/1/1/1
10	BMA	U	3	10	-	2/2/19/22	0/1/1/1
10	MAN	U	4	10	-	0/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
10	MAN	U	6	10	-	0/2/19/22	0/1/1/1
10	MAN	U	7	10	-	0/2/19/22	0/1/1/1
10	MAN	U	8	10	-	0/2/19/22	0/1/1/1
10	MAN	U	9	10	-	0/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
8	NAG	W	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
9	NAG	X	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	0/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	0/2/19/22	0/1/1/1
11	NAG	Y	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	Y	10	11	-	0/2/19/22	0/1/1/1
11	NAG	Y	2	11	-	4/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	4	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	Y	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	6	11	-	1/2/19/22	0/1/1/1
11	MAN	Y	7	11	-	2/2/19/22	0/1/1/1
11	MAN	Y	8	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	9	11	-	0/2/19/22	1/1/1/1
8	NAG	Z	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
6	NAG	d	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	4/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
6	MAN	d	4	6	-	0/2/19/22	0/1/1/1
6	MAN	d	5	6	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	BMA	e	3	7	-	0/2/19/22	0/1/1/1
7	MAN	e	4	7	-	2/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
6	MAN	f	4	6	-	1/2/19/22	0/1/1/1
6	MAN	f	5	6	-	0/2/19/22	0/1/1/1
8	NAG	g	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	g	2	8	-	5/6/23/26	0/1/1/1
9	NAG	h	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
9	MAN	h	4	9	-	2/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	0/2/19/22	0/1/1/1
9	MAN	h	7	9	-	0/2/19/22	0/1/1/1
10	NAG	i	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	i	10	10	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	i	11	10	-	0/2/19/22	0/1/1/1
10	NAG	i	2	10	-	1/6/23/26	0/1/1/1
10	BMA	i	3	10	-	2/2/19/22	0/1/1/1
10	MAN	i	4	10	-	0/2/19/22	0/1/1/1
10	MAN	i	5	10	-	0/2/19/22	0/1/1/1
10	MAN	i	6	10	-	0/2/19/22	0/1/1/1
10	MAN	i	7	10	-	0/2/19/22	0/1/1/1
10	MAN	i	8	10	-	0/2/19/22	0/1/1/1
10	MAN	i	9	10	-	0/2/19/22	0/1/1/1
6	NAG	j	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	BMA	j	3	6	-	0/2/19/22	0/1/1/1
6	MAN	j	4	6	-	0/2/19/22	0/1/1/1
6	MAN	j	5	6	-	0/2/19/22	0/1/1/1
8	NAG	k	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
9	NAG	l	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	2/2/19/22	0/1/1/1
9	MAN	l	4	9	-	0/2/19/22	0/1/1/1
9	MAN	l	5	9	-	0/2/19/22	0/1/1/1
9	MAN	l	6	9	-	0/2/19/22	0/1/1/1
9	MAN	l	7	9	-	0/2/19/22	0/1/1/1
11	NAG	m	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	m	10	11	-	0/2/19/22	0/1/1/1
11	NAG	m	2	11	-	4/6/23/26	0/1/1/1
11	BMA	m	3	11	-	0/2/19/22	0/1/1/1
11	MAN	m	4	11	-	0/2/19/22	0/1/1/1
11	MAN	m	5	11	-	0/2/19/22	0/1/1/1
11	MAN	m	6	11	-	1/2/19/22	0/1/1/1
11	MAN	m	7	11	-	2/2/19/22	0/1/1/1
11	MAN	m	8	11	-	0/2/19/22	0/1/1/1
11	MAN	m	9	11	-	0/2/19/22	1/1/1/1
8	NAG	n	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	n	2	8	-	0/6/23/26	0/1/1/1
8	NAG	o	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
8	NAG	p	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	p	2	8	-	0/6/23/26	0/1/1/1
8	NAG	q	1	8,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
6	NAG	r	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	r	2	6	-	4/6/23/26	0/1/1/1
6	BMA	r	3	6	-	0/2/19/22	0/1/1/1
6	MAN	r	4	6	-	0/2/19/22	0/1/1/1
6	MAN	r	5	6	-	0/2/19/22	0/1/1/1
7	NAG	s	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	s	2	7	-	0/6/23/26	0/1/1/1
7	BMA	s	3	7	-	0/2/19/22	0/1/1/1
7	MAN	s	4	7	-	2/2/19/22	0/1/1/1
6	NAG	t	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	t	2	6	-	2/6/23/26	0/1/1/1
6	BMA	t	3	6	-	2/2/19/22	0/1/1/1
6	MAN	t	4	6	-	1/2/19/22	0/1/1/1
6	MAN	t	5	6	-	0/2/19/22	0/1/1/1
8	NAG	u	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	u	2	8	-	5/6/23/26	0/1/1/1
9	NAG	v	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
9	BMA	v	3	9	-	2/2/19/22	0/1/1/1
9	MAN	v	4	9	-	2/2/19/22	0/1/1/1
9	MAN	v	5	9	-	0/2/19/22	0/1/1/1
9	MAN	v	6	9	-	0/2/19/22	0/1/1/1
9	MAN	v	7	9	-	0/2/19/22	0/1/1/1
10	NAG	w	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	w	10	10	-	1/2/19/22	0/1/1/1
10	MAN	w	11	10	-	0/2/19/22	0/1/1/1
10	NAG	w	2	10	-	2/6/23/26	0/1/1/1
10	BMA	w	3	10	-	2/2/19/22	0/1/1/1
10	MAN	w	4	10	-	0/2/19/22	0/1/1/1
10	MAN	w	5	10	-	0/2/19/22	0/1/1/1
10	MAN	w	6	10	-	0/2/19/22	0/1/1/1
10	MAN	w	7	10	-	0/2/19/22	0/1/1/1
10	MAN	w	8	10	-	0/2/19/22	0/1/1/1
10	MAN	w	9	10	-	0/2/19/22	0/1/1/1
6	NAG	x	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	x	2	6	-	0/6/23/26	0/1/1/1
6	BMA	x	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	x	4	6	-	0/2/19/22	0/1/1/1
6	MAN	x	5	6	-	0/2/19/22	0/1/1/1
8	NAG	y	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
9	NAG	z	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	z	2	9	-	1/6/23/26	0/1/1/1
9	BMA	z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	z	5	9	-	0/2/19/22	0/1/1/1
9	MAN	z	6	9	-	0/2/19/22	0/1/1/1
9	MAN	z	7	9	-	0/2/19/22	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	x	1	NAG	O5-C1	-2.87	1.38	1.43
8	c	1	NAG	O5-C1	-2.77	1.39	1.43
6	V	1	NAG	O5-C1	-2.65	1.39	1.43
9	v	4	MAN	C2-C3	2.57	1.56	1.52
10	i	1	NAG	O5-C1	-2.55	1.39	1.43

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	r	2	NAG	C2-N2-C7	4.61	129.08	122.90
6	P	2	NAG	C2-N2-C7	4.60	129.07	122.90
6	d	2	NAG	C2-N2-C7	4.60	129.06	122.90
8	u	2	NAG	C2-N2-C7	4.58	129.04	122.90
8	g	2	NAG	C2-N2-C7	4.54	128.98	122.90

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	e	4	MAN	C4-C5-C6-O6
11	0	2	NAG	O5-C5-C6-O6
10	U	1	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
11	m	2	NAG	O5-C5-C6-O6

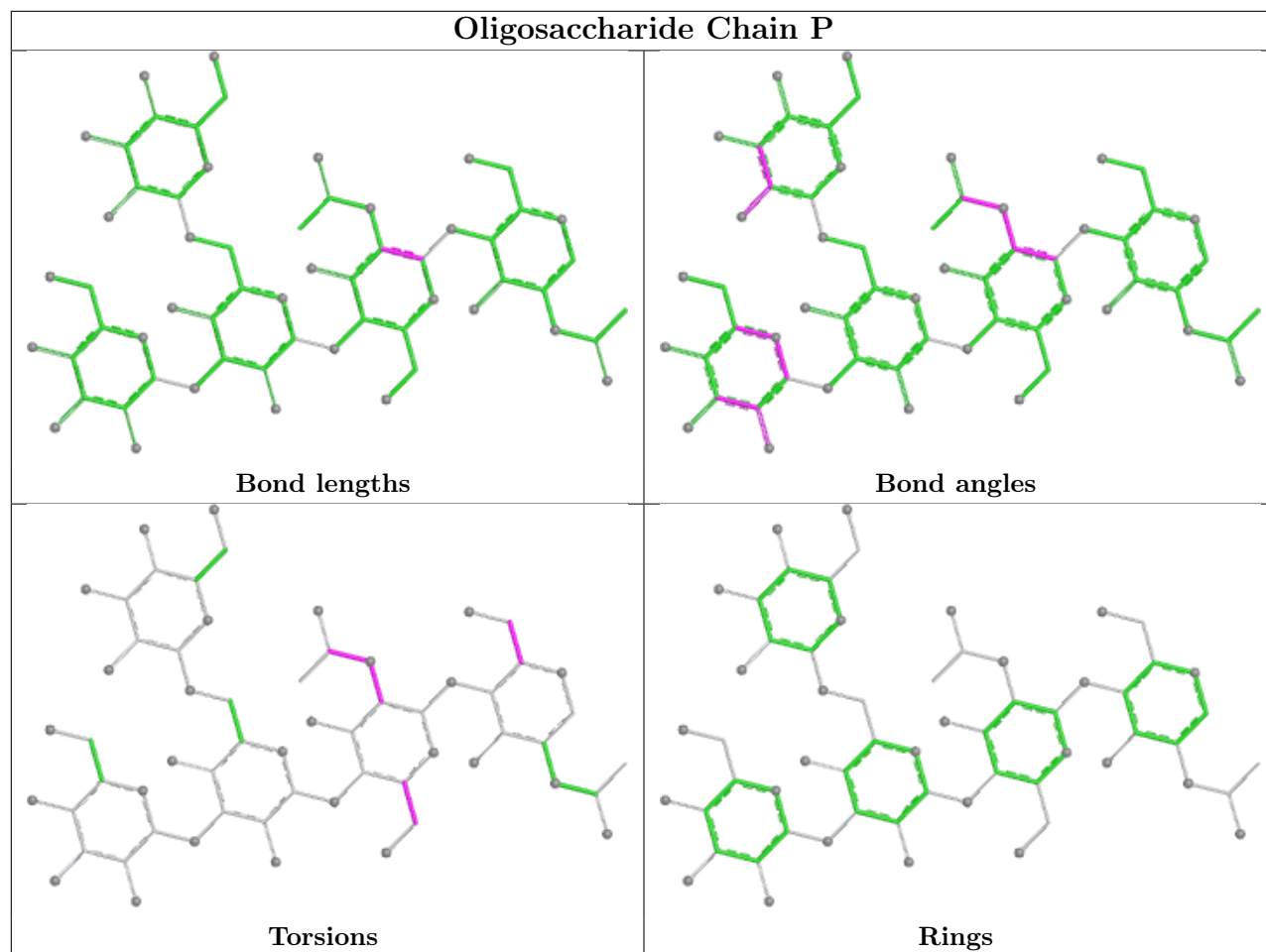
All (3) ring outliers are listed below:

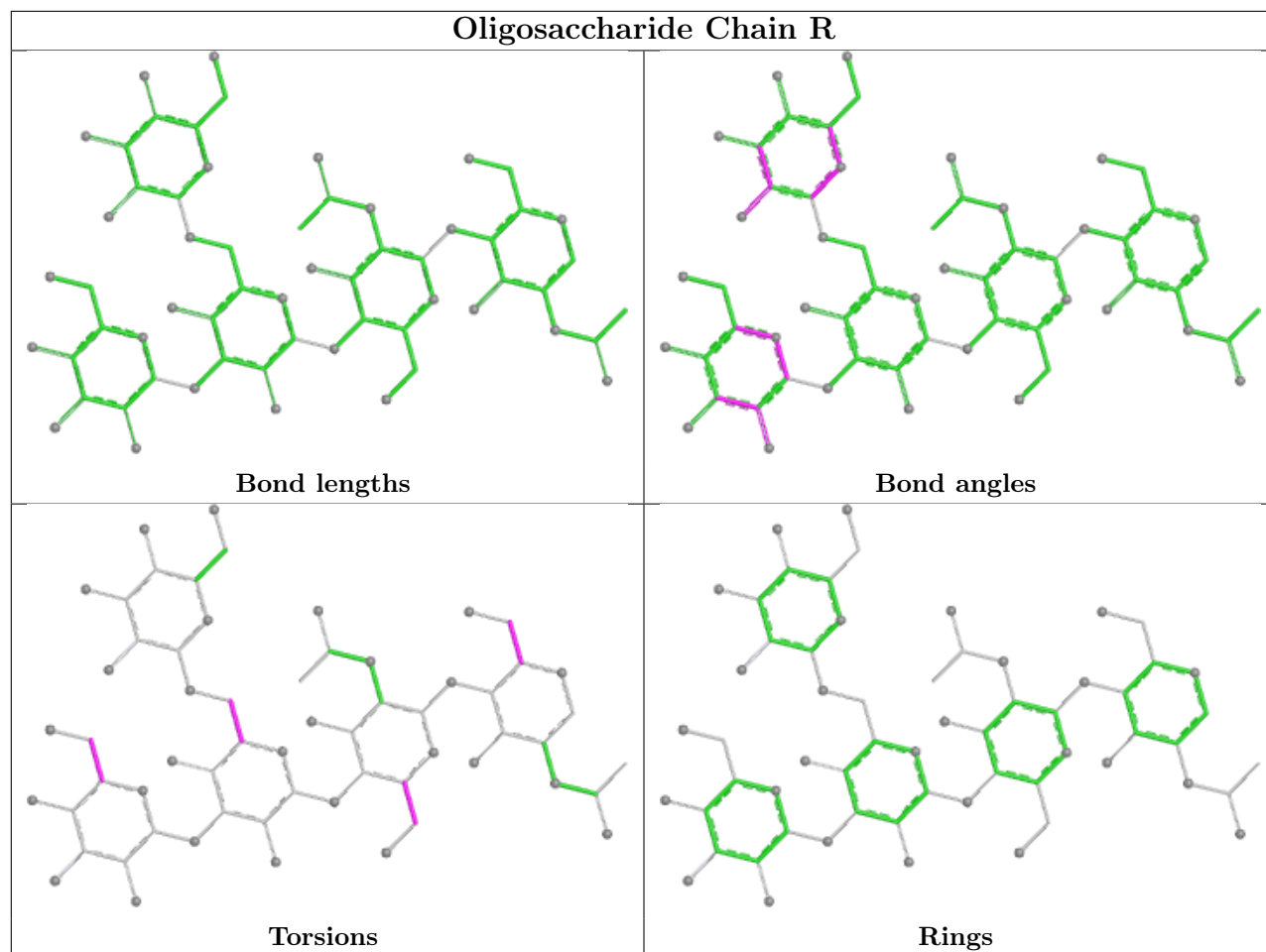
Mol	Chain	Res	Type	Atoms
11	m	9	MAN	C1-C2-C3-C4-C5-O5
11	Y	9	MAN	C1-C2-C3-C4-C5-O5
11	0	9	MAN	C1-C2-C3-C4-C5-O5

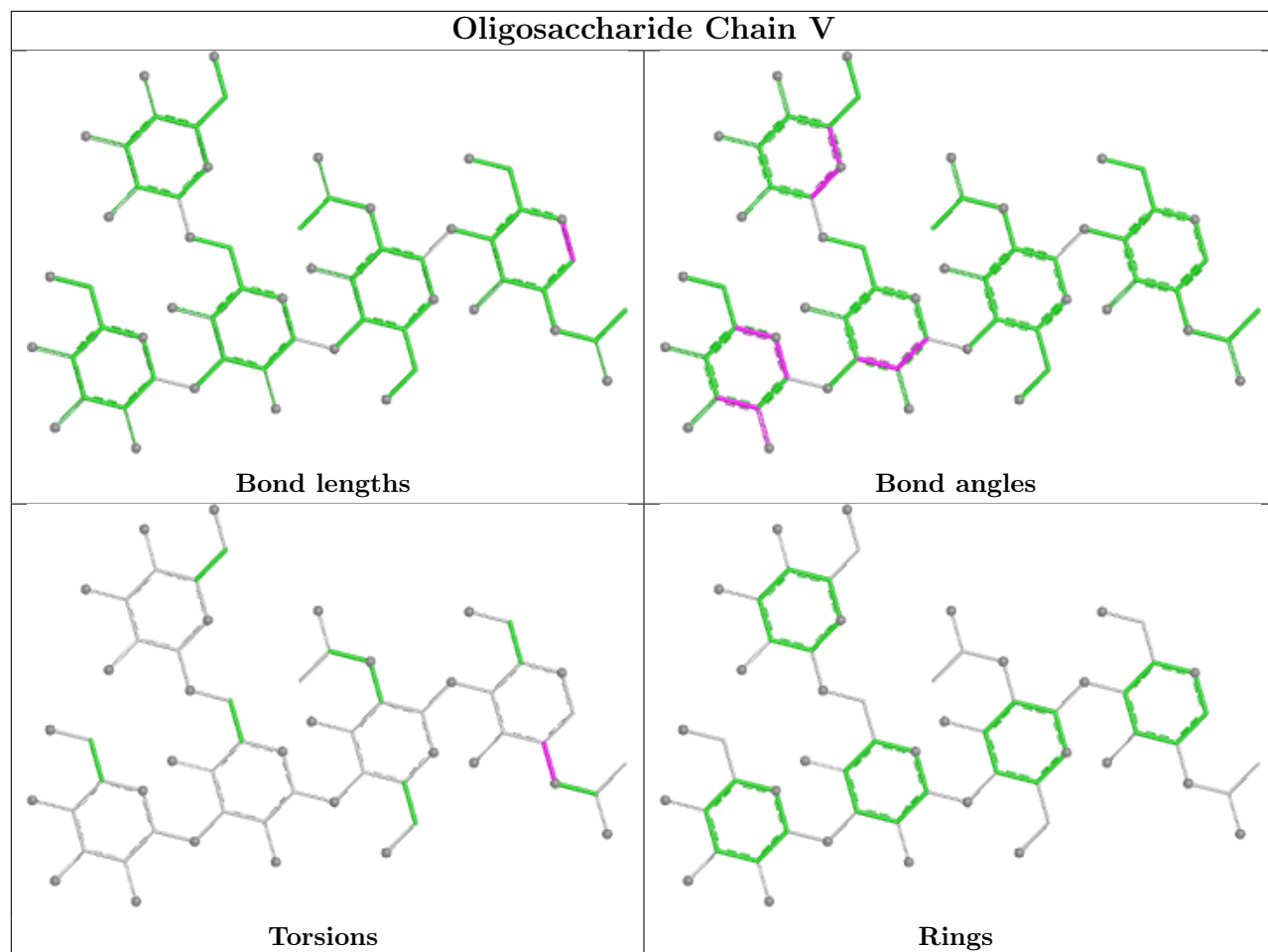
28 monomers are involved in 25 short contacts:

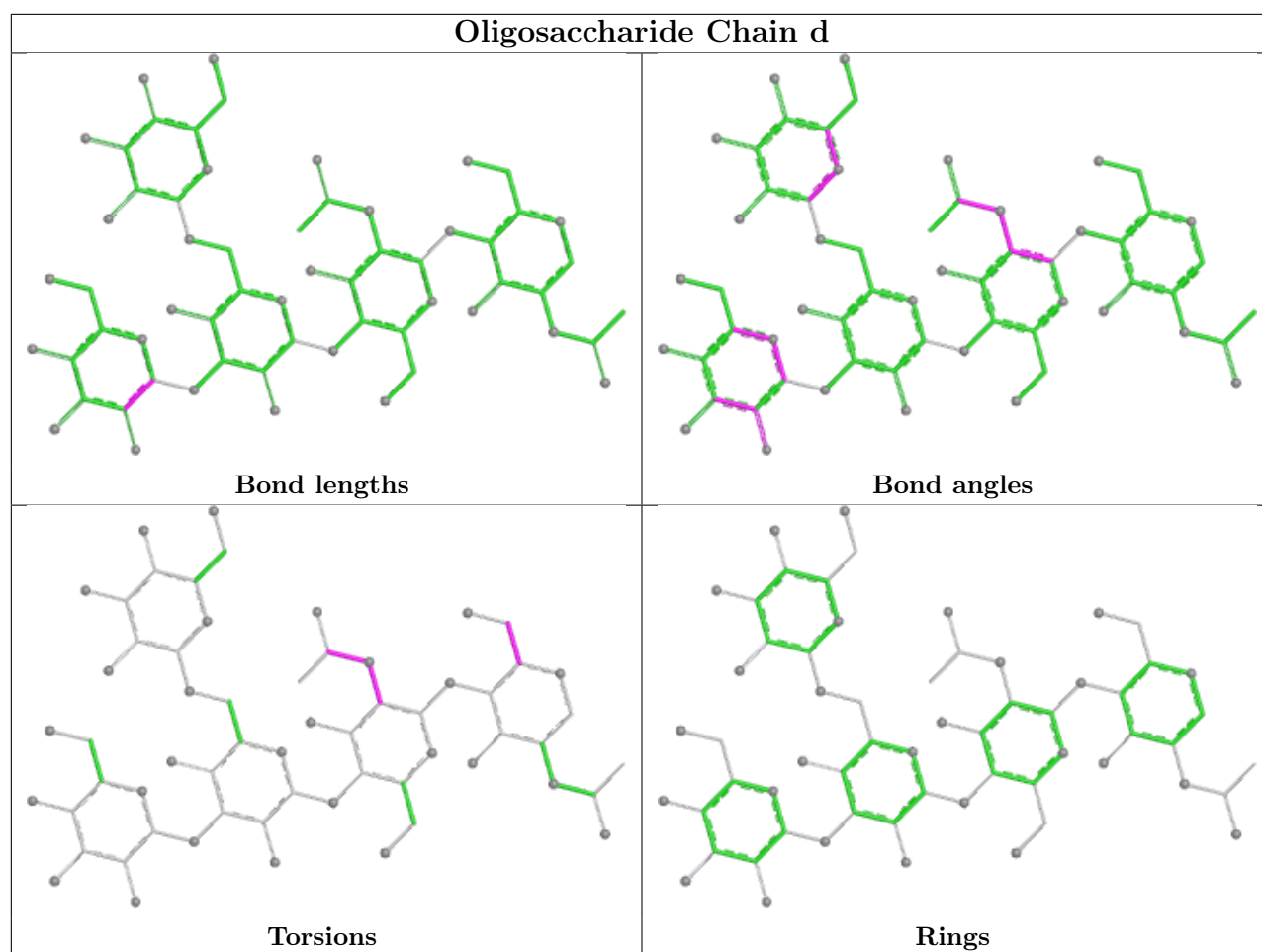
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	r	2	NAG	1	0
6	j	1	NAG	1	0
7	Q	4	MAN	1	0
8	Z	2	NAG	1	0
8	n	2	NAG	1	0
7	s	4	MAN	1	0
6	x	1	NAG	1	0
8	l	1	NAG	1	0
8	l	2	NAG	1	0
8	b	1	NAG	1	0
8	u	2	NAG	1	0
8	Z	1	NAG	1	0
9	v	7	MAN	1	0
8	n	1	NAG	1	0
8	g	2	NAG	2	0
6	P	2	NAG	1	0
11	m	2	NAG	1	0
6	d	2	NAG	1	0
9	T	7	MAN	1	0
7	s	2	NAG	1	0
8	g	1	NAG	1	0
7	e	2	NAG	1	0
7	Q	1	NAG	1	0
8	S	2	NAG	1	0
9	T	6	MAN	1	0
6	P	1	NAG	1	0
7	Q	2	NAG	1	0
6	r	1	NAG	1	0

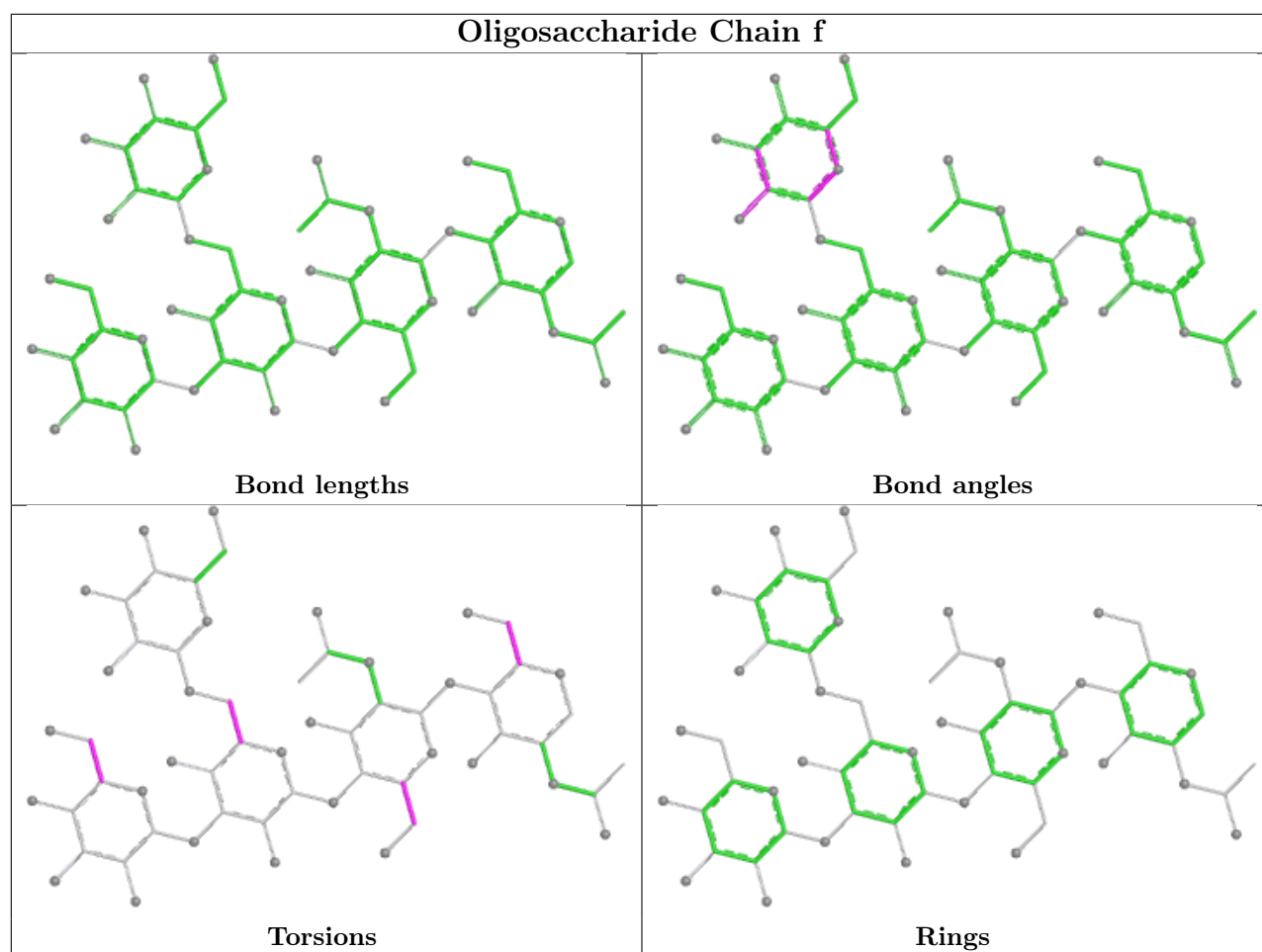
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

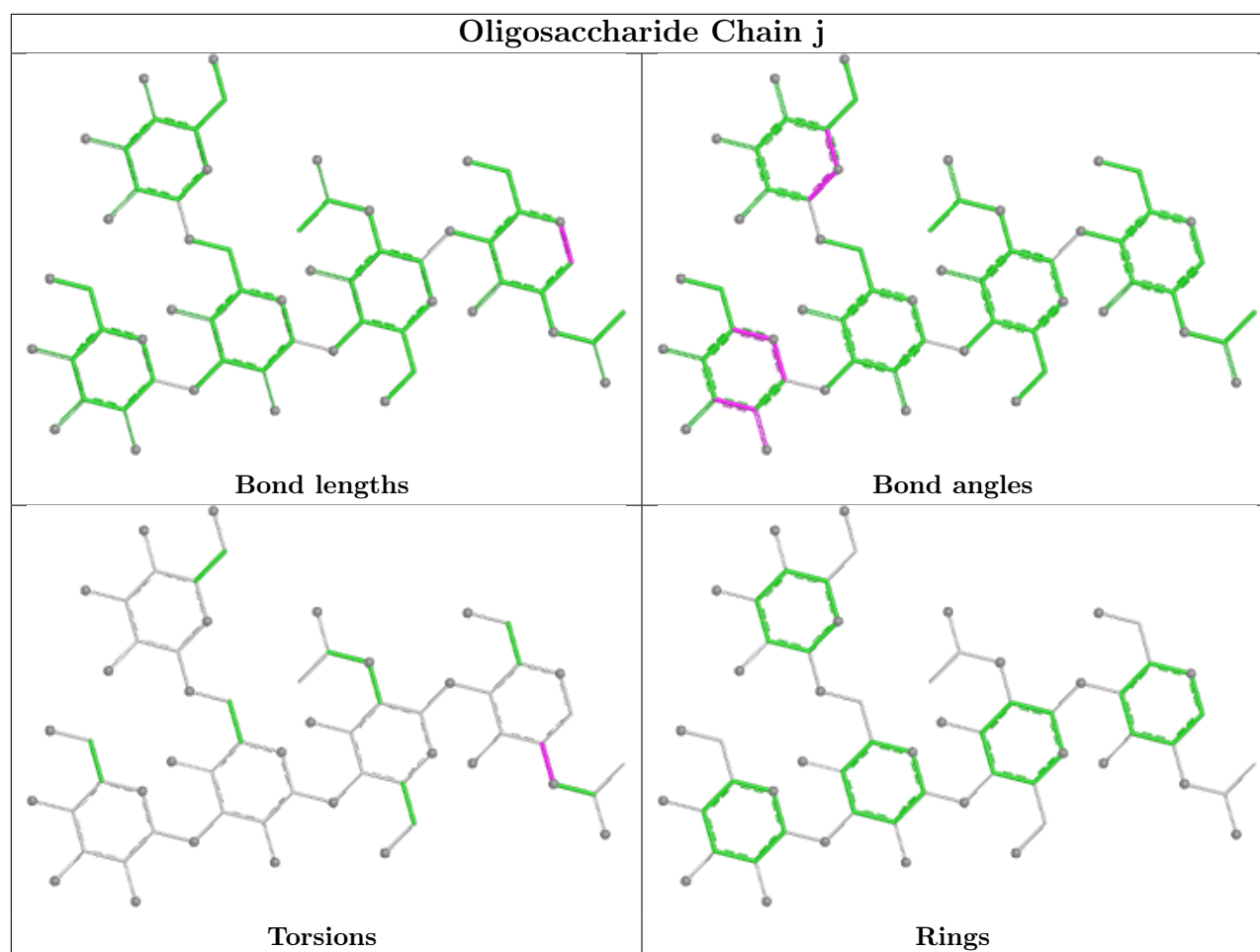


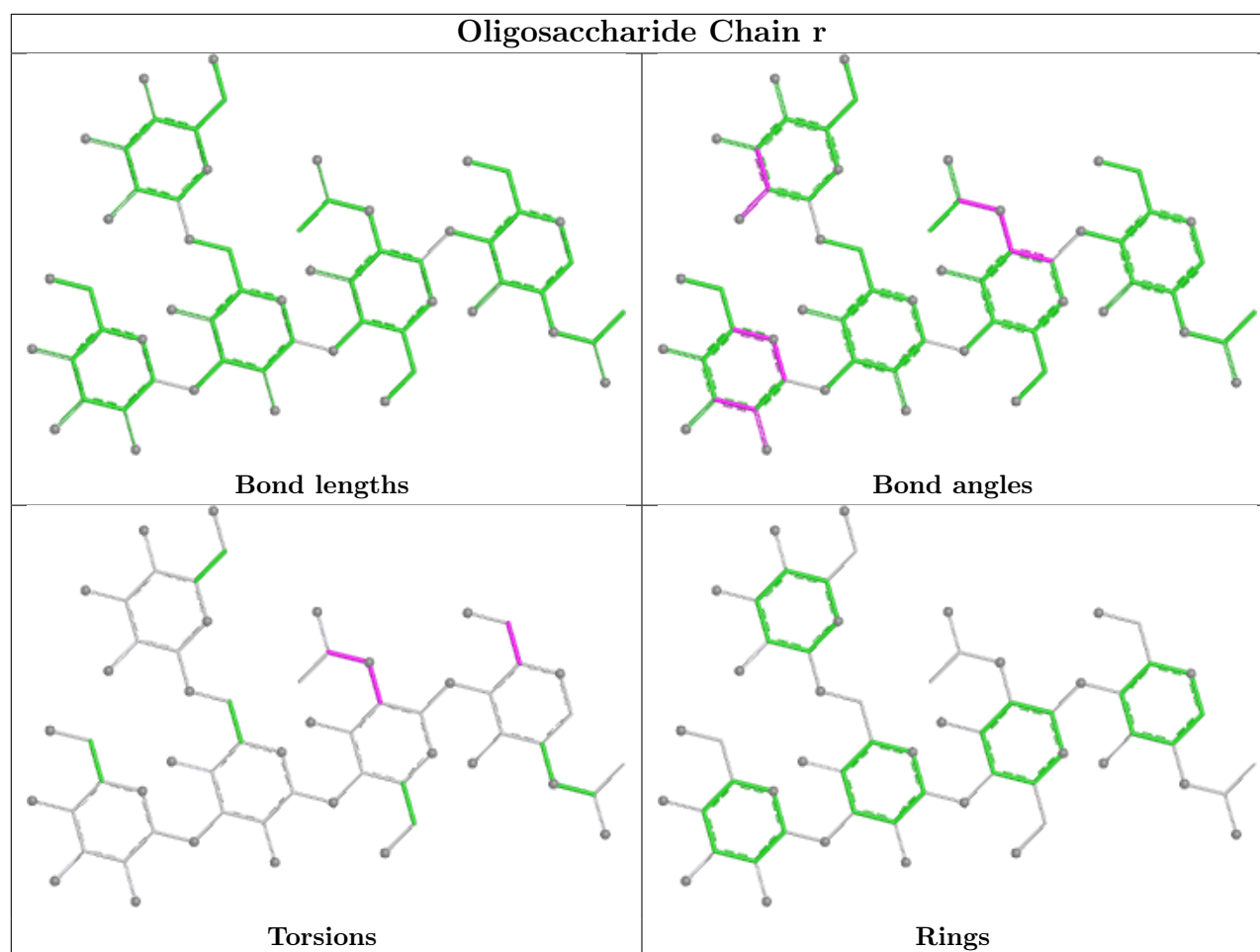


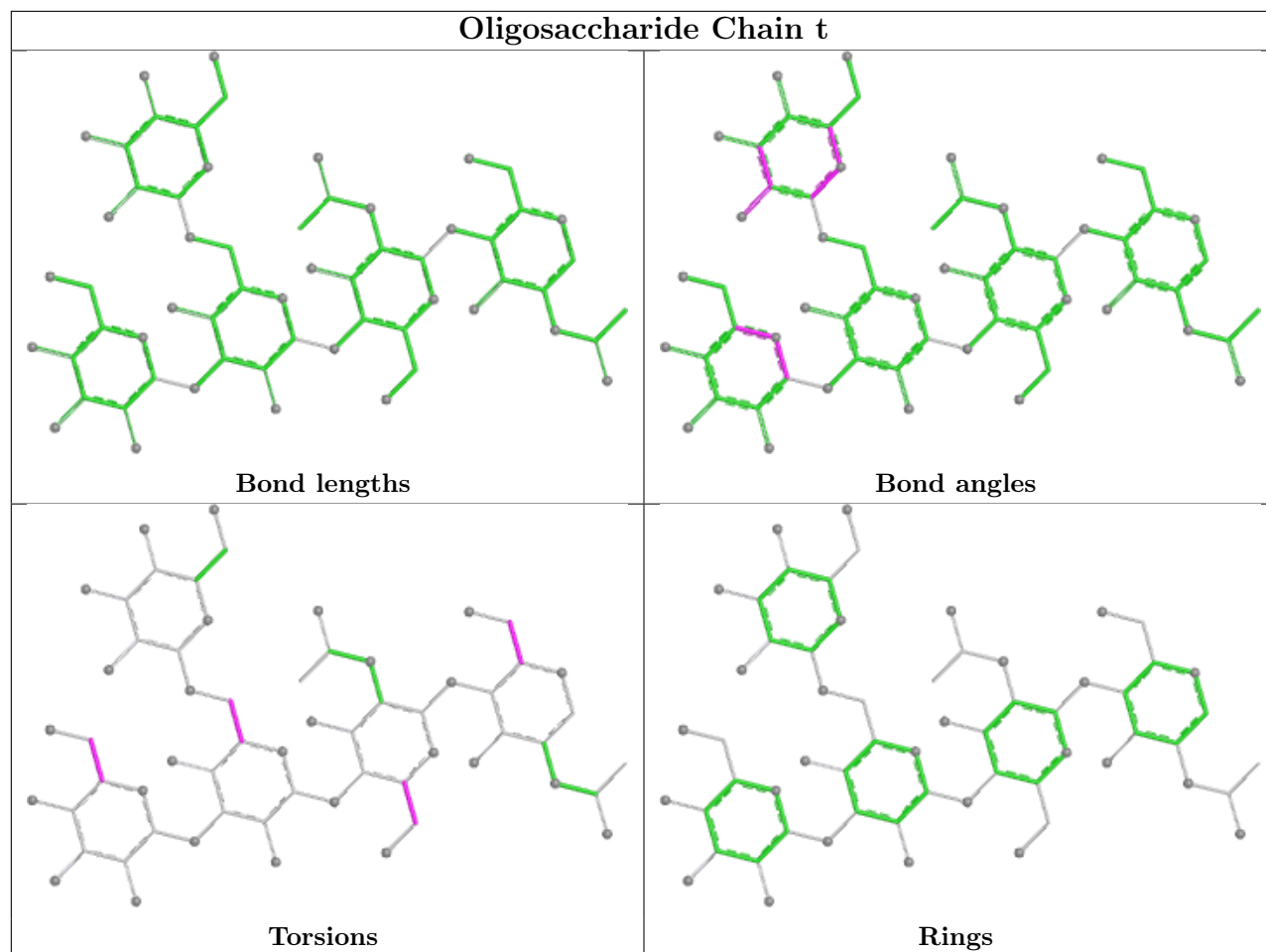


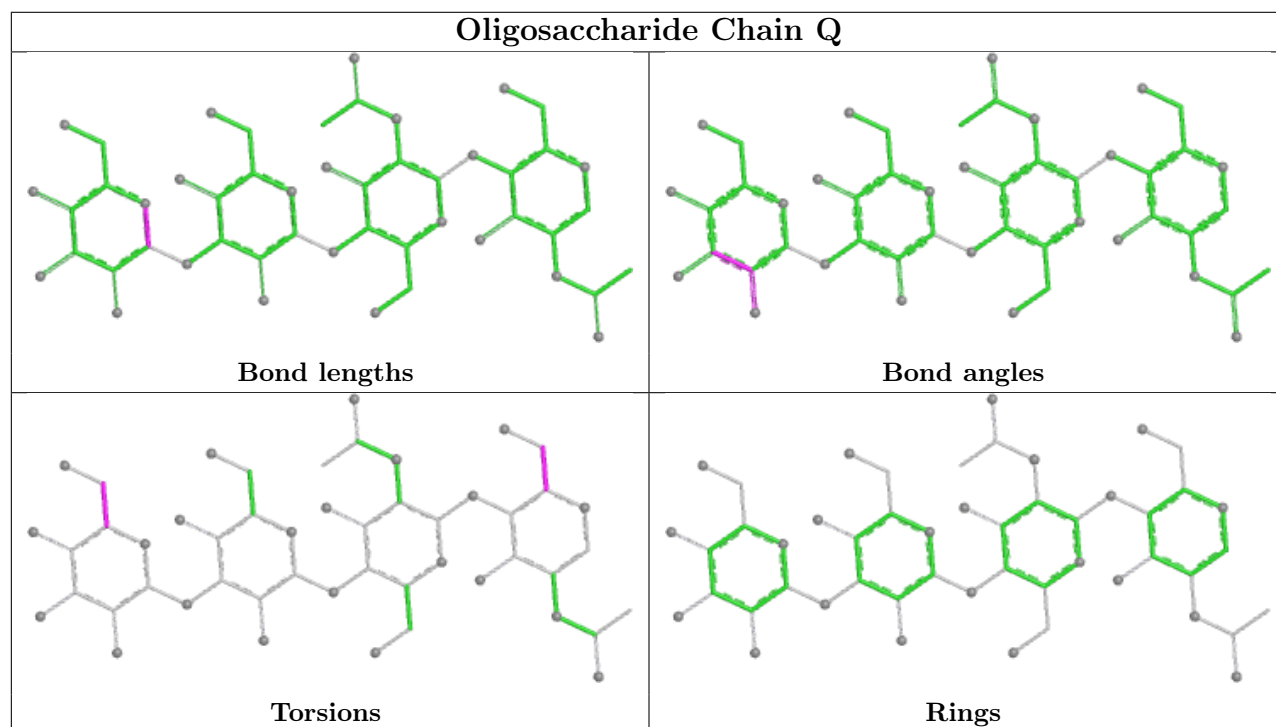
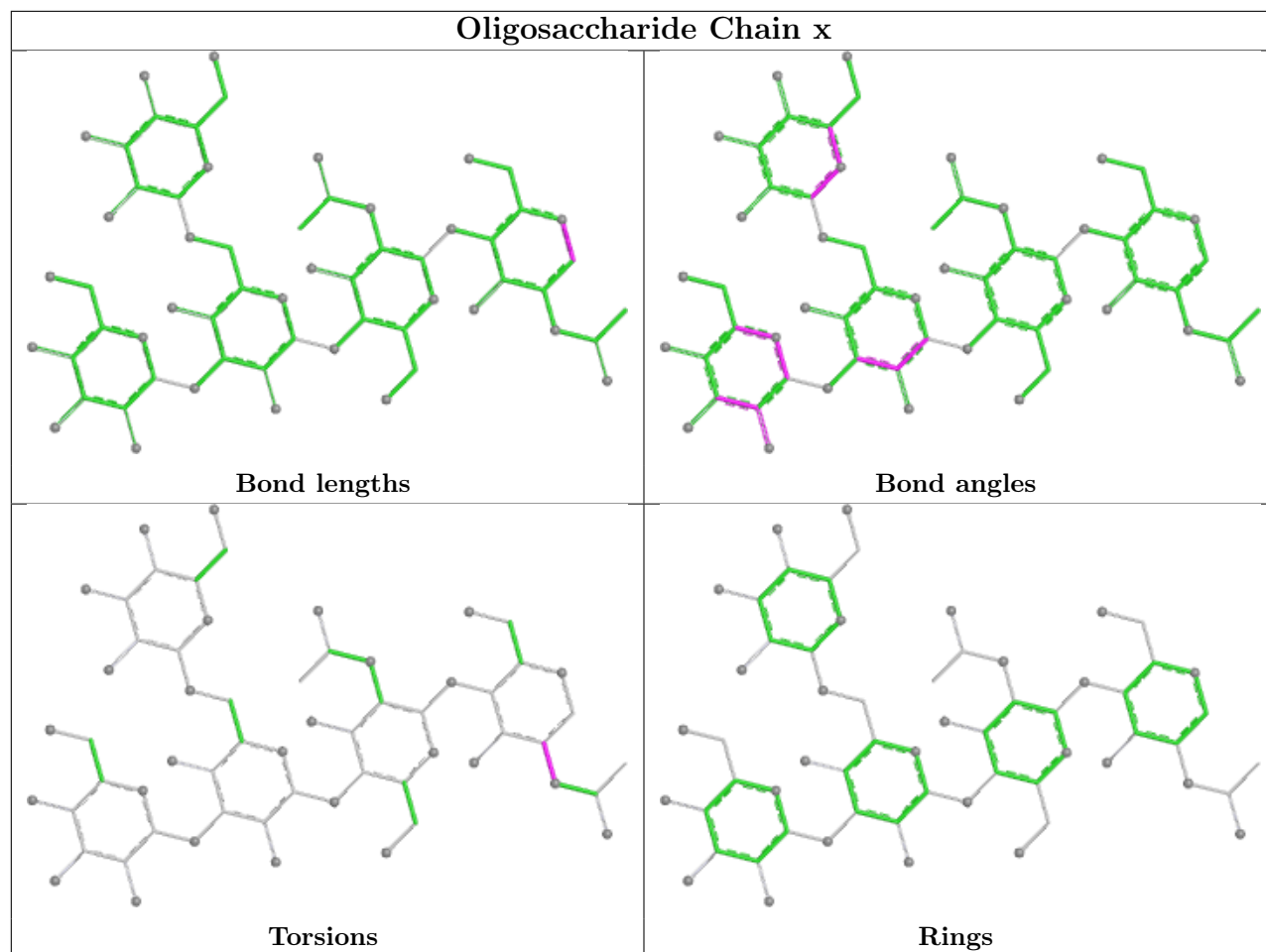


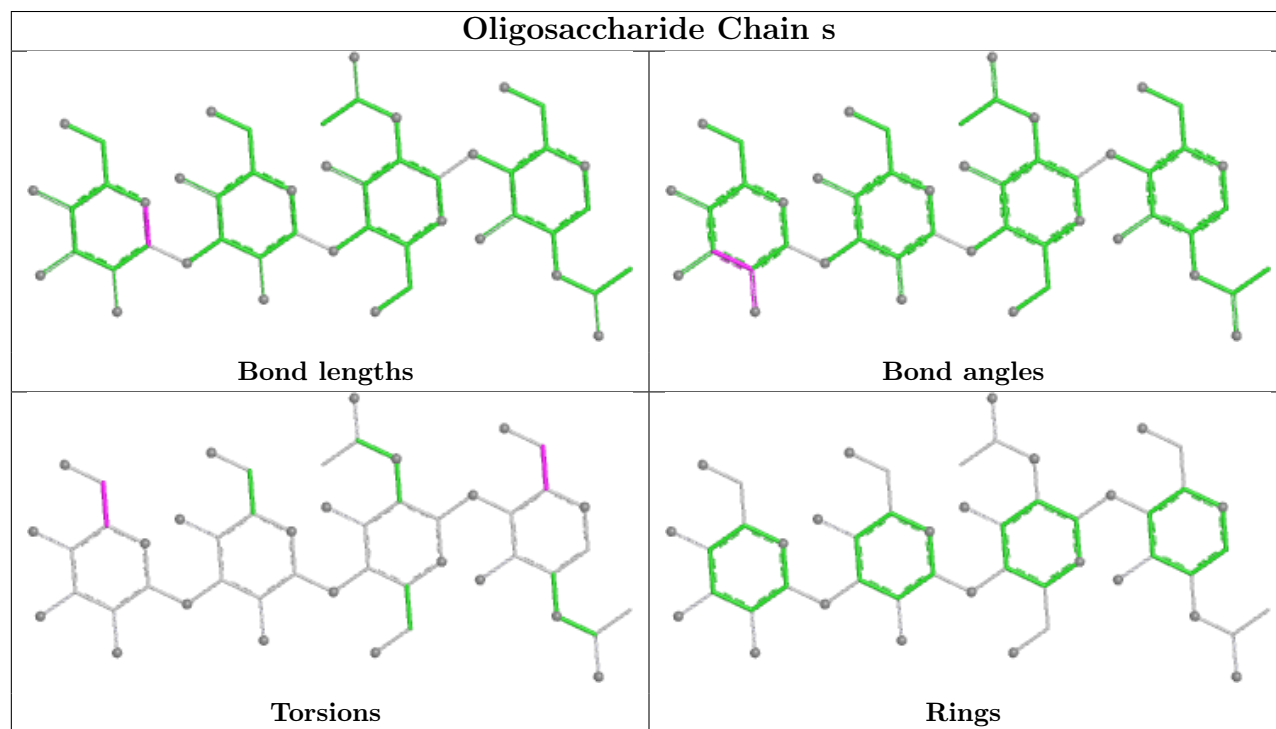
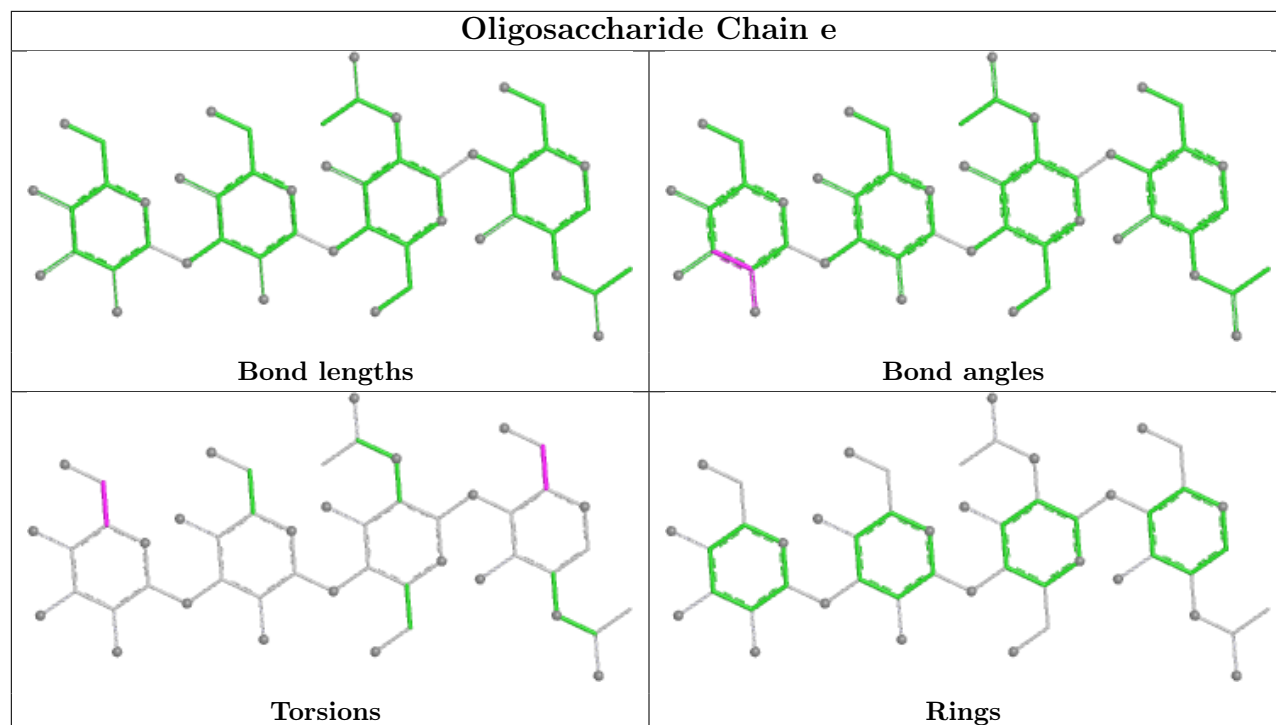


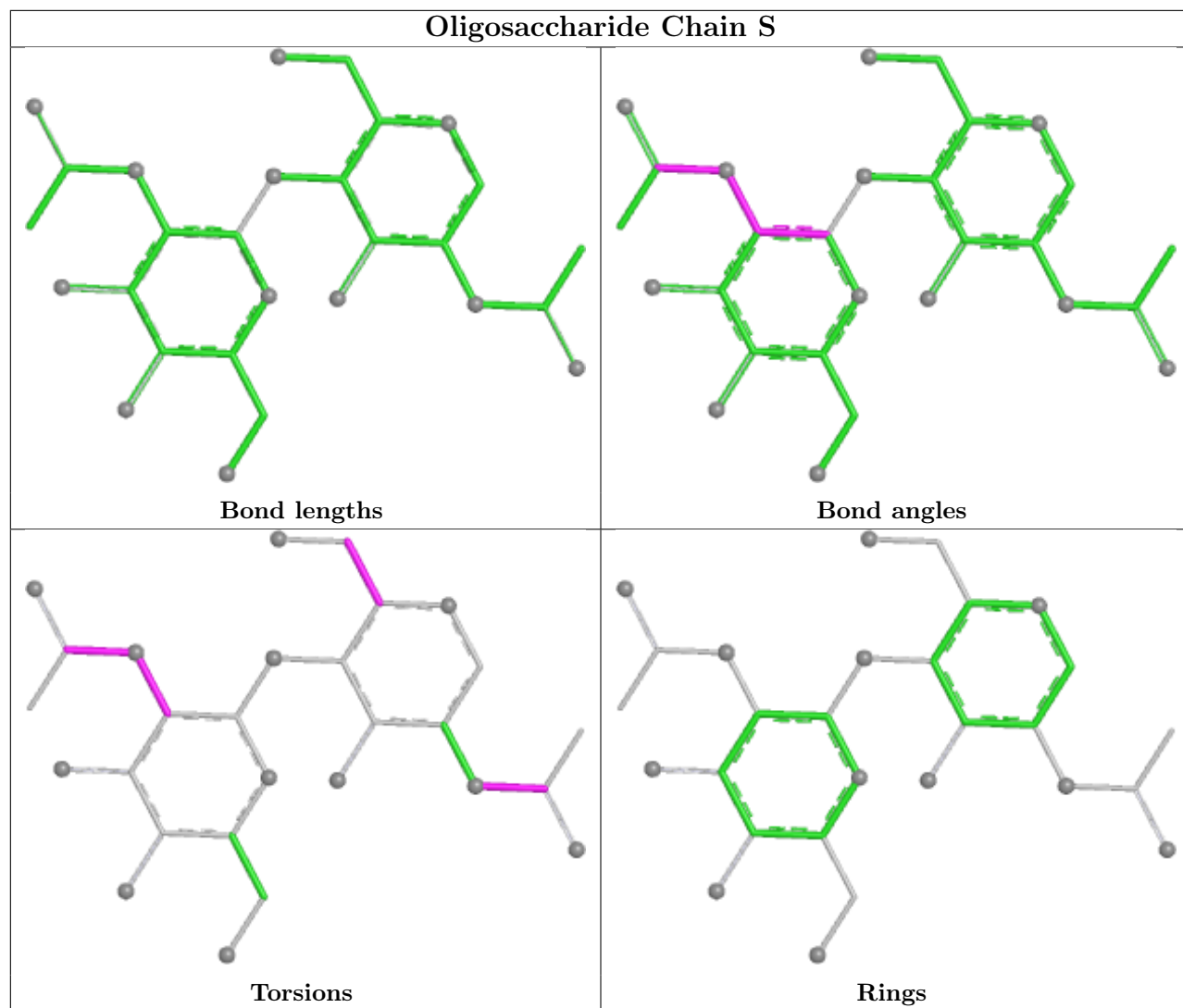


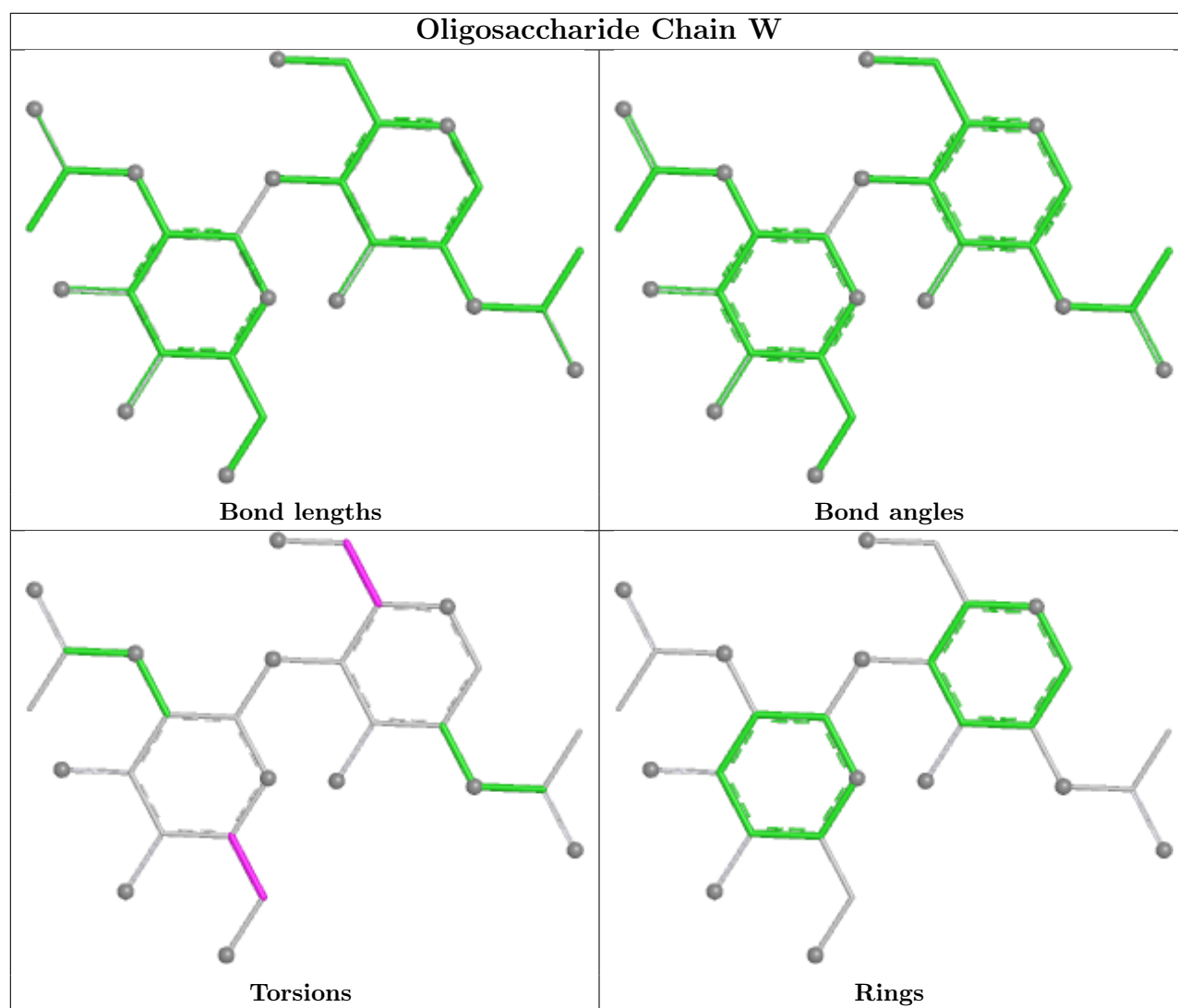


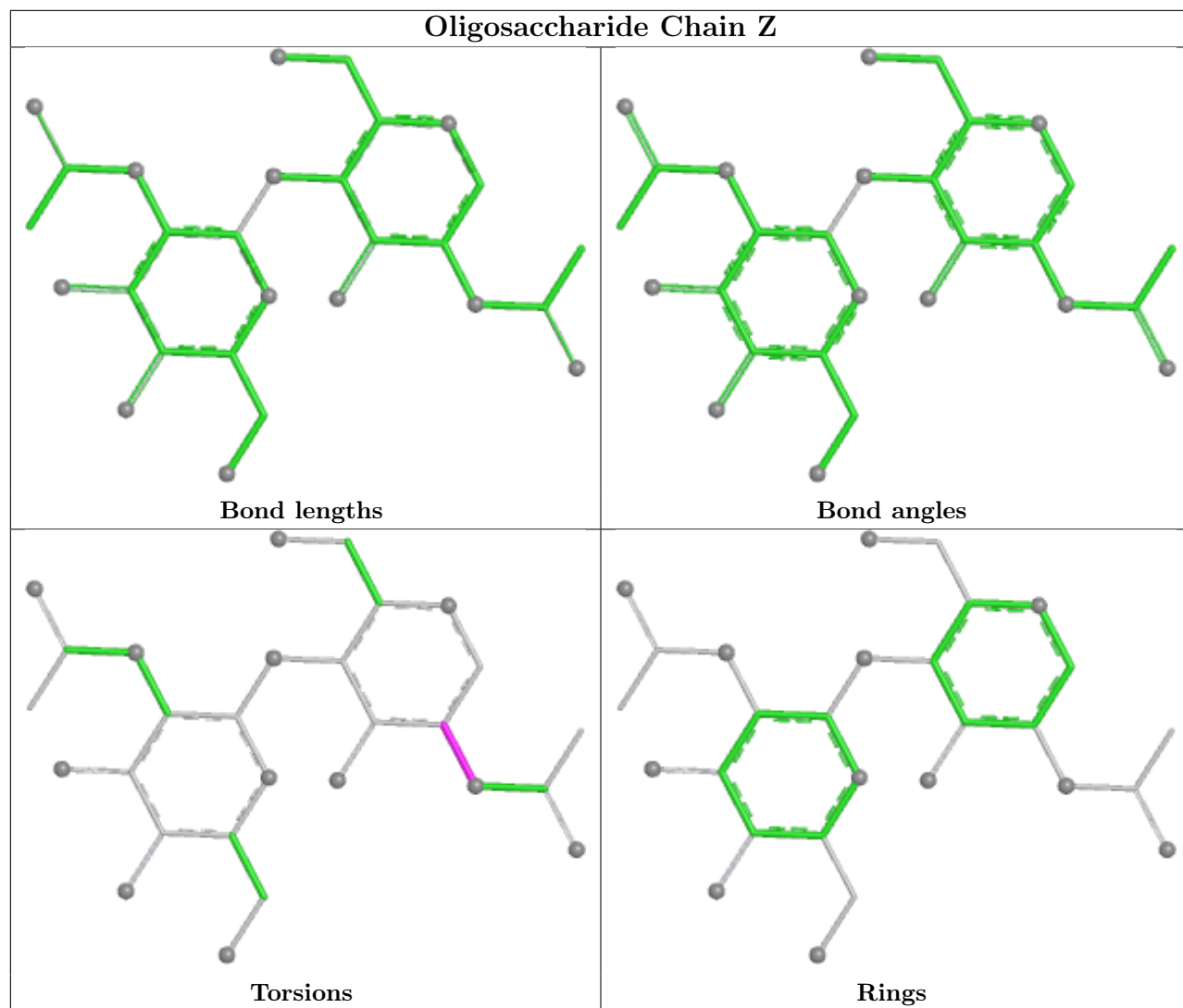


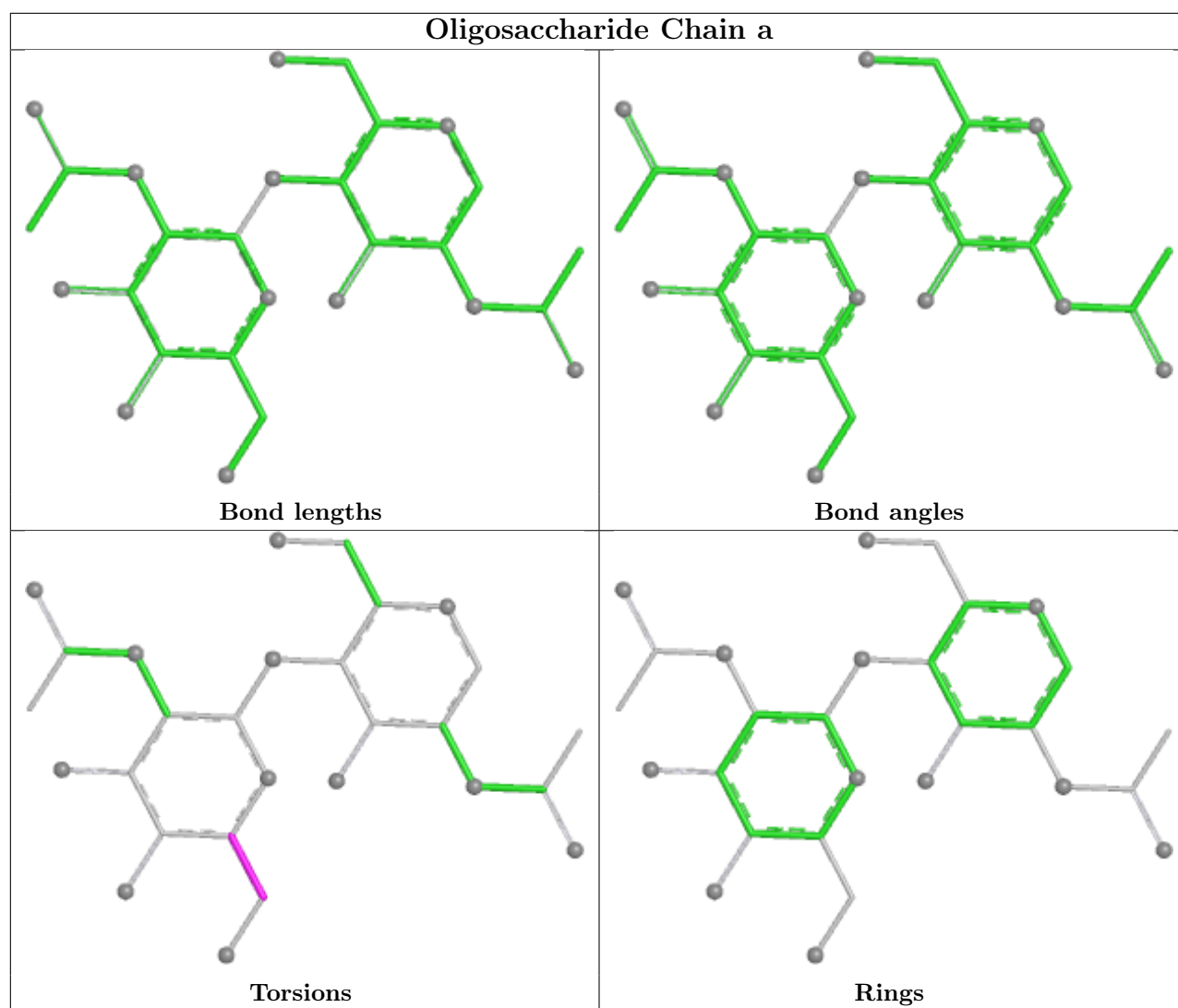


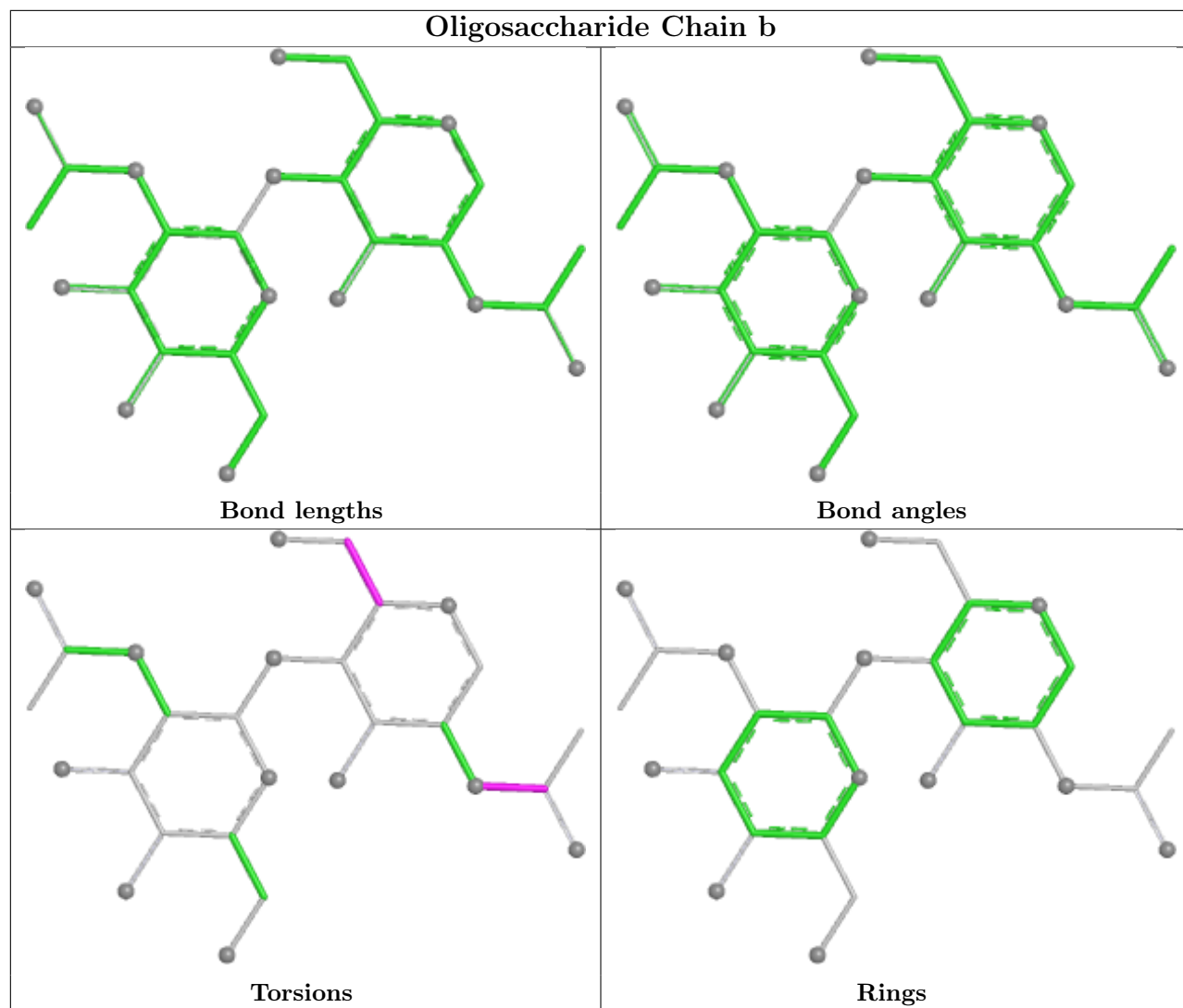


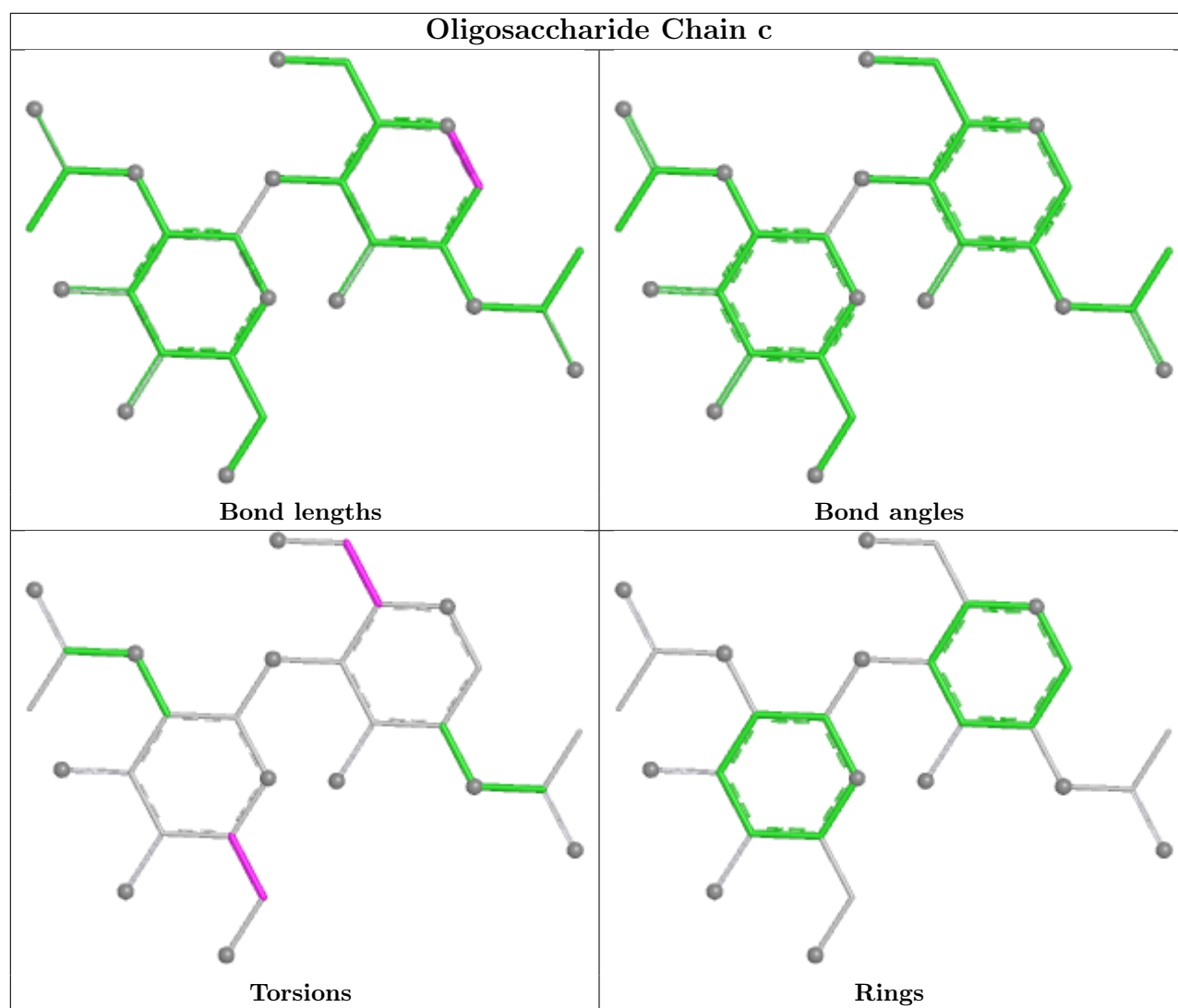


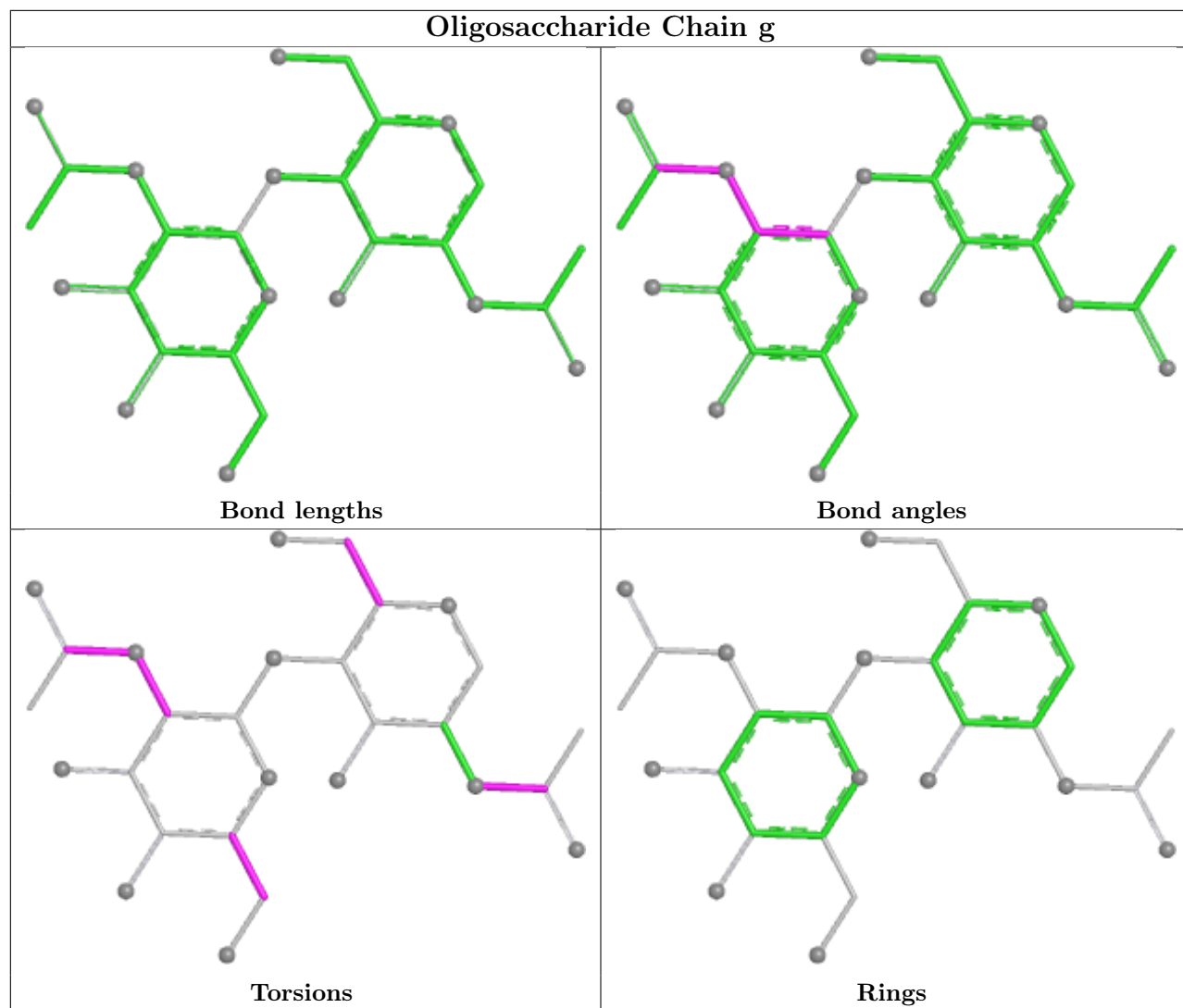


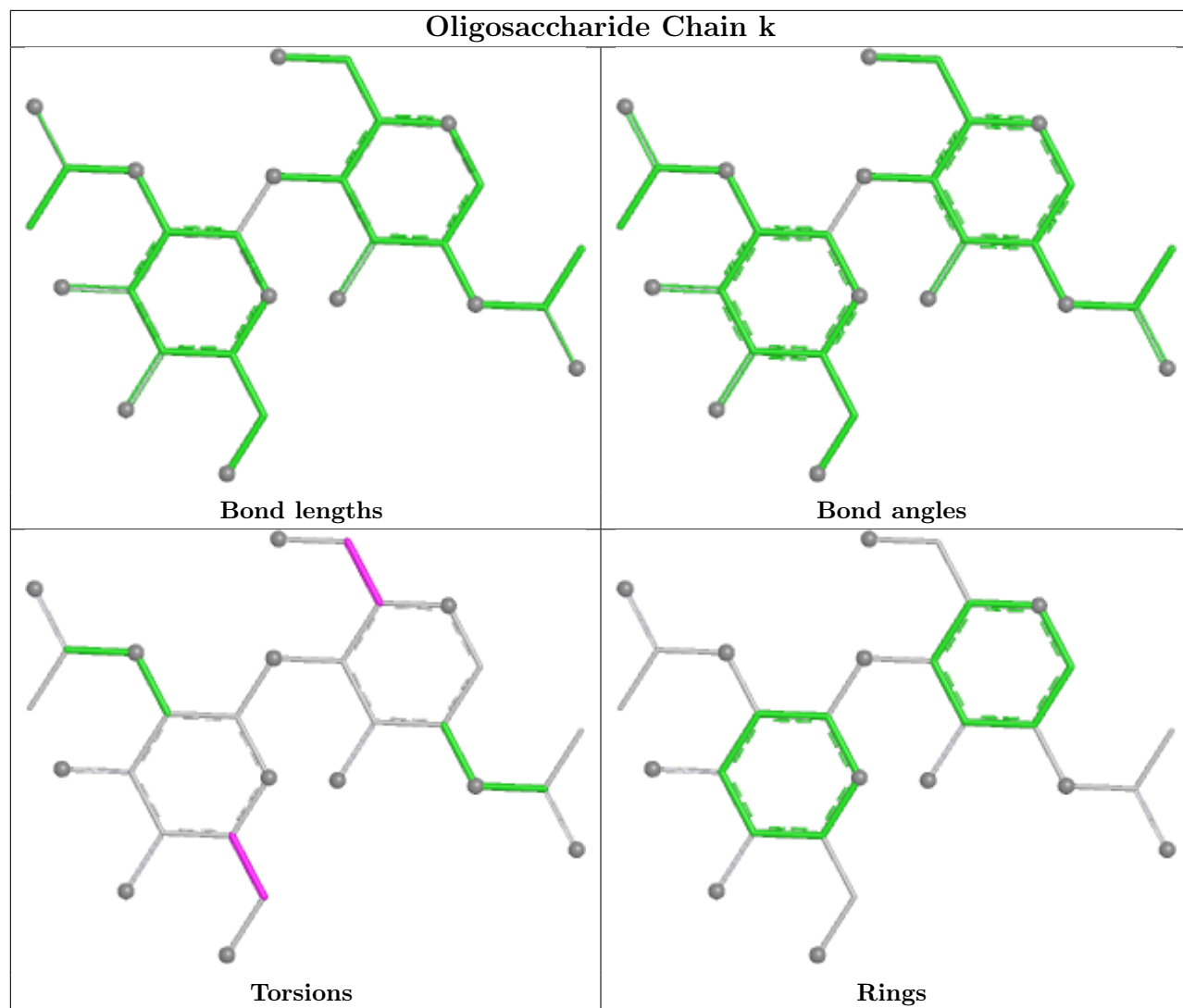


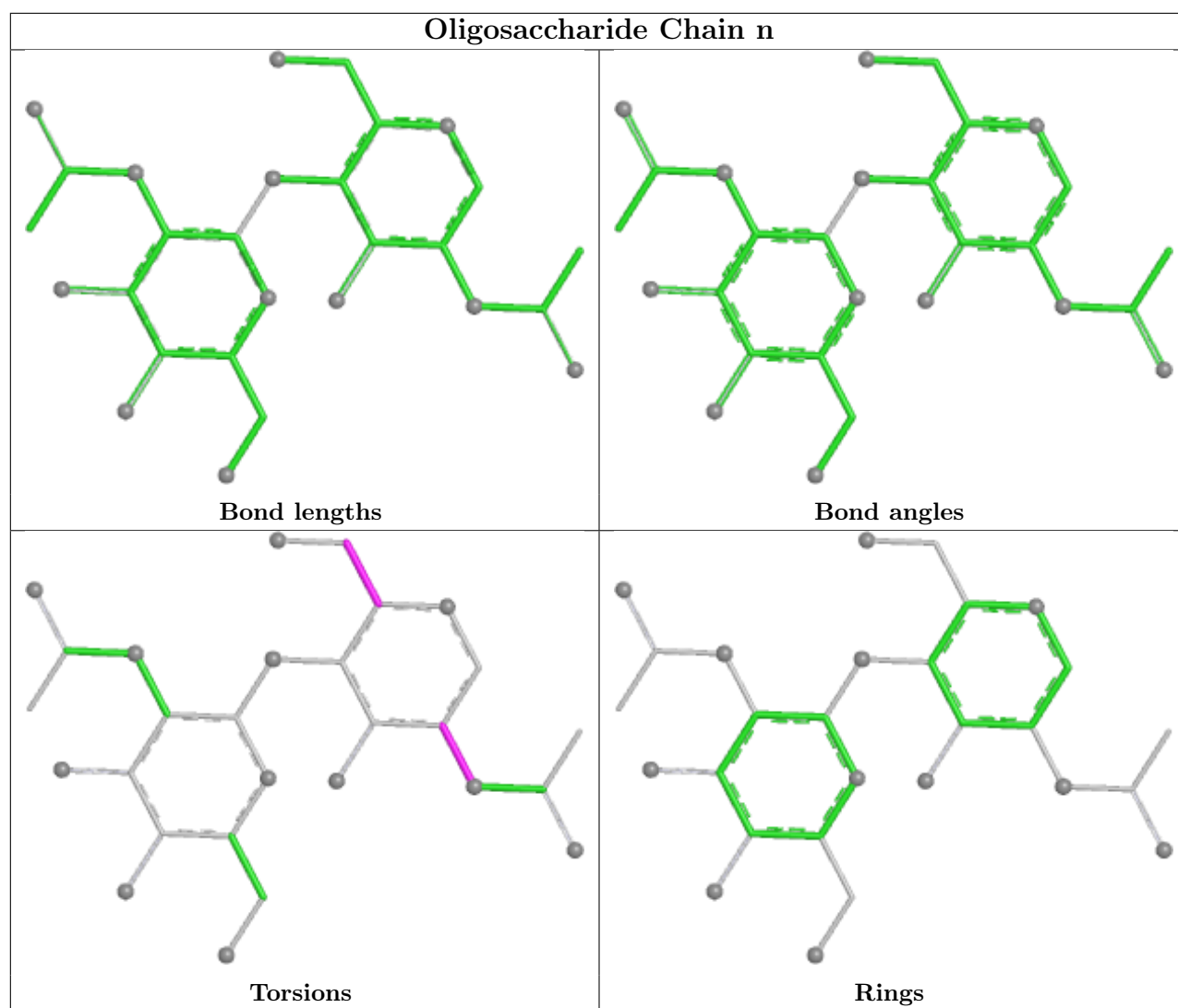


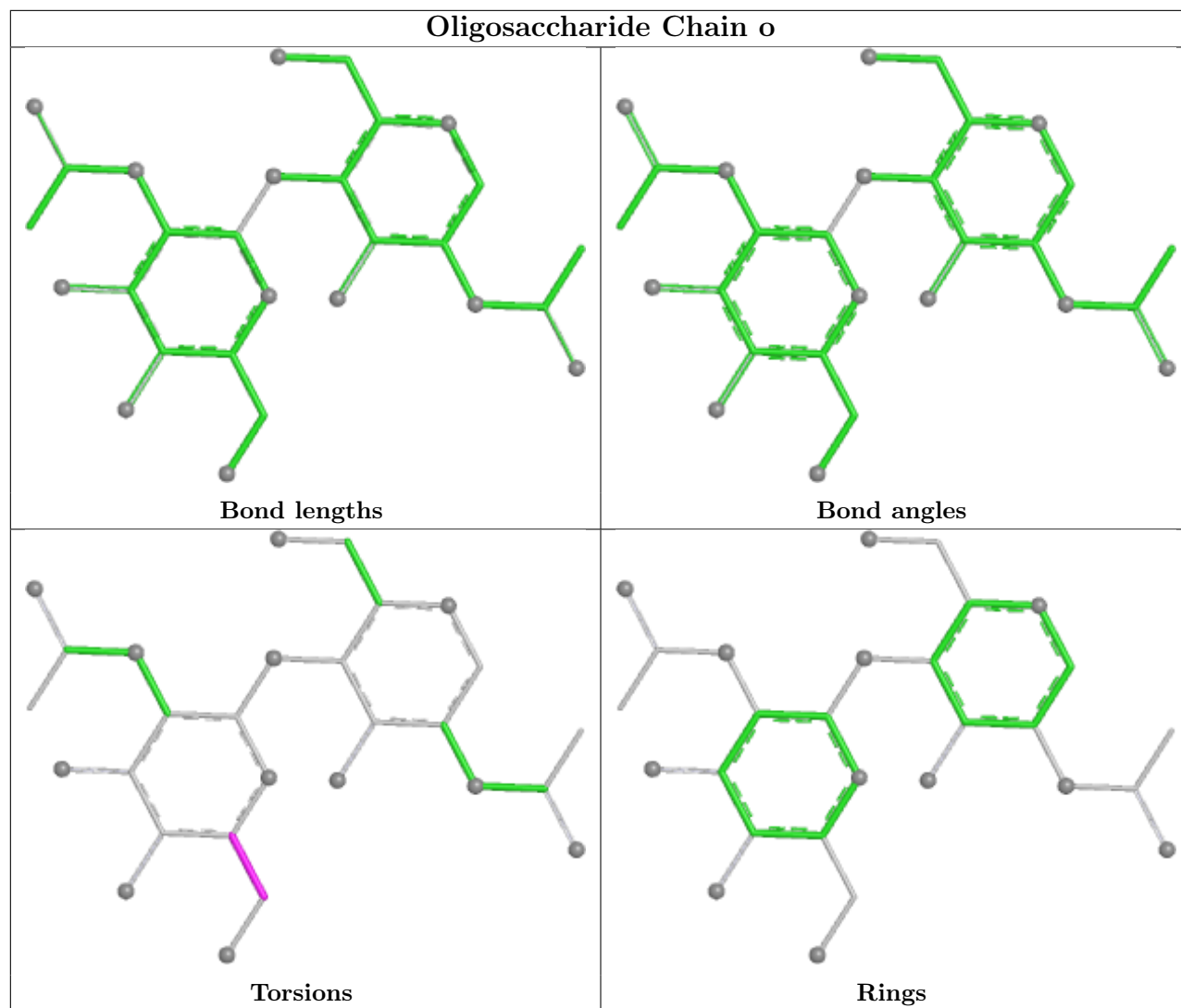


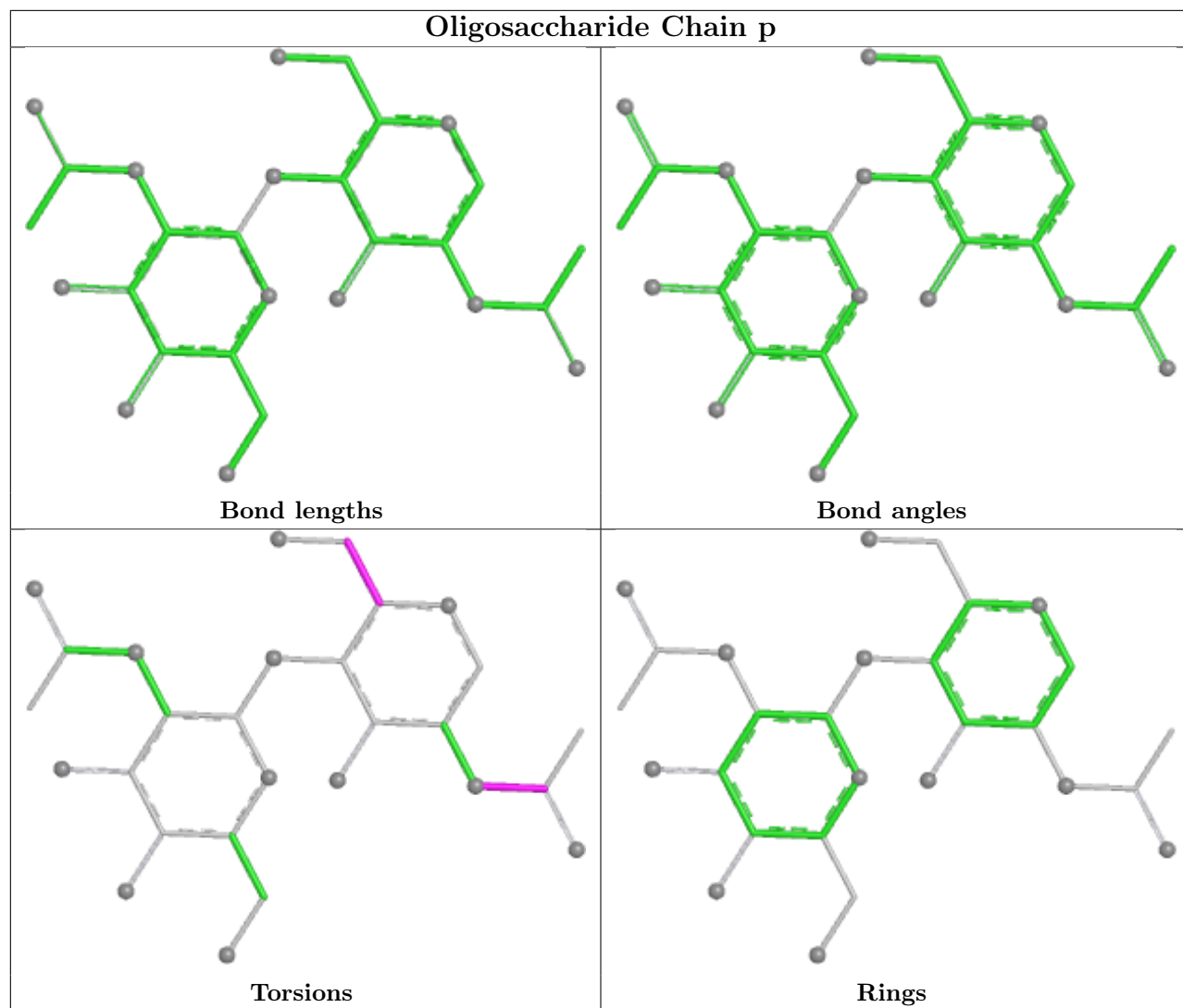


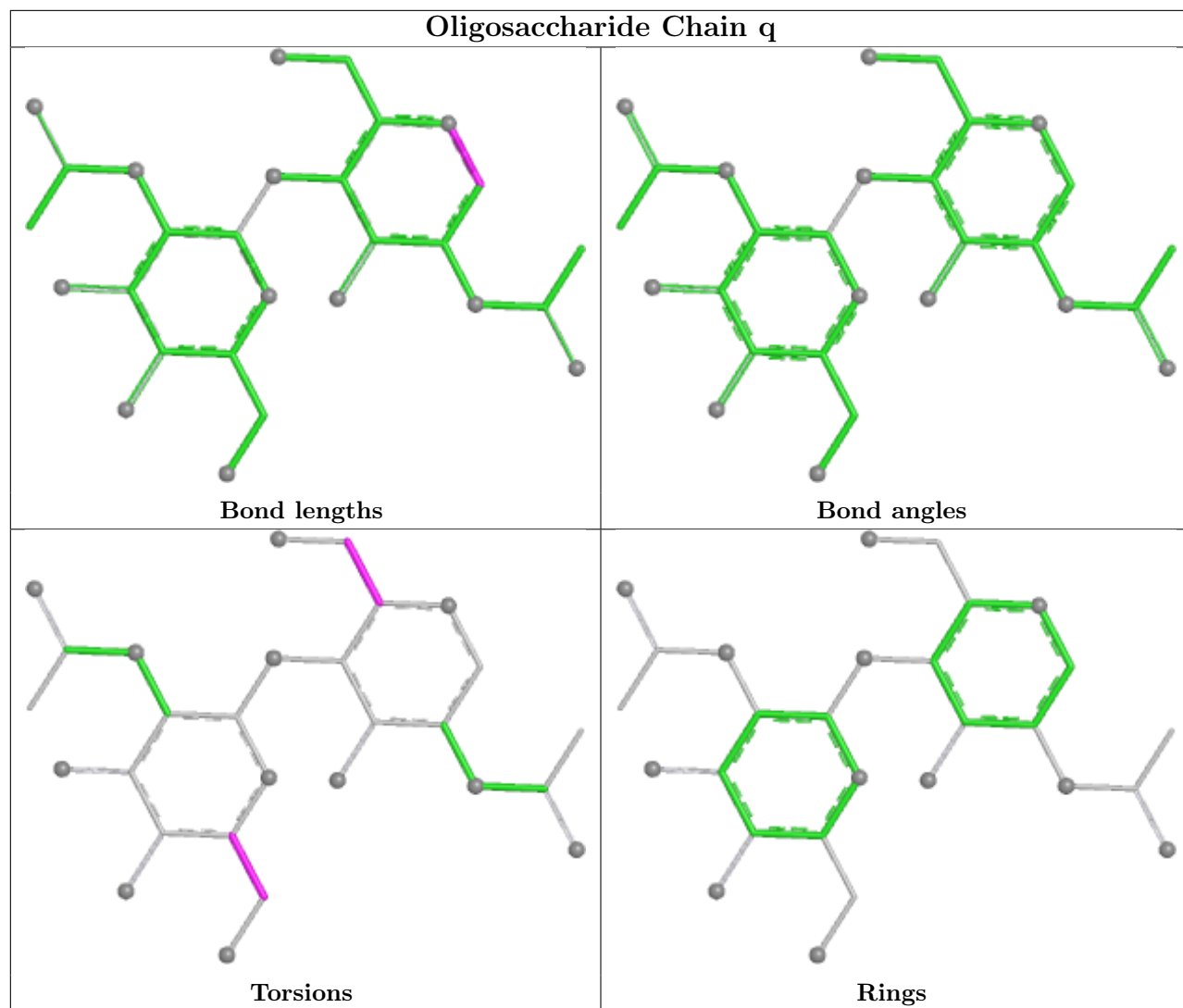


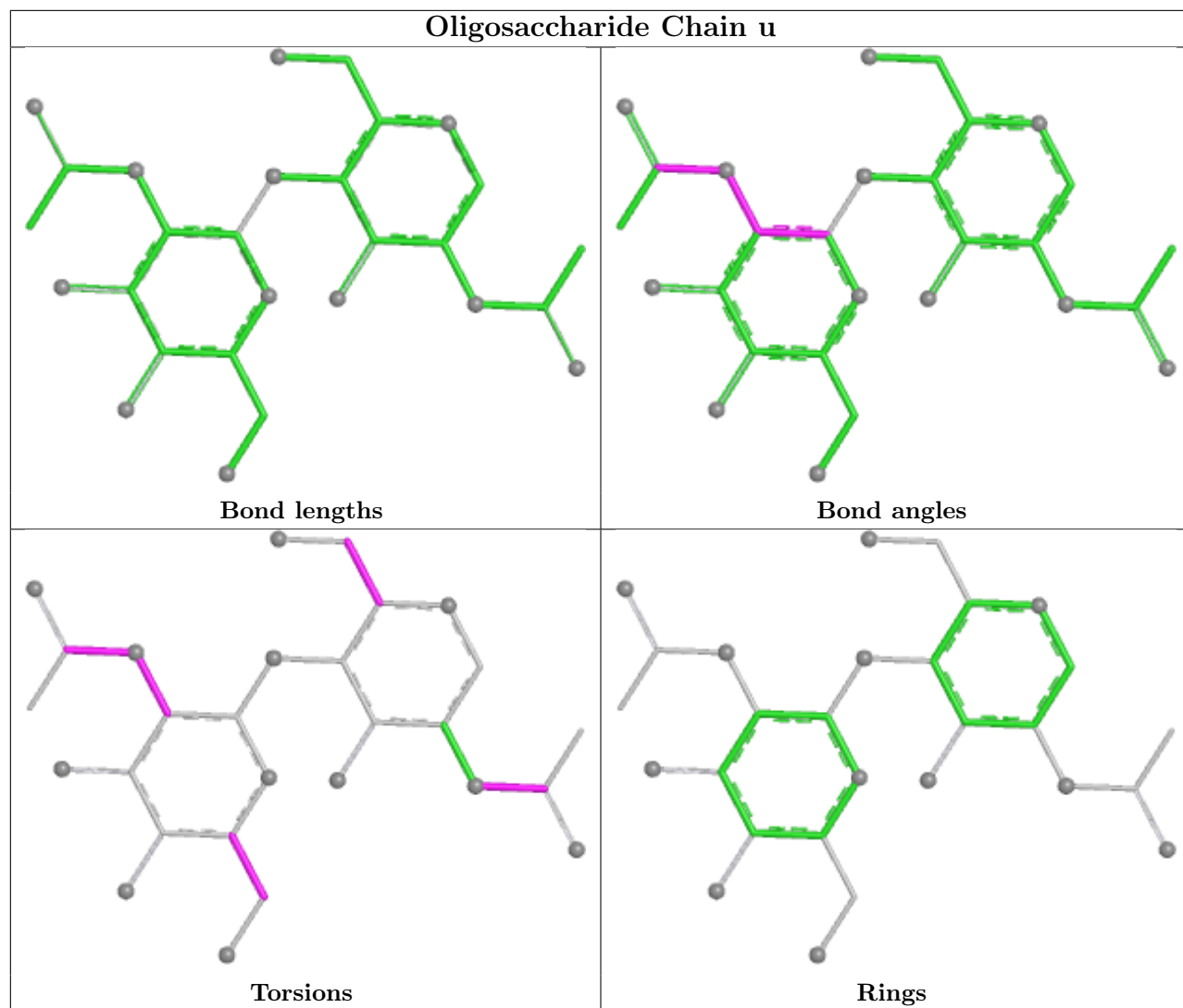


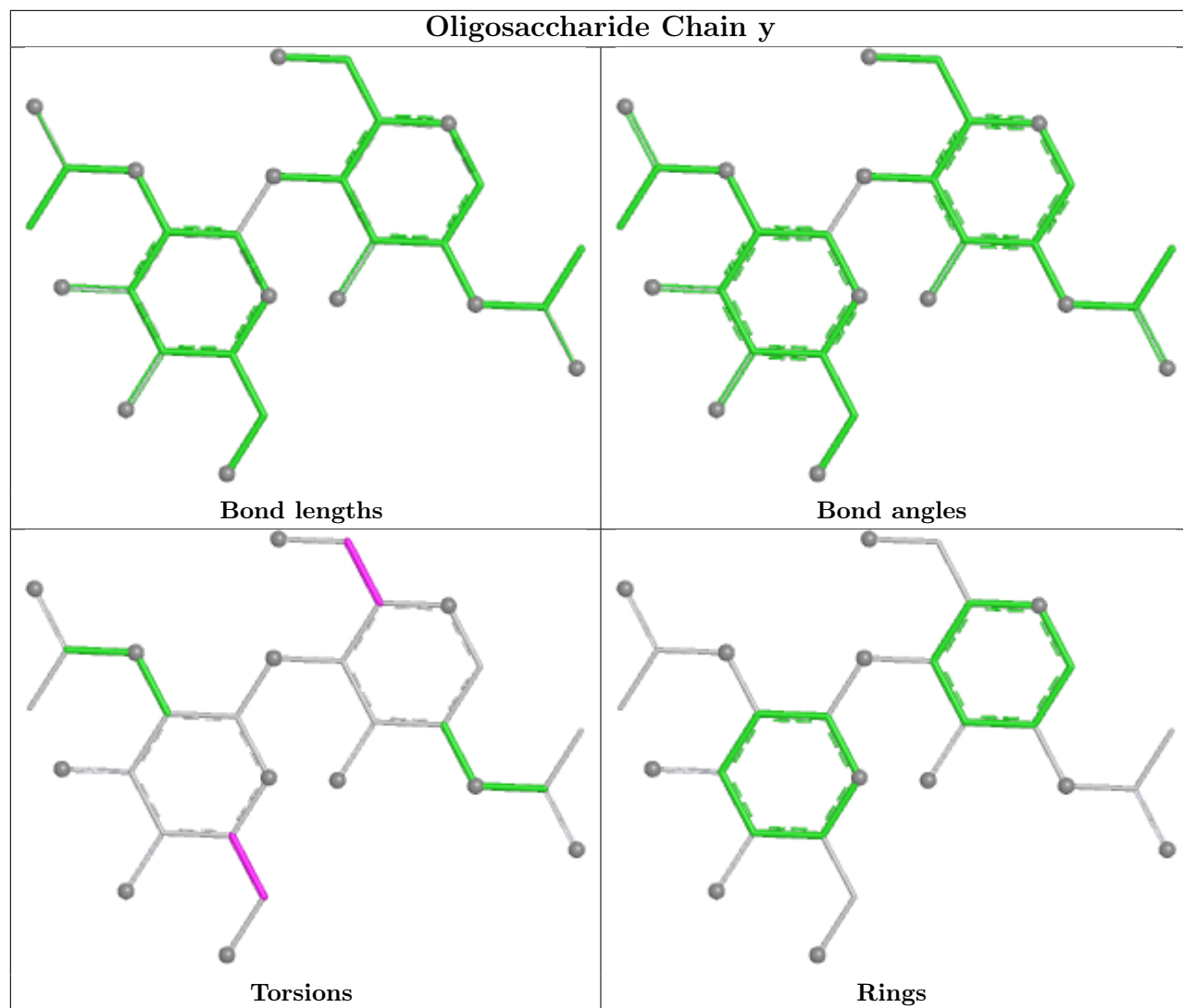


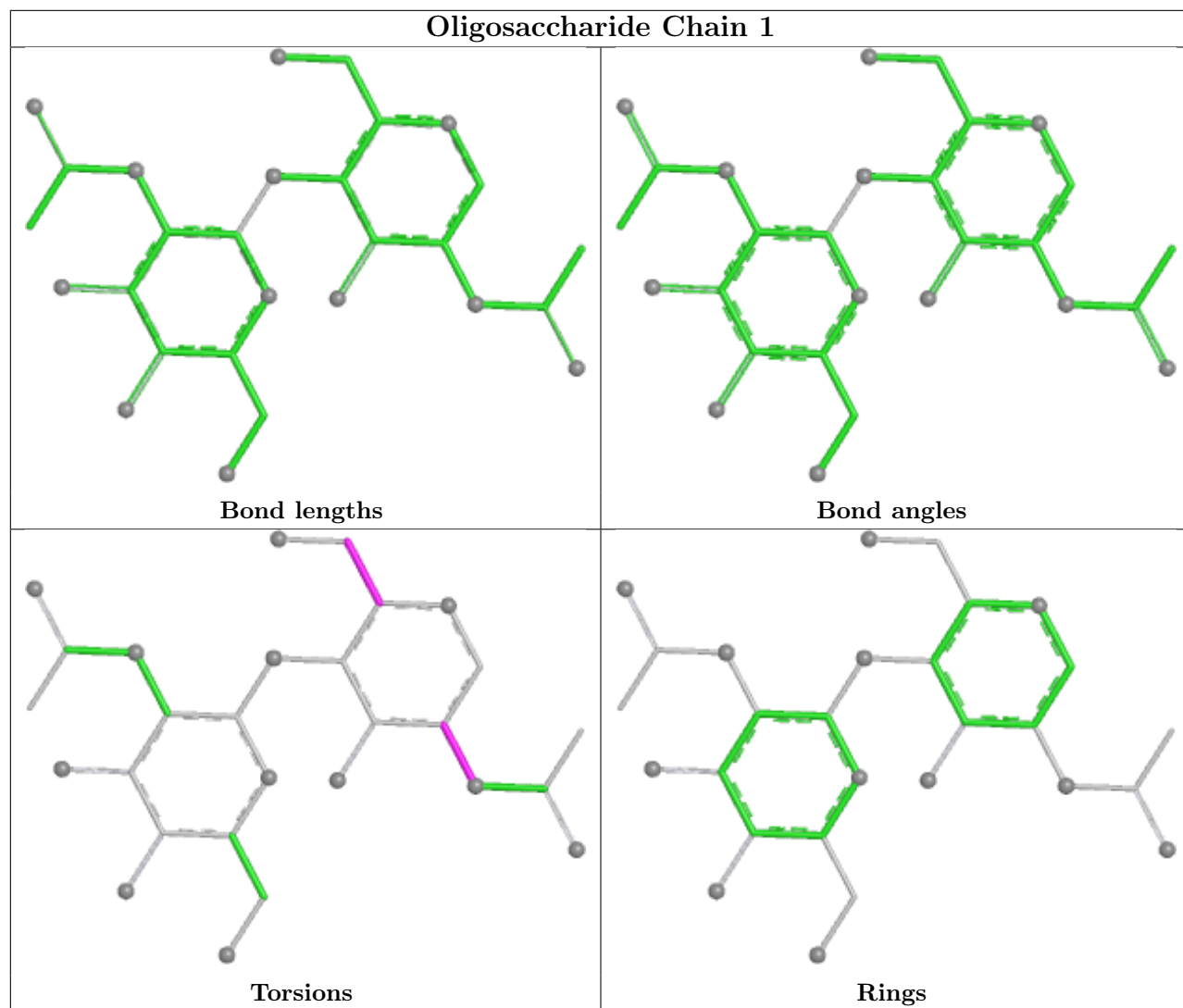


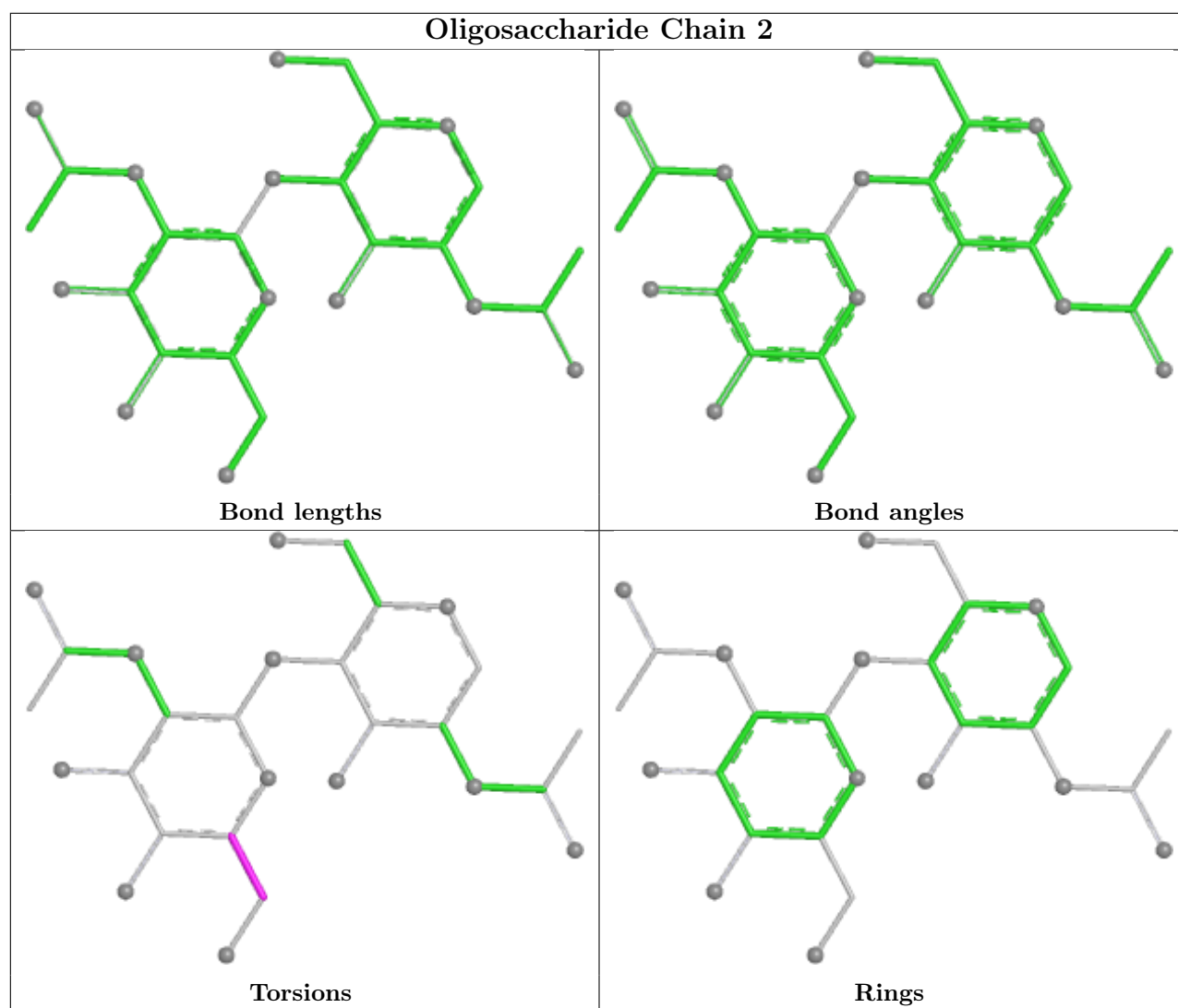


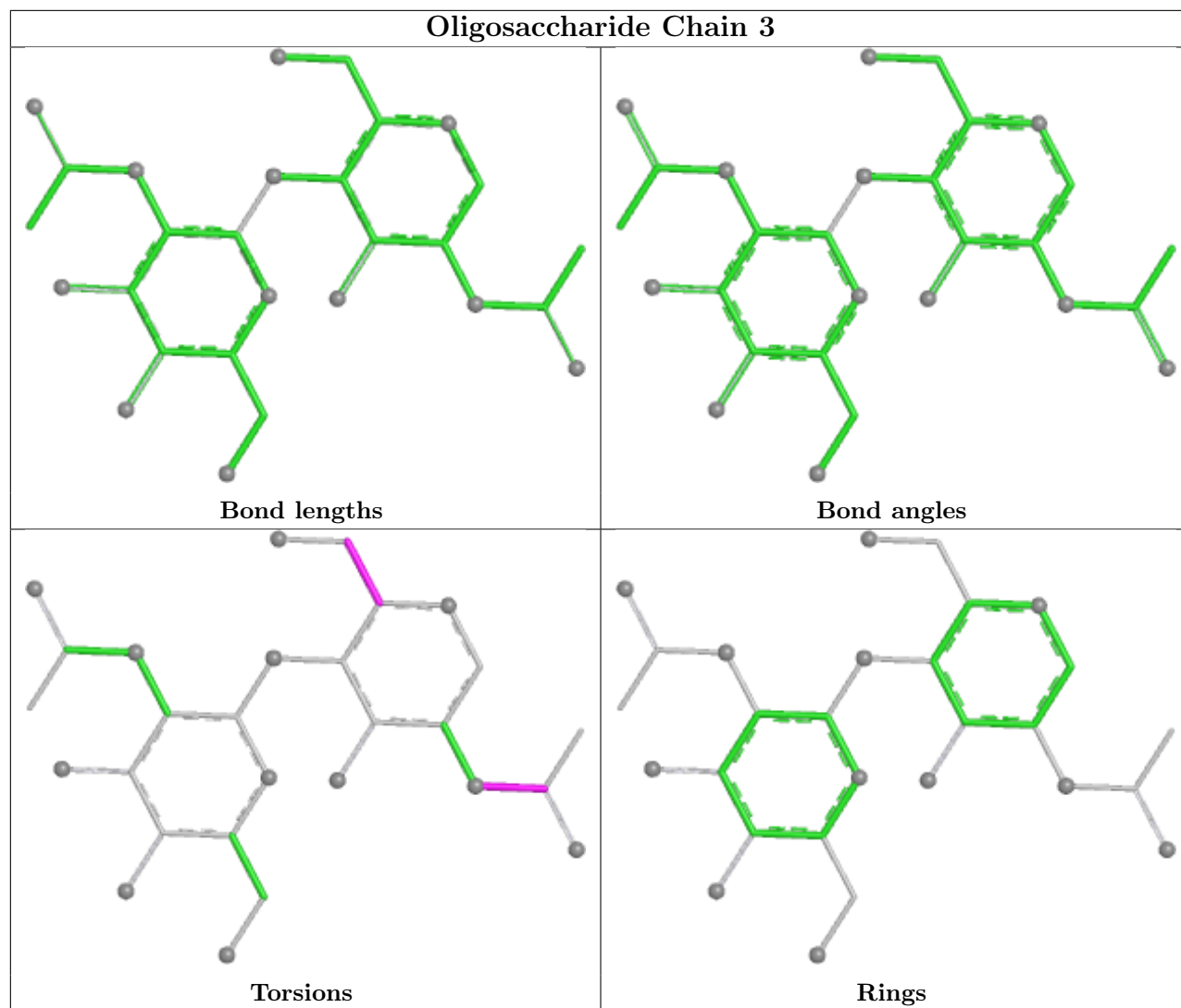


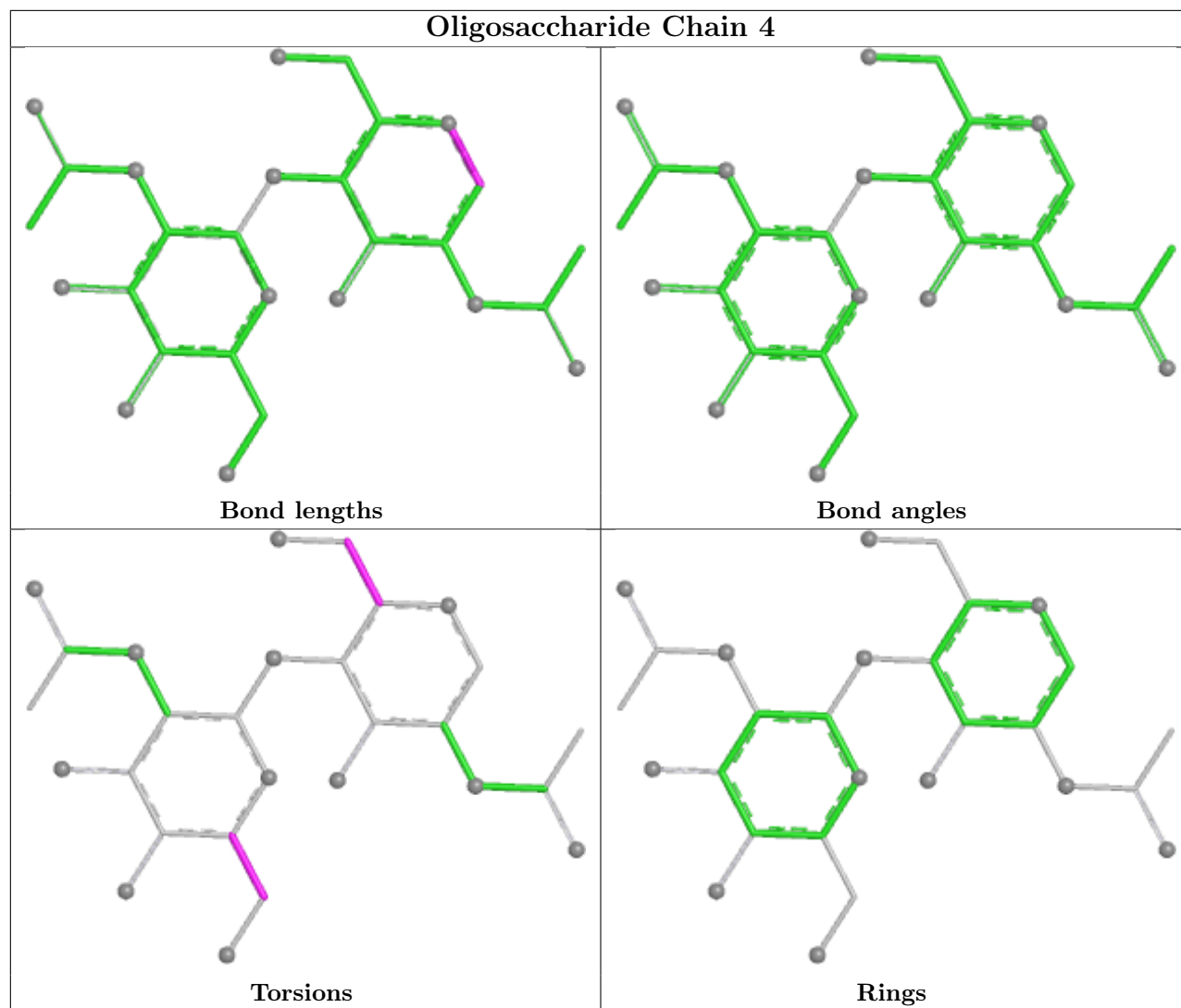


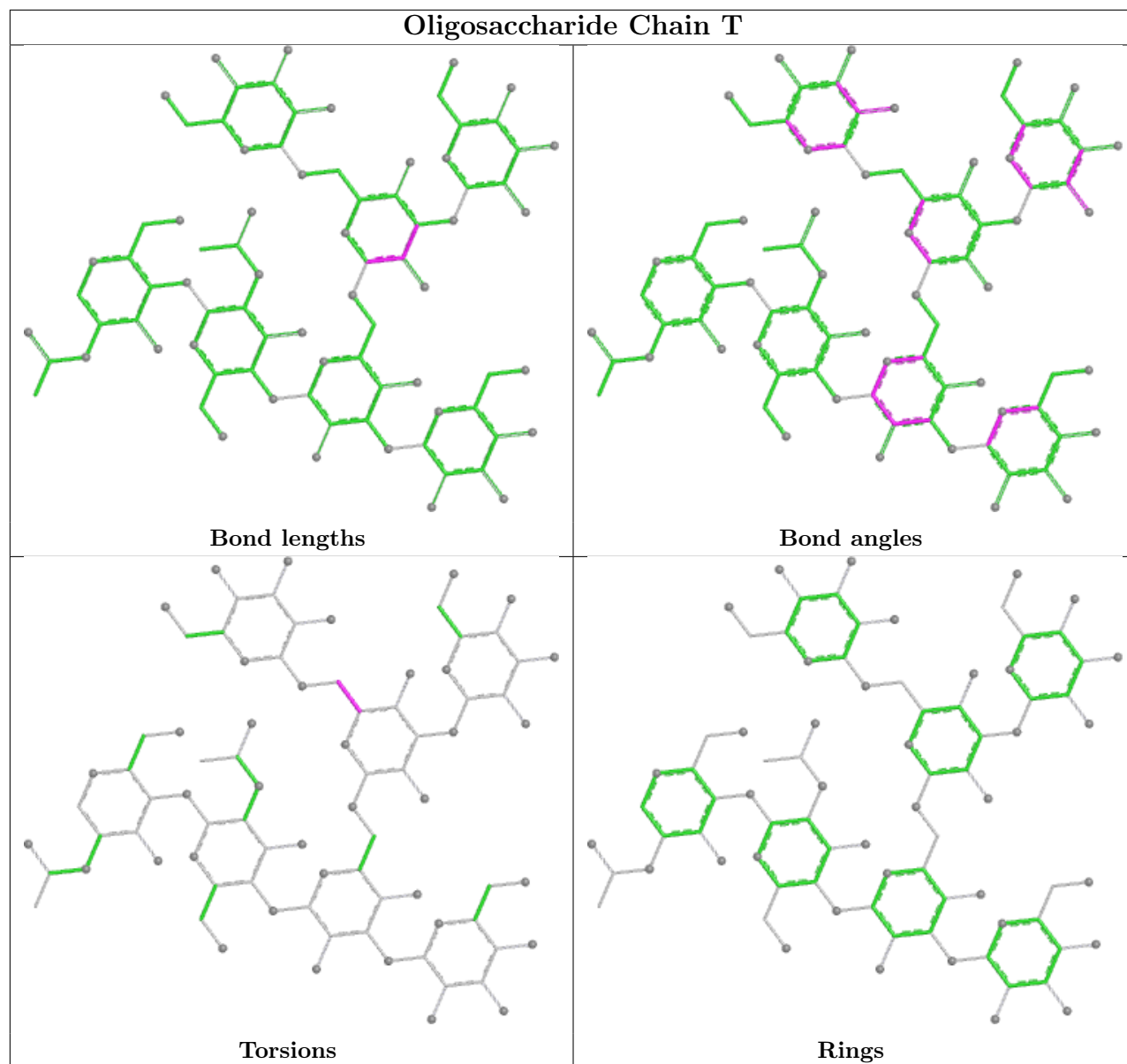


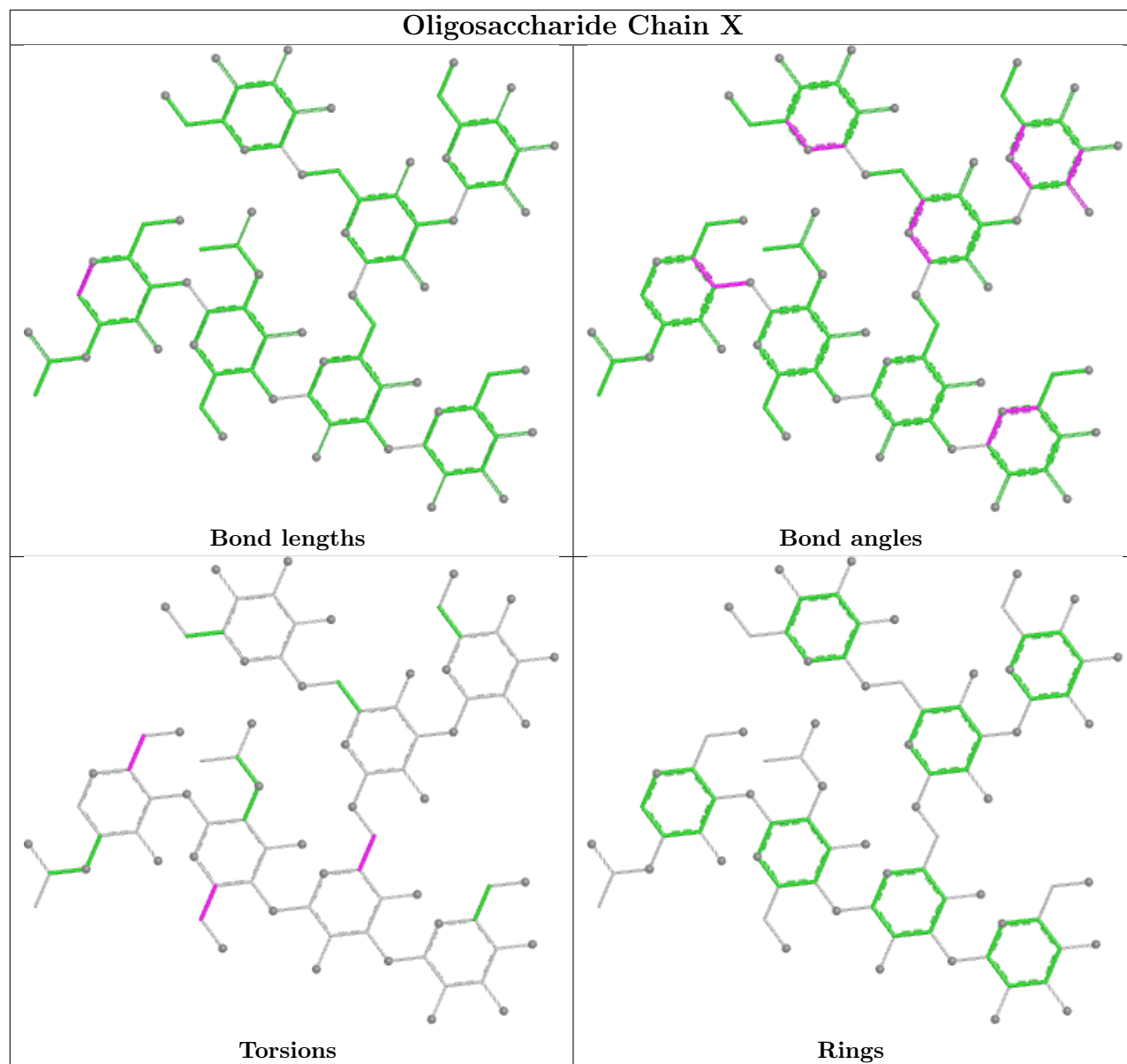


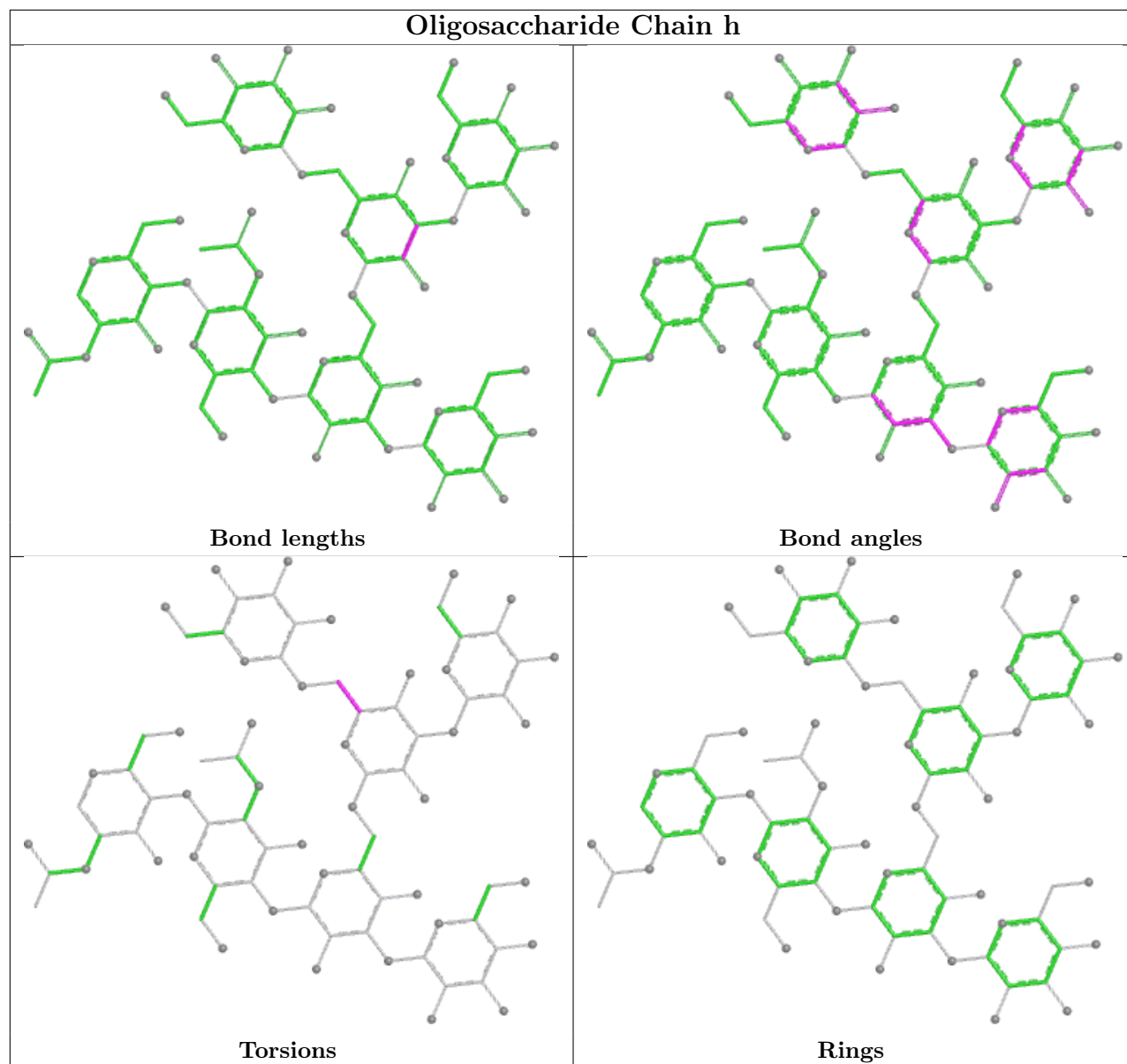


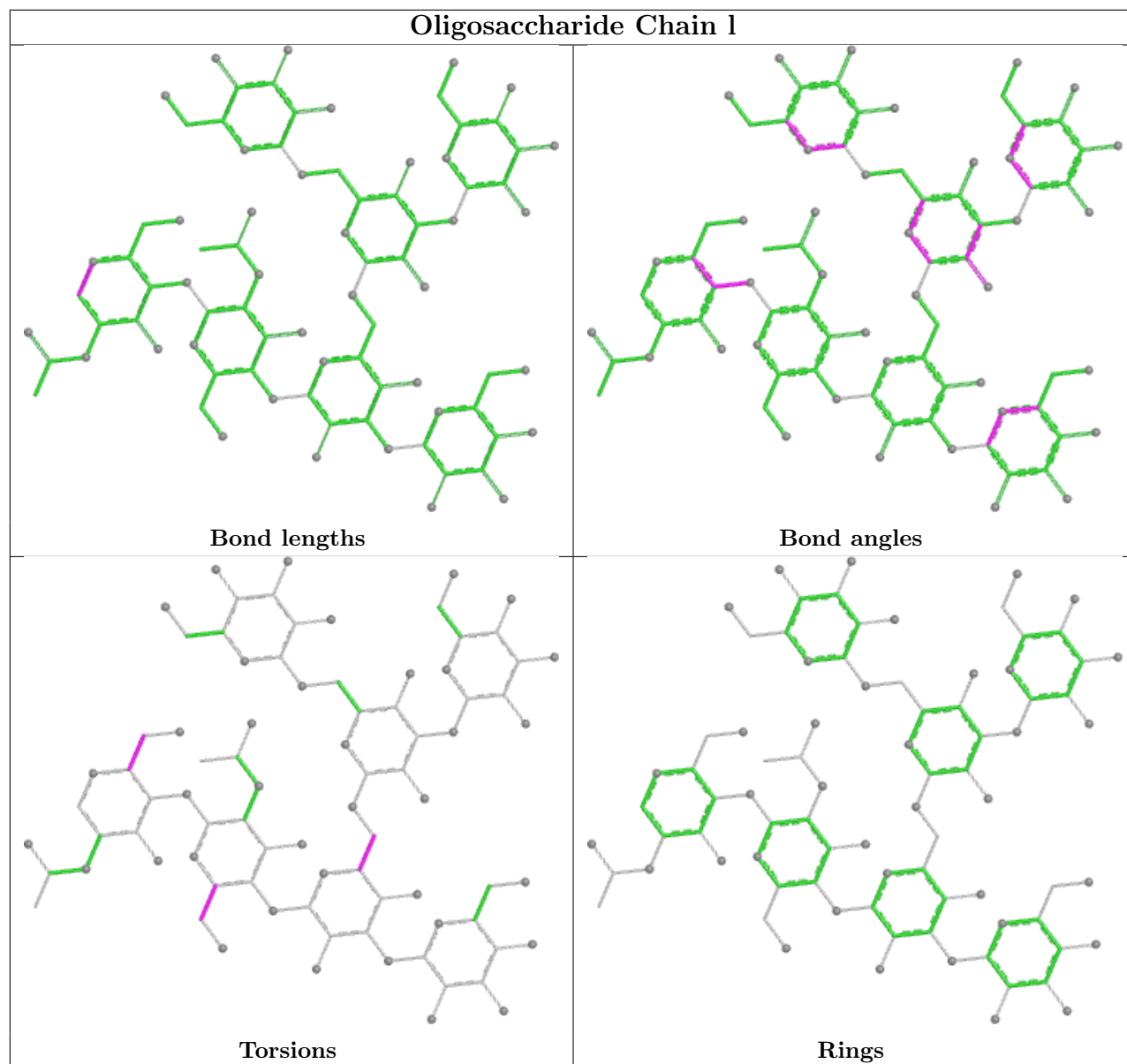


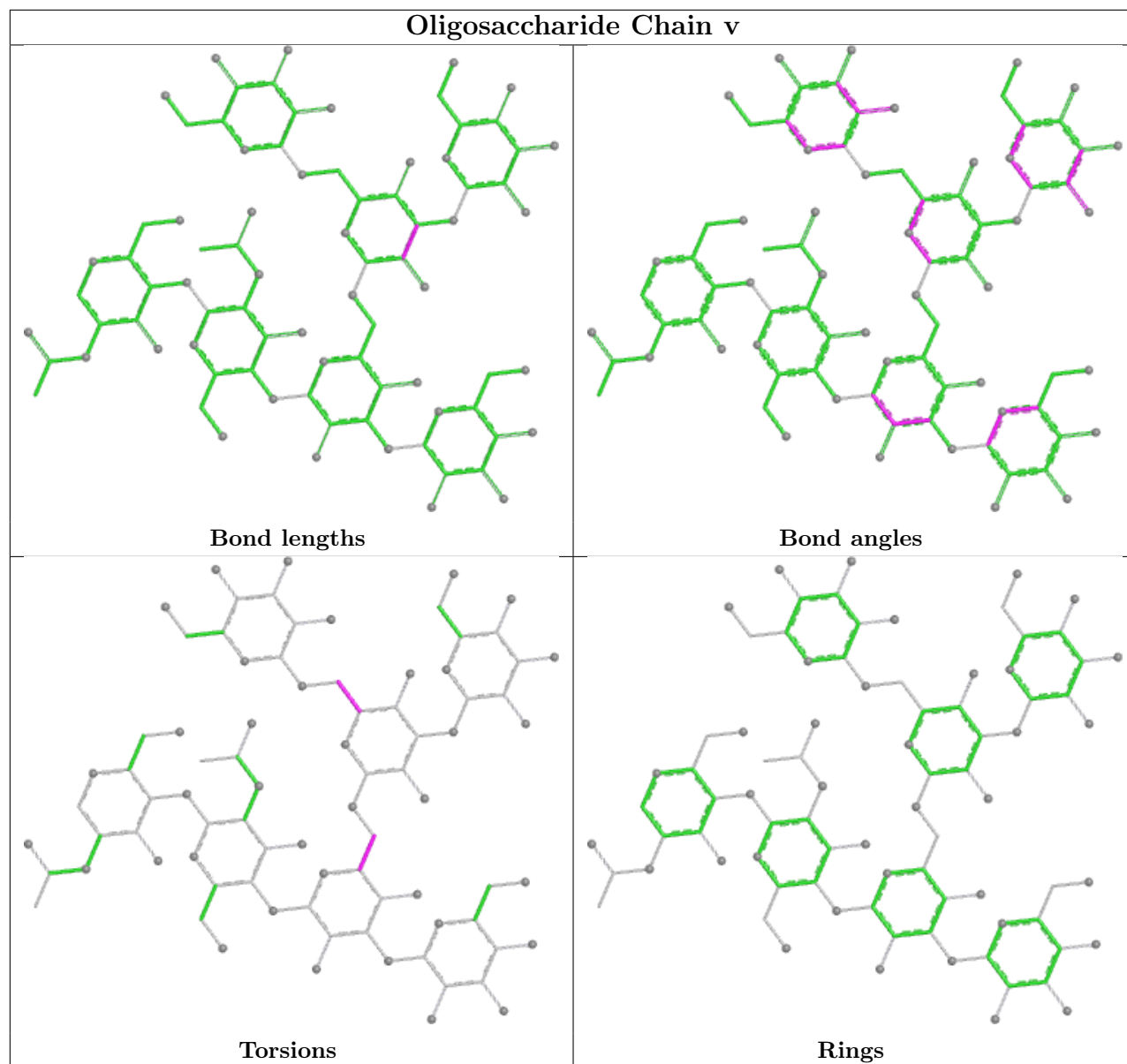


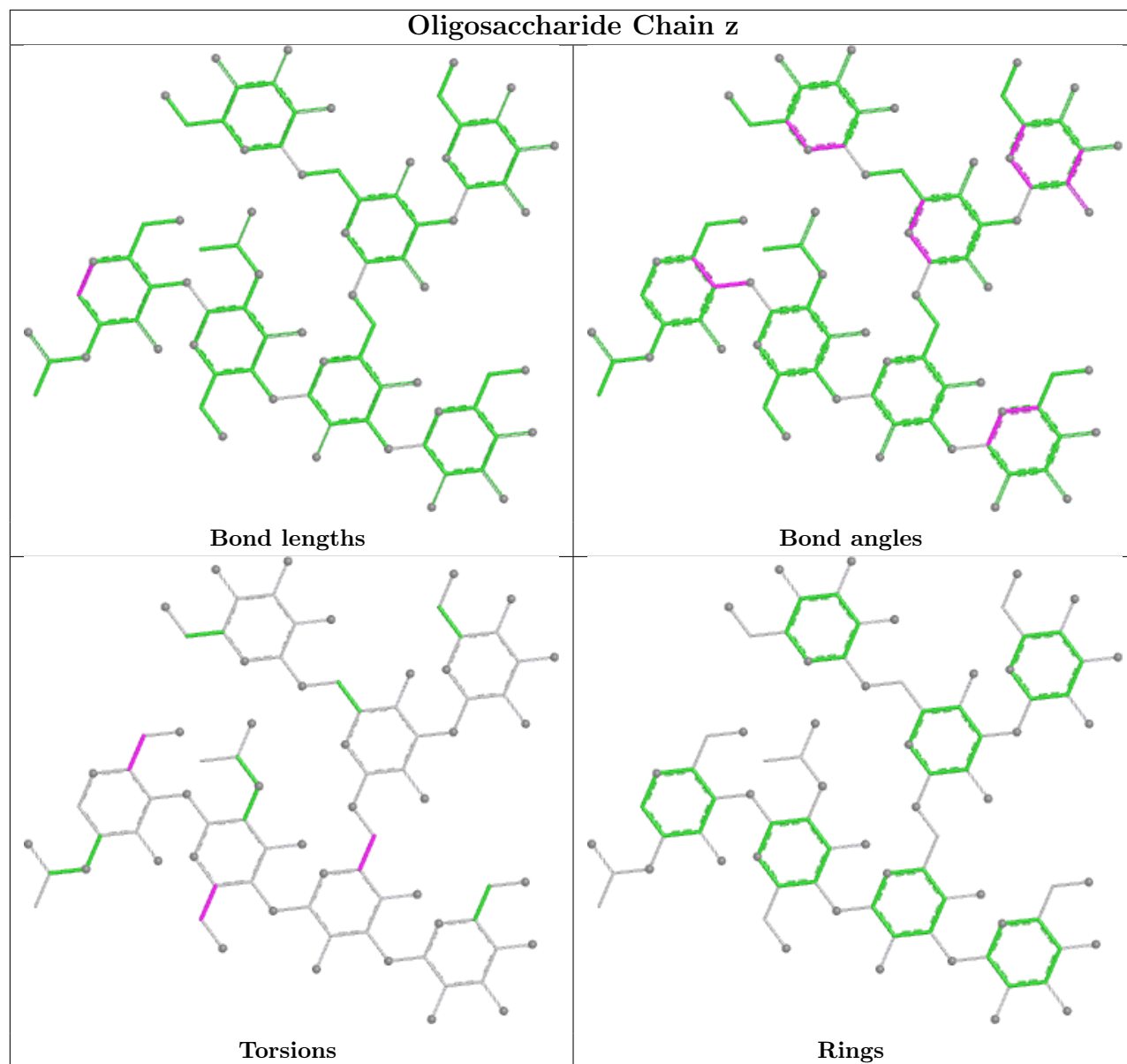


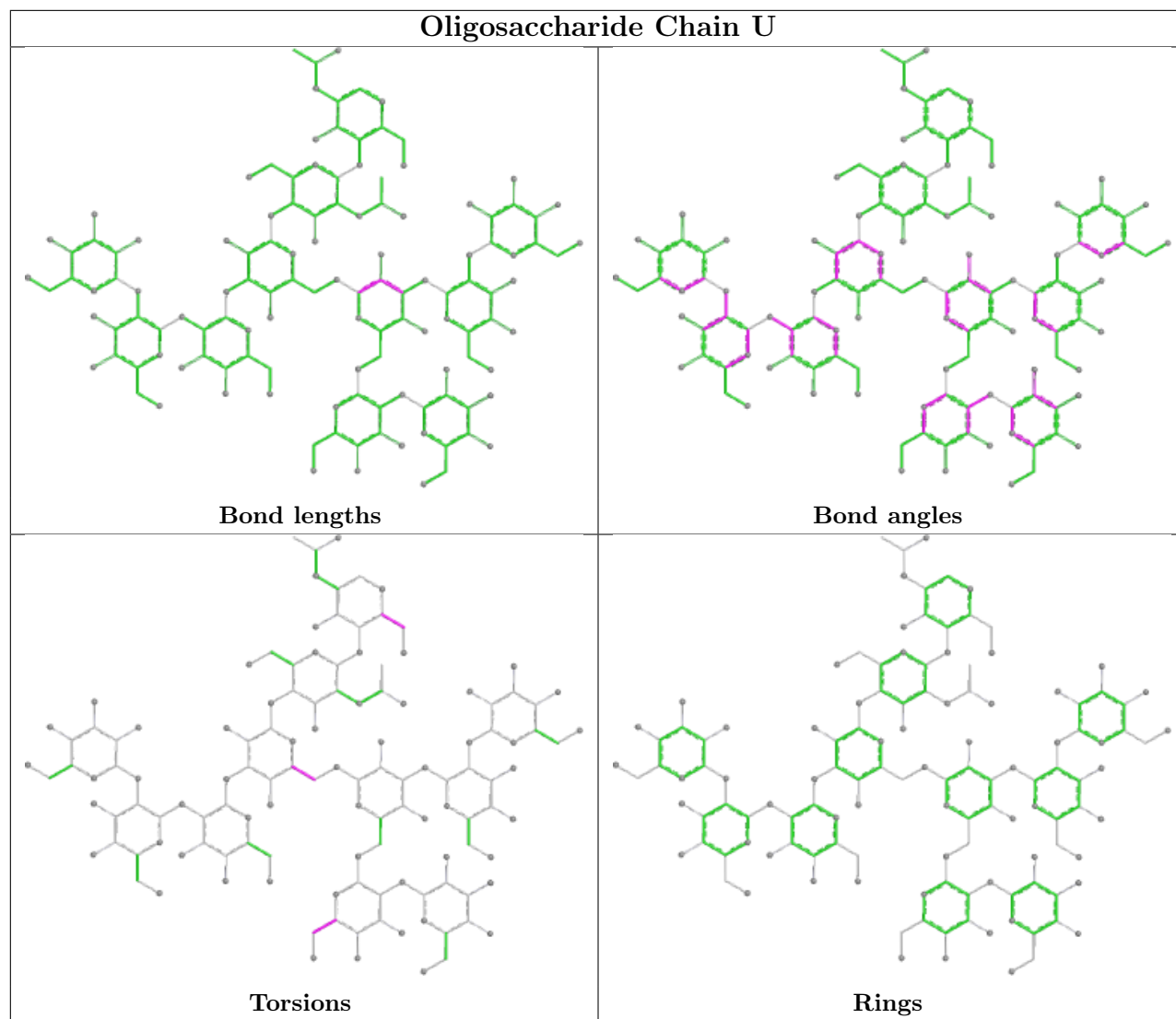


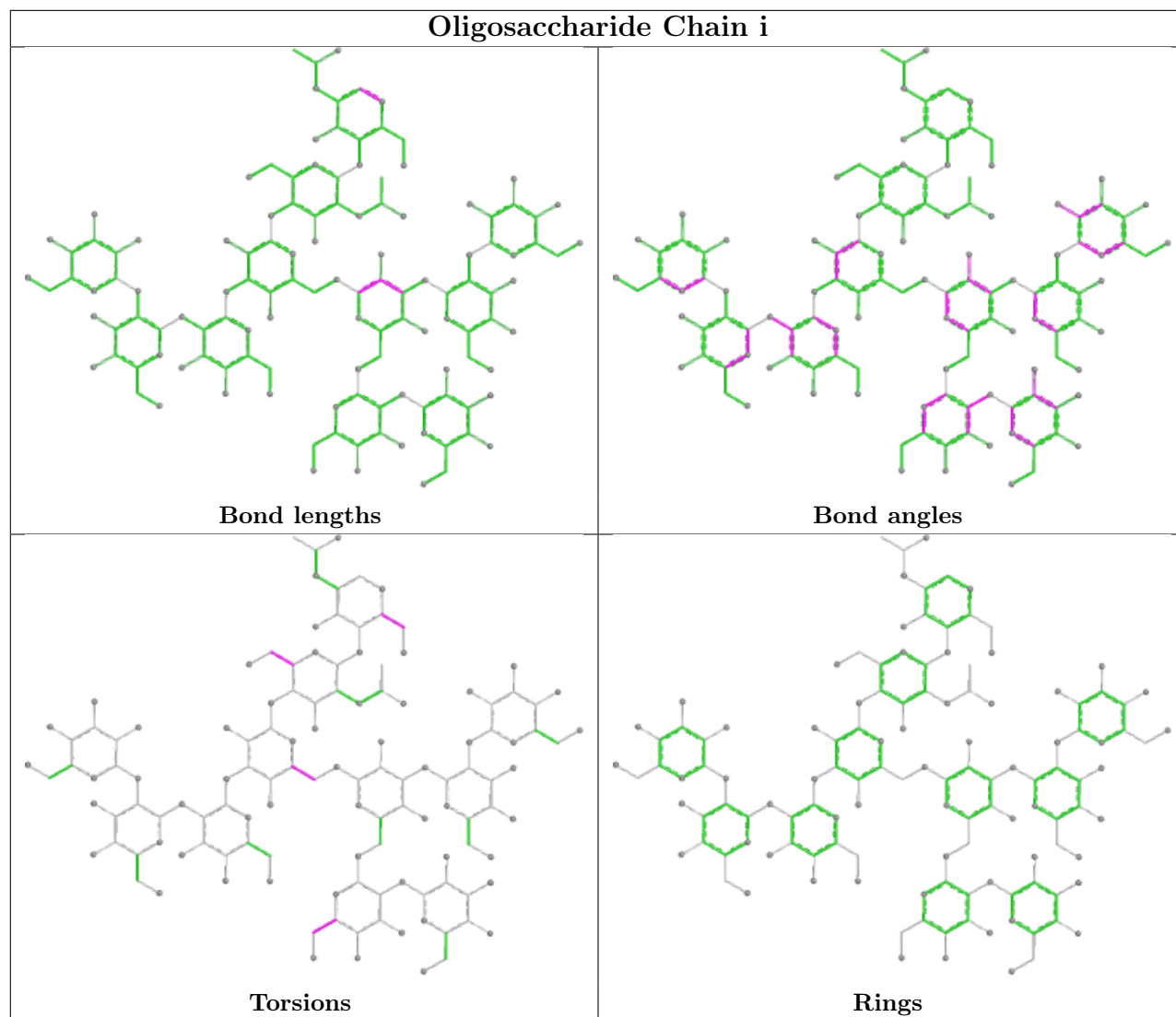


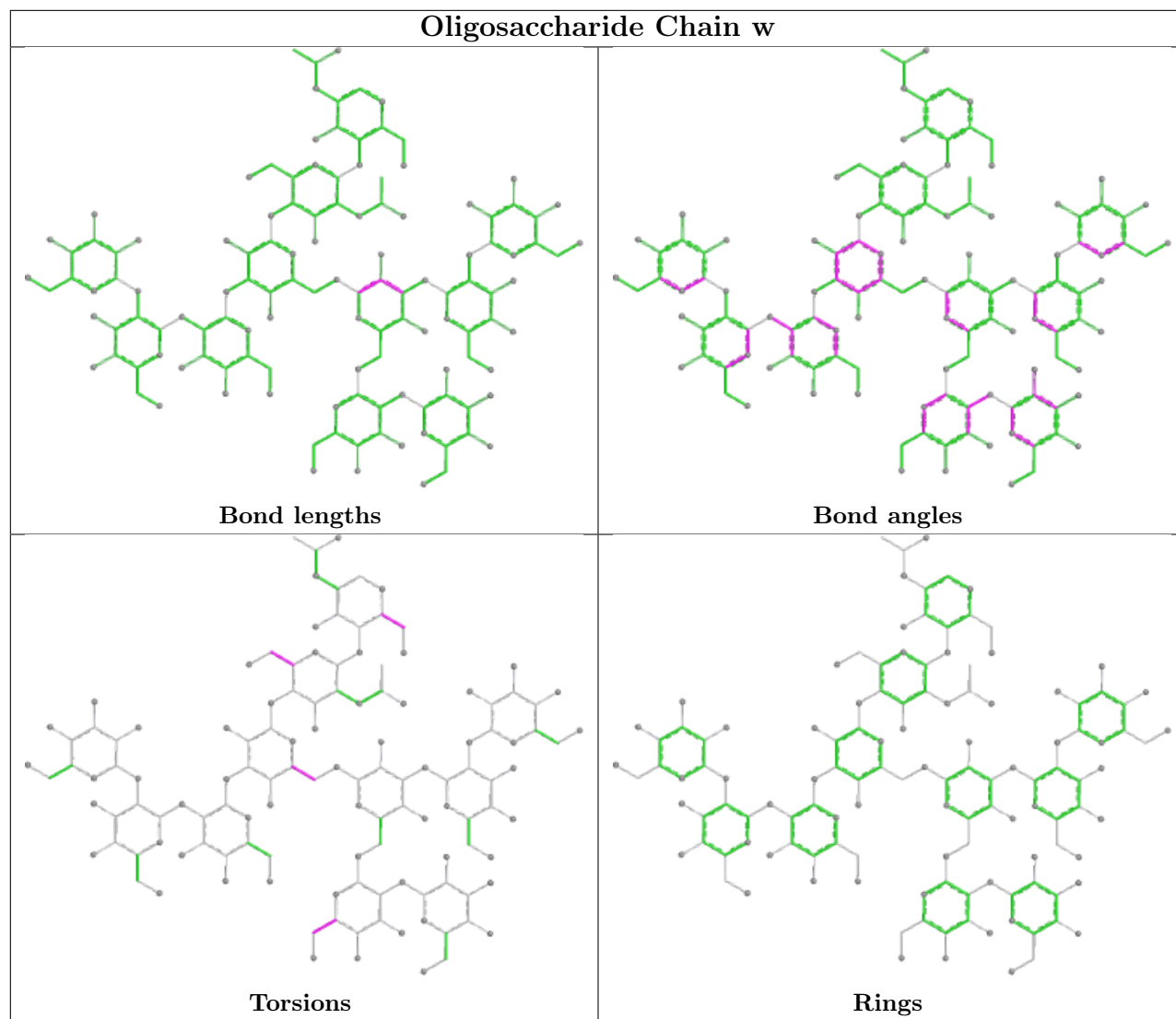


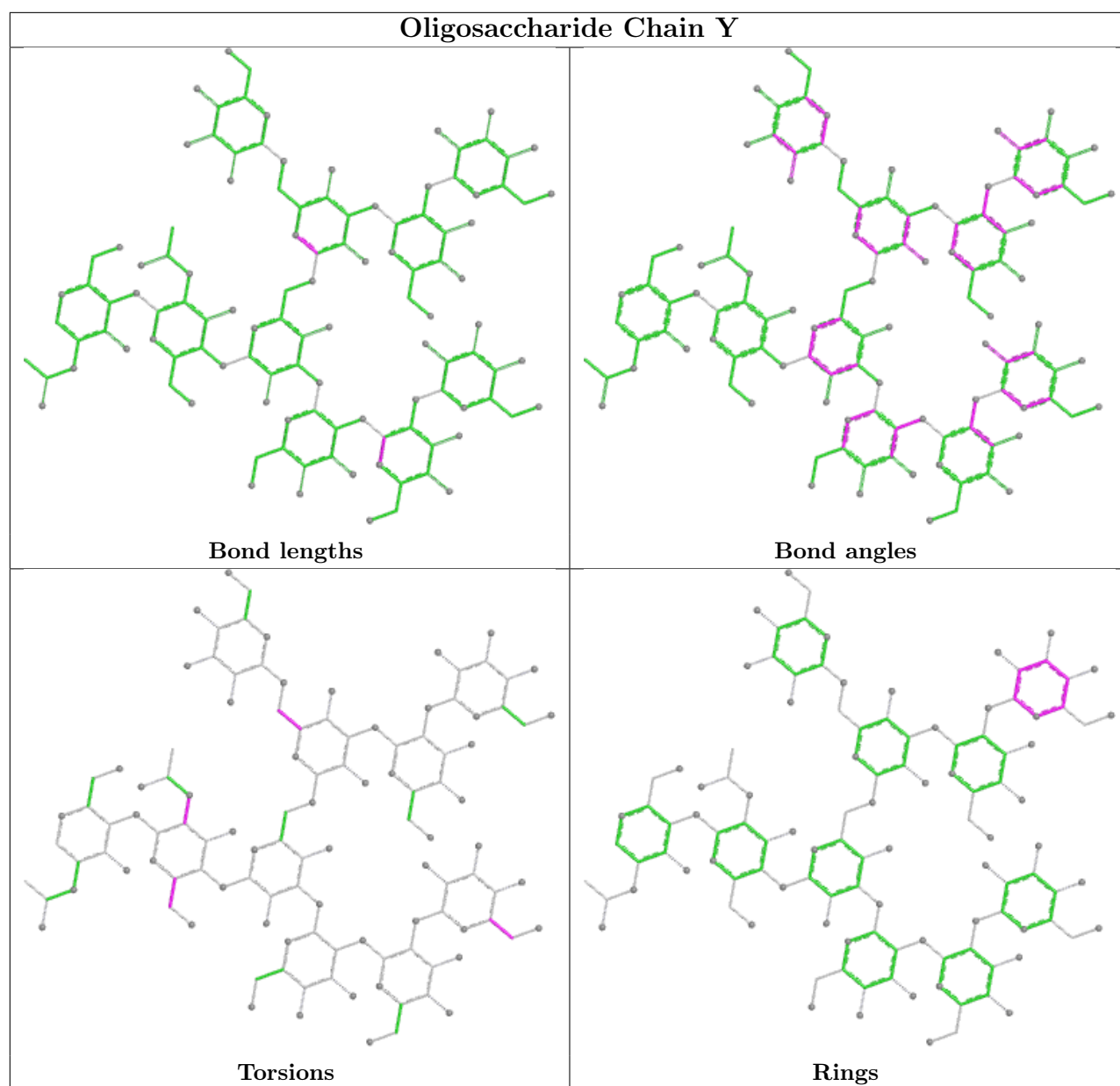


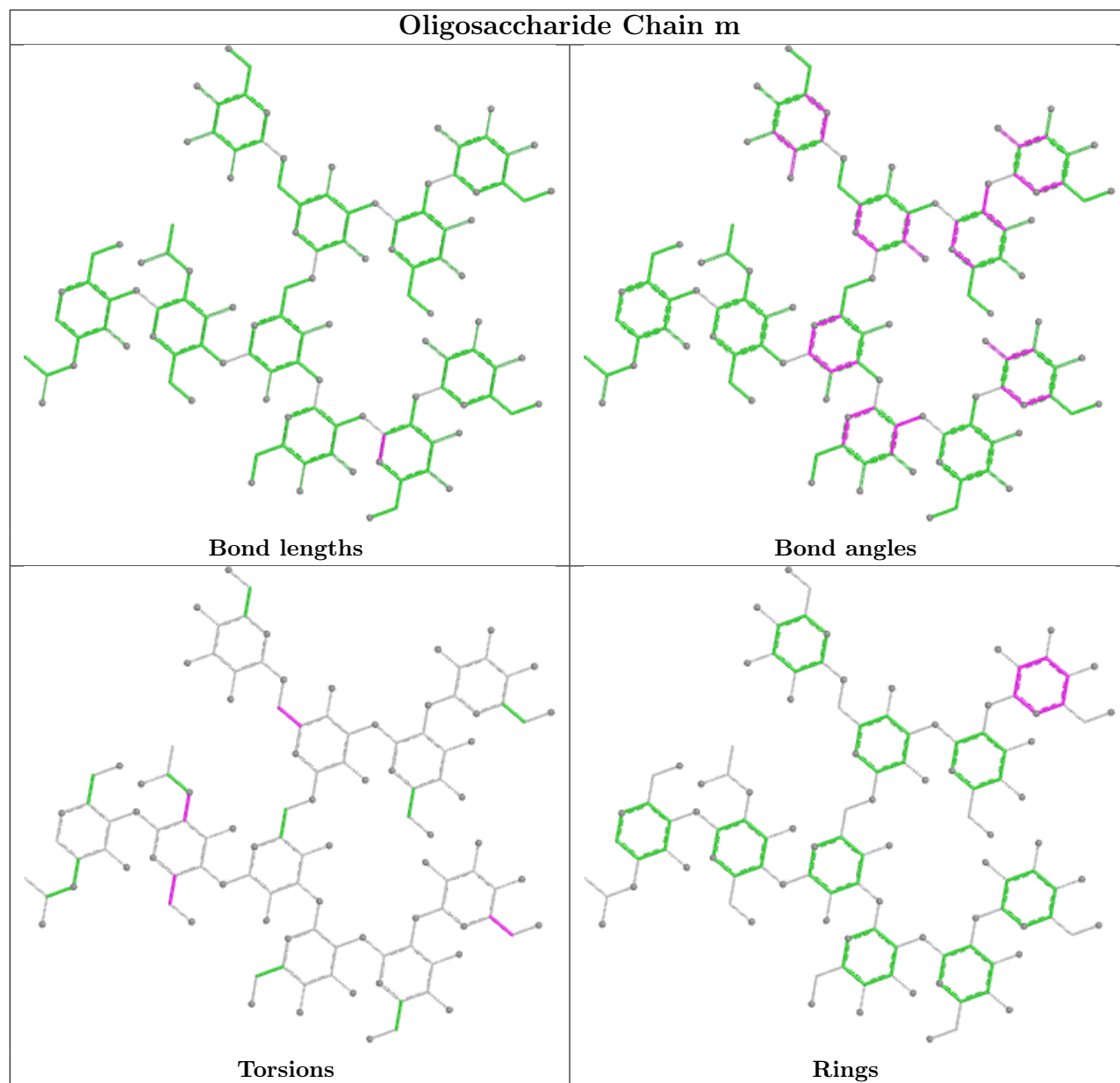


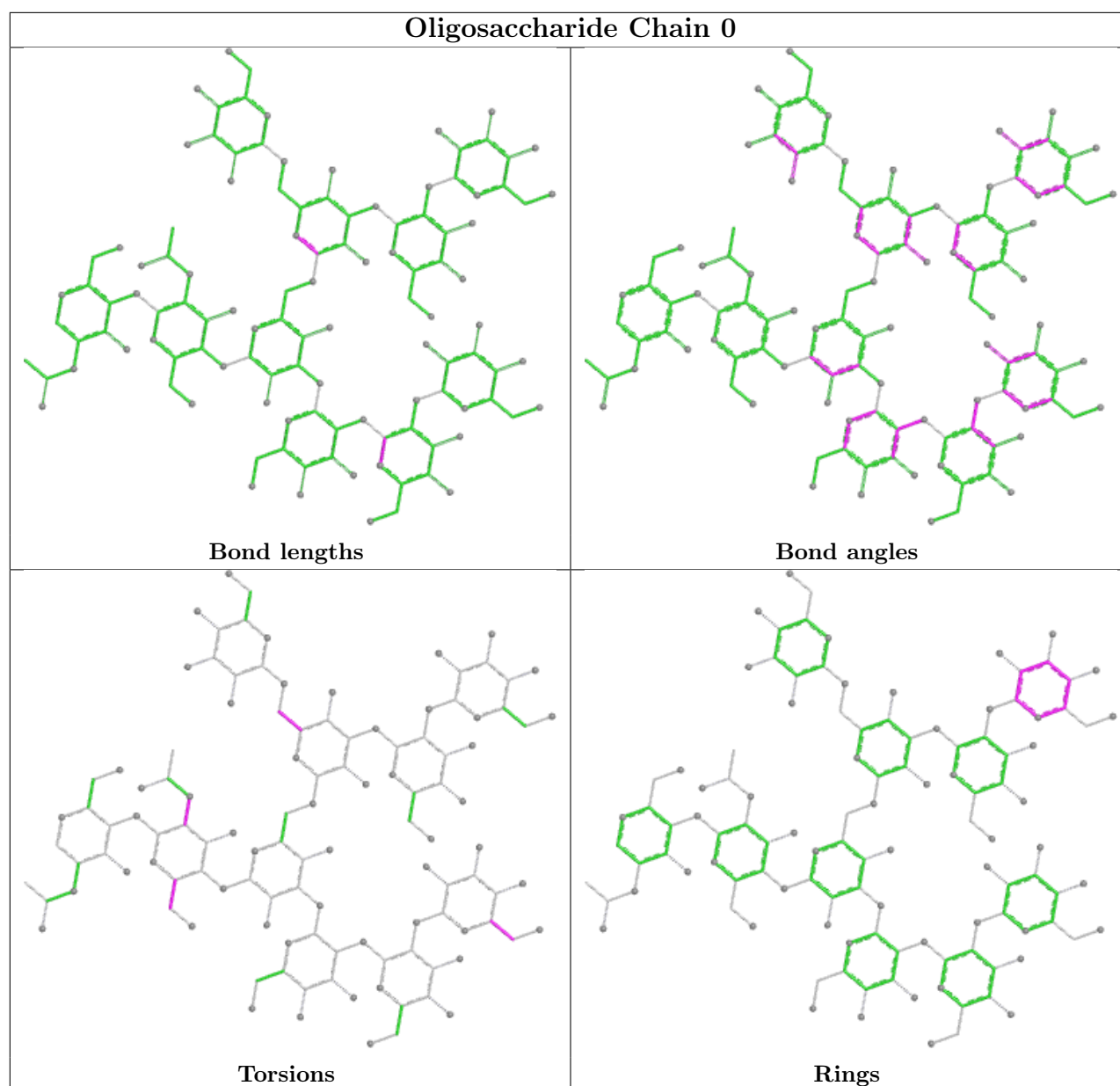












5.6 Ligand geometry [i](#)

18 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
12	NAG	A	662	1	14,14,15	0.34	0	17,19,21	0.46	0
12	NAG	G	641	1	14,14,15	0.26	0	17,19,21	0.41	0
12	NAG	K	702	2	14,14,15	0.20	0	17,19,21	0.43	0
12	NAG	G	606	1	14,14,15	0.24	0	17,19,21	0.45	0
12	NAG	C	702	2	14,14,15	0.20	0	17,19,21	0.44	0
12	NAG	C	701	2	14,14,15	0.22	0	17,19,21	0.47	0
12	NAG	B	702	2	14,14,15	0.19	0	17,19,21	0.46	0
12	NAG	A	606	1	14,14,15	0.22	0	17,19,21	0.44	0
12	NAG	G	661	1	14,14,15	0.22	0	17,19,21	0.43	0
12	NAG	A	641	1	14,14,15	0.22	0	17,19,21	0.38	0
12	NAG	B	701	2	14,14,15	0.18	0	17,19,21	0.53	0
12	NAG	G	662	1	14,14,15	0.35	0	17,19,21	0.50	0
12	NAG	A	661	1	14,14,15	0.23	0	17,19,21	0.43	0
12	NAG	J	606	1	14,14,15	0.22	0	17,19,21	0.43	0
12	NAG	J	641	1	14,14,15	0.24	0	17,19,21	0.41	0
12	NAG	J	661	1	14,14,15	0.24	0	17,19,21	0.44	0
12	NAG	J	662	1	14,14,15	0.29	0	17,19,21	0.45	0
12	NAG	K	701	2	14,14,15	0.26	0	17,19,21	0.50	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
12	NAG	A	662	1	-	0/6/23/26	0/1/1/1
12	NAG	G	641	1	-	2/6/23/26	0/1/1/1
12	NAG	K	702	2	-	2/6/23/26	0/1/1/1
12	NAG	G	606	1	-	1/6/23/26	0/1/1/1
12	NAG	C	702	2	-	2/6/23/26	0/1/1/1
12	NAG	C	701	2	-	1/6/23/26	0/1/1/1
12	NAG	B	702	2	-	2/6/23/26	0/1/1/1
12	NAG	A	606	1	-	1/6/23/26	0/1/1/1
12	NAG	G	661	1	-	1/6/23/26	0/1/1/1
12	NAG	A	641	1	-	2/6/23/26	0/1/1/1
12	NAG	B	701	2	-	1/6/23/26	0/1/1/1
12	NAG	G	662	1	-	0/6/23/26	0/1/1/1
12	NAG	A	661	1	-	0/6/23/26	0/1/1/1
12	NAG	J	606	1	-	2/6/23/26	0/1/1/1
12	NAG	J	641	1	-	2/6/23/26	0/1/1/1
12	NAG	J	661	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	J	662	1	-	0/6/23/26	0/1/1/1
12	NAG	K	701	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	641	NAG	O5-C5-C6-O6
12	G	641	NAG	O5-C5-C6-O6
12	J	641	NAG	O5-C5-C6-O6
12	G	641	NAG	C4-C5-C6-O6
12	A	641	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	641	NAG	1	0
12	J	641	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	448/472 (94%)	0.60	32 (7%) 22 24	138, 198, 269, 365	0
1	G	448/472 (94%)	0.54	32 (7%) 22 24	133, 193, 262, 390	0
1	J	448/472 (94%)	0.45	20 (4%) 38 33	113, 193, 270, 367	0
2	B	121/152 (79%)	0.70	11 (9%) 15 18	140, 200, 245, 279	0
2	C	121/152 (79%)	0.72	13 (10%) 11 15	132, 199, 244, 290	0
2	K	121/152 (79%)	0.61	7 (5%) 29 28	128, 205, 240, 274	0
3	E	208/211 (98%)	0.50	16 (7%) 19 22	159, 212, 241, 269	0
3	L	208/211 (98%)	0.60	17 (8%) 17 21	179, 234, 277, 291	0
3	M	208/211 (98%)	0.40	6 (2%) 53 42	148, 199, 250, 269	0
4	F	227/235 (96%)	0.62	14 (6%) 26 27	135, 192, 242, 301	0
4	H	227/235 (96%)	0.56	13 (5%) 29 29	167, 211, 278, 383	0
4	N	227/235 (96%)	0.46	8 (3%) 47 38	138, 188, 248, 275	0
5	D	221/241 (91%)	0.58	17 (7%) 19 22	178, 227, 270, 317	0
5	I	221/241 (91%)	0.53	18 (8%) 18 21	200, 267, 312, 339	0
5	O	221/241 (91%)	0.52	14 (6%) 26 27	210, 267, 301, 322	0
All	All	3675/3933 (93%)	0.55	238 (6%) 25 25	113, 208, 284, 390	0

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	71	LEU	8.0
3	L	80	ALA	6.4
3	L	82	ASP	5.9
4	F	29	VAL	5.8
5	D	249	GLY	5.5

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

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, 95th 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 ²)	Q<0.9
5	PCA	I	1	8/9	-0.25	0.27	267,277,289,294	0
5	PCA	O	1	8/9	0.47	0.19	222,231,268,273	0
5	PCA	D	1	8/9	0.71	0.16	184,193,214,219	0

6.3 Carbohydrates [i](#)

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, 95th 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 ²)	Q<0.9
9	MAN	T	7	11/12	-0.29	0.23	261,261,261,261	0
6	MAN	V	5	11/12	-0.02	0.18	261,261,261,261	0
6	MAN	P	5	11/12	-0.01	0.17	293,300,308,309	0
10	MAN	U	11	11/12	0.09	0.23	261,261,261,261	0
10	MAN	U	6	11/12	0.13	0.18	261,261,261,261	0
9	NAG	T	1	14/15	0.14	0.30	261,261,261,261	0
9	MAN	T	6	11/12	0.16	0.21	261,261,261,261	0
10	MAN	U	7	11/12	0.20	0.15	261,261,261,261	0
6	BMA	P	3	11/12	0.20	0.13	252,263,287,290	0
10	BMA	U	3	11/12	0.22	0.14	261,261,261,261	0
10	MAN	U	9	11/12	0.23	0.17	261,261,261,261	0
9	BMA	X	3	11/12	0.23	0.10	261,261,261,261	0
6	MAN	R	5	11/12	0.27	0.17	339,341,344,346	0
9	BMA	T	3	11/12	0.27	0.15	261,261,261,261	0
9	MAN	T	4	11/12	0.32	0.15	261,261,261,261	0
6	NAG	d	1	14/15	-	-	221,229,242,243	0
6	NAG	d	2	14/15	-	-	230,242,258,262	0
6	BMA	d	3	11/12	-	-	252,263,287,290	0
6	MAN	d	4	11/12	-	-	253,260,277,291	0
6	MAN	d	5	11/12	-	-	293,300,308,309	0
6	NAG	f	1	14/15	-	-	213,259,277,280	0
6	NAG	f	2	14/15	-	-	277,291,302,313	0
6	BMA	f	3	11/12	-	-	312,321,331,341	0
6	MAN	f	4	11/12	-	-	296,308,312,313	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	f	5	11/12	-	-	339,341,344,346	0
6	NAG	j	1	14/15	-	-	261,261,261,261	0
6	NAG	j	2	14/15	-	-	261,261,261,261	0
6	BMA	j	3	11/12	-	-	261,261,261,261	0
6	MAN	j	4	11/12	-	-	261,261,261,261	0
6	MAN	j	5	11/12	-	-	261,261,261,261	0
6	NAG	r	1	14/15	-	-	221,229,242,243	0
6	NAG	r	2	14/15	-	-	230,242,258,262	0
6	BMA	r	3	11/12	-	-	252,263,287,290	0
6	MAN	r	4	11/12	-	-	253,260,277,291	0
6	MAN	r	5	11/12	-	-	293,300,308,309	0
6	NAG	t	1	14/15	-	-	213,259,277,280	0
6	NAG	t	2	14/15	-	-	277,291,302,313	0
6	BMA	t	3	11/12	-	-	312,321,331,341	0
6	MAN	t	4	11/12	-	-	296,308,312,313	0
6	MAN	t	5	11/12	-	-	339,341,344,346	0
6	NAG	x	1	14/15	-	-	261,261,261,261	0
6	NAG	x	2	14/15	-	-	261,261,261,261	0
6	BMA	x	3	11/12	-	-	261,261,261,261	0
6	MAN	x	4	11/12	-	-	261,261,261,261	0
6	MAN	x	5	11/12	-	-	261,261,261,261	0
9	MAN	X	7	11/12	0.35	0.13	261,261,261,261	0
11	MAN	Y	9	11/12	0.39	0.17	327,335,339,340	0
9	MAN	T	5	11/12	0.43	0.16	261,261,261,261	0
10	MAN	U	5	11/12	0.48	0.15	261,261,261,261	0
7	NAG	e	1	14/15	-	-	258,284,302,304	0
7	NAG	e	2	14/15	-	-	295,304,312,313	0
7	BMA	e	3	11/12	-	-	309,319,327,335	0
7	MAN	e	4	11/12	-	-	325,342,352,353	0
7	NAG	s	1	14/15	-	-	258,284,302,304	0
7	NAG	s	2	14/15	-	-	295,304,312,313	0
7	BMA	s	3	11/12	-	-	309,319,327,335	0
7	MAN	s	4	11/12	-	-	325,342,352,353	0
8	NAG	S	2	14/15	0.48	0.17	279,293,304,311	0
6	BMA	R	3	11/12	0.49	0.09	312,321,331,341	0
9	MAN	X	6	11/12	0.53	0.26	261,261,261,261	0
9	NAG	X	1	14/15	0.62	0.33	261,261,261,261	0
6	NAG	P	1	14/15	0.64	0.15	221,229,242,243	0
8	NAG	Z	2	14/15	0.68	0.24	317,335,342,344	0
8	NAG	a	1	14/15	-	-	296,306,323,326	0
8	NAG	a	2	14/15	-	-	307,328,330,330	0
8	NAG	b	1	14/15	-	-	259,277,289,292	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	b	2	14/15	-	-	288,310,336,363	0
8	NAG	c	1	14/15	-	-	261,261,261,261	0
8	NAG	c	2	14/15	-	-	261,261,261,261	0
8	NAG	g	1	14/15	-	-	252,275,284,297	0
8	NAG	g	2	14/15	-	-	279,293,304,311	0
8	NAG	k	1	14/15	-	-	245,261,286,296	0
8	NAG	k	2	14/15	-	-	303,317,328,336	0
8	NAG	n	1	14/15	-	-	260,297,316,323	0
8	NAG	n	2	14/15	-	-	317,335,342,344	0
8	NAG	o	1	14/15	-	-	296,306,323,326	0
8	NAG	o	2	14/15	-	-	307,328,330,330	0
8	NAG	p	1	14/15	-	-	259,277,289,292	0
8	NAG	p	2	14/15	-	-	288,310,336,363	0
8	NAG	q	1	14/15	-	-	261,261,261,261	0
8	NAG	q	2	14/15	-	-	261,261,261,261	0
8	NAG	u	1	14/15	-	-	252,275,284,297	0
8	NAG	u	2	14/15	-	-	279,293,304,311	0
8	NAG	y	1	14/15	-	-	245,261,286,296	0
8	NAG	y	2	14/15	-	-	303,317,328,336	0
8	NAG	1	1	14/15	-	-	260,297,316,323	0
8	NAG	1	2	14/15	-	-	317,335,342,344	0
8	NAG	2	1	14/15	-	-	296,306,323,326	0
8	NAG	2	2	14/15	-	-	307,328,330,330	0
8	NAG	3	1	14/15	-	-	259,277,289,292	0
8	NAG	3	2	14/15	-	-	288,310,336,363	0
8	NAG	4	1	14/15	-	-	261,261,261,261	0
8	NAG	4	2	14/15	-	-	261,261,261,261	0
6	MAN	R	4	11/12	0.68	0.14	296,308,312,313	0
11	MAN	Y	6	11/12	0.70	0.16	301,306,311,311	0
6	MAN	P	4	11/12	0.70	0.17	253,260,277,291	0
7	BMA	Q	3	11/12	0.71	0.17	309,319,327,335	0
10	MAN	U	8	11/12	0.72	0.25	261,261,261,261	0
10	MAN	U	10	11/12	0.73	0.11	261,261,261,261	0
6	BMA	V	3	11/12	0.73	0.09	261,261,261,261	0
9	MAN	X	5	11/12	0.73	0.12	261,261,261,261	0
10	NAG	U	1	14/15	0.73	0.16	261,261,261,261	0
11	MAN	Y	7	11/12	0.74	0.10	286,303,309,318	0
7	MAN	Q	4	11/12	0.74	0.21	325,342,352,353	0
11	MAN	Y	10	11/12	0.75	0.15	280,295,301,303	0
7	NAG	Q	2	14/15	0.76	0.20	295,304,312,313	0
9	MAN	X	4	11/12	0.76	0.14	261,261,261,261	0
9	NAG	h	1	14/15	-	-	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	h	2	14/15	-	-	261,261,261,261	0
9	BMA	h	3	11/12	-	-	261,261,261,261	0
9	MAN	h	4	11/12	-	-	261,261,261,261	0
9	MAN	h	5	11/12	-	-	261,261,261,261	0
9	MAN	h	6	11/12	-	-	261,261,261,261	0
9	MAN	h	7	11/12	-	-	261,261,261,261	0
9	NAG	l	1	14/15	-	-	261,261,261,261	0
9	NAG	l	2	14/15	-	-	261,261,261,261	0
9	BMA	l	3	11/12	-	-	261,261,261,261	0
9	MAN	l	4	11/12	-	-	261,261,261,261	0
9	MAN	l	5	11/12	-	-	261,261,261,261	0
9	MAN	l	6	11/12	-	-	261,261,261,261	0
9	MAN	l	7	11/12	-	-	261,261,261,261	0
9	NAG	v	1	14/15	-	-	261,261,261,261	0
9	NAG	v	2	14/15	-	-	261,261,261,261	0
9	BMA	v	3	11/12	-	-	261,261,261,261	0
9	MAN	v	4	11/12	-	-	261,261,261,261	0
9	MAN	v	5	11/12	-	-	261,261,261,261	0
9	MAN	v	6	11/12	-	-	261,261,261,261	0
9	MAN	v	7	11/12	-	-	261,261,261,261	0
9	NAG	z	1	14/15	-	-	261,261,261,261	0
9	NAG	z	2	14/15	-	-	261,261,261,261	0
9	BMA	z	3	11/12	-	-	261,261,261,261	0
9	MAN	z	4	11/12	-	-	261,261,261,261	0
9	MAN	z	5	11/12	-	-	261,261,261,261	0
9	MAN	z	6	11/12	-	-	261,261,261,261	0
9	MAN	z	7	11/12	-	-	261,261,261,261	0
6	NAG	P	2	14/15	0.77	0.12	230,242,258,262	0
8	NAG	W	2	14/15	0.77	0.21	303,317,328,336	0
10	MAN	U	4	11/12	0.78	0.15	261,261,261,261	0
9	NAG	X	2	14/15	0.80	0.15	261,261,261,261	0
9	NAG	T	2	14/15	0.83	0.17	261,261,261,261	0
7	NAG	Q	1	14/15	0.83	0.18	258,284,302,304	0
6	NAG	R	2	14/15	0.83	0.15	277,291,302,313	0
11	MAN	Y	8	11/12	0.84	0.23	321,323,332,338	0
11	NAG	Y	2	14/15	0.87	0.21	257,273,294,300	0
11	BMA	Y	3	11/12	0.87	0.11	251,268,283,285	0
11	MAN	Y	5	11/12	0.87	0.12	262,265,279,286	0
10	NAG	i	1	14/15	-	-	261,261,261,261	0
10	NAG	i	2	14/15	-	-	261,261,261,261	0
10	BMA	i	3	11/12	-	-	261,261,261,261	0
10	MAN	i	4	11/12	-	-	261,261,261,261	0

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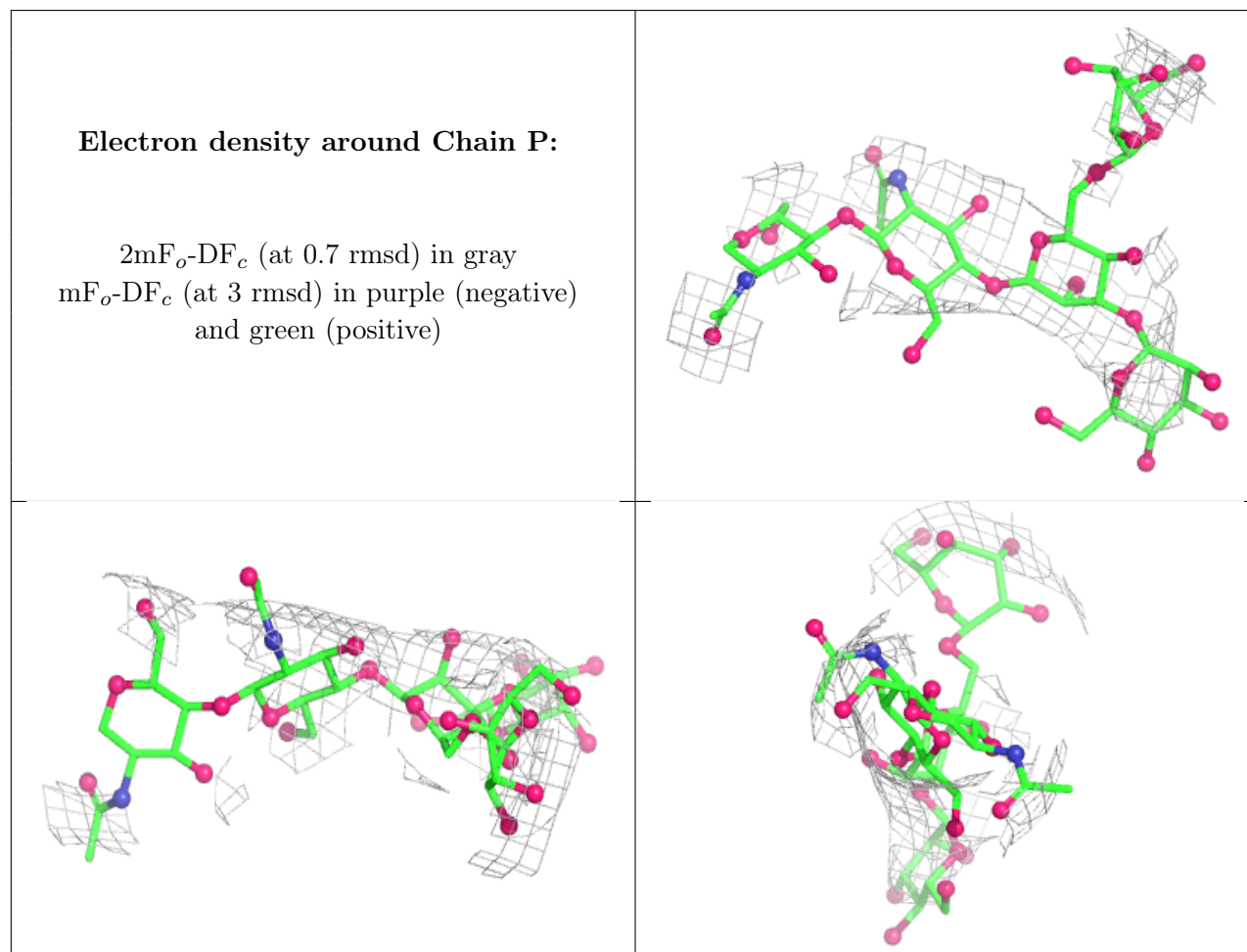
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MAN	i	5	11/12	-	-	261,261,261,261	0
10	MAN	i	6	11/12	-	-	261,261,261,261	0
10	MAN	i	7	11/12	-	-	261,261,261,261	0
10	MAN	i	8	11/12	-	-	261,261,261,261	0
10	MAN	i	9	11/12	-	-	261,261,261,261	0
10	MAN	i	10	11/12	-	-	261,261,261,261	0
10	MAN	i	11	11/12	-	-	261,261,261,261	0
10	NAG	w	1	14/15	-	-	261,261,261,261	0
10	NAG	w	2	14/15	-	-	261,261,261,261	0
10	BMA	w	3	11/12	-	-	261,261,261,261	0
10	MAN	w	4	11/12	-	-	261,261,261,261	0
10	MAN	w	5	11/12	-	-	261,261,261,261	0
10	MAN	w	6	11/12	-	-	261,261,261,261	0
10	MAN	w	7	11/12	-	-	261,261,261,261	0
10	MAN	w	8	11/12	-	-	261,261,261,261	0
10	MAN	w	9	11/12	-	-	261,261,261,261	0
10	MAN	w	10	11/12	-	-	261,261,261,261	0
10	MAN	w	11	11/12	-	-	261,261,261,261	0
8	NAG	W	1	14/15	0.87	0.13	245,261,286,296	0
8	NAG	S	1	14/15	0.89	0.15	252,275,284,297	0
11	NAG	Y	1	14/15	0.90	0.18	237,248,265,270	0
6	MAN	V	4	11/12	0.91	0.12	261,261,261,261	0
6	NAG	V	2	14/15	0.91	0.15	261,261,261,261	0
8	NAG	Z	1	14/15	0.92	0.14	260,297,316,323	0
11	MAN	Y	4	11/12	0.95	0.12	235,240,258,278	0
6	NAG	R	1	14/15	0.96	0.16	213,259,277,280	0
10	NAG	U	2	14/15	0.96	0.12	261,261,261,261	0
6	NAG	V	1	14/15	0.96	0.12	261,261,261,261	0
11	NAG	m	1	14/15	-	-	237,248,265,270	0
11	NAG	m	2	14/15	-	-	257,273,294,300	0
11	BMA	m	3	11/12	-	-	251,268,283,285	0
11	MAN	m	4	11/12	-	-	235,240,258,278	0
11	MAN	m	5	11/12	-	-	262,265,279,286	0
11	MAN	m	6	11/12	-	-	301,306,311,311	0
11	MAN	m	7	11/12	-	-	286,303,309,318	0
11	MAN	m	8	11/12	-	-	321,323,332,338	0
11	MAN	m	9	11/12	-	-	327,335,339,340	0
11	MAN	m	10	11/12	-	-	280,295,301,303	0
11	NAG	0	1	14/15	-	-	237,248,265,270	0
11	NAG	0	2	14/15	-	-	257,273,294,300	0
11	BMA	0	3	11/12	-	-	251,268,283,285	0
11	MAN	0	4	11/12	-	-	235,240,258,278	0

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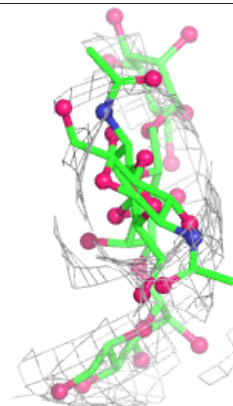
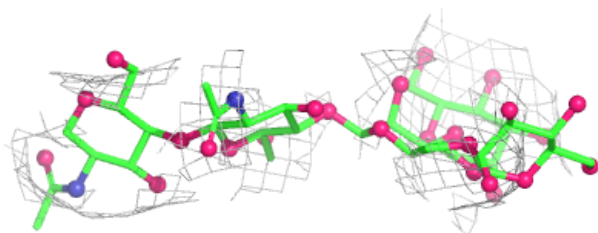
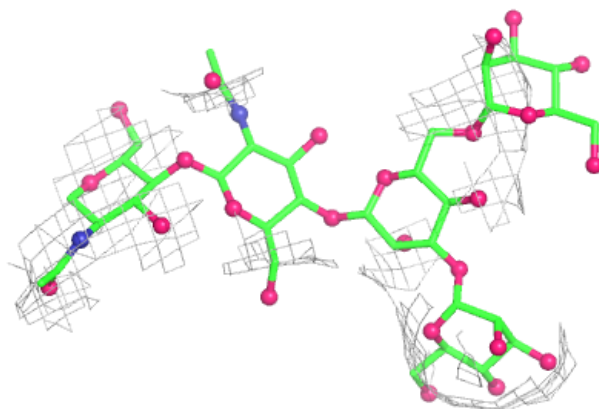
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MAN	0	5	11/12	-	-	262,265,279,286	0
11	MAN	0	6	11/12	-	-	301,306,311,311	0
11	MAN	0	7	11/12	-	-	286,303,309,318	0
11	MAN	0	8	11/12	-	-	321,323,332,338	0
11	MAN	0	9	11/12	-	-	327,335,339,340	0
11	MAN	0	10	11/12	-	-	280,295,301,303	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



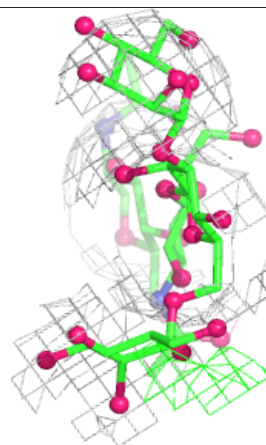
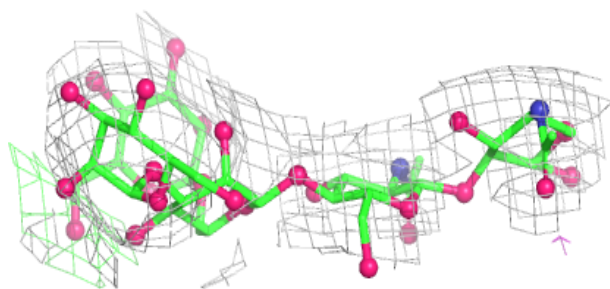
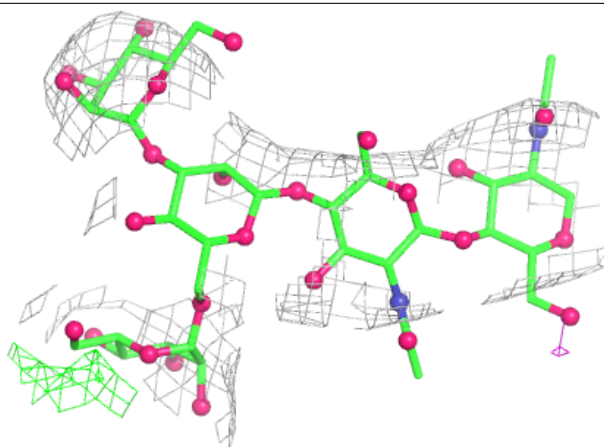
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



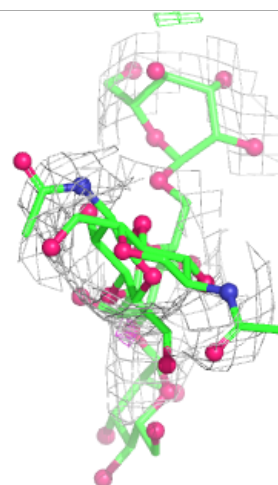
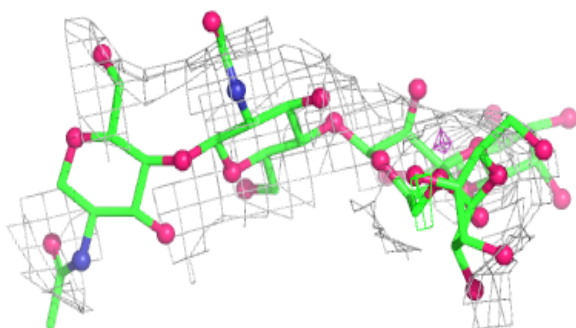
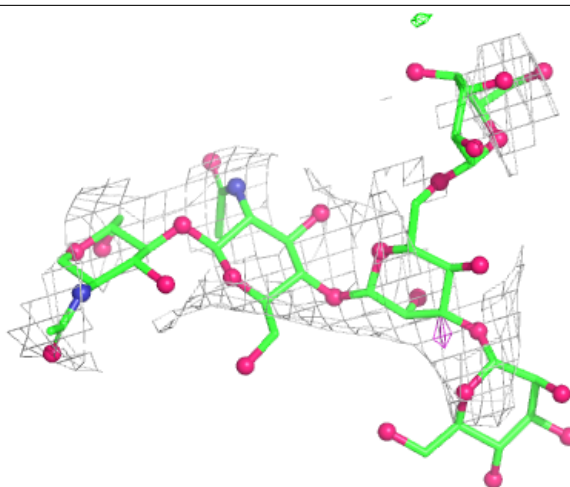
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



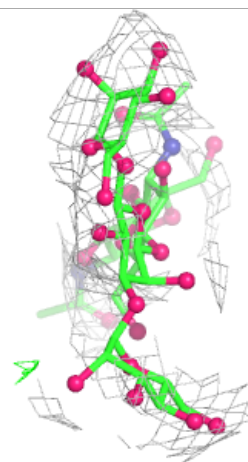
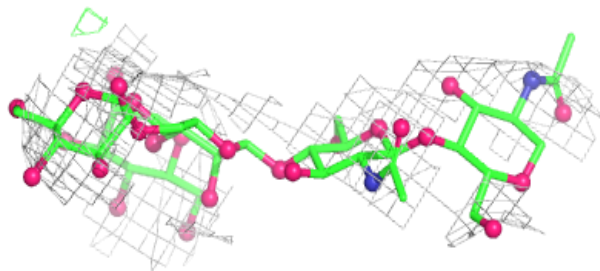
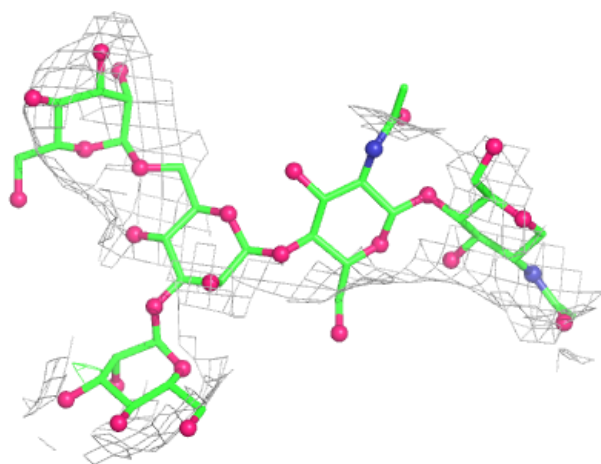
Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



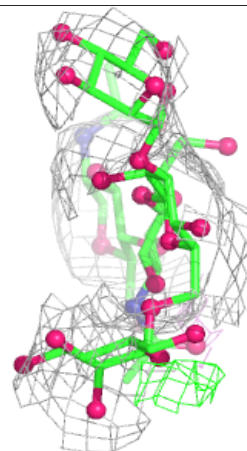
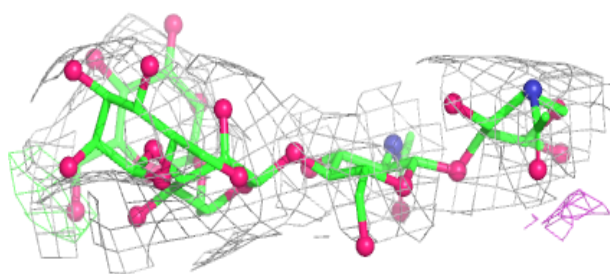
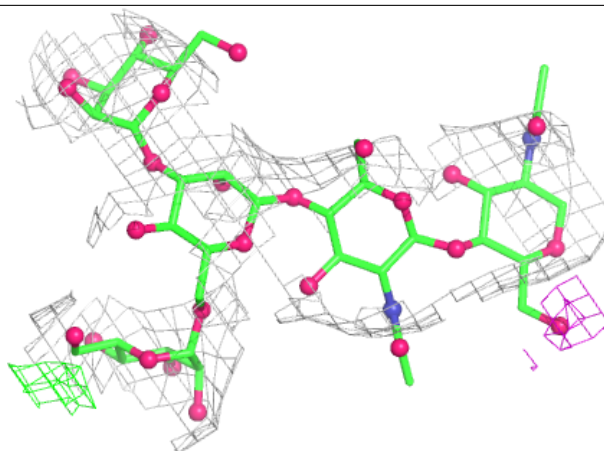
Electron density around Chain f:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



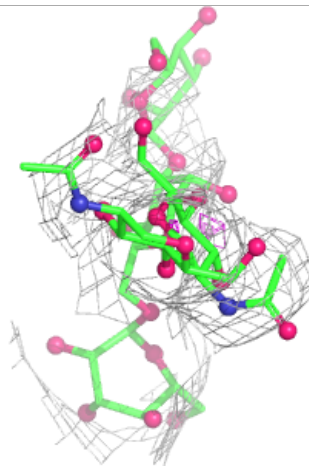
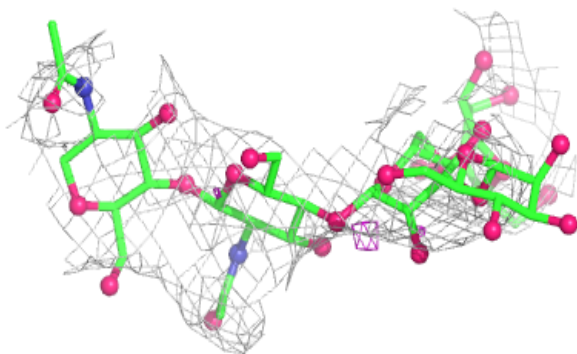
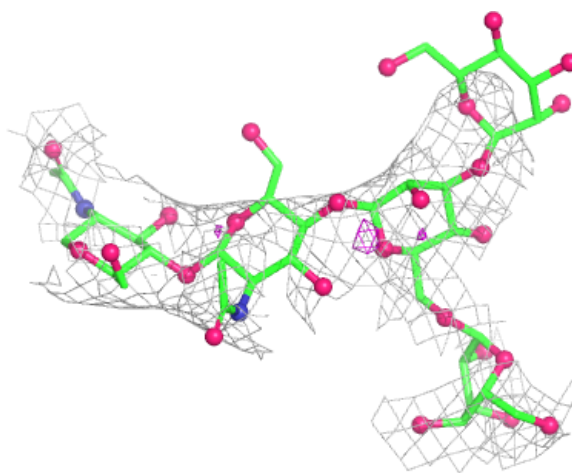
Electron density around Chain j:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



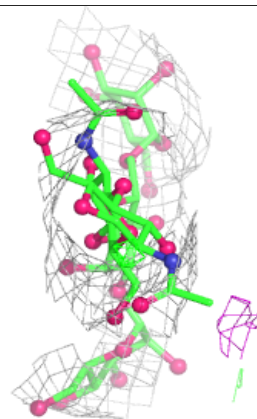
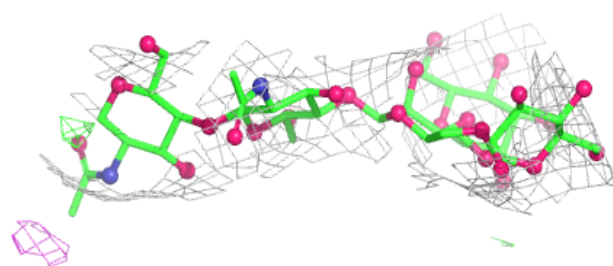
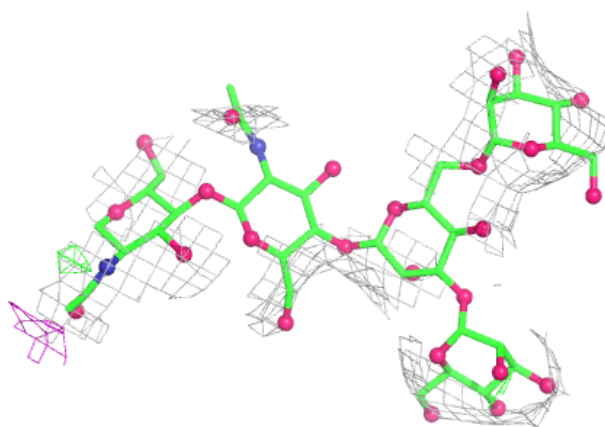
Electron density around Chain r:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



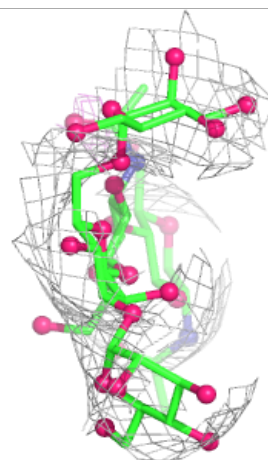
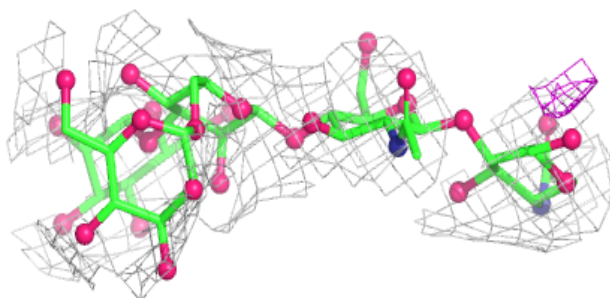
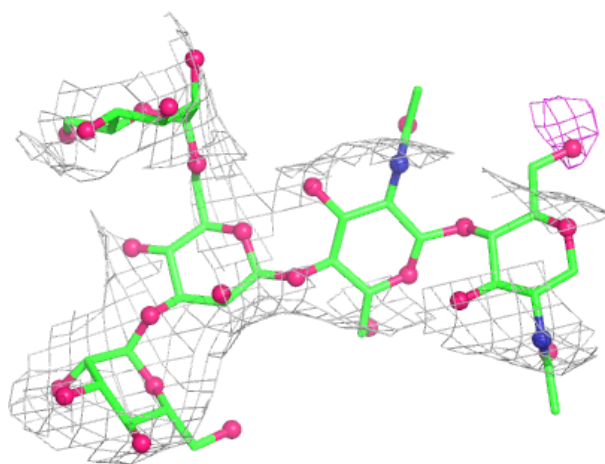
Electron density around Chain t:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



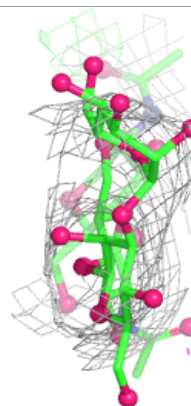
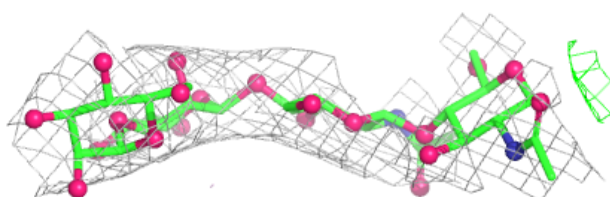
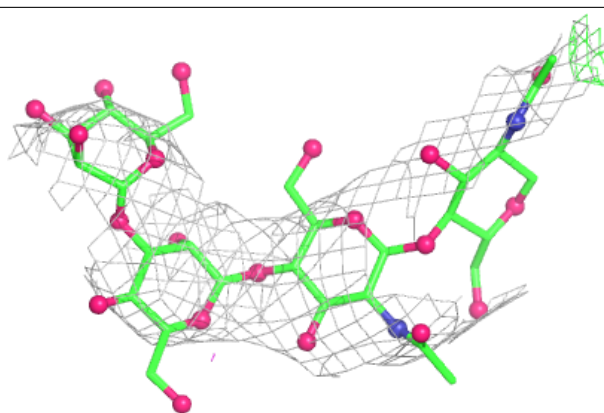
Electron density around Chain x:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

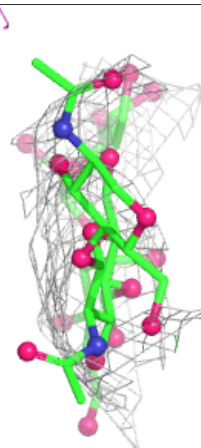
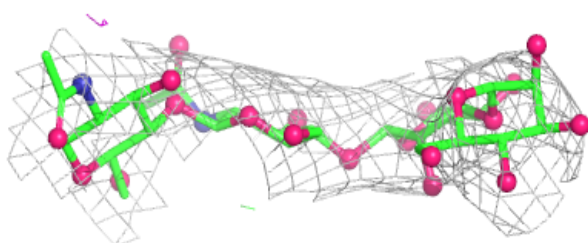
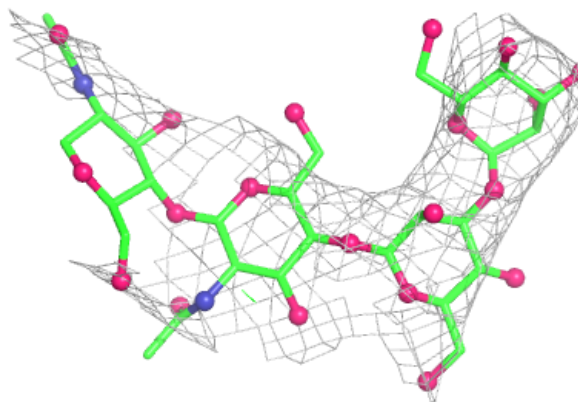


Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

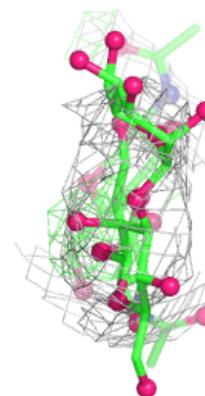
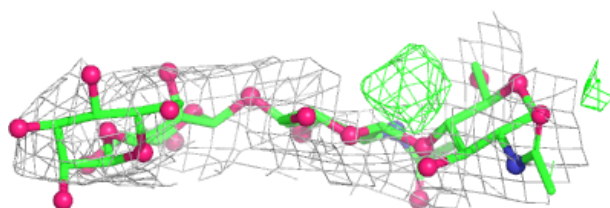
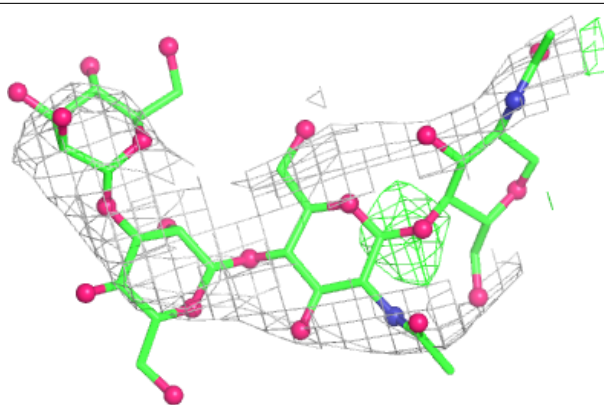
**Electron density around Chain e:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

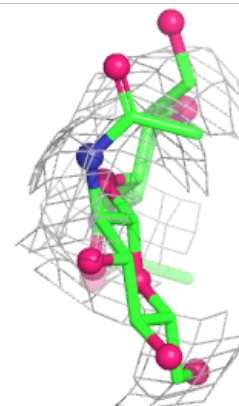
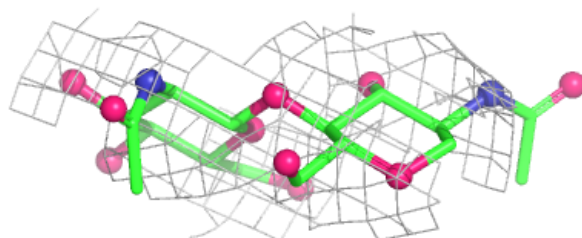
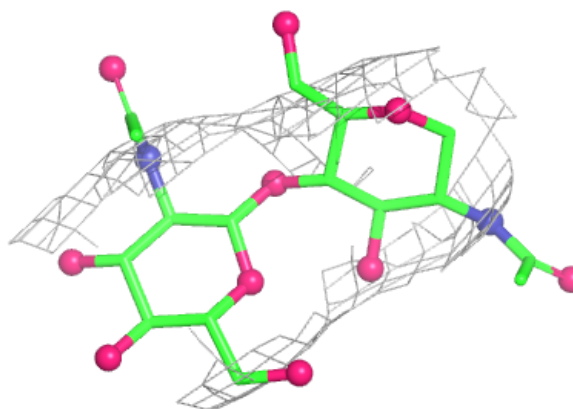


Electron density around Chain s:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

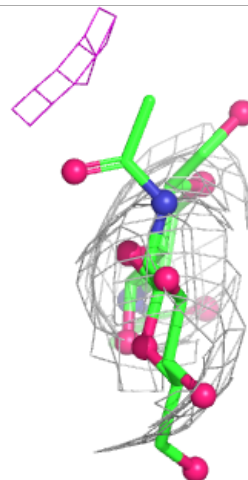
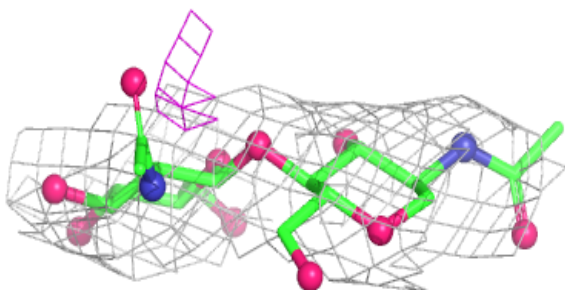
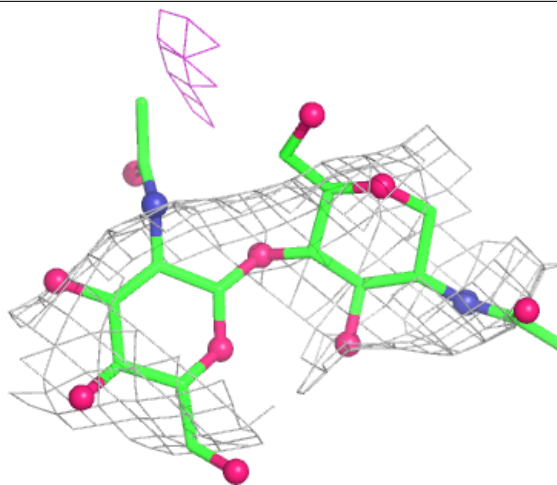
**Electron density around Chain S:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



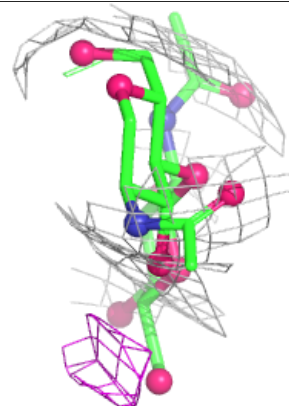
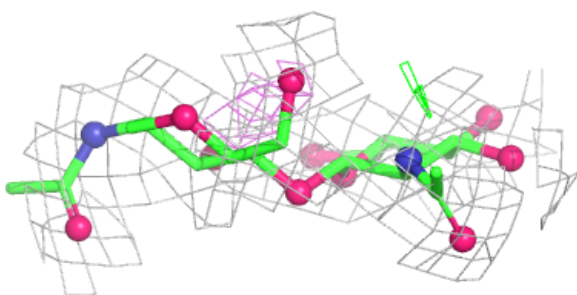
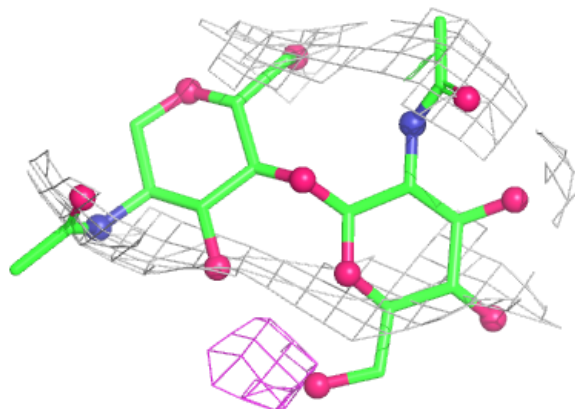
Electron density around Chain W:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



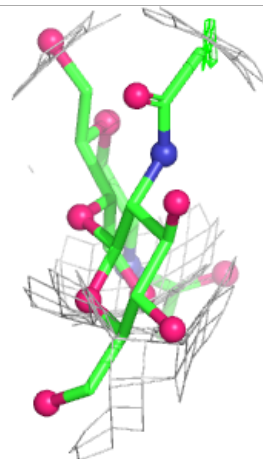
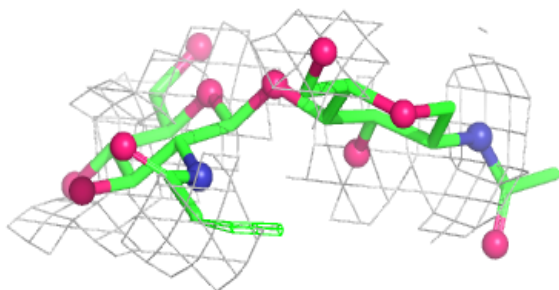
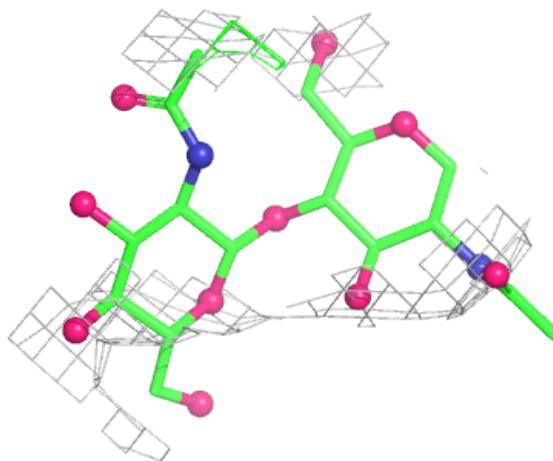
Electron density around Chain Z:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



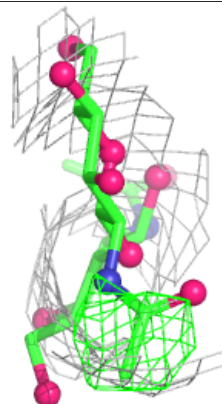
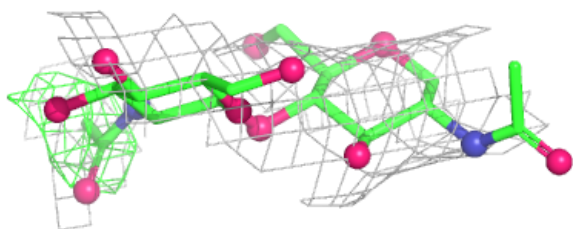
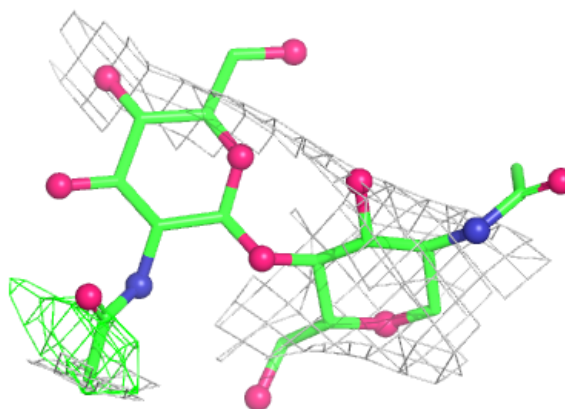
Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



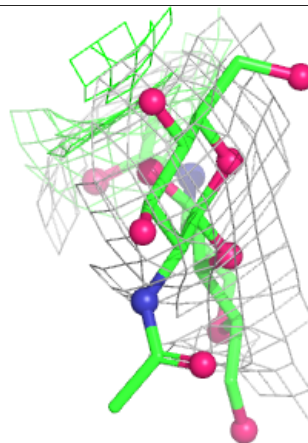
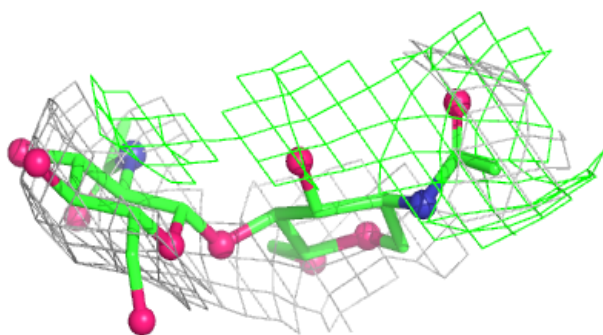
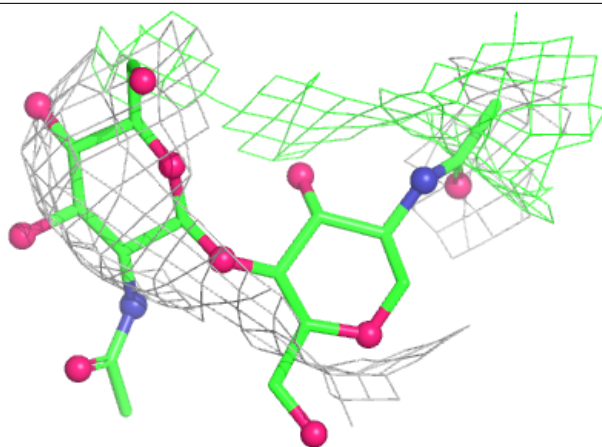
Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



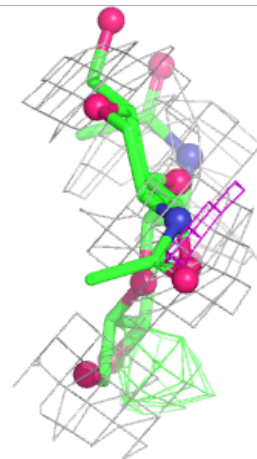
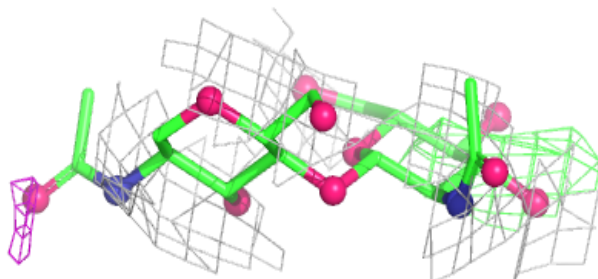
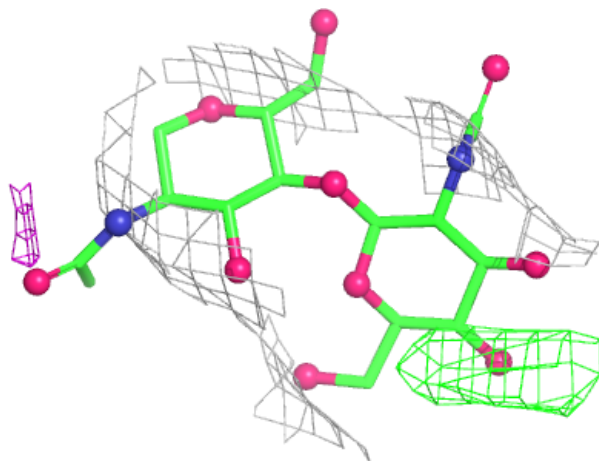
Electron density around Chain c:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



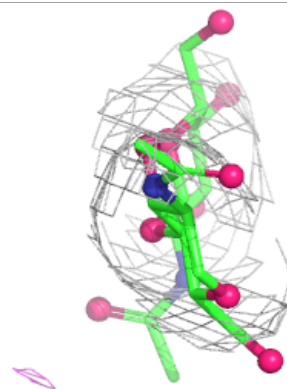
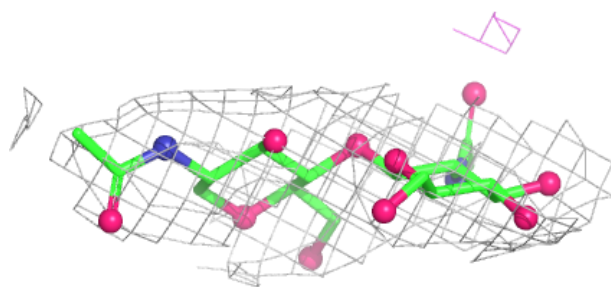
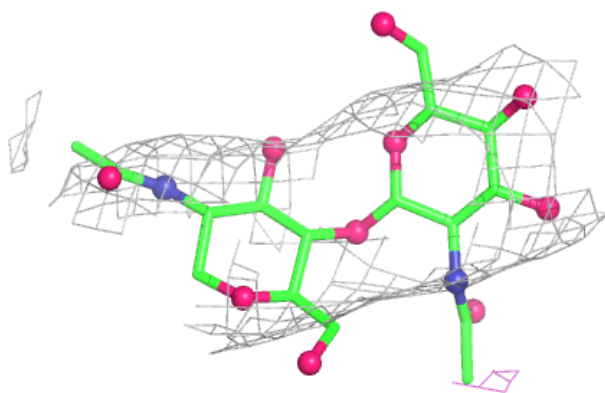
Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

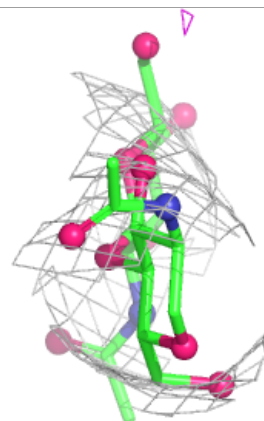
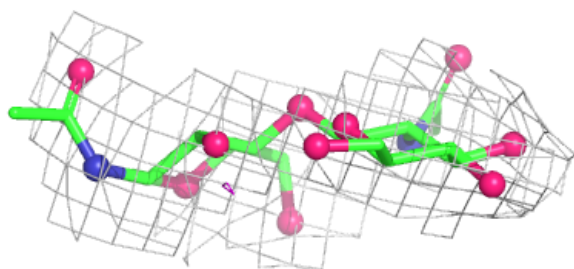
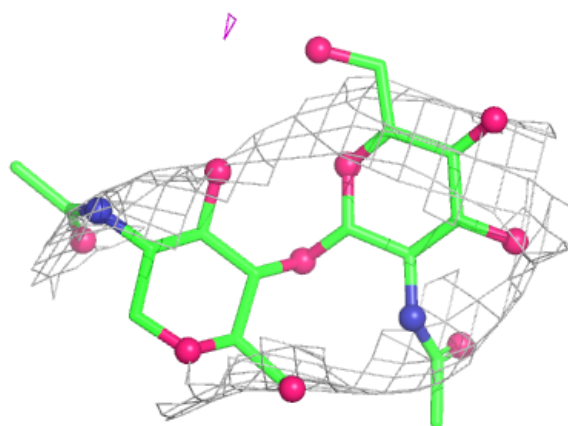


Electron density around Chain k:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

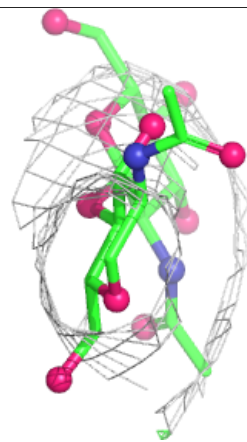
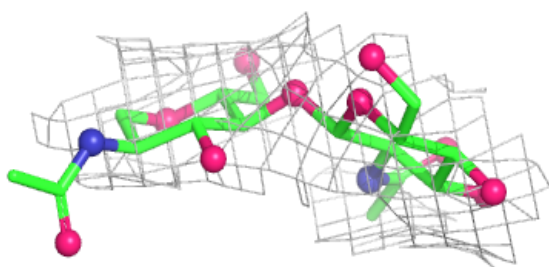
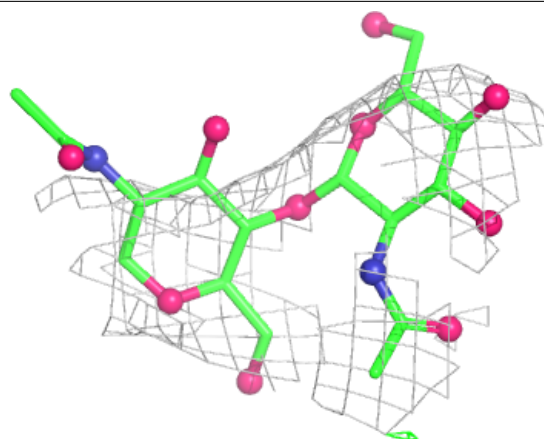
**Electron density around Chain n:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



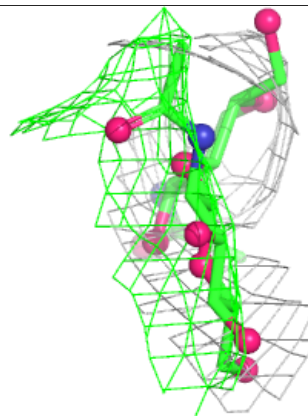
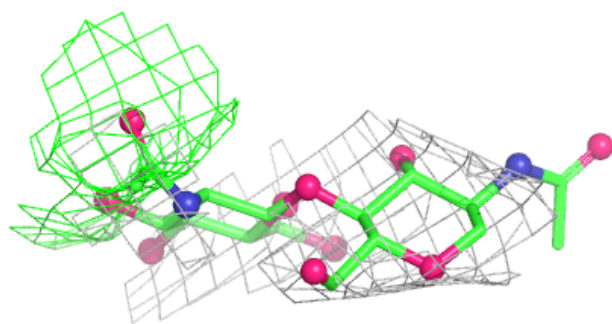
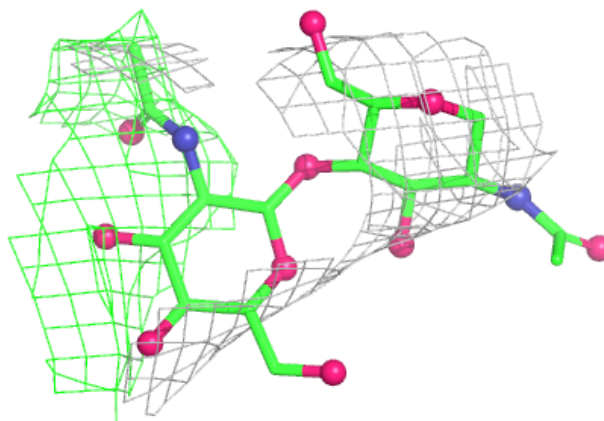
Electron density around Chain o:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



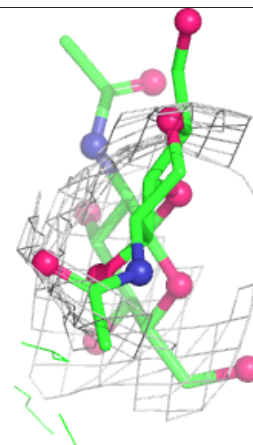
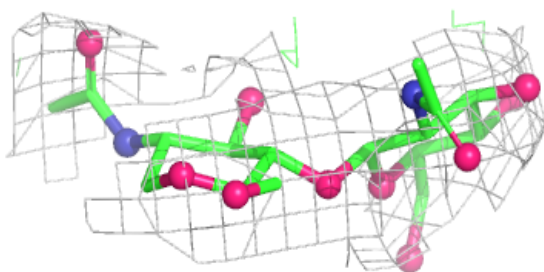
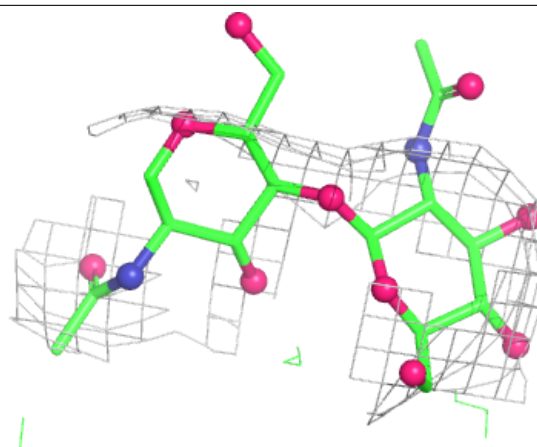
Electron density around Chain p:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



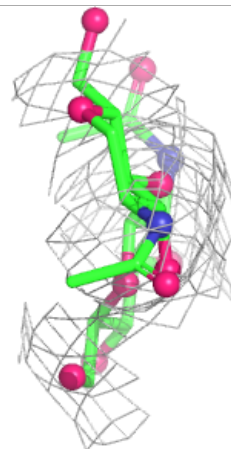
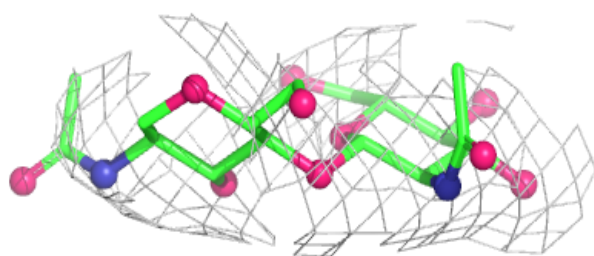
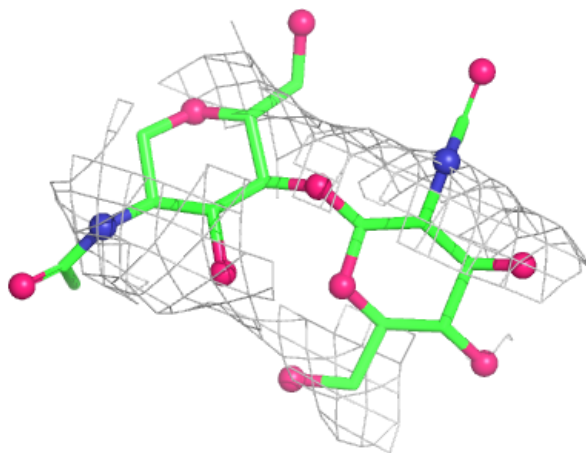
Electron density around Chain q:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



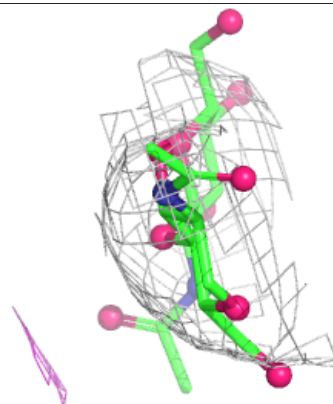
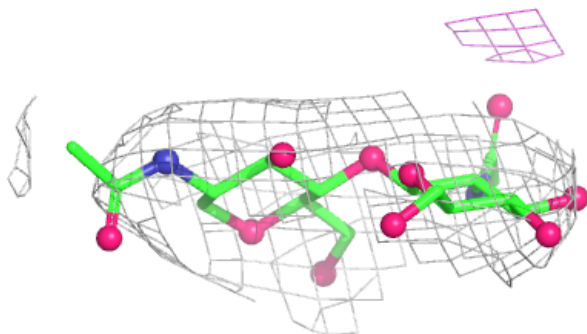
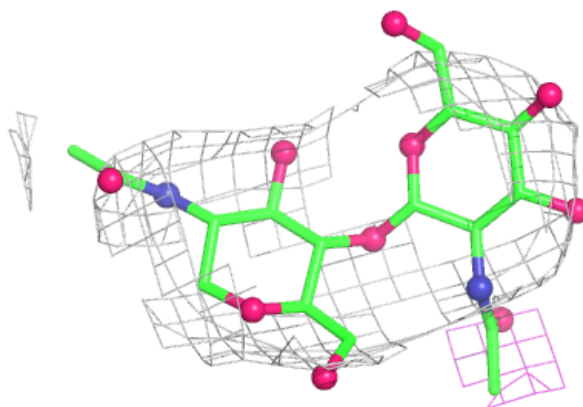
Electron density around Chain u:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



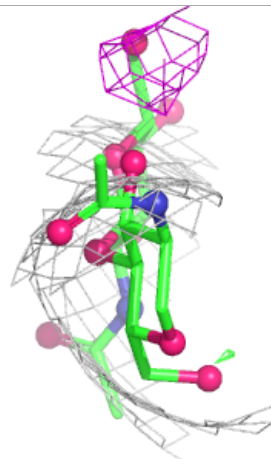
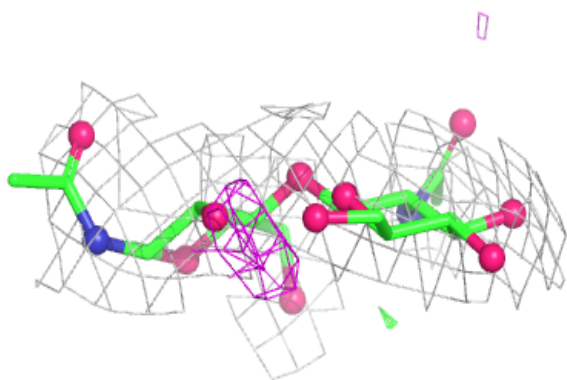
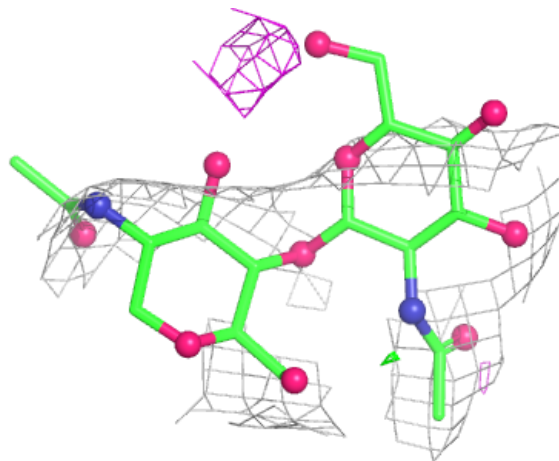
Electron density around Chain y:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



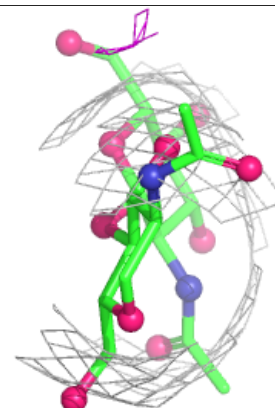
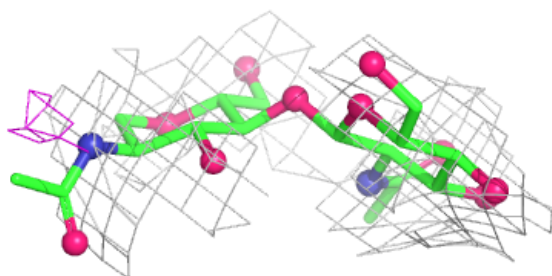
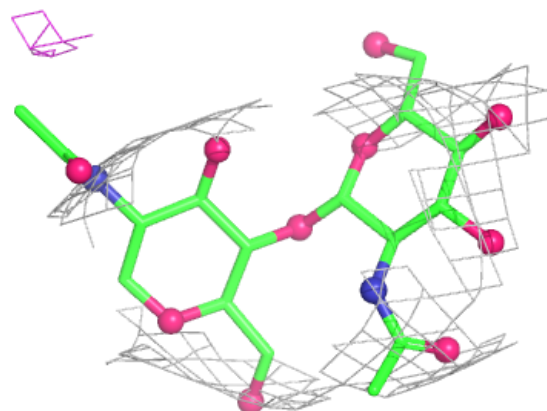
Electron density around Chain 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

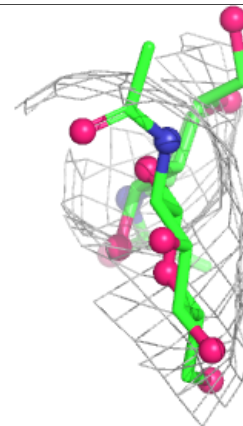
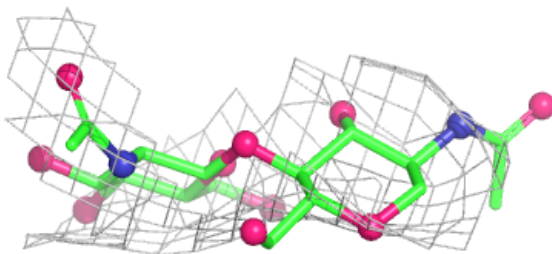
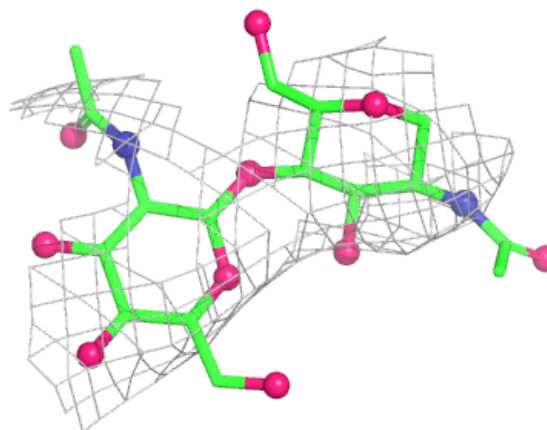


Electron density around Chain 2:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

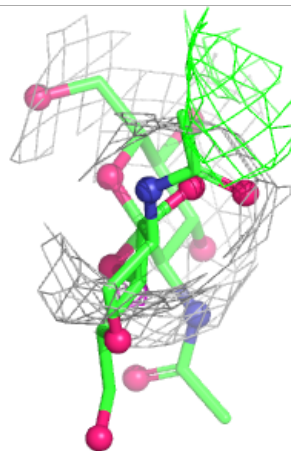
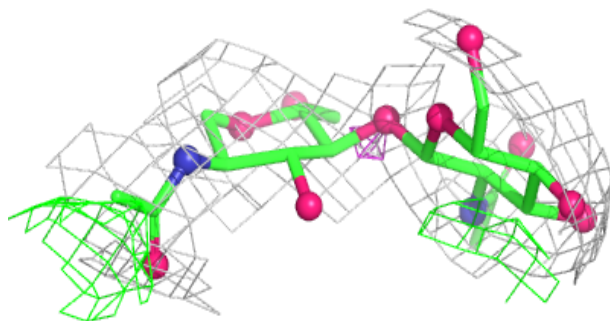
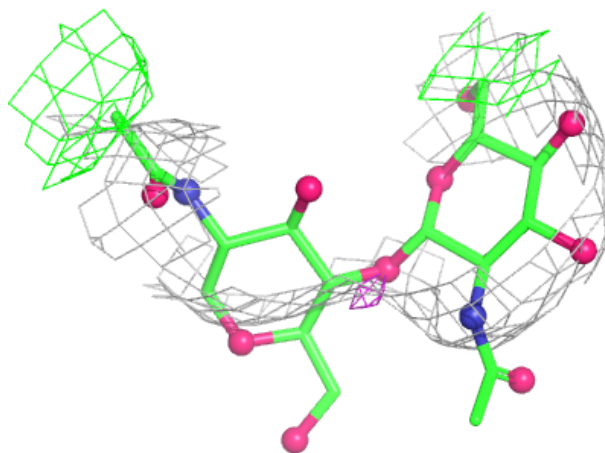
**Electron density around Chain 3:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



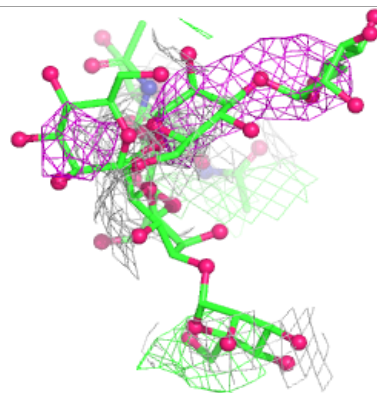
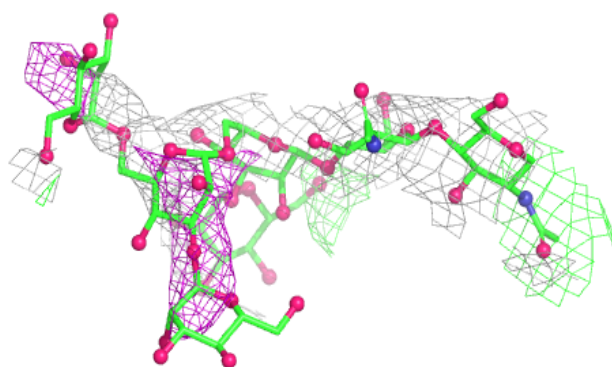
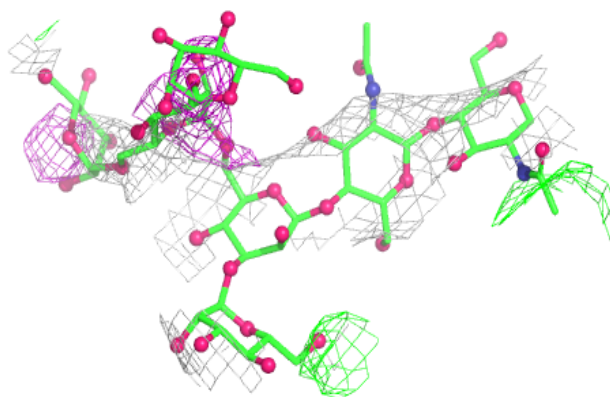
Electron density around Chain 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

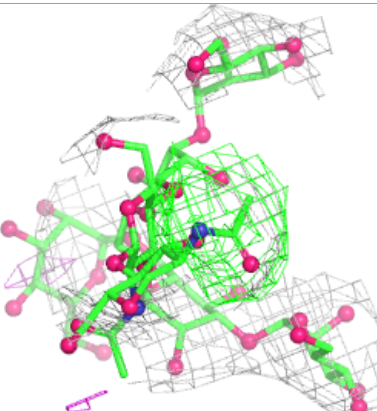
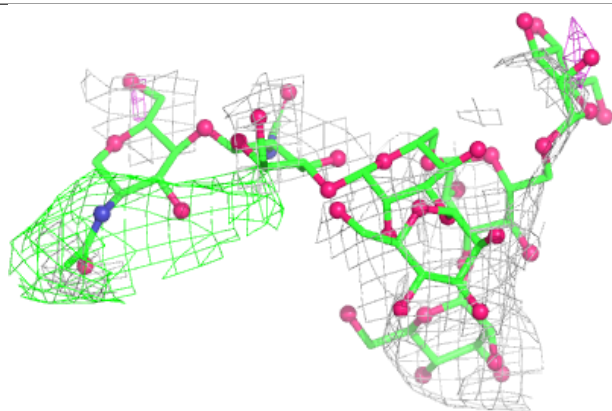
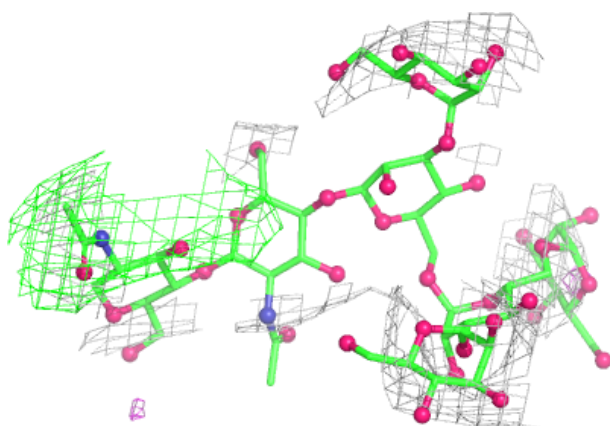


Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

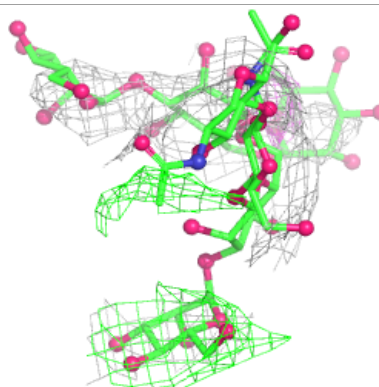
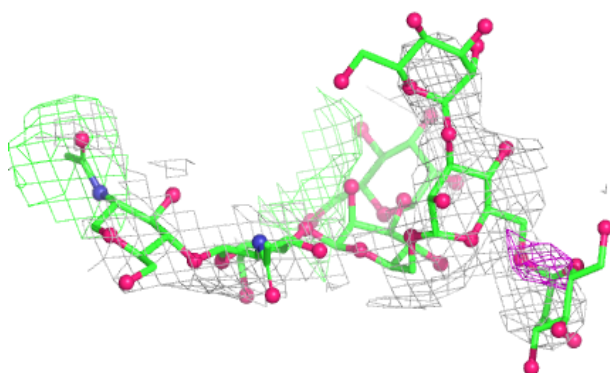
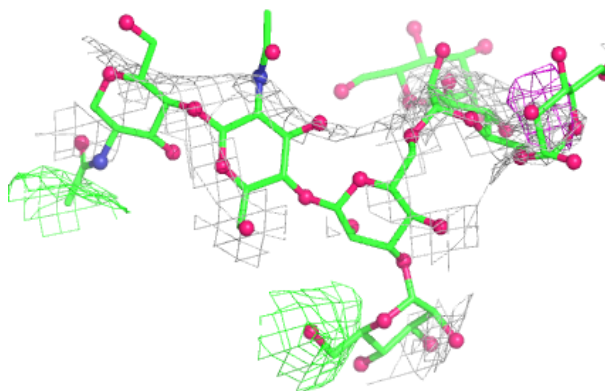
**Electron density around Chain X:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

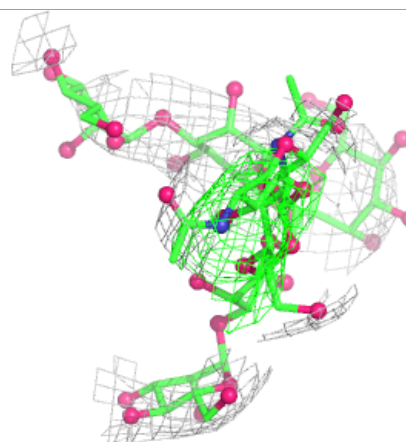
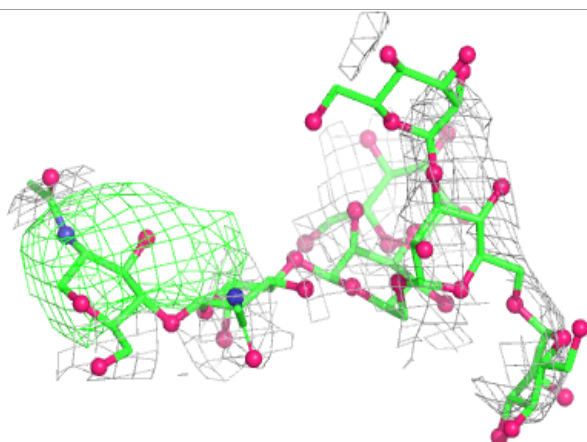
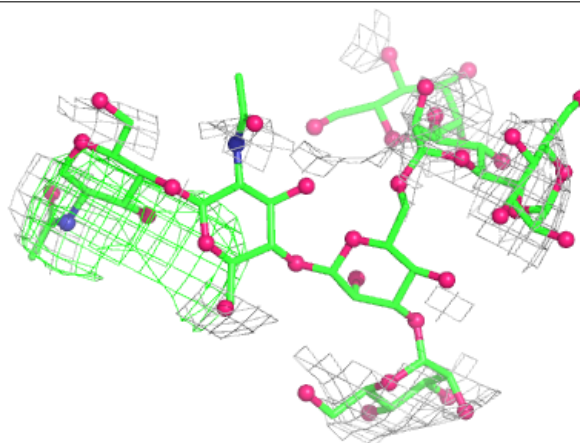


Electron density around Chain h:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

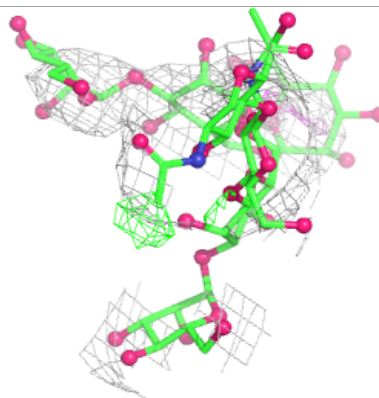
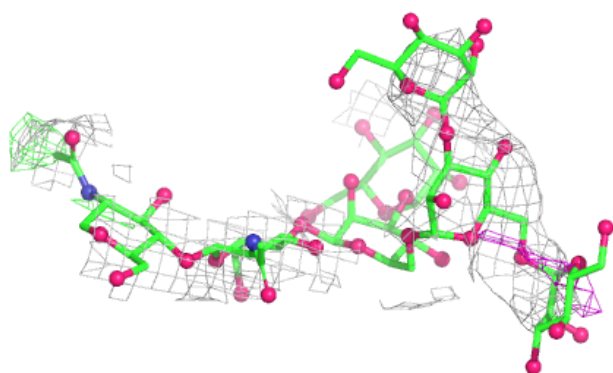
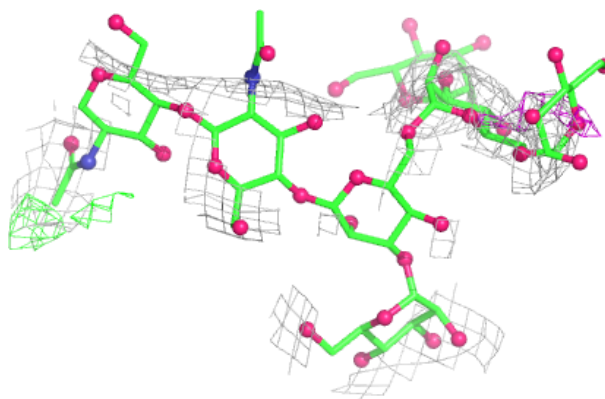
**Electron density around Chain i:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

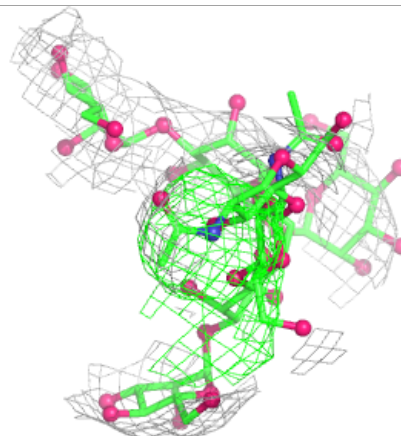
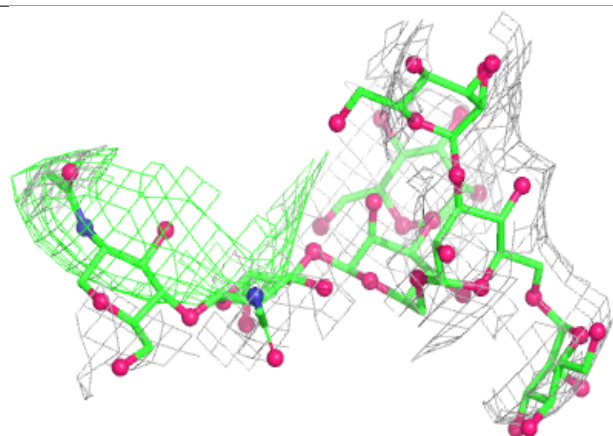
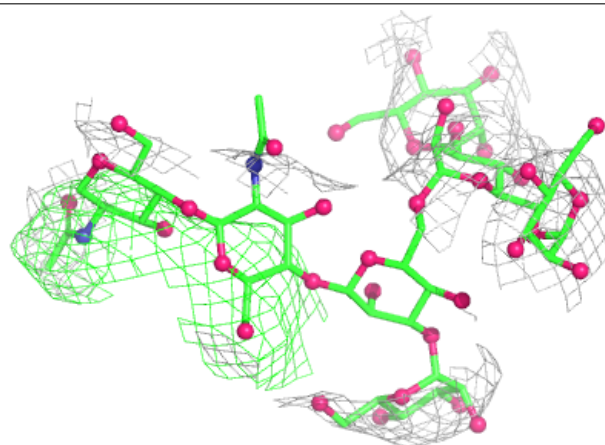


Electron density around Chain v:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

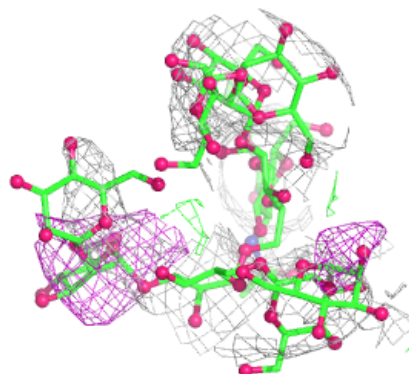
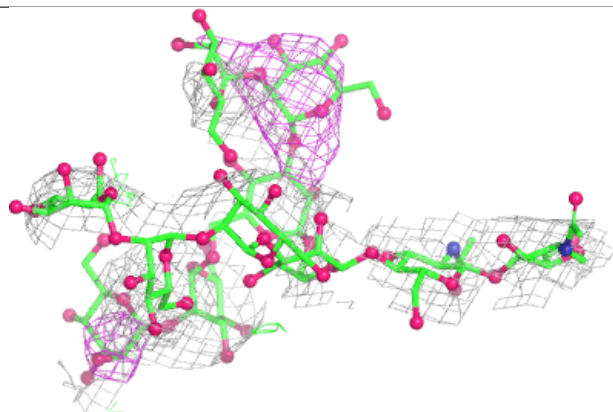
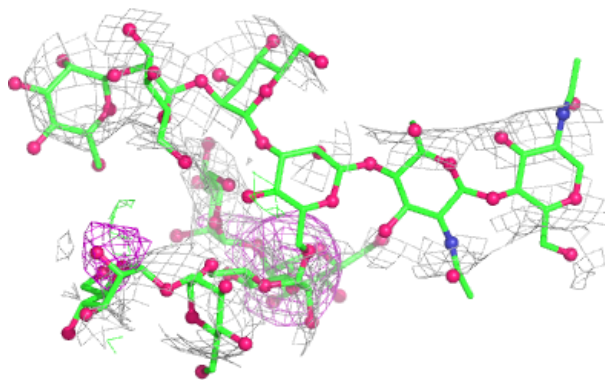
**Electron density around Chain z:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

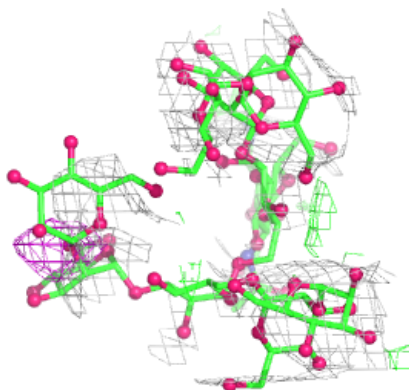
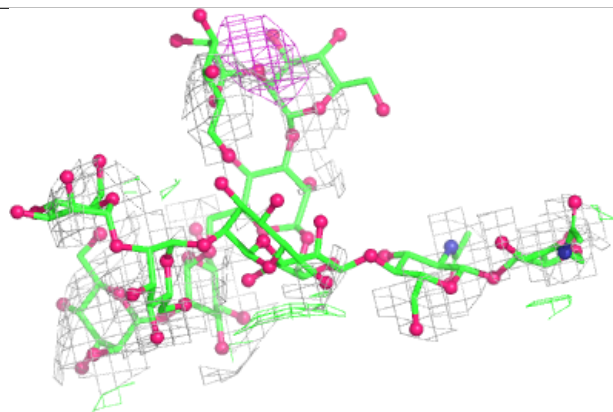
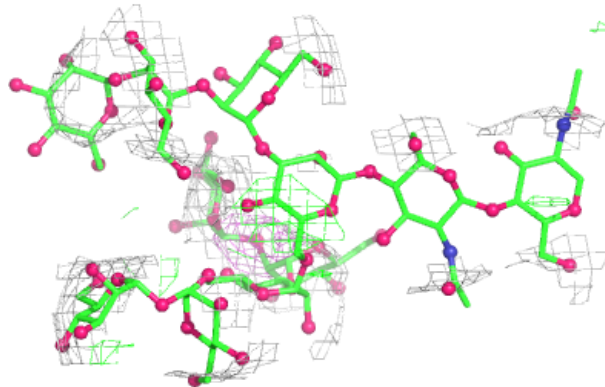


Electron density around Chain U:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

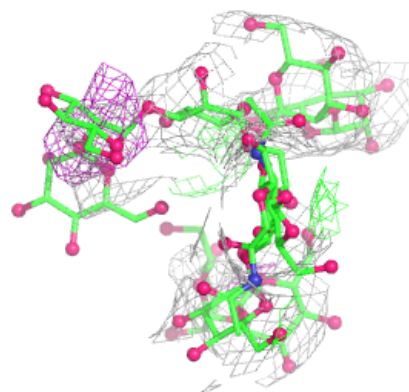
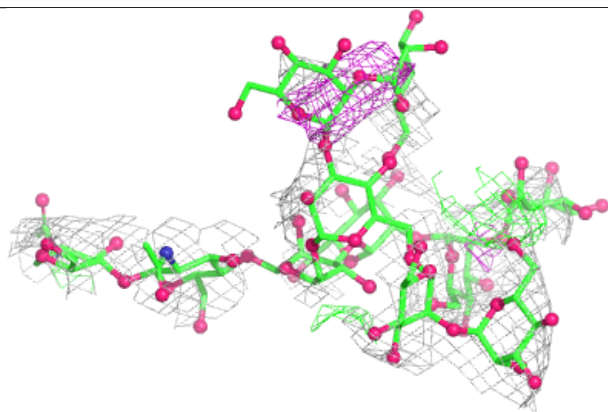
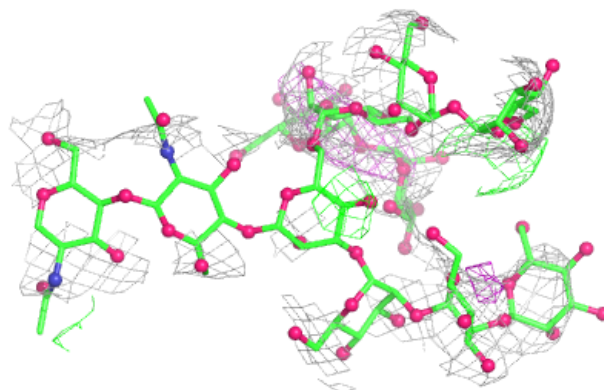
**Electron density around Chain i:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



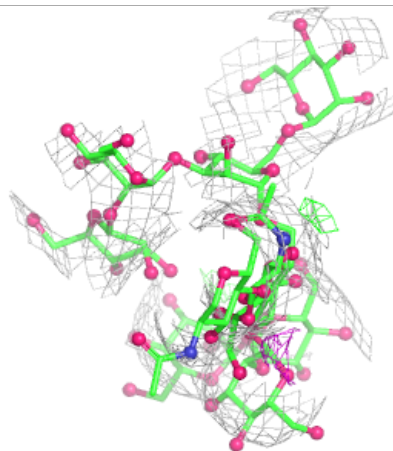
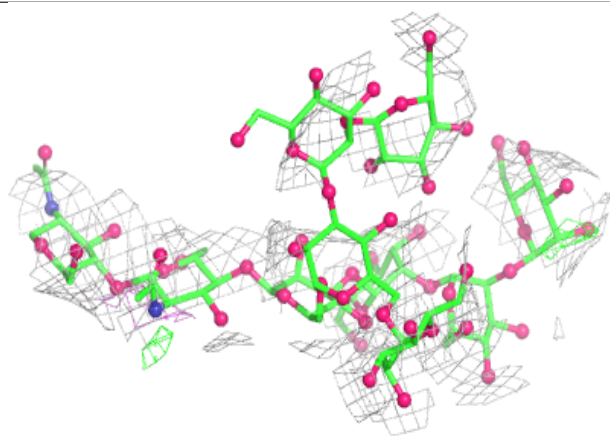
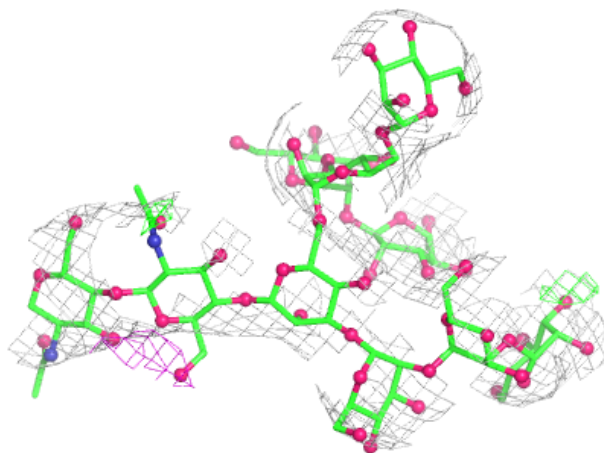
Electron density around Chain w:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



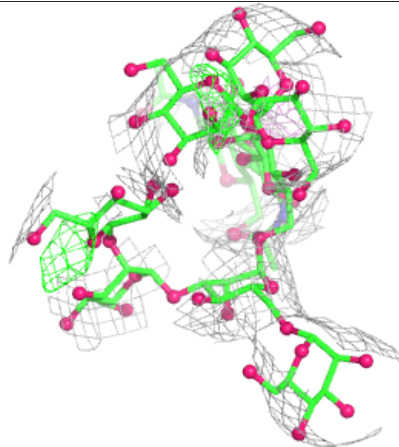
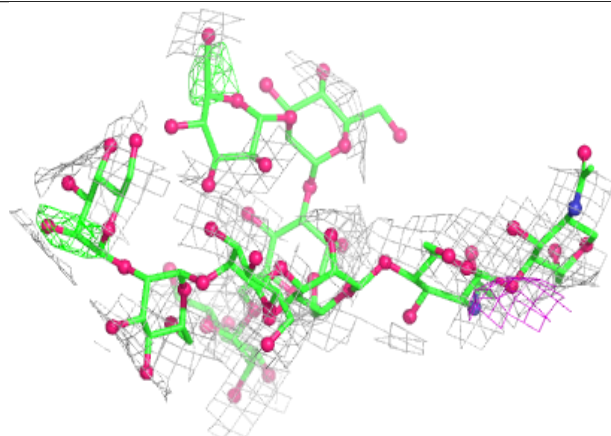
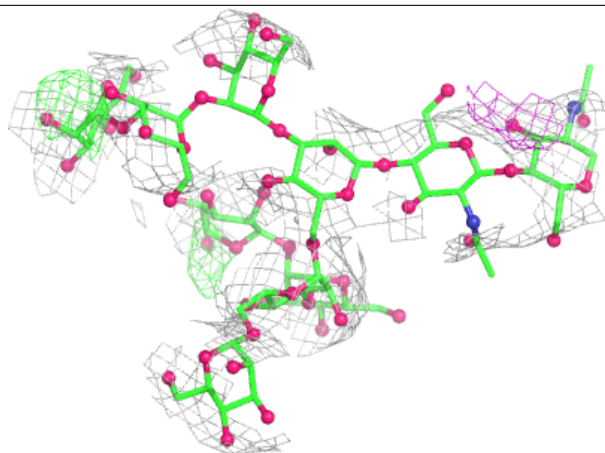
Electron density around Chain Y:

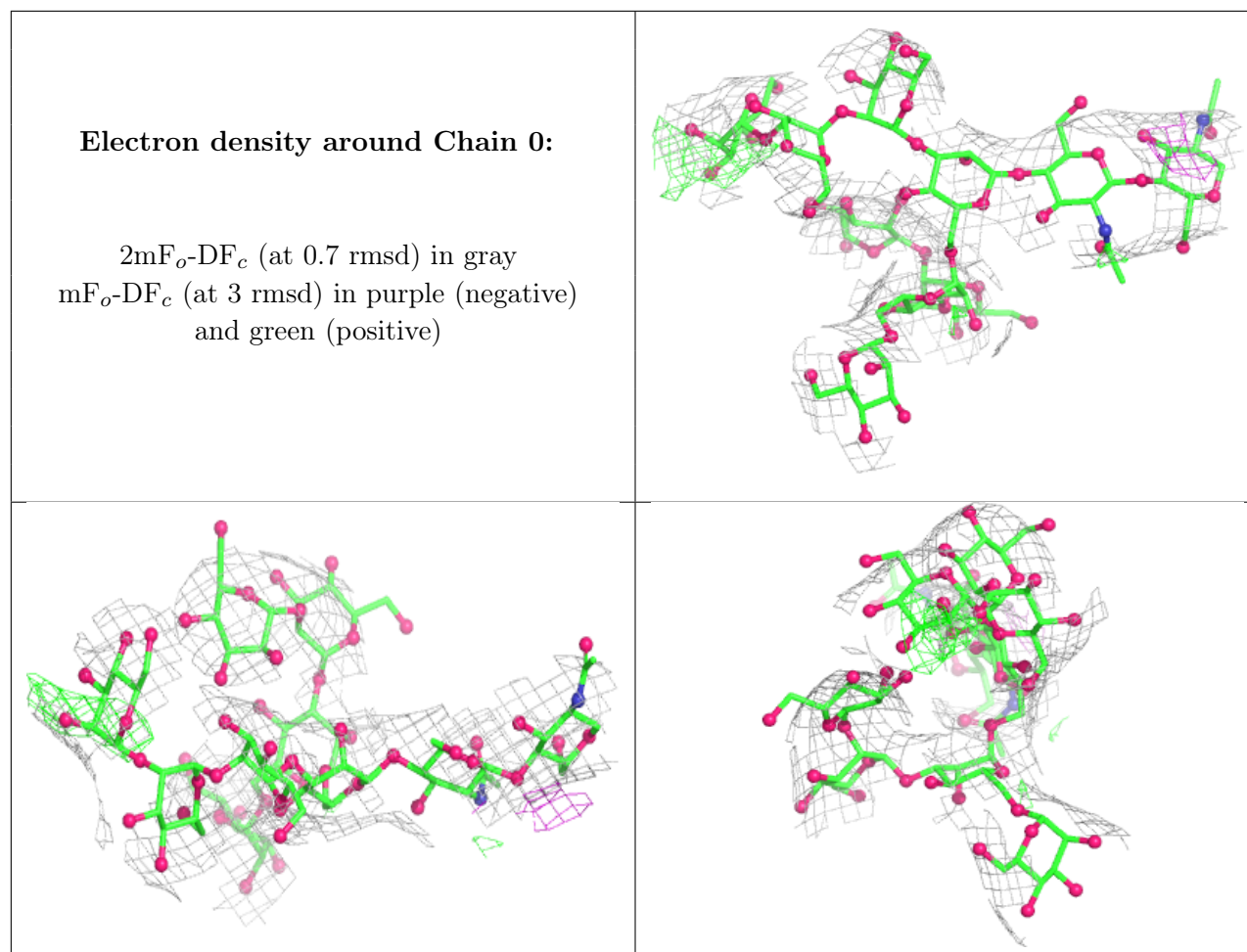
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain m:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
12	NAG	B	702	14/15	0.41	0.17	285,303,316,317	0
12	NAG	G	606	14/15	0.61	0.22	290,305,316,319	0
12	NAG	A	661	14/15	0.65	0.28	293,311,318,323	0
12	NAG	C	702	14/15	0.66	0.11	285,303,316,317	0
12	NAG	A	662	14/15	0.73	0.27	267,275,300,318	0
12	NAG	J	661	14/15	0.73	0.31	293,311,318,323	0
12	NAG	G	662	14/15	0.75	0.27	267,275,300,318	0
12	NAG	A	641	14/15	0.75	0.24	261,261,261,261	0
12	NAG	A	606	14/15	0.77	0.16	290,305,316,319	0
12	NAG	J	641	14/15	0.78	0.21	261,261,261,261	0
12	NAG	J	606	14/15	0.81	0.18	290,305,316,319	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	NAG	J	662	14/15	0.81	0.17	267,275,300,318	0
12	NAG	B	701	14/15	0.82	0.24	296,313,326,330	0
12	NAG	K	702	14/15	0.82	0.11	285,303,316,317	0
12	NAG	C	701	14/15	0.85	0.24	296,313,326,330	0
12	NAG	G	661	14/15	0.86	0.17	293,311,318,323	0
12	NAG	K	701	14/15	0.87	0.22	296,313,326,330	0
12	NAG	G	641	14/15	0.88	0.20	261,261,261,261	0

6.5 Other polymers [i](#)

There are no such residues in this entry.