



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 1ZPU / pdb_00001zpu
Title : Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import
Authors : Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.
Deposited on : 2005-05-17
Resolution : 2.80 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

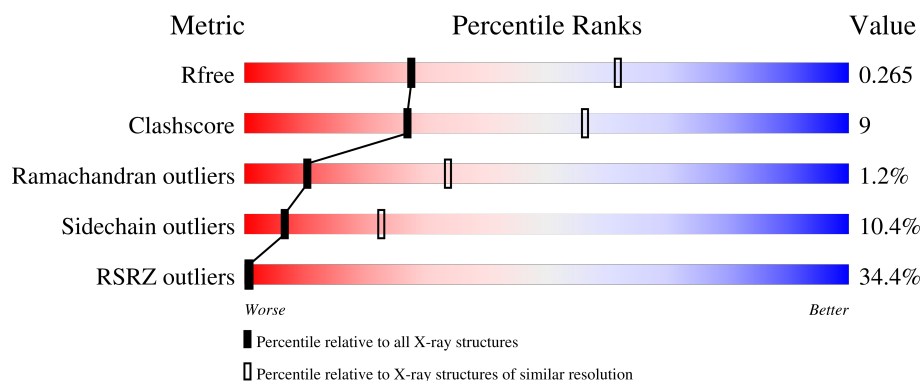
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	534	30% 72% 22% ..
1	B	534	13% 68% 26% 5% .
1	C	534	40% 71% 23% ..
1	D	534	25% 71% 24% ..
1	E	534	28% 75% 21% ..

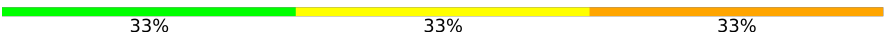
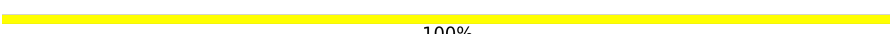
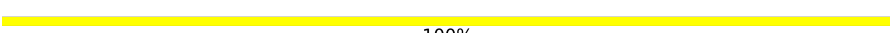
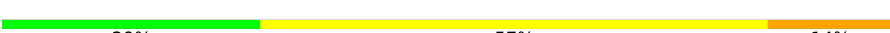
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Mol	Chain	Length	Quality of chain
1	F	534	
2	G	5	
2	J	5	
2	M	5	
2	O	5	
2	S	5	
2	U	5	
2	Y	5	
2	a	5	
2	d	5	
2	f	5	
2	i	5	
2	k	5	
3	H	6	
3	N	6	
3	Z	6	
3	j	6	
4	I	2	
4	P	2	
4	Q	2	
4	V	2	
4	b	2	
4	g	2	
5	K	3	
5	L	3	

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Mol	Chain	Length	Quality of chain
5	W	3	
5	X	3	
5	c	3	
5	h	3	
5	l	3	
6	R	4	
7	T	7	
7	e	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	a	1	X	-	-	-
2	NAG	f	1	X	-	-	-
3	NAG	H	1	X	-	-	-
3	NAG	N	1	X	-	-	-
3	NAG	Z	1	X	-	-	-
3	NAG	j	1	X	-	-	-
4	NAG	b	1	X	-	-	-
5	NAG	L	1	X	-	-	-
5	NAG	X	1	X	-	-	-
5	NAG	c	1	X	-	-	-
5	NAG	h	1	X	-	-	-
5	NAG	l	1	X	-	-	-
6	NAG	R	1	X	-	-	-
7	NAG	T	1	X	-	-	-
7	NAG	e	1	X	-	-	-
8	NAG	A	2006	X	-	-	-
8	NAG	A	2012	X	-	-	-
8	NAG	A	2018	X	-	-	-
8	NAG	B	2006	X	-	-	-
8	NAG	B	2012	X	-	-	-
8	NAG	B	2018	X	-	-	-
8	NAG	C	2012	X	-	-	-
8	NAG	C	2018	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	D	2006	X	-	-	-
8	NAG	E	2012	X	-	-	-
8	NAG	F	2005	X	-	-	-
8	NAG	F	2006	X	-	-	-
8	NAG	F	2009	X	-	-	-
8	NAG	F	2012	X	-	-	-

2 Entry composition [i](#)

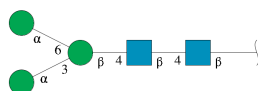
There are 9 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

- Molecule 2 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.



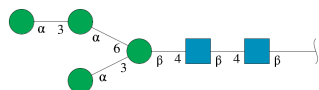
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	k	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



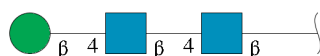
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	N	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	Z	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	j	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



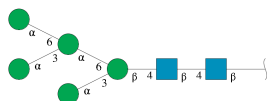
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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.



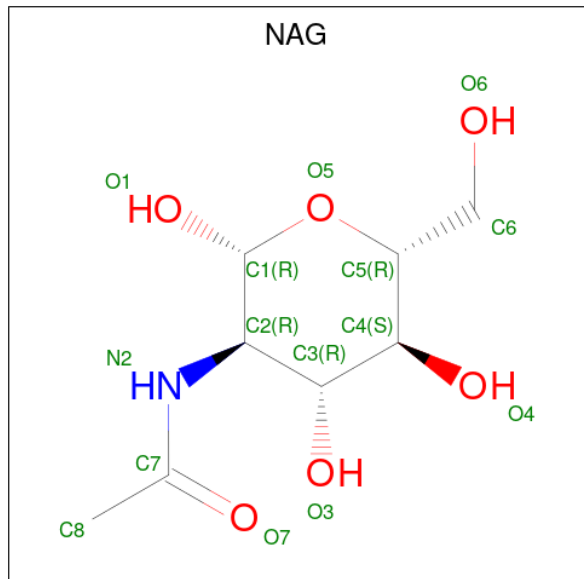
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 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
7	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	e	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



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

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

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

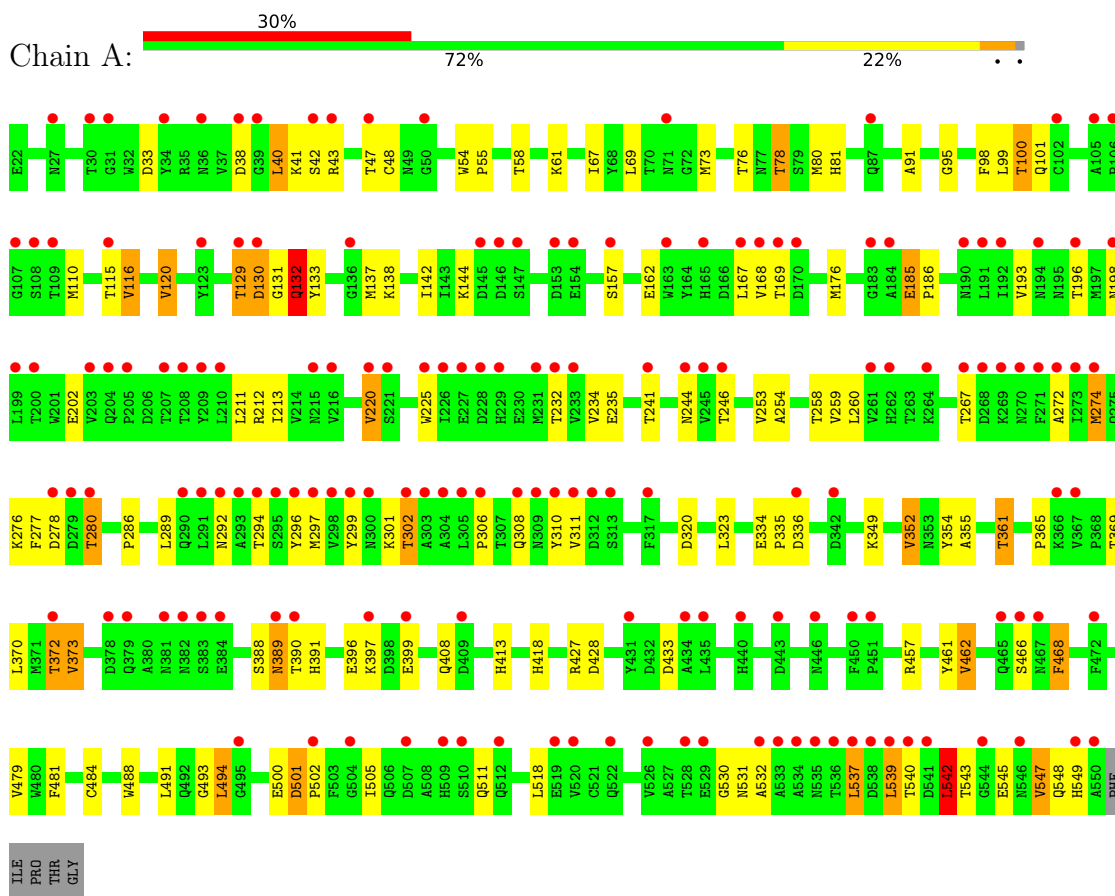
- Molecule 9 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cu	0	0
			4	4		
9	B	4	Total	Cu	0	0
			4	4		
9	C	4	Total	Cu	0	0
			4	4		
9	D	4	Total	Cu	0	0
			4	4		
9	E	4	Total	Cu	0	0
			4	4		
9	F	4	Total	Cu	0	0
			4	4		

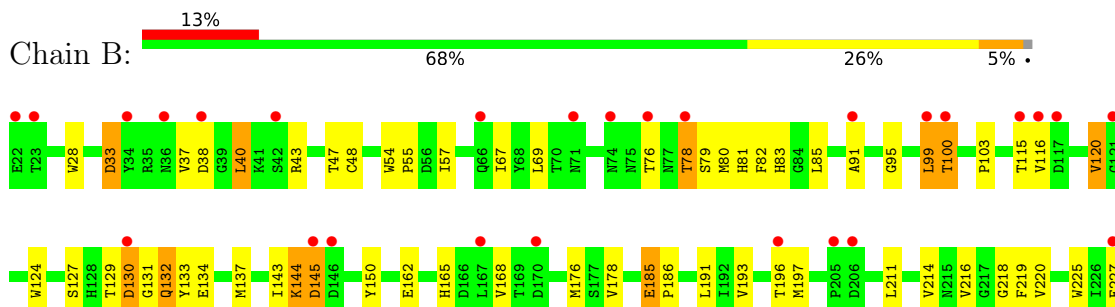
3 Residue-property plots

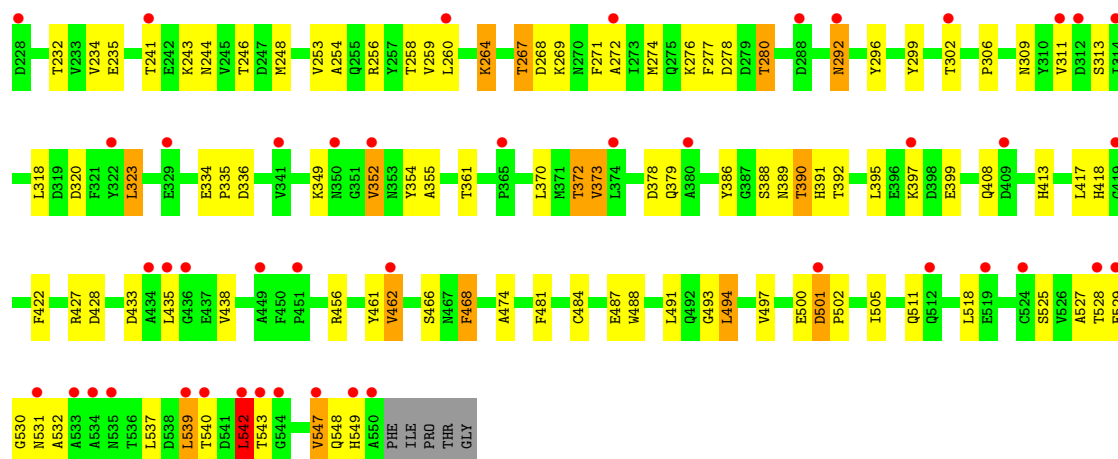
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Iron transport multicopper oxidase FET3

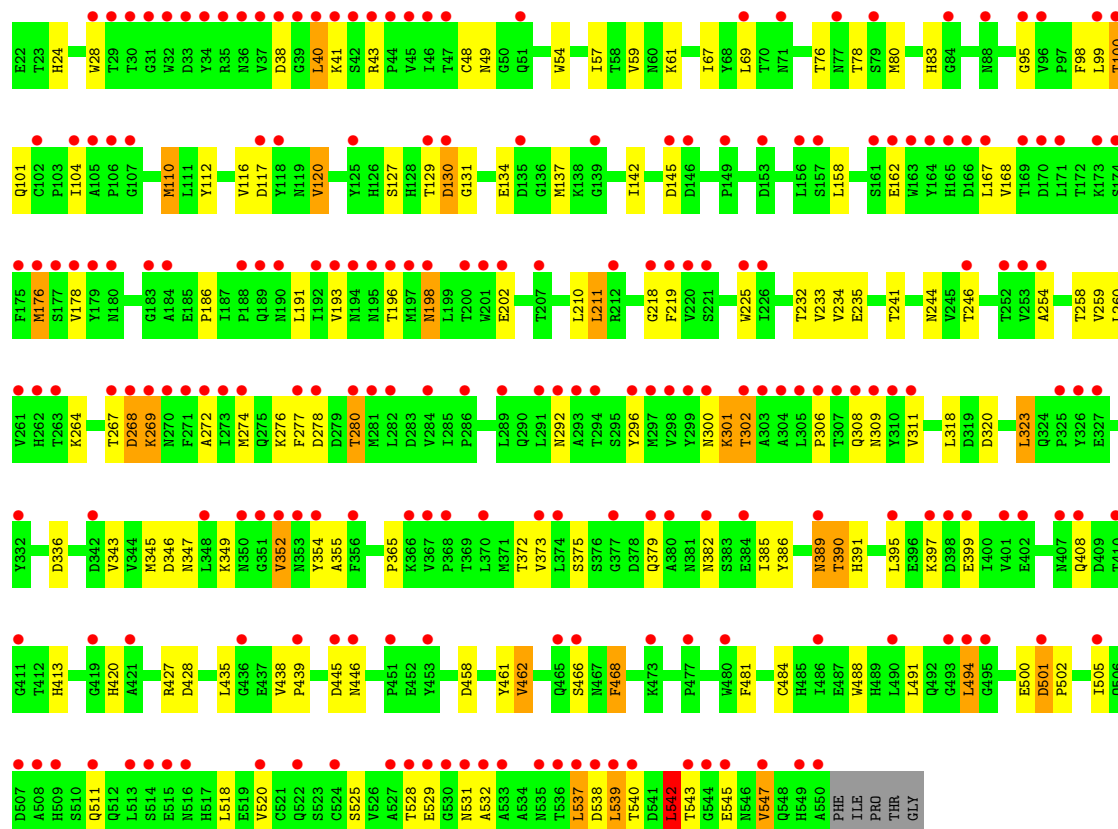


- Molecule 1: Iron transport multicopper oxidase FET3

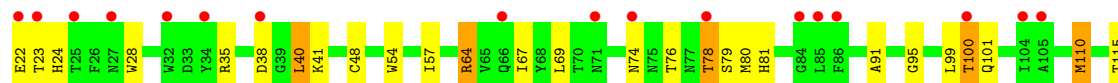
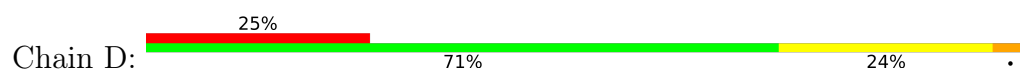


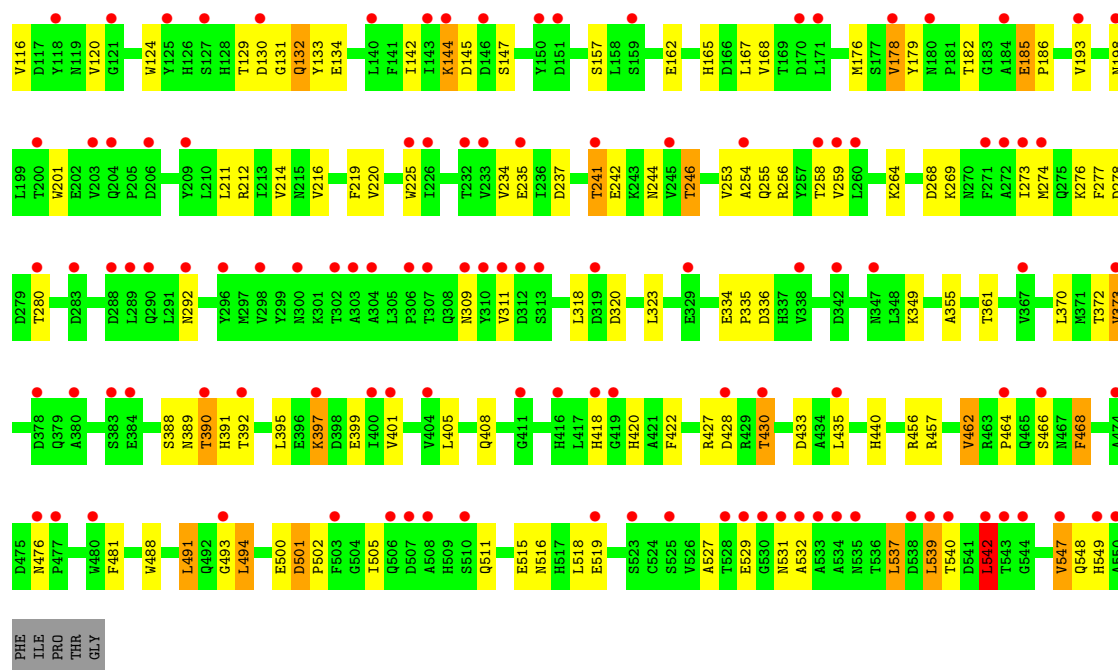


• Molecule 1: Iron transport multicopper oxidase FET3

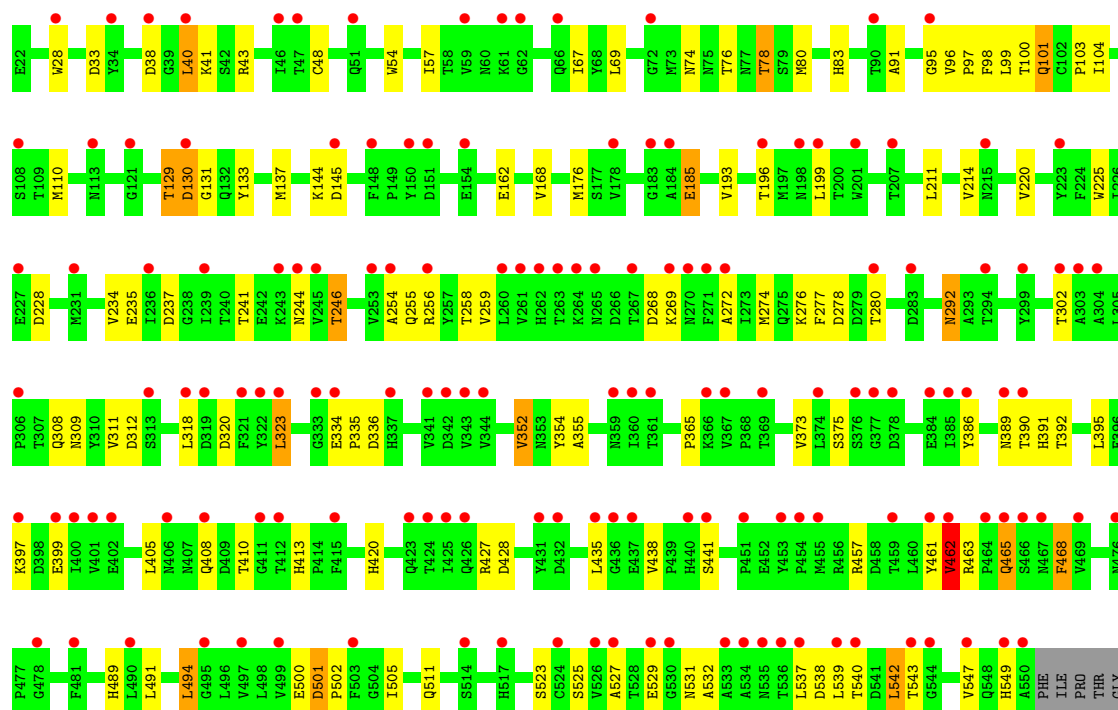
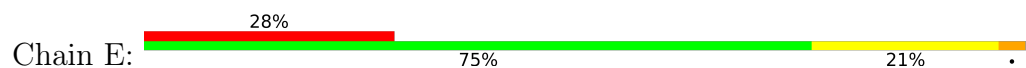


• Molecule 1: Iron transport multicopper oxidase FET3



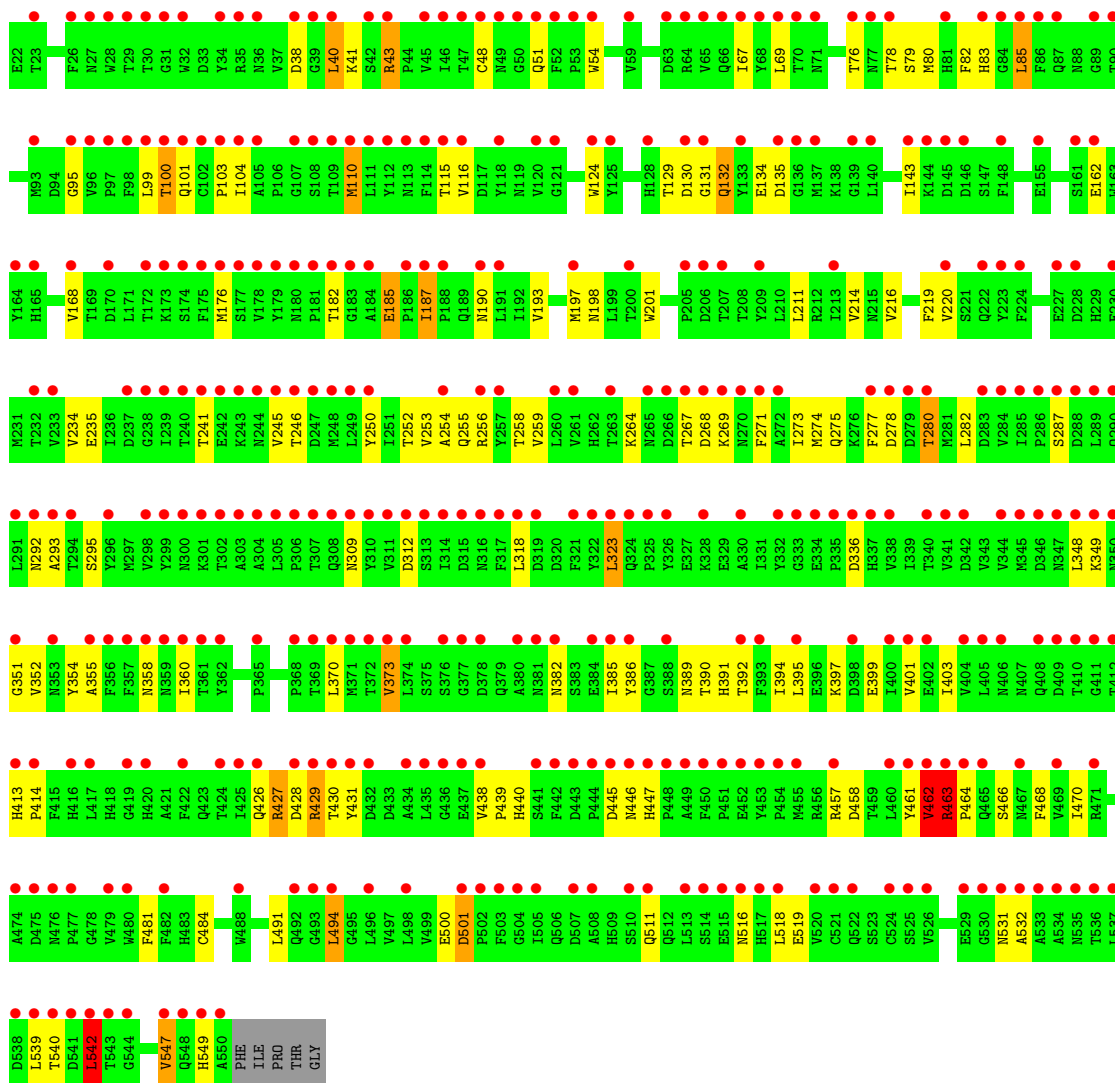


• Molecule 1: Iron transport multicopper oxidase FET3



• Molecule 1: Iron transport multicopper oxidase FET3





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

Chain G: 60%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain J: 80%

MAG1
MAG2
BMA3
MAN4
MAN5

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

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

Chain M:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain O:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain S:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain U:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain Y:  60% 40%

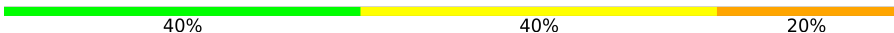
MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain a:  100%

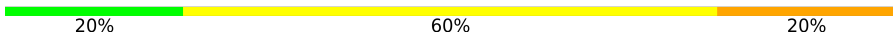
MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain d: 



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

Chain f: 

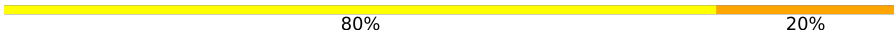


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 

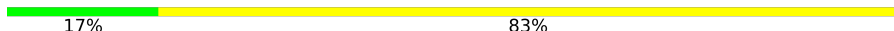


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 

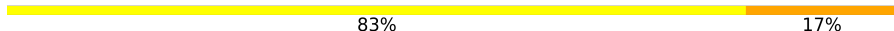


- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 



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

Chain N: 



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

Chain Z: 100%



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

Chain j: 83% 17%



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

Chain I: 50% 50%



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

Chain P: 50% 50%



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

Chain Q: 100%



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

Chain V: 100%

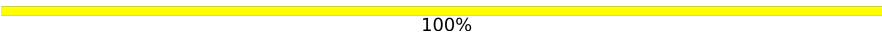


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: A horizontal bar divided into two equal 50% segments. The left segment is green and the right segment is yellow.

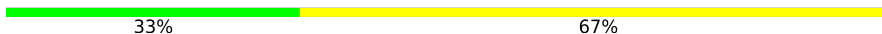


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: A horizontal bar that is entirely yellow, representing 100%.

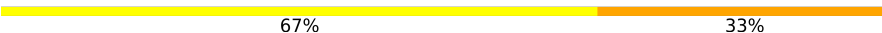


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: A horizontal bar divided into two segments: a green segment on the left representing 33%, and a yellow segment on the right representing 67%.



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

Chain L: A horizontal bar divided into two segments: a yellow segment on the left representing 67%, and an orange segment on the right representing 33%.

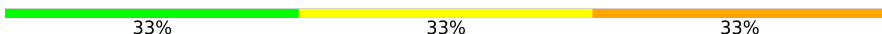


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: A horizontal bar divided into two segments: a yellow segment on the left representing 33%, and an orange segment on the right representing 67%.



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

Chain X: A horizontal bar divided into three equal 33% segments: green on the left, yellow in the middle, and orange on the right.

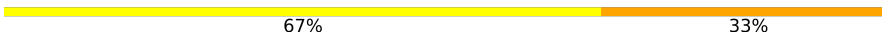


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  33% 67%

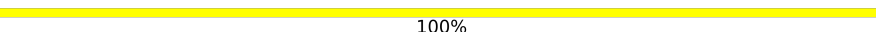
NAG1
NAG2
BMA3

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

Chain h:  67% 33%

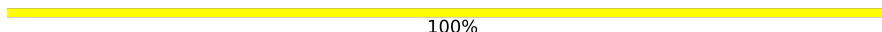
NAG1
NAG2
BMA3

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

Chain l:  100%

NAG1
NAG2
BMA3

- Molecule 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 R:  100%

NAG1
NAG2
BMA3
MAN4

- Molecule 7: 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% 57% 14%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 7: 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 e:  71% 29%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.257 0.235 , 0.265	Depositor DCC
R_{free} test set	6726 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, NAG, MAN, BMA

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	0.59	0/4373	0.88	2/5981 (0.0%)
1	B	0.59	2/4373 (0.0%)	0.87	4/5981 (0.1%)
1	C	0.62	5/4373 (0.1%)	0.86	4/5981 (0.1%)
1	D	0.53	3/4373 (0.1%)	0.80	1/5981 (0.0%)
1	E	0.52	2/4373 (0.0%)	0.80	4/5981 (0.1%)
1	F	0.96	19/4373 (0.4%)	0.86	7/5981 (0.1%)
All	All	0.65	31/26238 (0.1%)	0.85	22/35886 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	37.41	1.85	1.32
1	F	358	ASN	CG-OD1	12.49	1.47	1.23
1	F	445	ASP	CG-OD2	11.82	1.47	1.25
1	C	538	ASP	CG-OD2	11.39	1.47	1.25
1	F	312	ASP	CG-OD2	9.52	1.43	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	463	ARG	NE-CZ-NH2	-13.17	107.34	119.20
1	E	465	GLN	OE1-CD-NE2	-8.63	113.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	VAL	CB-CA-C	-7.61	100.79	111.21
1	C	458	ASP	CB-CA-C	-7.28	96.35	110.11
1	E	465	GLN	CG-CD-NE2	7.13	127.10	116.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

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	4254	0	3960	78	0
1	B	4254	0	3960	99	0
1	C	4254	0	3961	83	0
1	D	4254	0	3960	79	0
1	E	4254	0	3962	69	0
1	F	4254	0	3960	82	0
2	G	61	0	52	1	0
2	J	61	0	52	1	0
2	M	61	0	52	0	0
2	O	61	0	52	1	0
2	S	61	0	52	1	0
2	U	61	0	52	0	0
2	Y	61	0	52	2	0
2	a	61	0	52	0	0
2	d	61	0	52	1	0
2	f	61	0	52	1	0
2	i	61	0	52	0	0
2	k	61	0	52	1	0
3	H	72	0	61	0	0
3	N	72	0	61	1	0
3	Z	72	0	61	0	0
3	j	72	0	61	1	0
4	I	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
4	b	28	0	25	0	0
4	g	28	0	25	0	0
5	K	39	0	34	0	0
5	L	39	0	34	2	0
5	W	39	0	34	3	0
5	X	39	0	34	1	0
5	c	39	0	34	0	0
5	h	39	0	34	1	0
5	l	39	0	34	0	0
6	R	50	0	43	0	0
7	T	83	0	70	1	0
7	e	83	0	70	2	0
8	A	70	0	65	0	0
8	B	70	0	65	3	0
8	C	70	0	65	2	0
8	D	70	0	64	2	0
8	E	70	0	65	2	0
8	F	84	0	78	4	0
9	A	4	0	0	0	0
9	B	4	0	0	0	0
9	C	4	0	0	0	0
9	D	4	0	0	0	0
9	E	4	0	0	0	0
9	F	4	0	0	0	0
All	All	27659	0	25604	491	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 9.

The worst 5 of 491 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)
8:F:2006:NAG:C7	8:F:2006:NAG:C8	1.80	1.60
1:F:463:ARG:CZ	1:F:463:ARG:NH1	1.85	1.37
8:F:2005:NAG:O6	8:F:2005:NAG:C6	1.74	1.32
5:W:3:BMA:O6	5:W:3:BMA:C6	1.75	1.32
1:F:427:ARG:HD2	1:F:463:ARG:NH1	1.56	1.20

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	9	31
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	11	36
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	14	41
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	8	28
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	11	36
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	11	36
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	10	34

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	477/481 (99%)	427 (90%)	50 (10%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	477/481 (99%)	424 (89%)	53 (11%)	6	20
1	C	477/481 (99%)	426 (89%)	51 (11%)	6	21
1	D	477/481 (99%)	422 (88%)	55 (12%)	5	18
1	E	477/481 (99%)	434 (91%)	43 (9%)	9	28
1	F	477/481 (99%)	430 (90%)	47 (10%)	7	24
All	All	2862/2886 (99%)	2563 (90%)	299 (10%)	7	22

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	292	ASN
1	F	391	HIS
1	E	391	HIS
1	F	100	THR
1	B	528	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	465	GLN
1	F	51	GLN
1	D	492	GLN
1	E	347	ASN
1	F	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

135 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	2,1	14,14,15	0.71	0	17,19,21	1.37	3 (17%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
2	BMA	G	3	2	11,11,12	0.81	0	15,15,17	1.71	2 (13%)
2	MAN	G	4	2	11,11,12	0.58	0	15,15,17	1.33	1 (6%)
2	MAN	G	5	2	11,11,12	0.73	0	15,15,17	2.09	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.78	0	17,19,21	2.11	4 (23%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.85	0
3	BMA	H	3	3	11,11,12	0.73	0	15,15,17	1.82	3 (20%)
3	MAN	H	4	3	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
3	MAN	H	5	3	11,11,12	0.71	0	15,15,17	1.09	1 (6%)
3	MAN	H	6	3	11,11,12	0.67	0	15,15,17	1.54	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.63	0	17,19,21	2.17	5 (29%)
4	NAG	I	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.32	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.72	0	17,19,21	1.73	4 (23%)
2	NAG	J	2	2	14,14,15	0.62	0	17,19,21	2.05	3 (17%)
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	1.30	2 (13%)
2	MAN	J	4	2	11,11,12	0.72	0	15,15,17	1.59	2 (13%)
2	MAN	J	5	2	11,11,12	0.69	0	15,15,17	1.74	1 (6%)
5	NAG	K	1	5,1	14,14,15	0.51	0	17,19,21	2.04	3 (17%)
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.94	0
5	BMA	K	3	5	11,11,12	0.92	0	15,15,17	1.07	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.49	0	17,19,21	1.88	5 (29%)
5	NAG	L	2	5	14,14,15	0.54	0	17,19,21	1.14	2 (11%)
5	BMA	L	3	5	11,11,12	0.63	0	15,15,17	1.92	2 (13%)
2	NAG	M	1	2,1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
2	NAG	M	2	2	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
2	BMA	M	3	2	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
2	MAN	M	4	2	11,11,12	0.70	0	15,15,17	2.65	5 (33%)
2	MAN	M	5	2	11,11,12	0.45	0	15,15,17	1.34	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	3,1	14,14,15	0.69	0	17,19,21	1.53	4 (23%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
3	BMA	N	3	3	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	2.08	2 (13%)
3	MAN	N	5	3	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
3	MAN	N	6	3	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.56	0	17,19,21	1.68	3 (17%)
2	NAG	O	2	2	14,14,15	0.74	0	17,19,21	1.28	3 (17%)
2	BMA	O	3	2	11,11,12	0.75	0	15,15,17	1.51	4 (26%)
2	MAN	O	4	2	11,11,12	0.61	0	15,15,17	1.93	5 (33%)
2	MAN	O	5	2	11,11,12	1.67	2 (18%)	15,15,17	2.23	4 (26%)
4	NAG	P	1	4,1	14,14,15	0.56	0	17,19,21	0.96	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.47	0	17,19,21	1.87	4 (23%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	NAG	R	1	6,1	14,14,15	0.73	0	17,19,21	1.61	2 (11%)
6	NAG	R	2	6	14,14,15	0.62	0	17,19,21	1.21	2 (11%)
6	BMA	R	3	6	11,11,12	0.54	0	15,15,17	0.90	1 (6%)
6	MAN	R	4	6	11,11,12	0.53	0	15,15,17	2.04	4 (26%)
2	NAG	S	1	2,1	14,14,15	0.74	0	17,19,21	1.37	5 (29%)
2	NAG	S	2	2	14,14,15	0.61	0	17,19,21	1.36	3 (17%)
2	BMA	S	3	2	11,11,12	0.56	0	15,15,17	1.77	3 (20%)
2	MAN	S	4	2	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
2	MAN	S	5	2	11,11,12	0.62	0	15,15,17	1.18	1 (6%)
7	NAG	T	1	7,1	14,14,15	0.91	1 (7%)	17,19,21	2.10	7 (41%)
7	NAG	T	2	7	14,14,15	0.44	0	17,19,21	0.94	0
7	BMA	T	3	7	11,11,12	0.58	0	15,15,17	1.80	3 (20%)
7	MAN	T	4	7	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
7	MAN	T	5	7	11,11,12	0.70	0	15,15,17	0.75	0
7	MAN	T	6	7	11,11,12	0.55	0	15,15,17	2.10	1 (6%)
7	MAN	T	7	7	11,11,12	0.75	0	15,15,17	1.72	3 (20%)
2	NAG	U	1	2,1	14,14,15	0.48	0	17,19,21	1.98	2 (11%)
2	NAG	U	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.30	4 (23%)
2	BMA	U	3	2	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
2	MAN	U	4	2	11,11,12	0.77	0	15,15,17	1.43	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	U	5	2	11,11,12	0.59	0	15,15,17	1.61	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
4	NAG	V	2	4	14,14,15	1.20	2 (14%)	17,19,21	1.46	2 (11%)
5	NAG	W	1	5,1	14,14,15	1.99	3 (21%)	17,19,21	0.92	0
5	NAG	W	2	5	14,14,15	1.77	3 (21%)	17,19,21	2.25	4 (23%)
5	BMA	W	3	5	11,11,12	2.48	1 (9%)	15,15,17	1.70	4 (26%)
5	NAG	X	1	5,1	14,14,15	0.49	0	17,19,21	1.80	5 (29%)
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.21	2 (11%)
5	BMA	X	3	5	11,11,12	0.66	0	15,15,17	0.88	0
2	NAG	Y	1	2,1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	Y	2	2	14,14,15	0.58	0	17,19,21	1.23	3 (17%)
2	BMA	Y	3	2	11,11,12	0.57	0	15,15,17	1.29	2 (13%)
2	MAN	Y	4	2	11,11,12	0.57	0	15,15,17	1.25	1 (6%)
2	MAN	Y	5	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
3	NAG	Z	1	3,1	14,14,15	0.62	0	17,19,21	1.77	3 (17%)
3	NAG	Z	2	3	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
3	BMA	Z	3	3	11,11,12	0.70	0	15,15,17	1.75	4 (26%)
3	MAN	Z	4	3	11,11,12	0.59	0	15,15,17	1.09	1 (6%)
3	MAN	Z	5	3	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
3	MAN	Z	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.83	3 (20%)
2	NAG	a	1	2,1	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	NAG	a	2	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
2	BMA	a	3	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
2	MAN	a	4	2	11,11,12	0.54	0	15,15,17	1.46	1 (6%)
2	MAN	a	5	2	11,11,12	0.60	0	15,15,17	1.53	2 (13%)
4	NAG	b	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	1.66	3 (17%)
4	NAG	b	2	4	14,14,15	0.50	0	17,19,21	0.69	0
5	NAG	c	1	5,1	14,14,15	0.53	0	17,19,21	1.38	2 (11%)
5	NAG	c	2	5	14,14,15	0.54	0	17,19,21	0.82	0
5	BMA	c	3	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	d	1	2,1	14,14,15	0.60	0	17,19,21	1.11	1 (5%)
2	NAG	d	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	d	3	2	11,11,12	0.76	0	15,15,17	1.91	4 (26%)
2	MAN	d	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	MAN	d	5	2	11,11,12	0.54	0	15,15,17	1.38	1 (6%)
7	NAG	e	1	7,1	14,14,15	0.56	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	e	2	7	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
7	BMA	e	3	7	11,11,12	0.61	0	15,15,17	1.41	4 (26%)
7	MAN	e	4	7	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	MAN	e	5	7	11,11,12	0.55	0	15,15,17	0.98	1 (6%)
7	MAN	e	6	7	11,11,12	0.70	0	15,15,17	1.54	2 (13%)
7	MAN	e	7	7	11,11,12	0.52	0	15,15,17	1.52	1 (6%)
2	NAG	f	1	2,1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
2	NAG	f	2	2	14,14,15	0.50	0	17,19,21	0.95	0
2	BMA	f	3	2	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
2	MAN	f	4	2	11,11,12	0.56	0	15,15,17	1.34	1 (6%)
2	MAN	f	5	2	11,11,12	0.56	0	15,15,17	1.37	1 (6%)
4	NAG	g	1	4,1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
4	NAG	g	2	4	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
5	NAG	h	1	5,1	14,14,15	0.60	0	17,19,21	1.68	4 (23%)
5	NAG	h	2	5	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
5	BMA	h	3	5	11,11,12	0.86	0	15,15,17	1.78	3 (20%)
2	NAG	i	1	2,1	14,14,15	0.60	0	17,19,21	0.96	0
2	NAG	i	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	i	3	2	11,11,12	0.64	0	15,15,17	1.31	3 (20%)
2	MAN	i	4	2	11,11,12	0.64	0	15,15,17	1.79	3 (20%)
2	MAN	i	5	2	11,11,12	0.49	0	15,15,17	1.57	1 (6%)
3	NAG	j	1	3,1	14,14,15	0.63	0	17,19,21	1.49	3 (17%)
3	NAG	j	2	3	14,14,15	0.75	0	17,19,21	1.50	2 (11%)
3	BMA	j	3	3	11,11,12	0.78	0	15,15,17	0.90	2 (13%)
3	MAN	j	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.42	2 (13%)
3	MAN	j	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.92	1 (6%)
3	MAN	j	6	3	11,11,12	0.58	0	15,15,17	1.55	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
2	NAG	k	2	2	14,14,15	0.55	0	17,19,21	1.07	2 (11%)
2	BMA	k	3	2	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
2	MAN	k	4	2	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
2	MAN	k	5	2	11,11,12	1.57	1 (9%)	15,15,17	1.70	2 (13%)
5	NAG	l	1	5,1	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
5	NAG	l	2	5	14,14,15	0.57	0	17,19,21	1.52	4 (23%)
5	BMA	l	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.98	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
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	1/1/1/1
3	NAG	H	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	5/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	MAN	J	5	2	-	1/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	1/2/19/22	0/1/1/1
2	MAN	M	5	2	-	1/2/19/22	1/1/1/1
3	NAG	N	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1

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

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

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

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	O6-C6	7.78	1.75	1.42
2	k	5	MAN	O6-C6	4.89	1.63	1.42
5	l	3	BMA	O6-C6	4.81	1.62	1.42
5	W	1	NAG	C8-C7	4.59	1.60	1.50
5	W	2	NAG	C8-C7	4.54	1.60	1.50

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MAN	C1-O5-C5	7.27	121.93	112.19
2	M	4	MAN	C1-O5-C5	7.15	121.77	112.19
2	O	5	MAN	C1-O5-C5	6.84	121.35	112.19
2	U	1	NAG	C1-O5-C5	6.74	121.22	112.19
7	T	6	MAN	C1-O5-C5	6.61	121.04	112.19

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	a	1	NAG	C1
2	f	1	NAG	C1
3	H	1	NAG	C1
3	N	1	NAG	C1
3	Z	1	NAG	C1

5 of 250 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	5	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	f	4	MAN	C1-C2-C3-C4-C5-O5
2	i	5	MAN	C1-C2-C3-C4-C5-O5
2	M	5	MAN	C1-C2-C3-C4-C5-O5

21 monomers are involved in 23 short contacts:

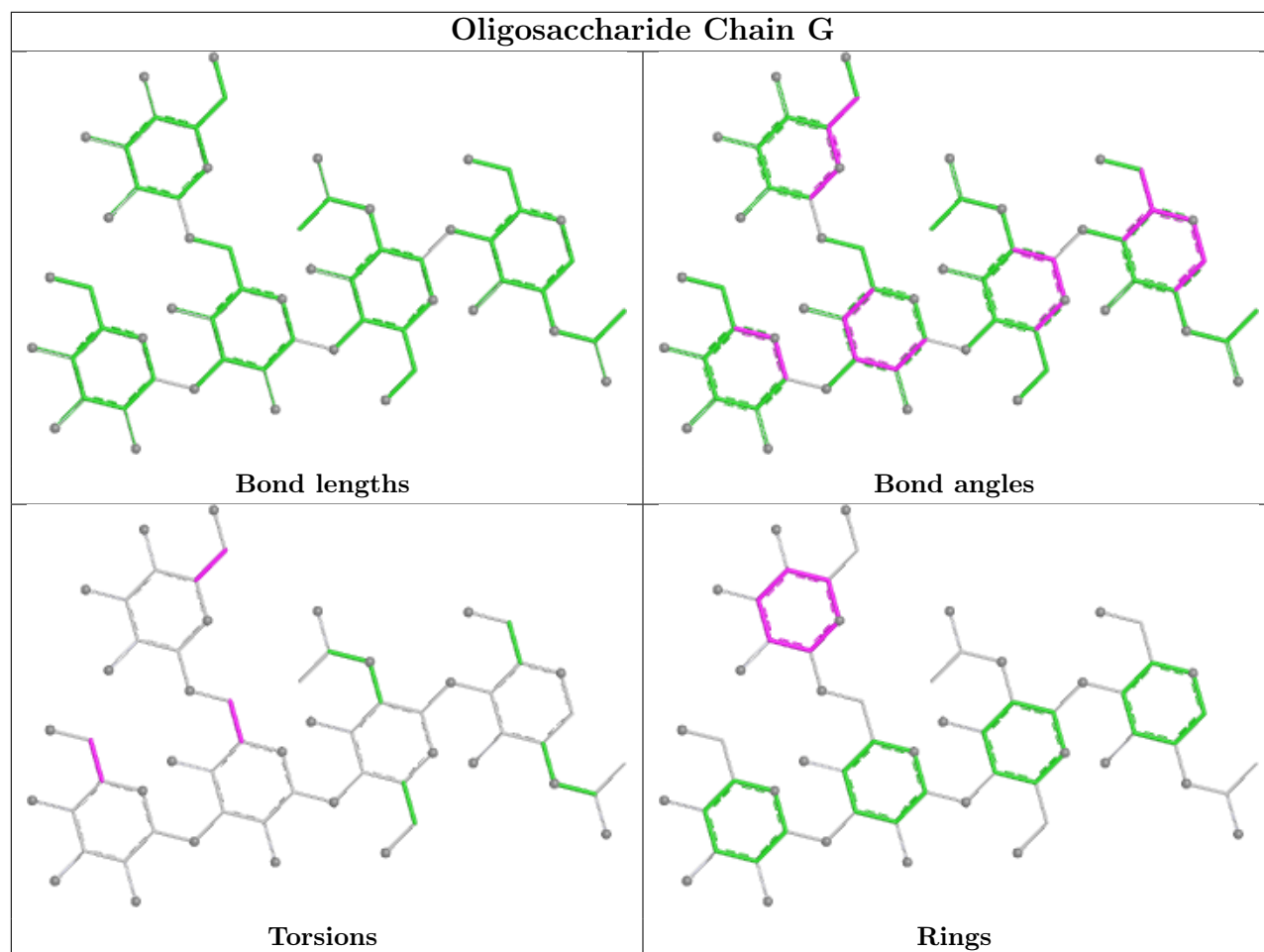
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	BMA	1	0
3	j	1	NAG	1	0
2	G	4	MAN	1	0
2	J	2	NAG	1	0
3	N	1	NAG	1	0

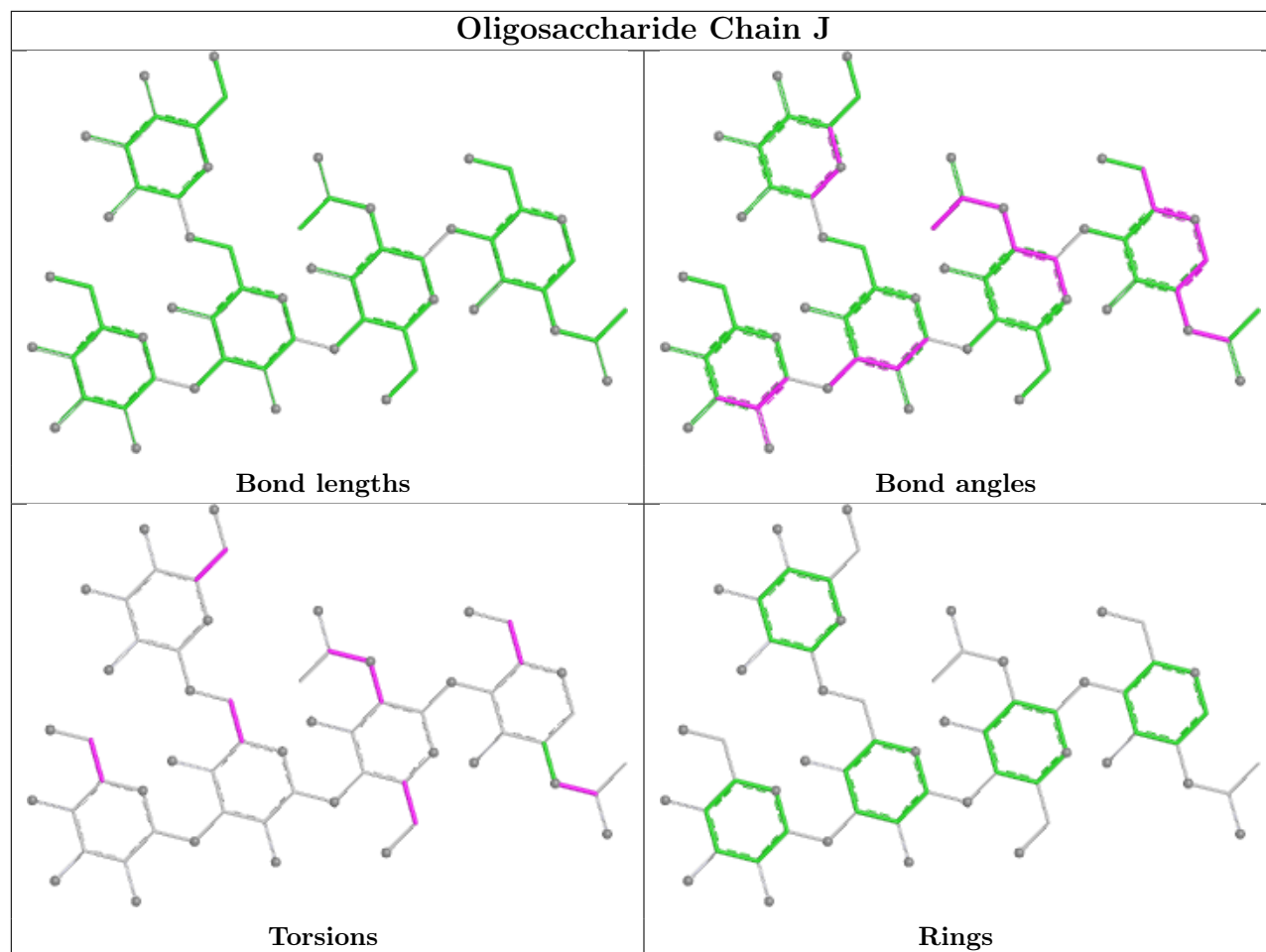
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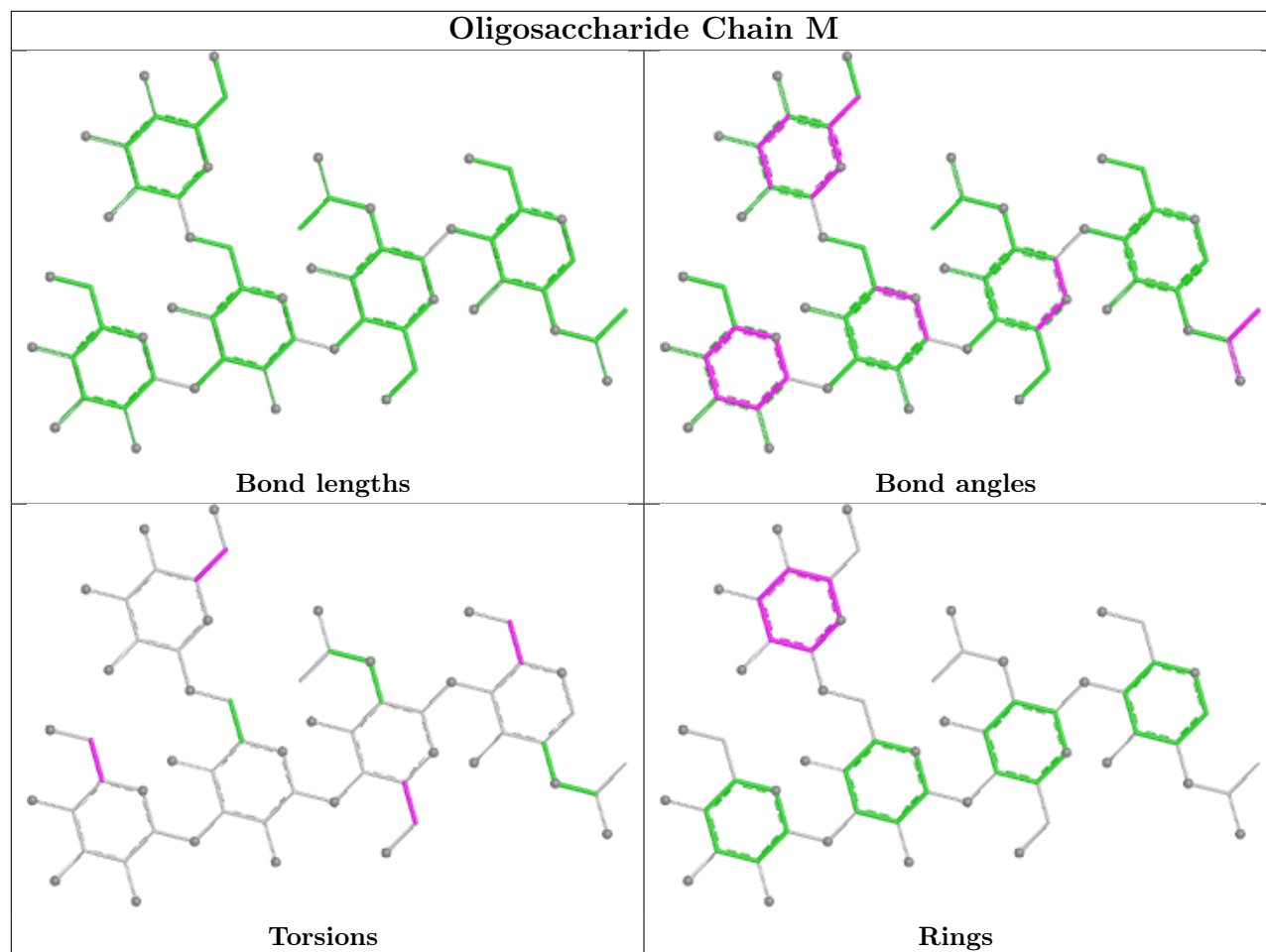
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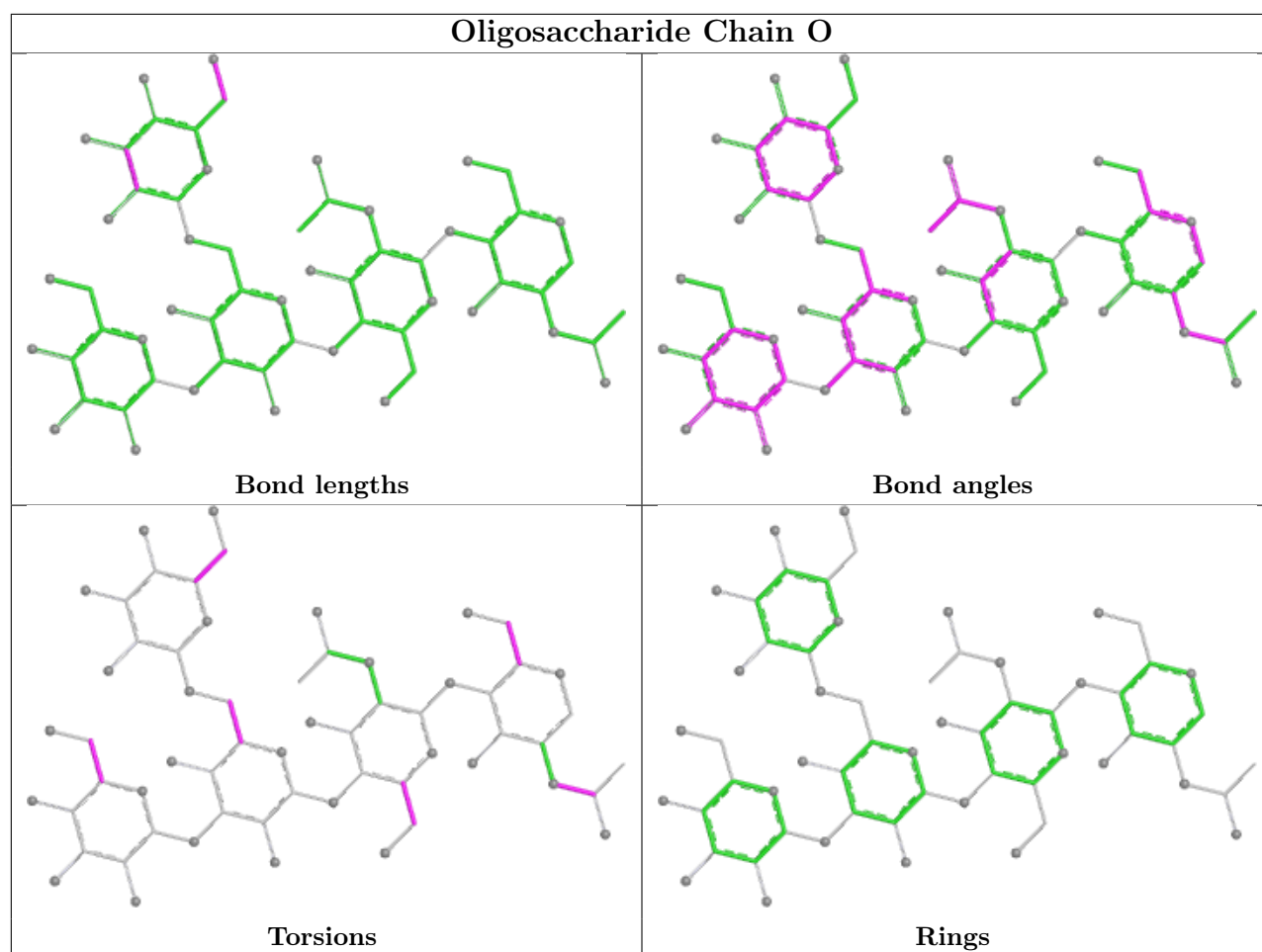
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	2	NAG	1	0
4	I	1	NAG	2	0
7	e	1	NAG	1	0
5	L	1	NAG	2	0
2	S	2	NAG	1	0
5	W	3	BMA	2	0
2	Y	2	NAG	1	0
2	Y	5	MAN	1	0
2	k	1	NAG	1	0
7	e	2	NAG	2	0
2	d	1	NAG	1	0
2	f	1	NAG	1	0
7	T	1	NAG	1	0
5	X	1	NAG	1	0
2	O	1	NAG	1	0
5	h	1	NAG	1	0

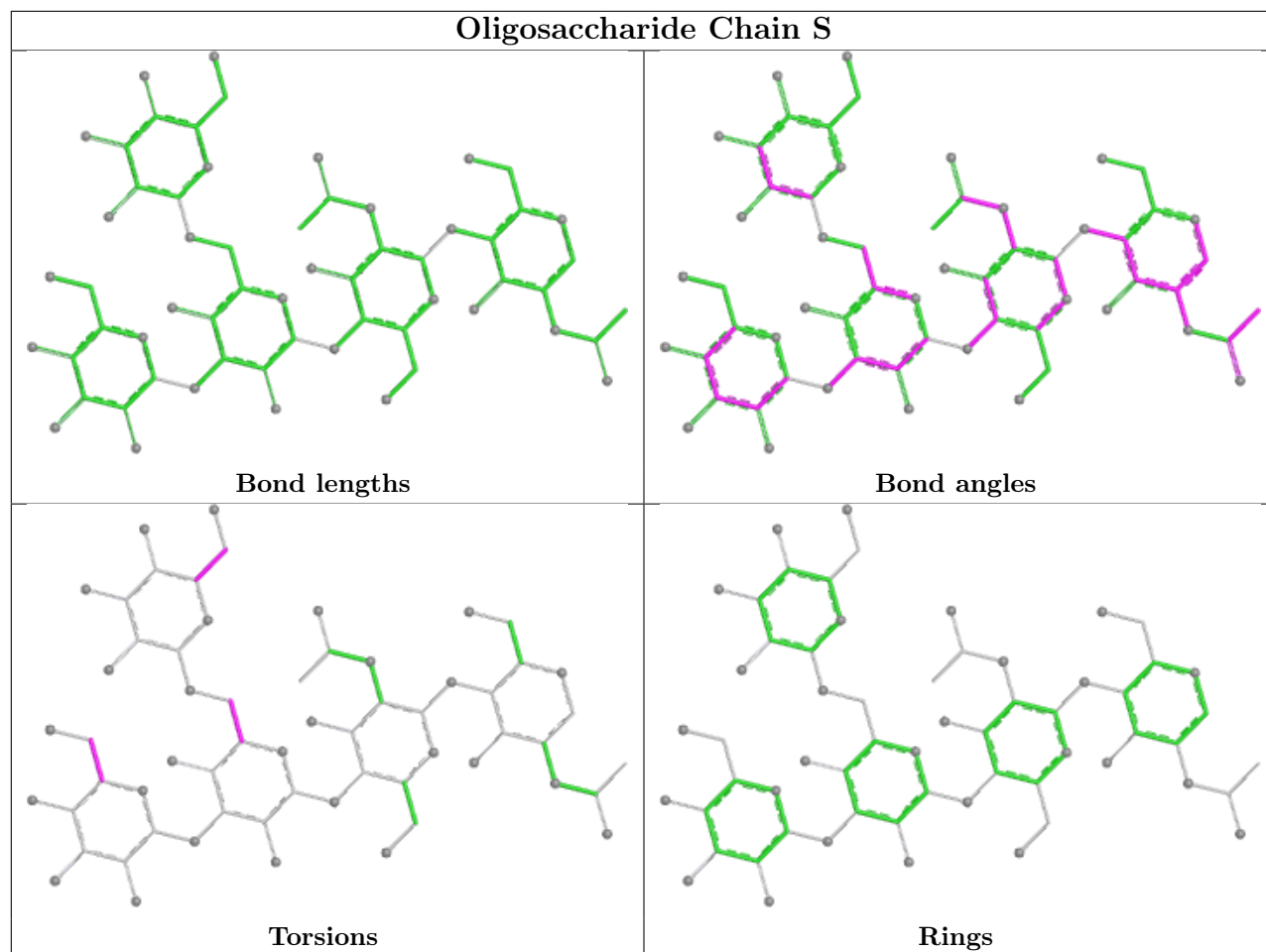
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

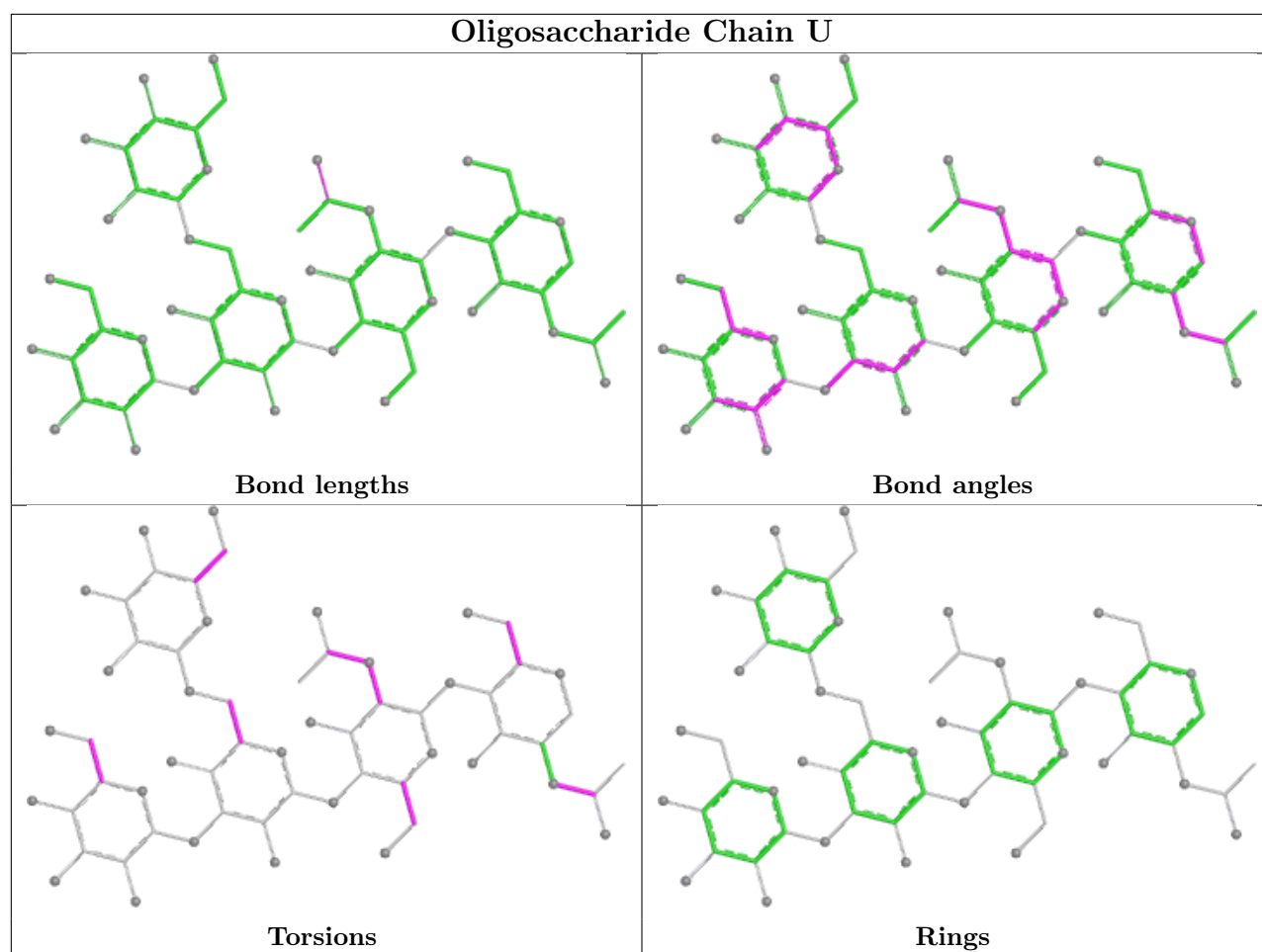


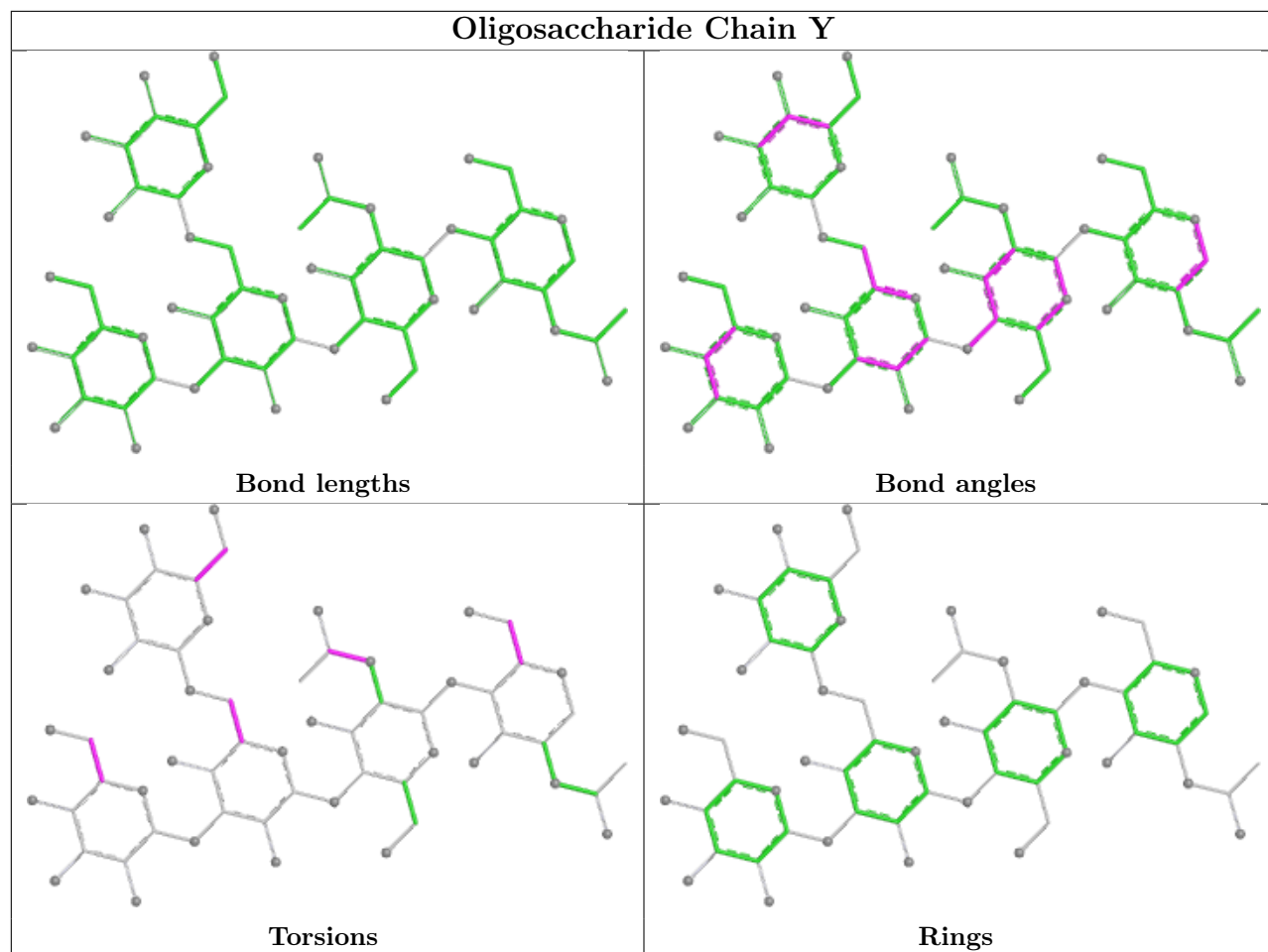


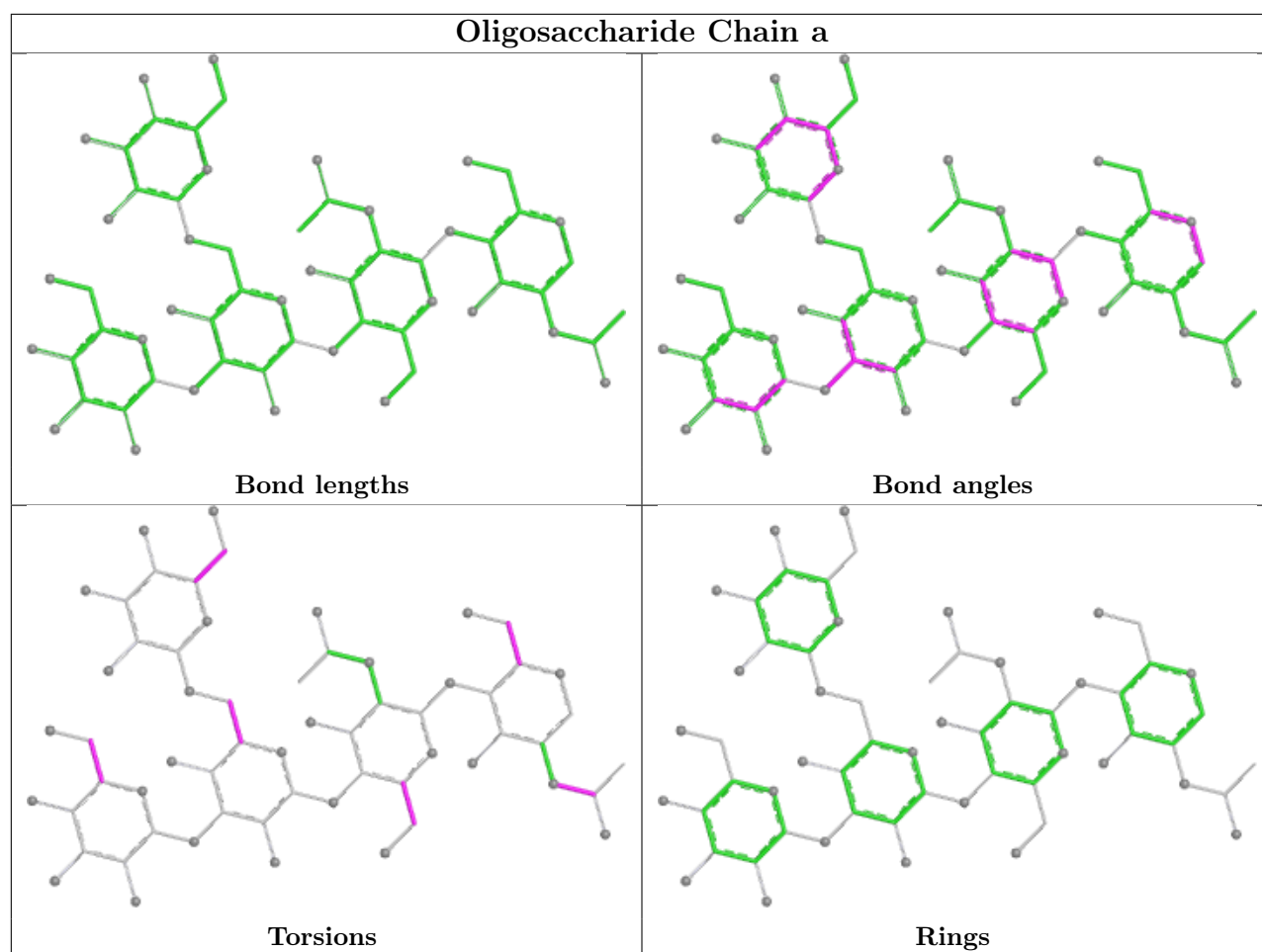


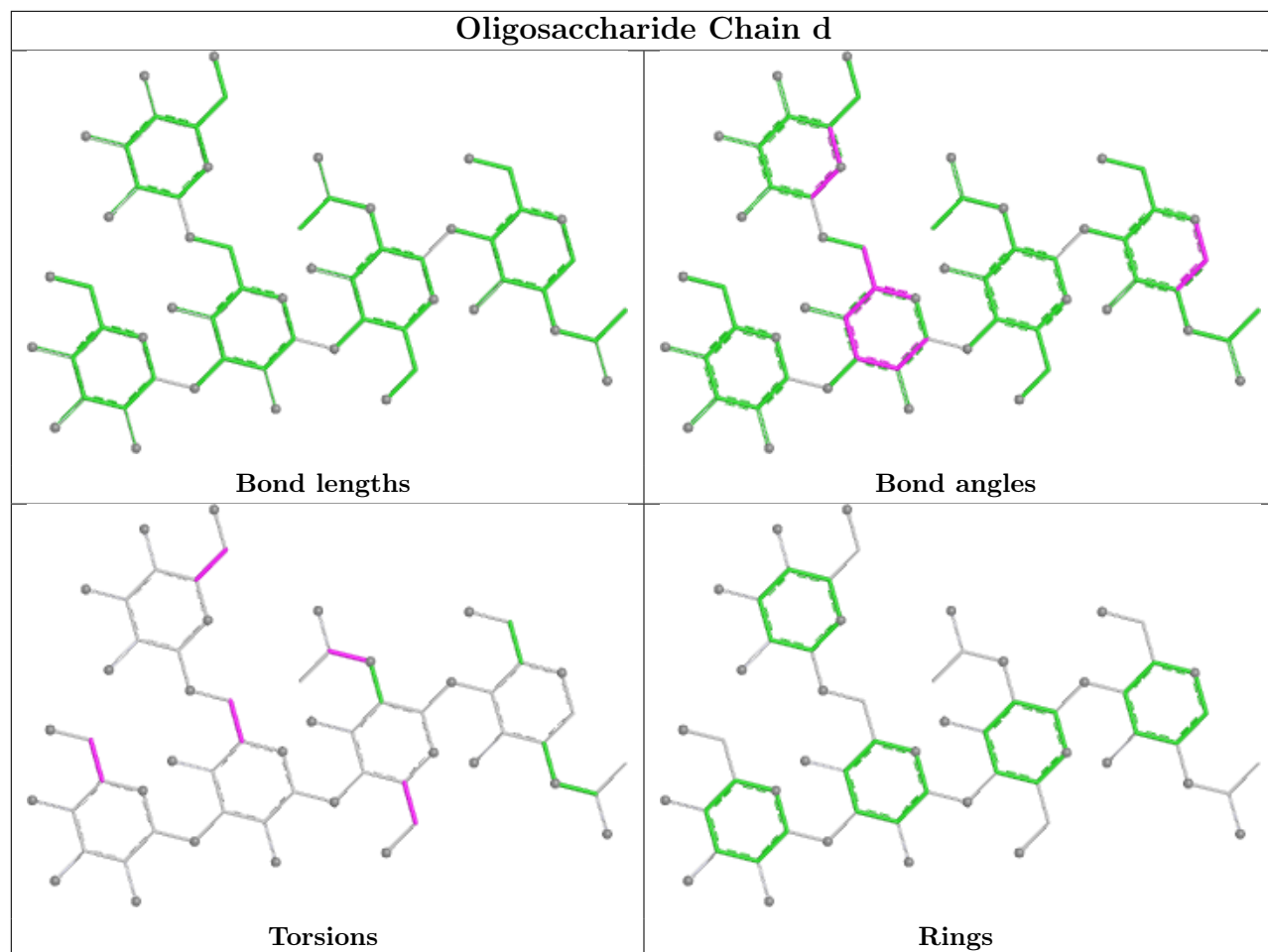


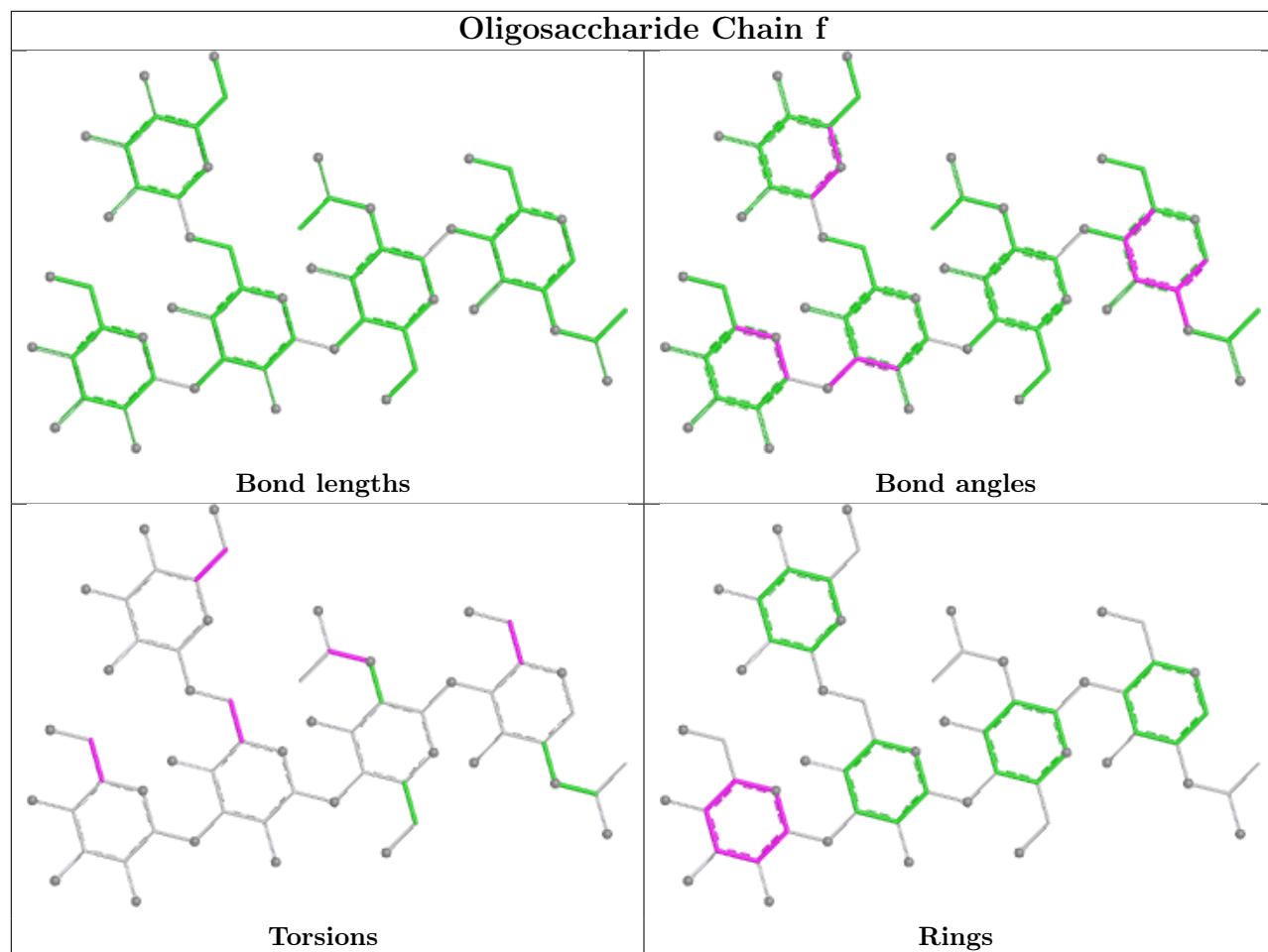


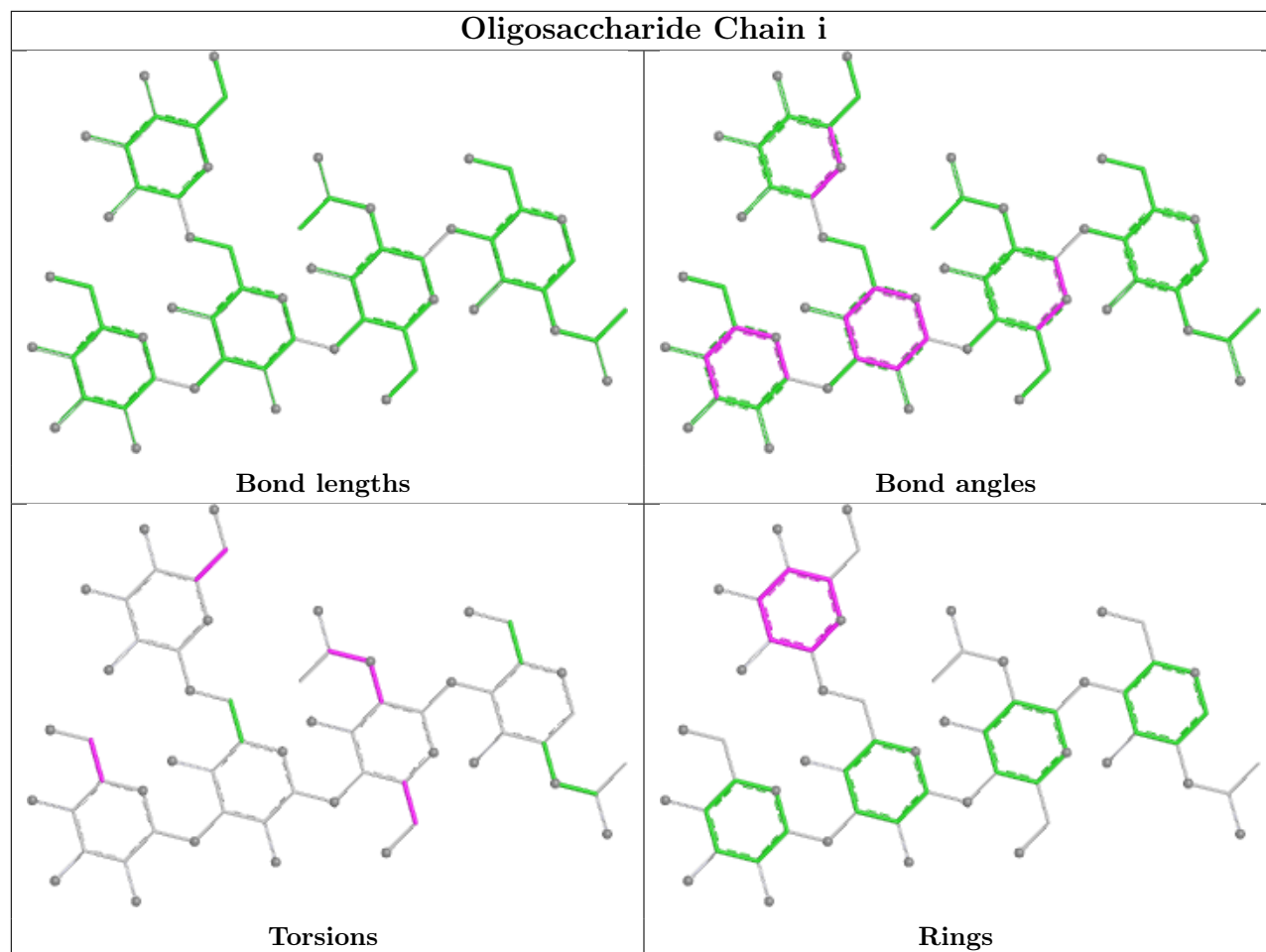


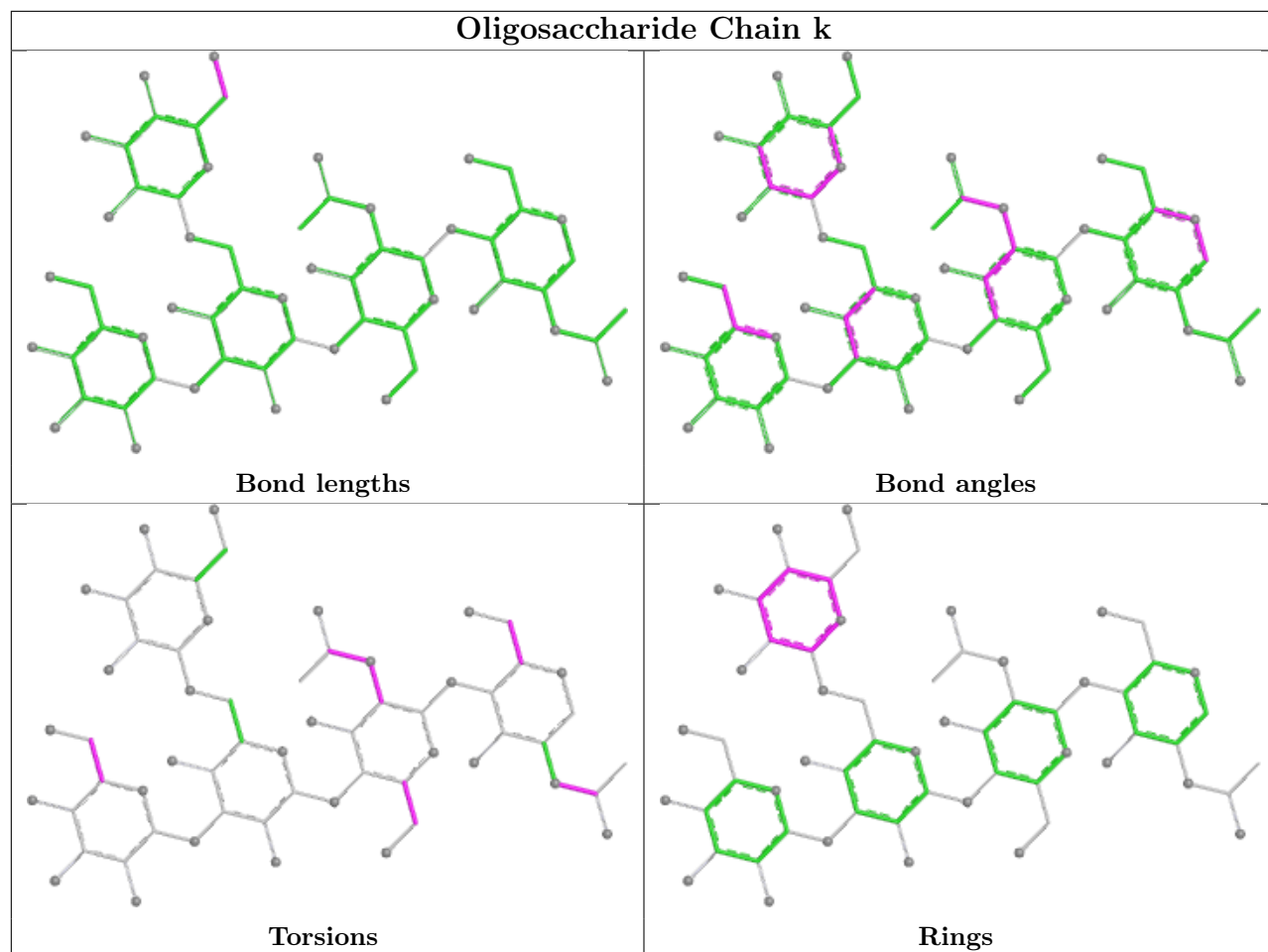


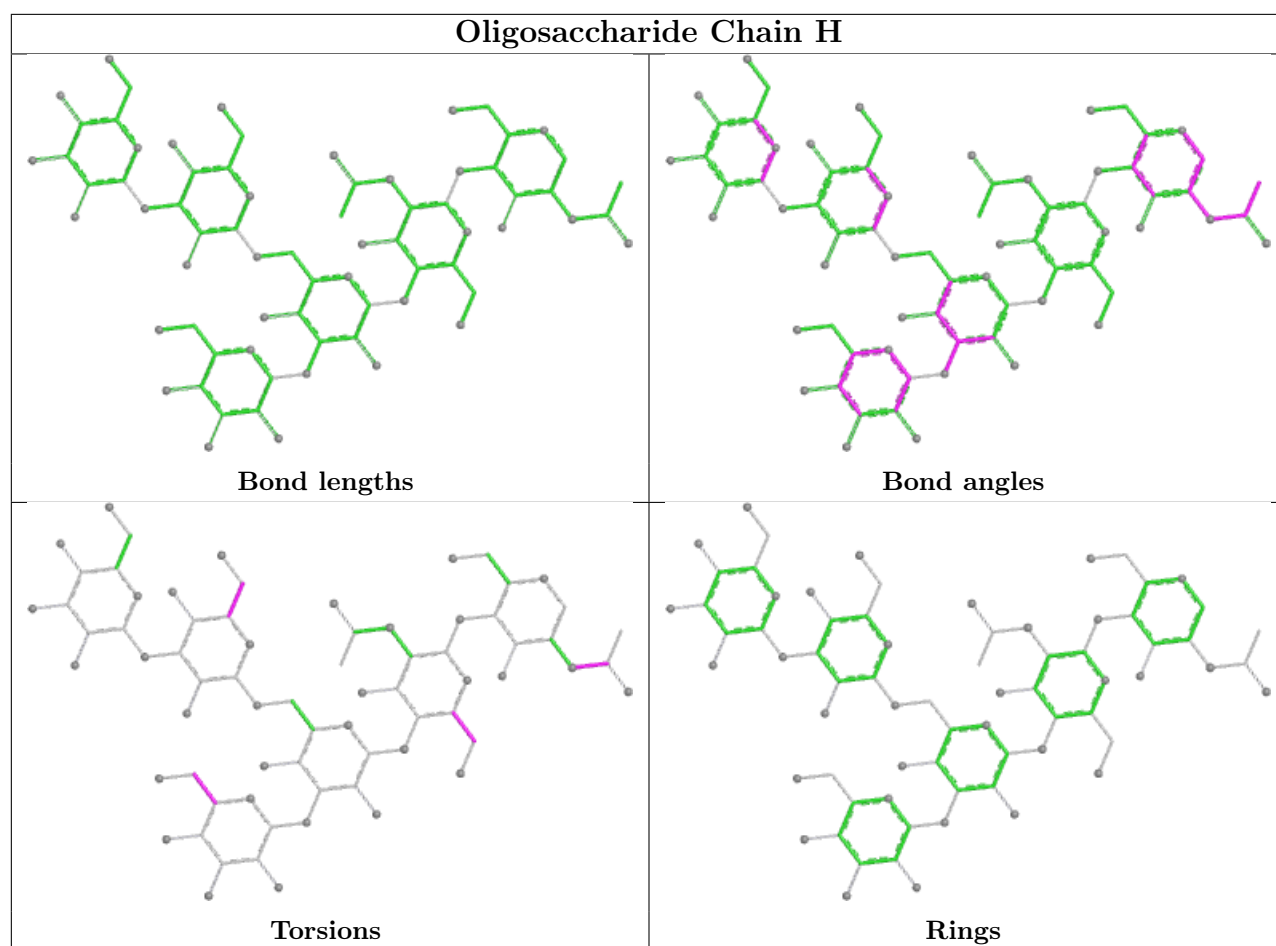


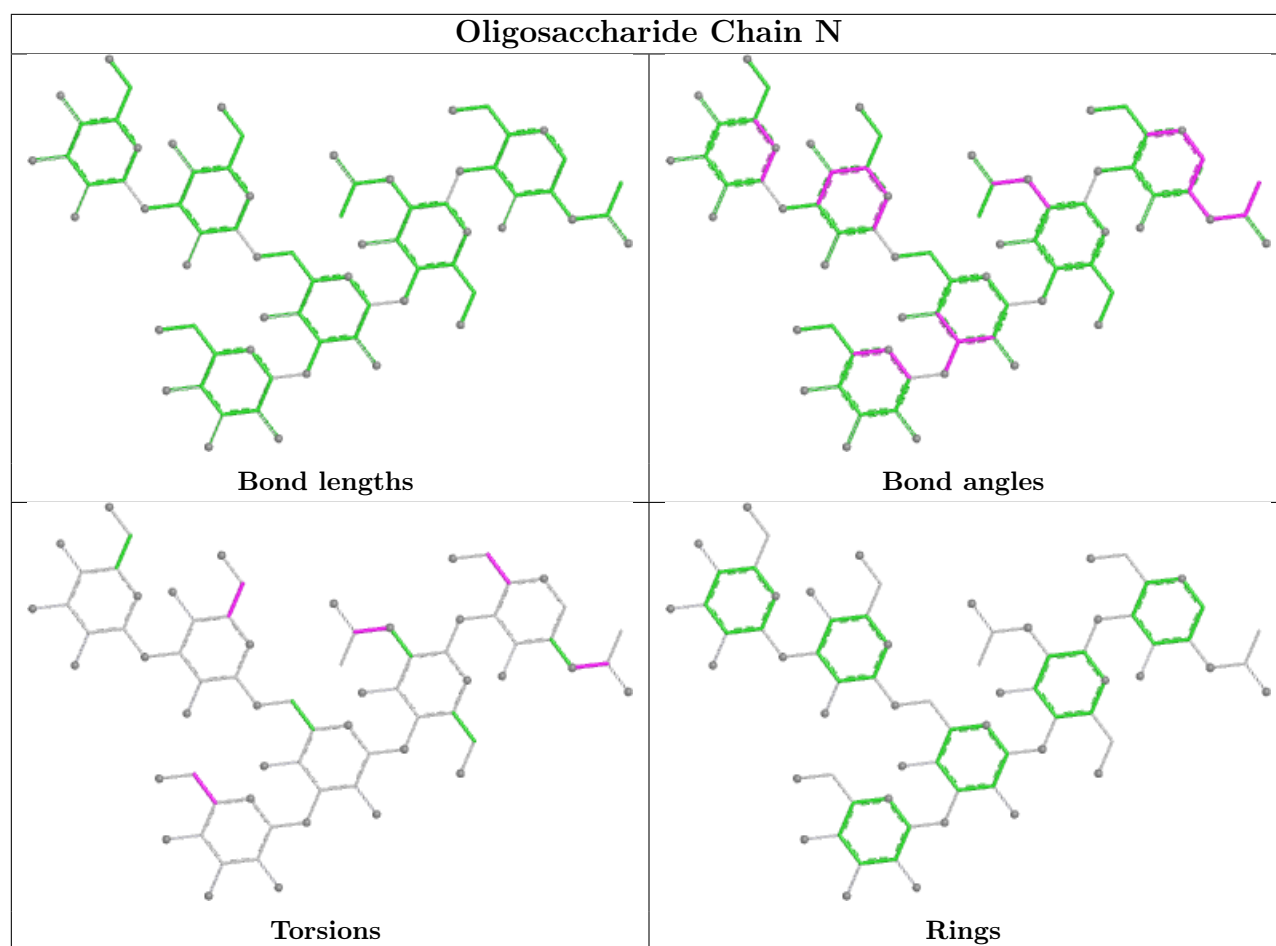


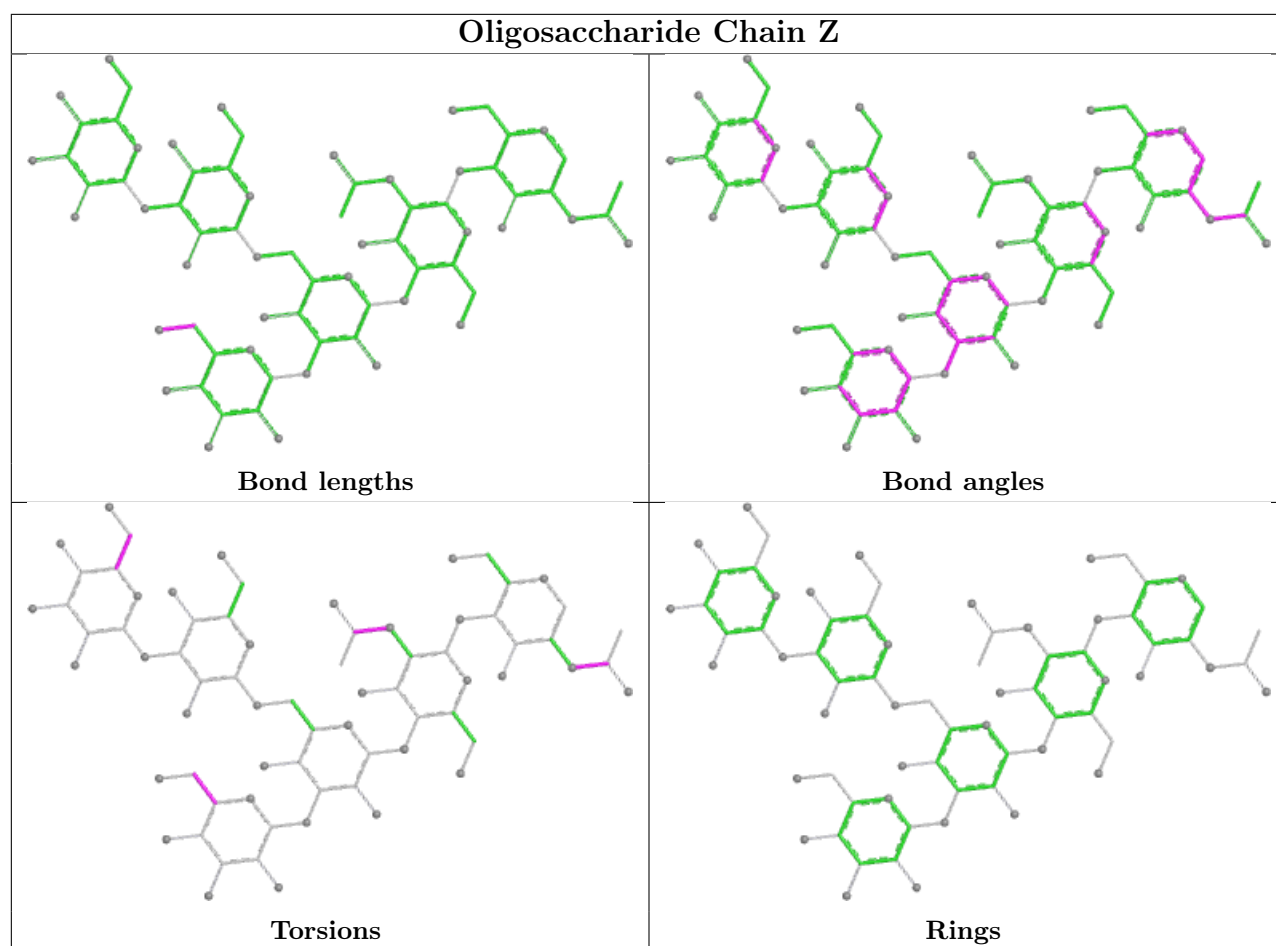


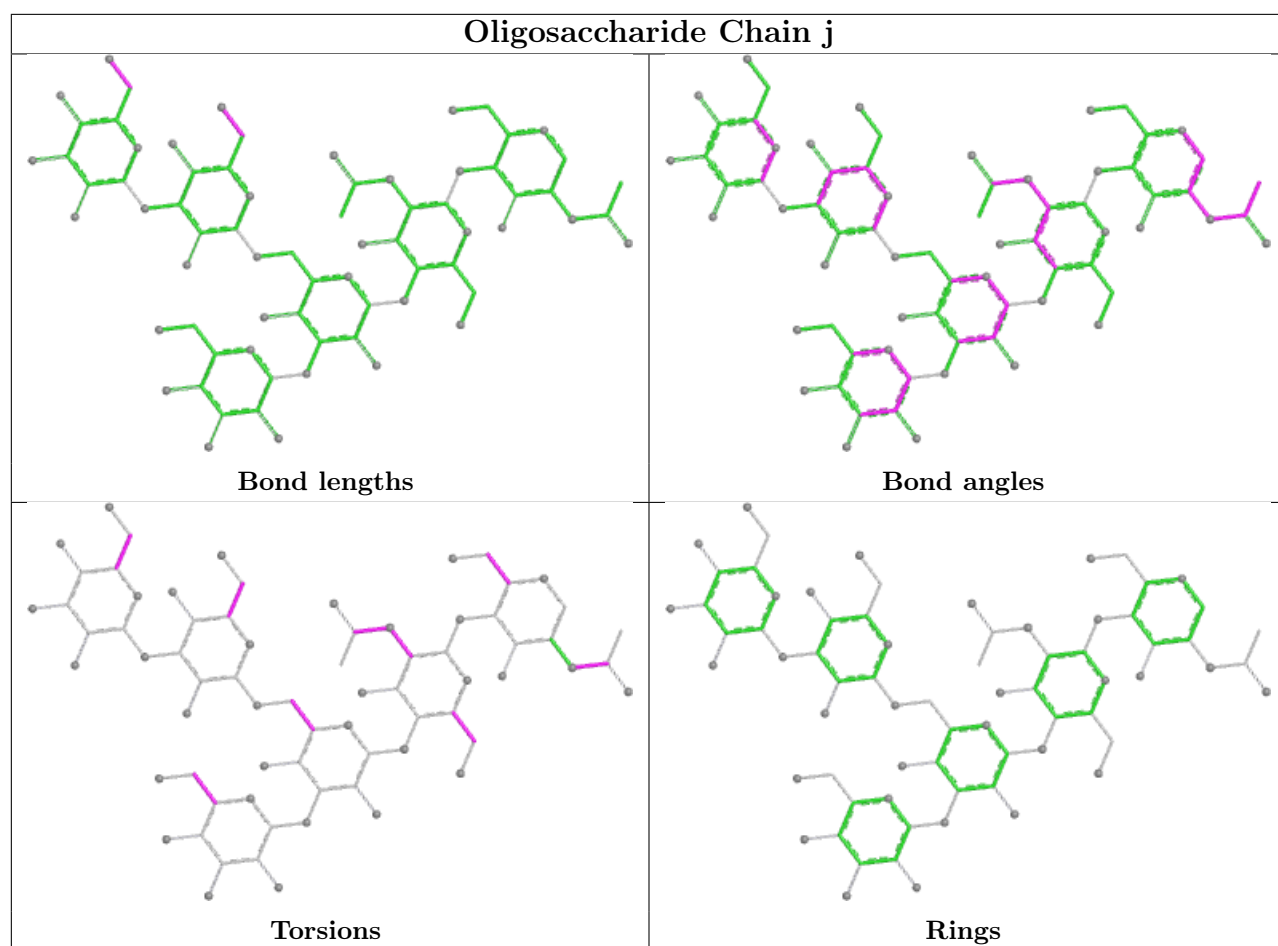


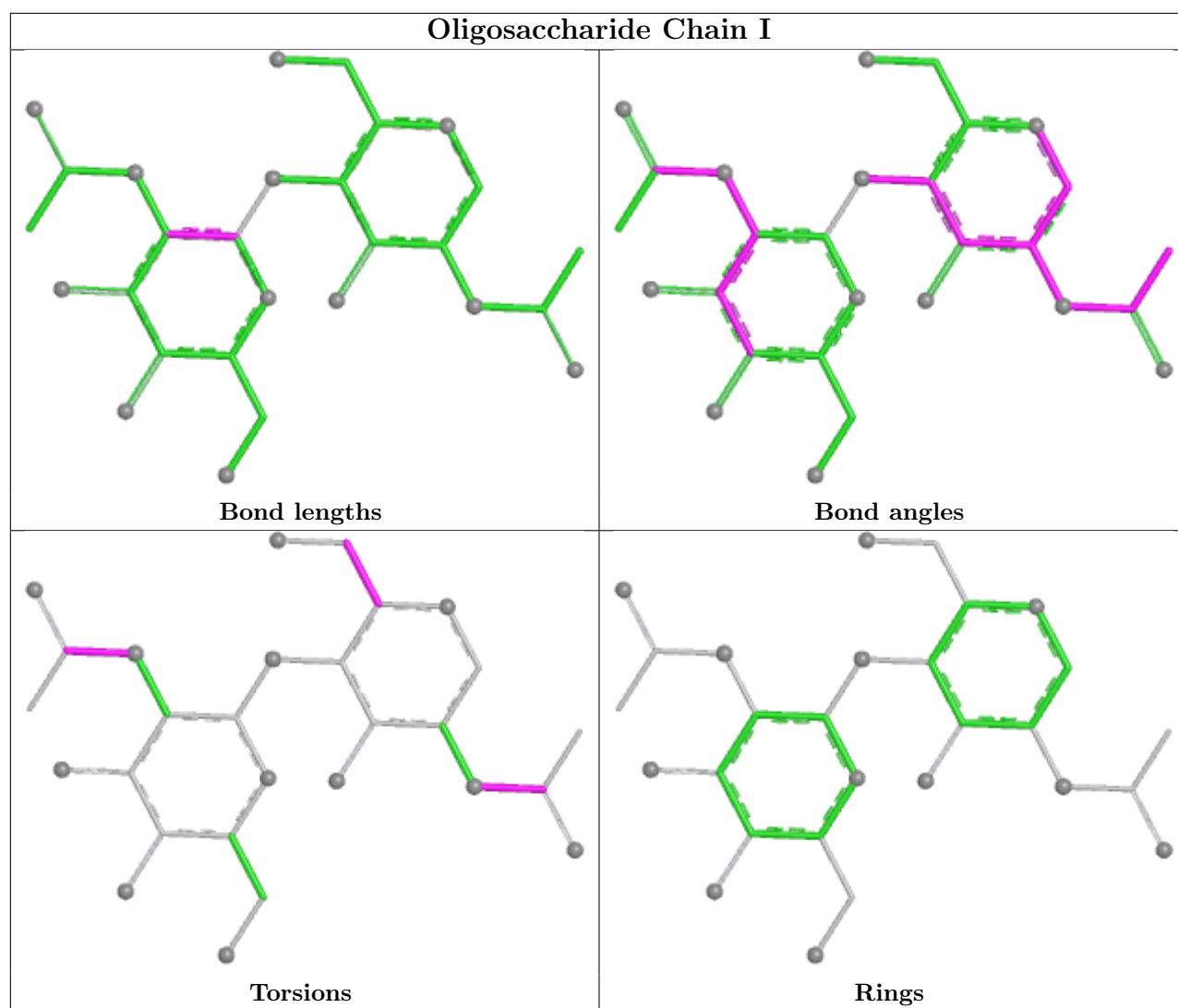


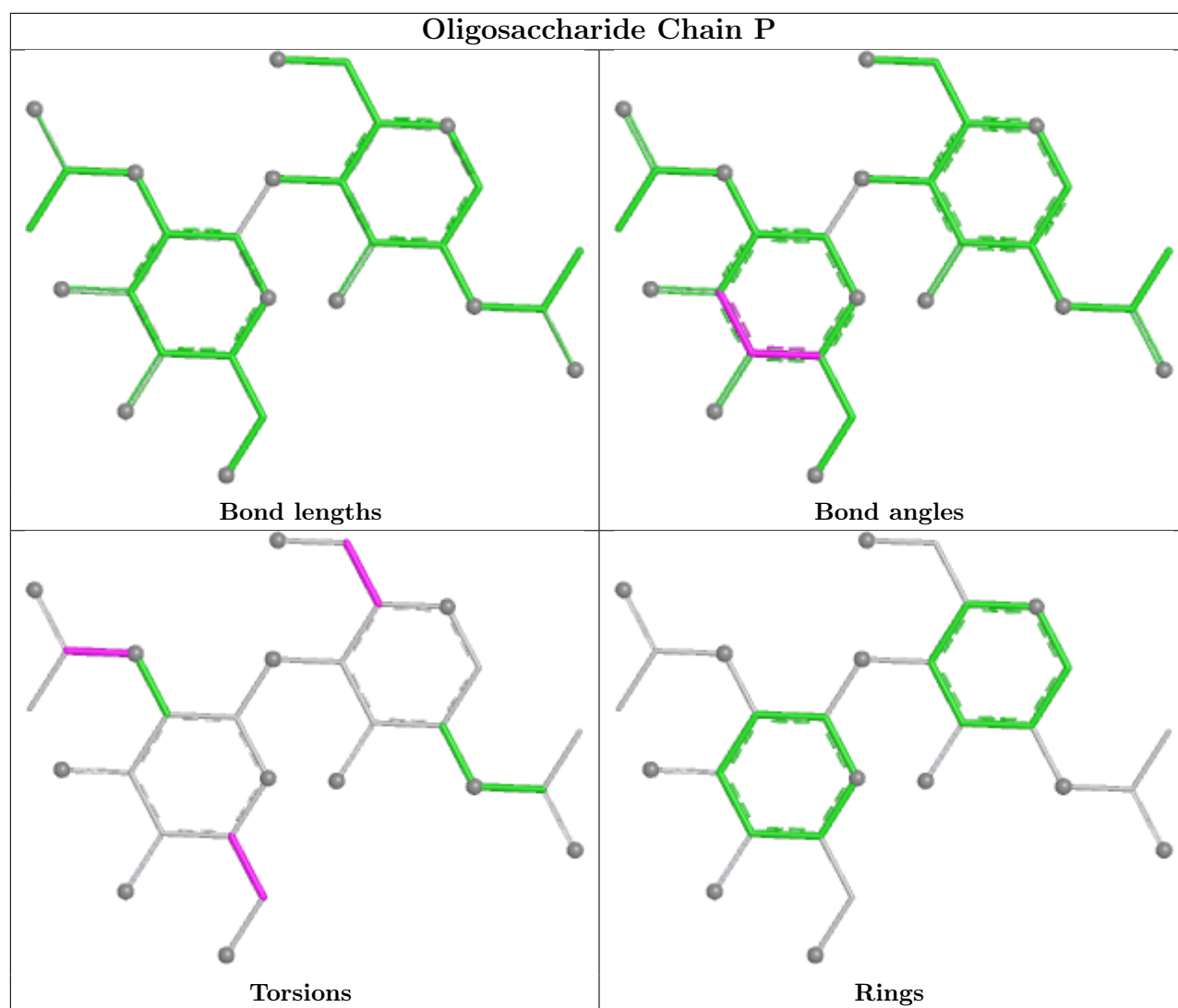


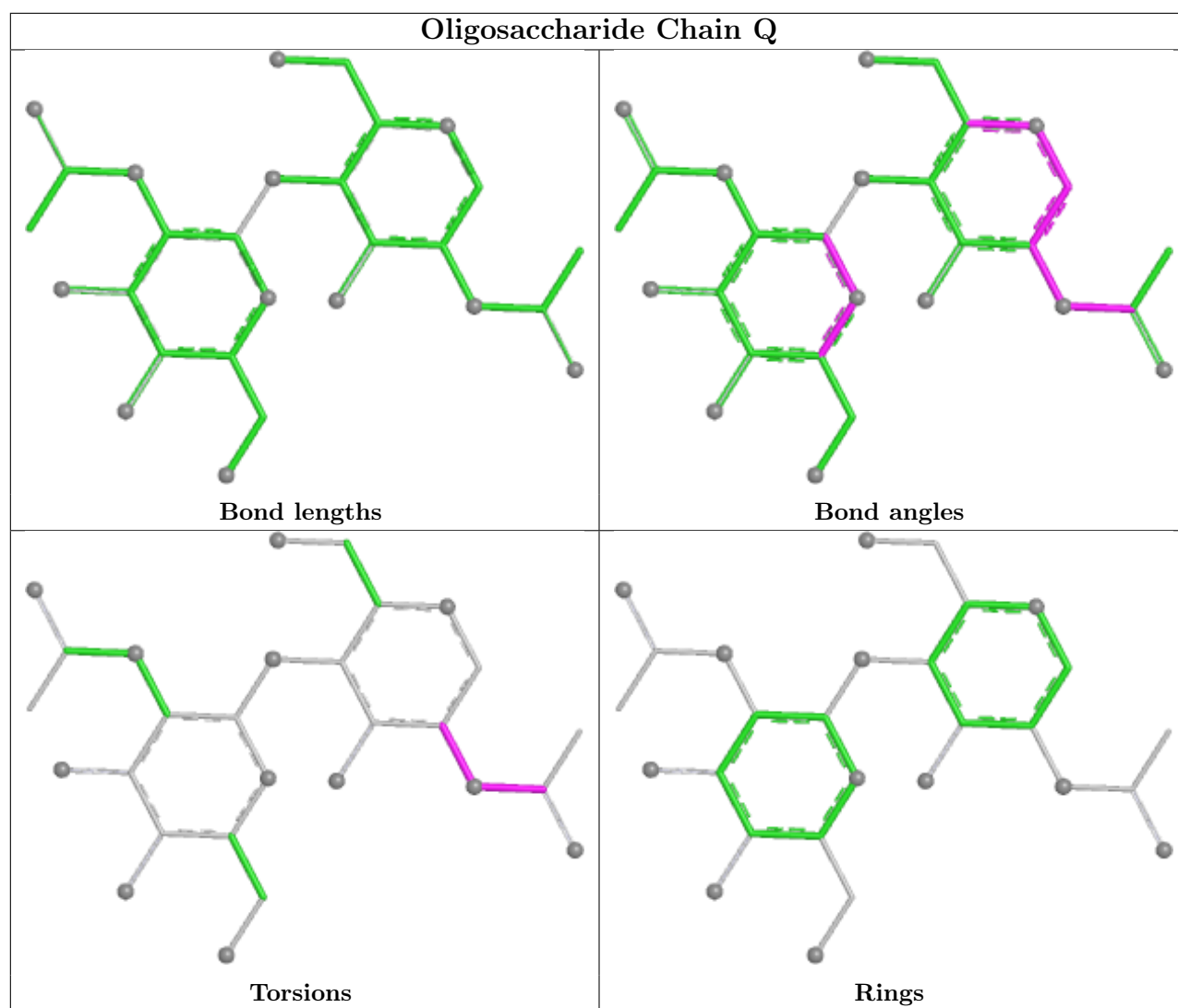


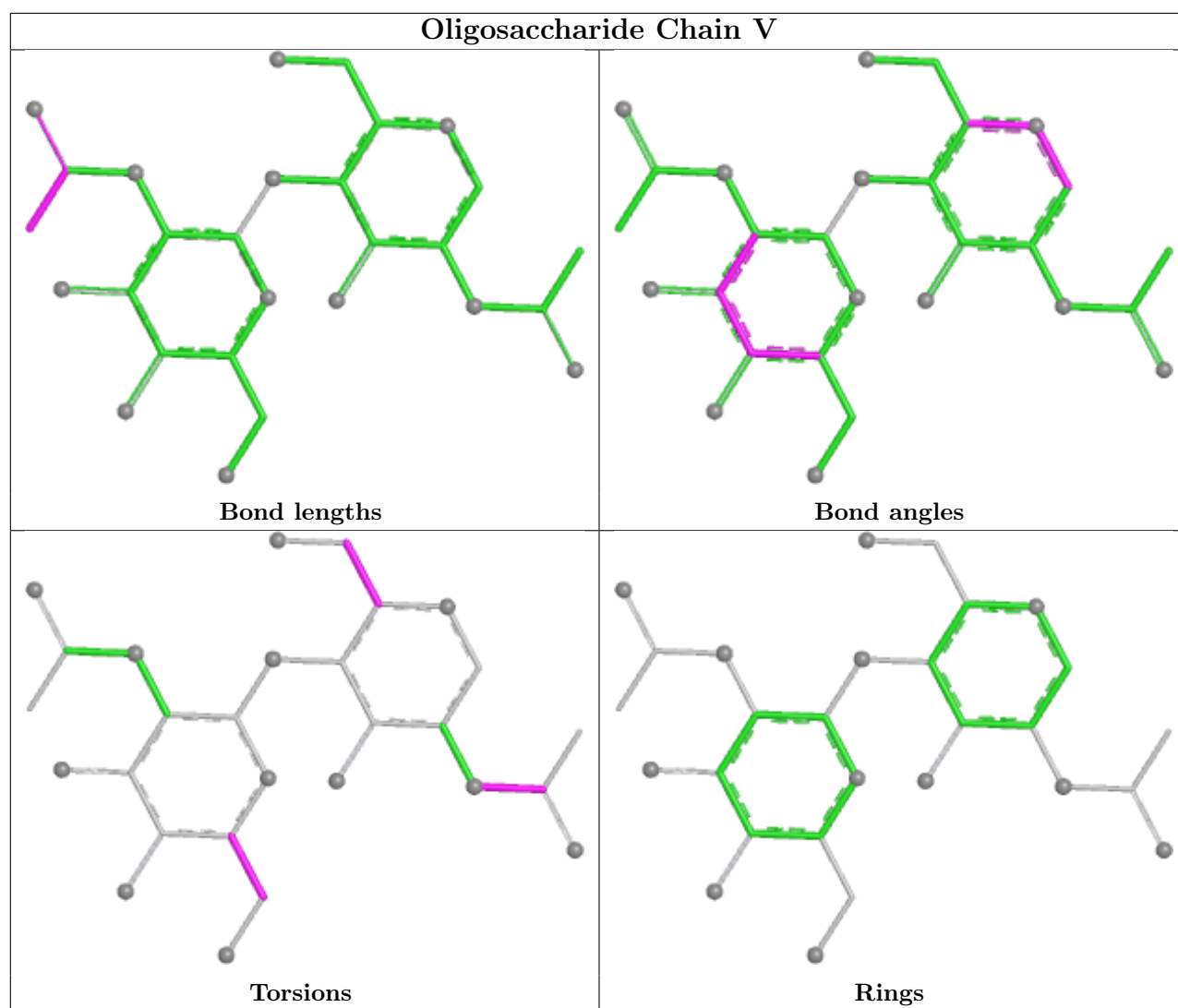


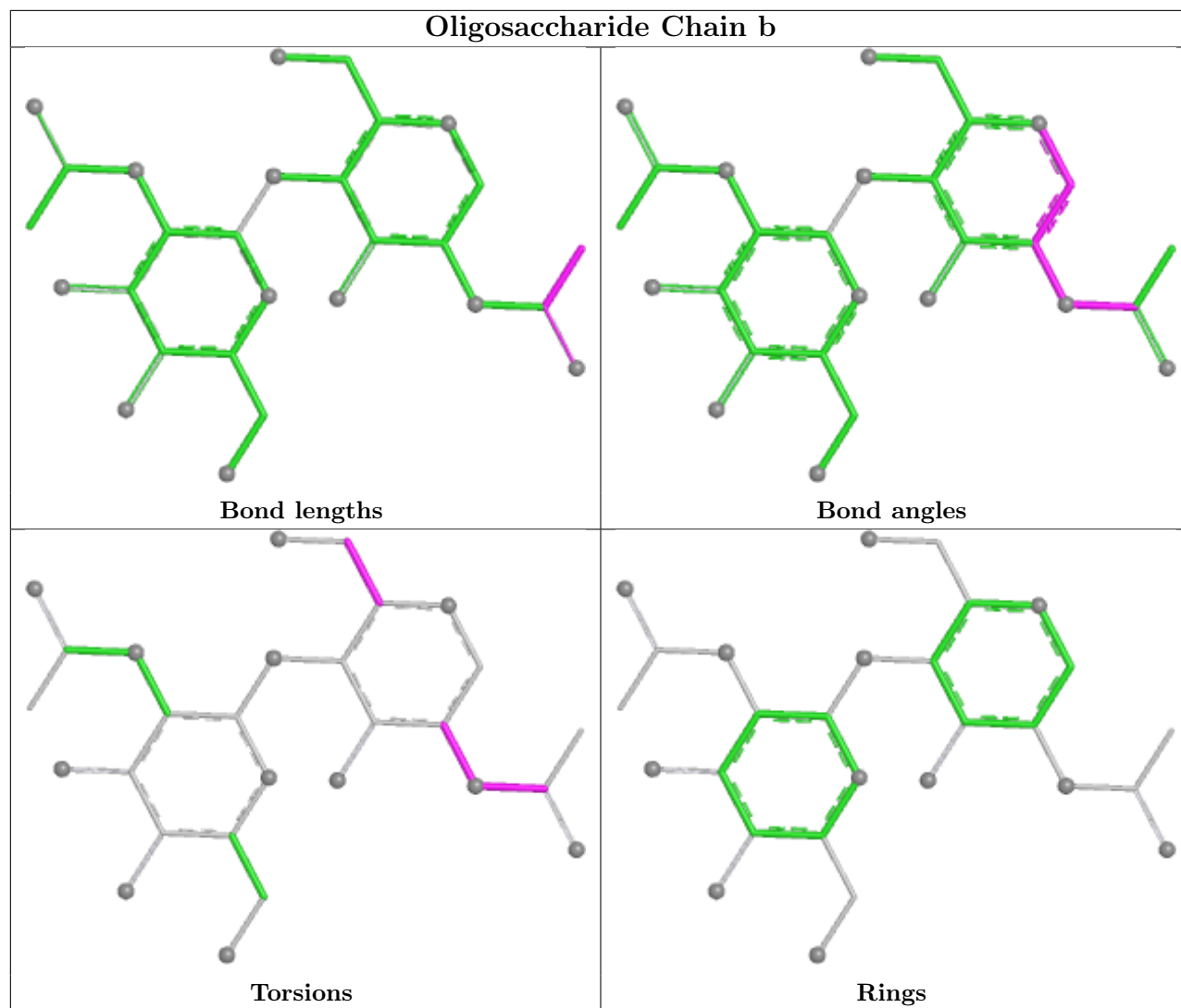


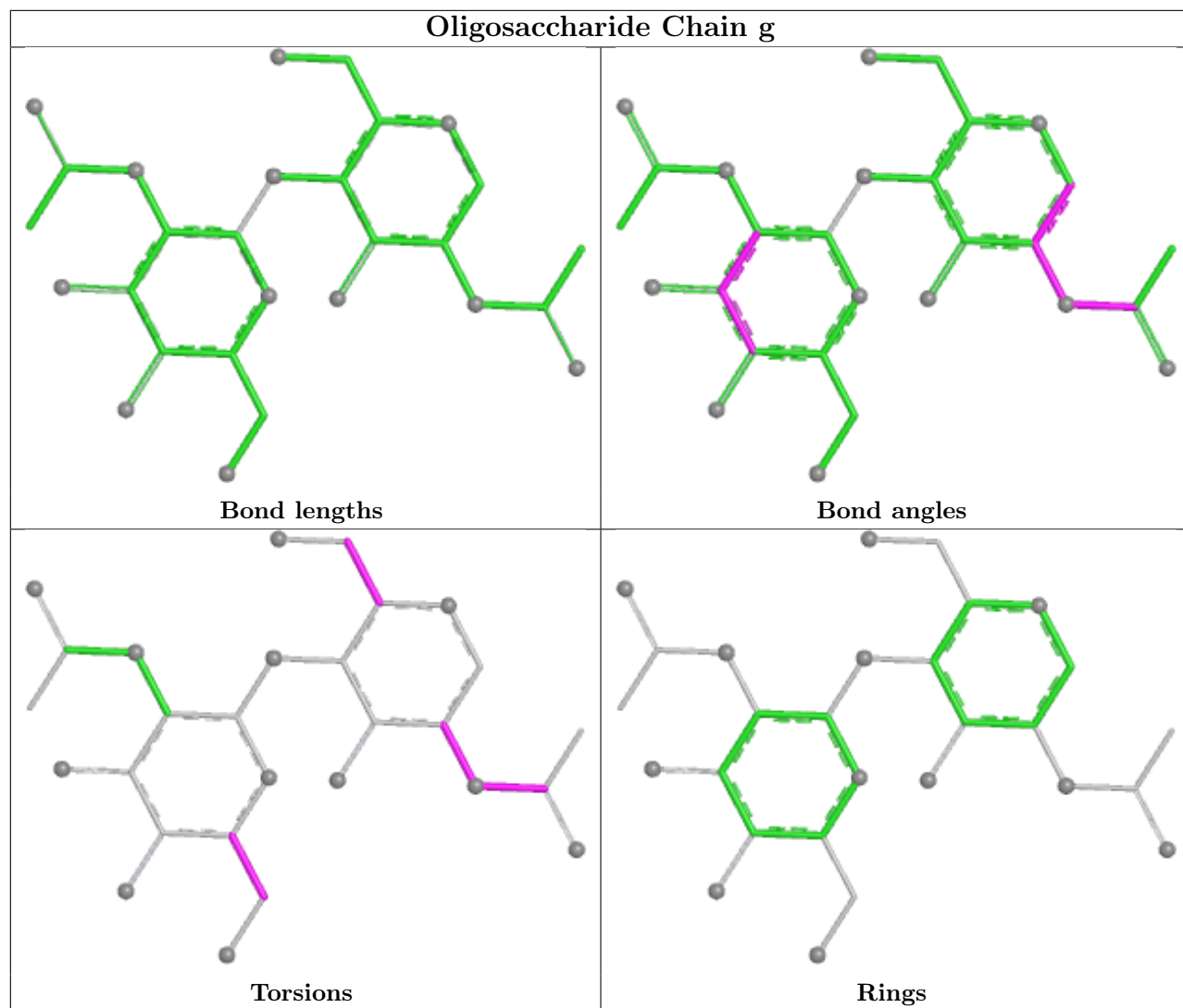


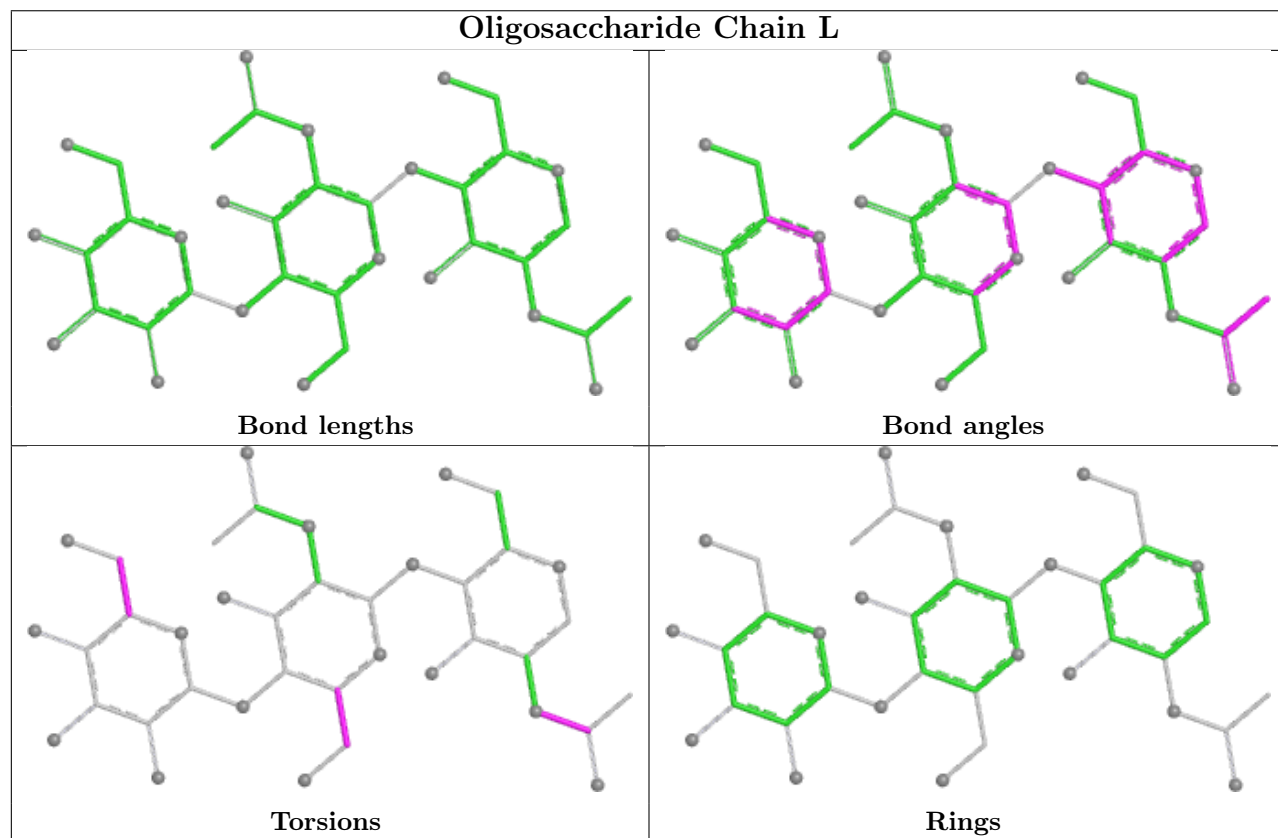
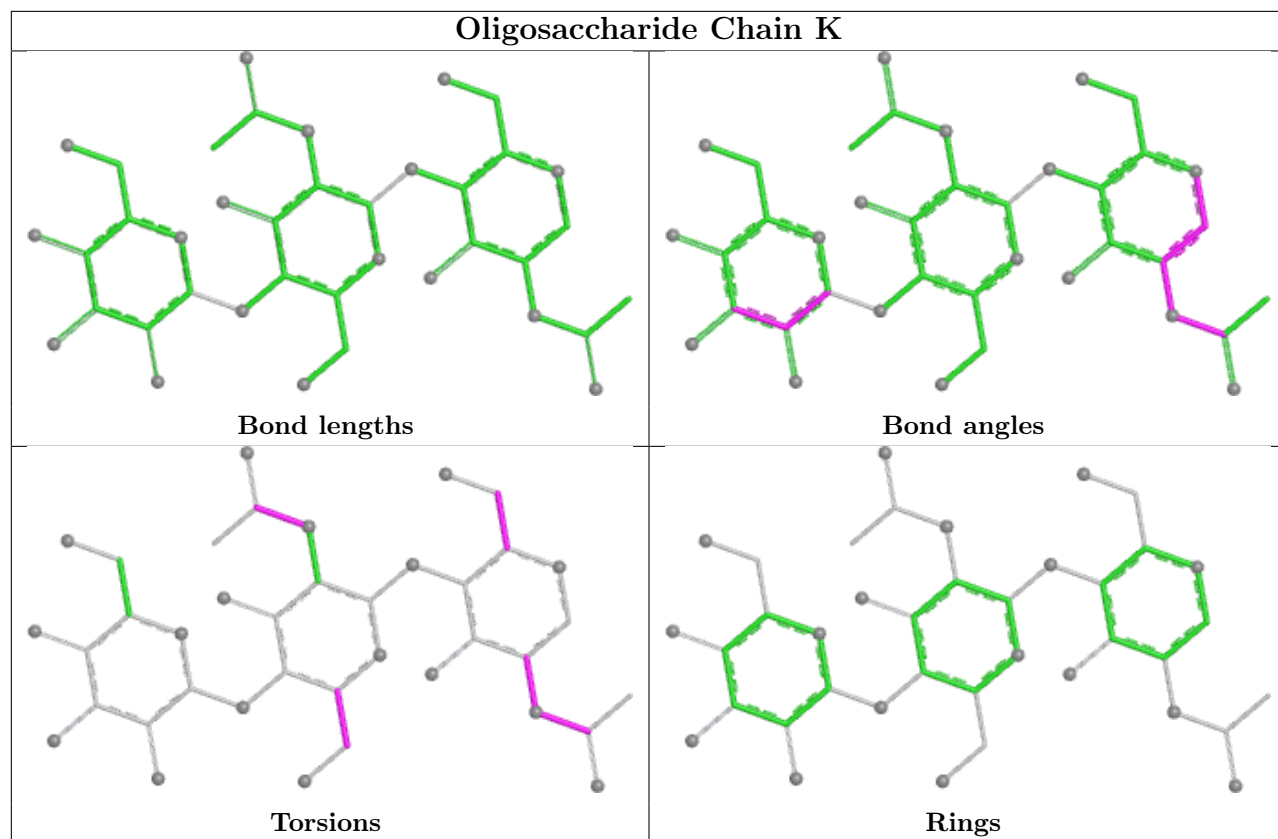


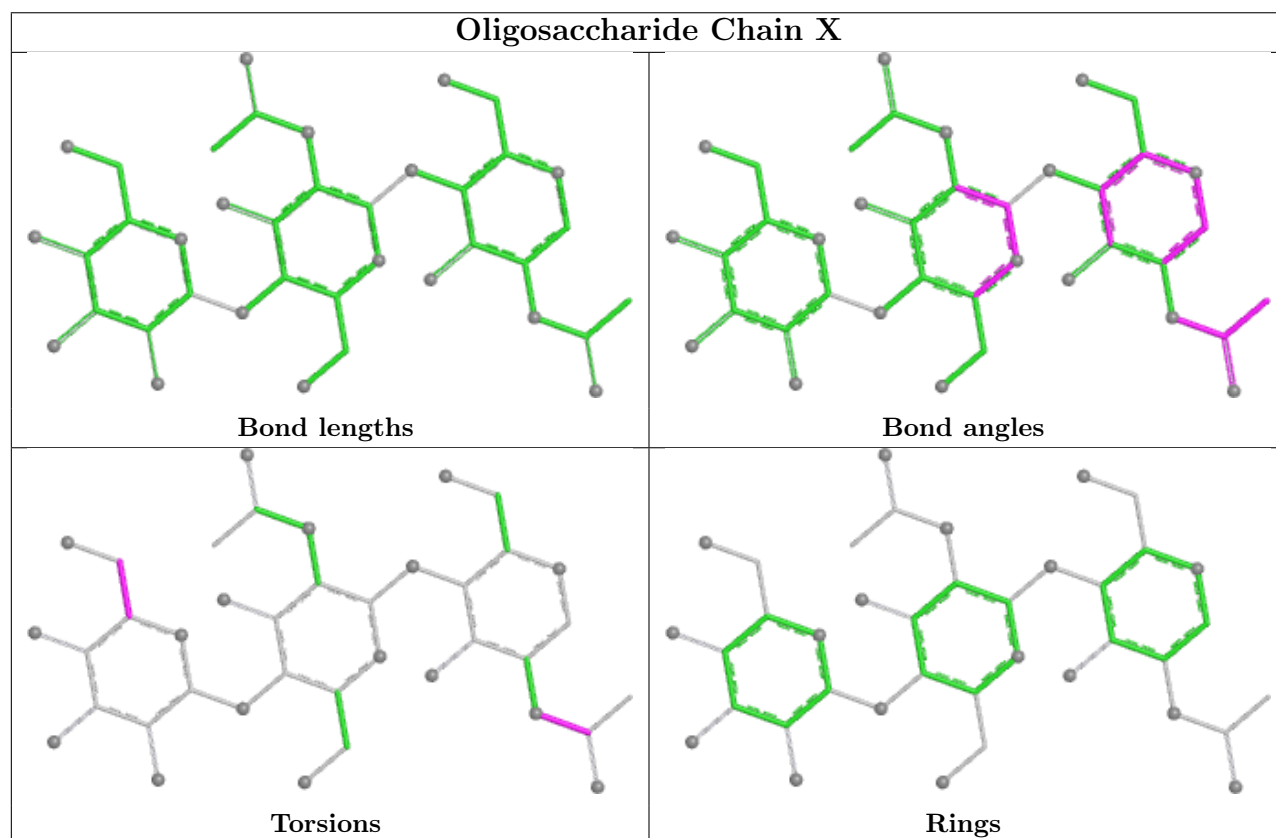
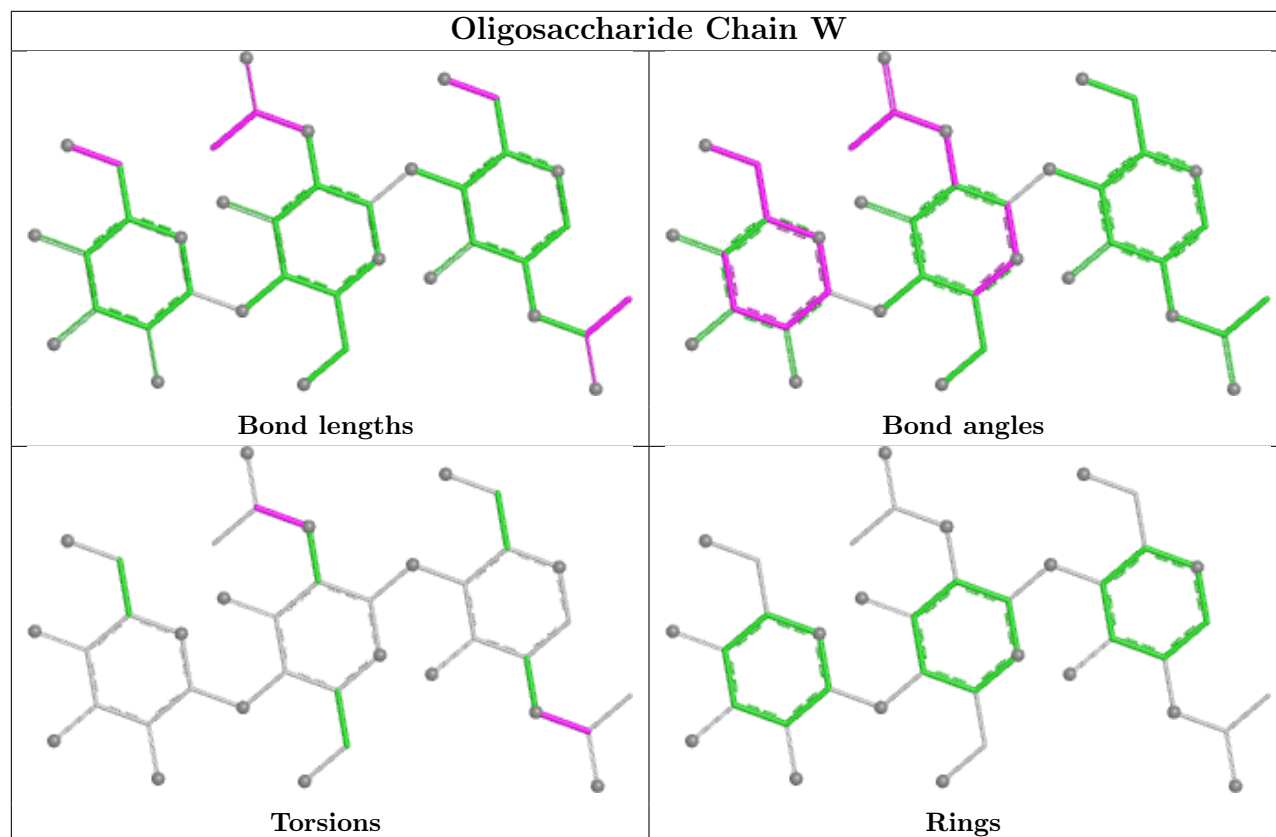


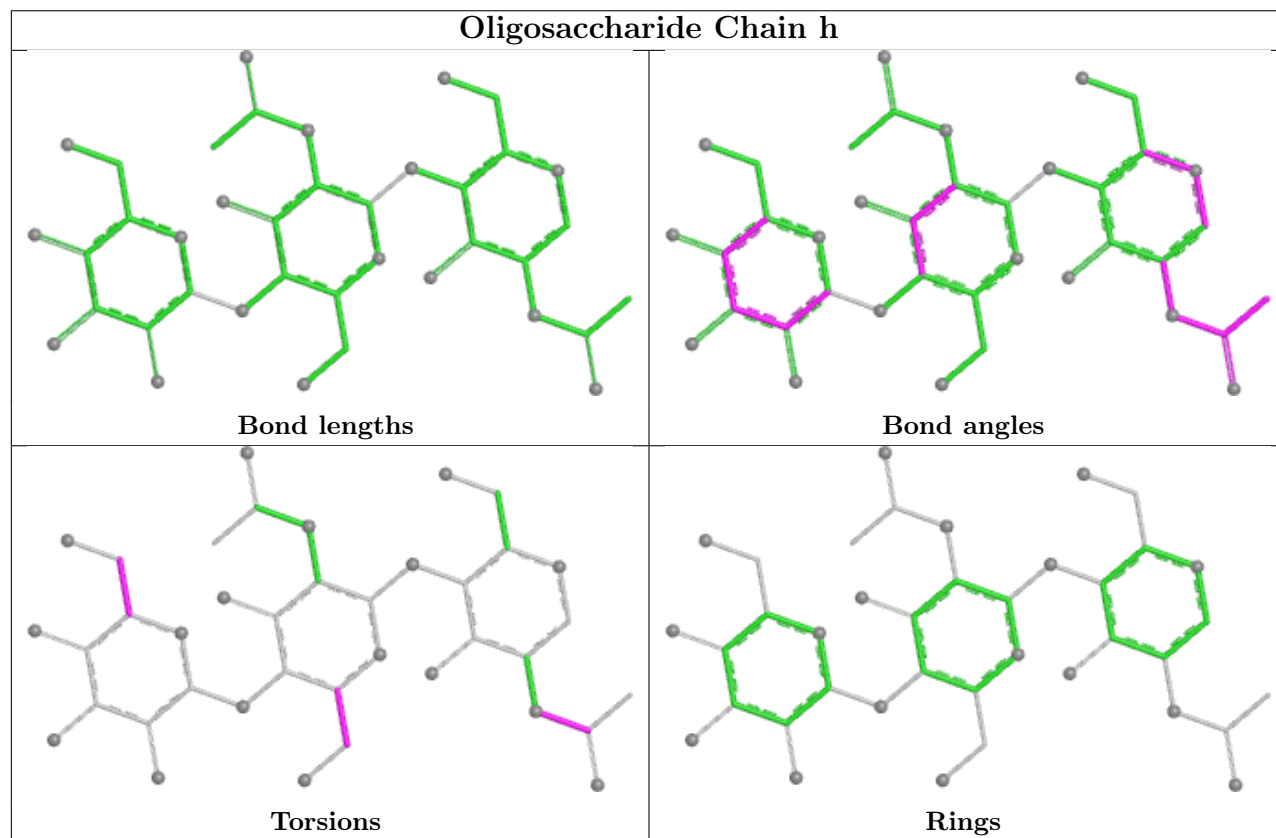
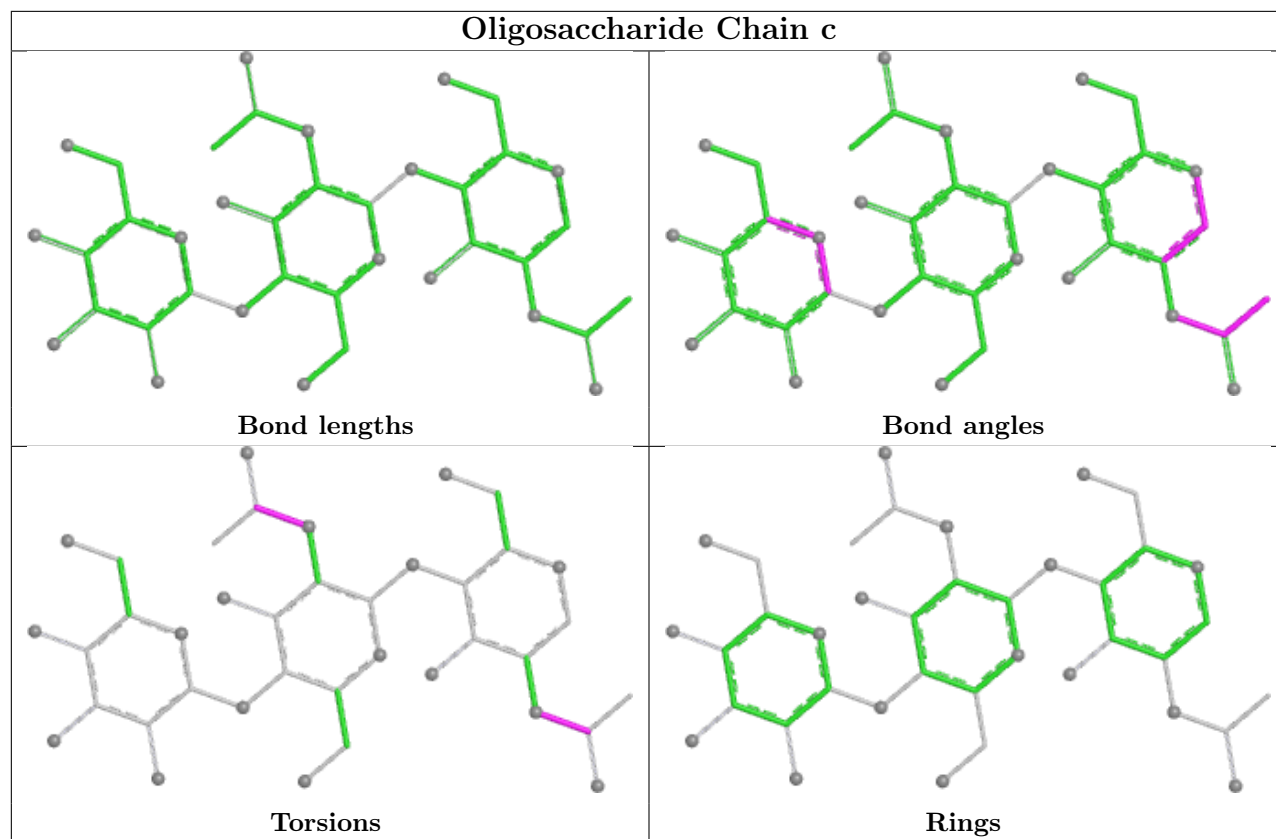


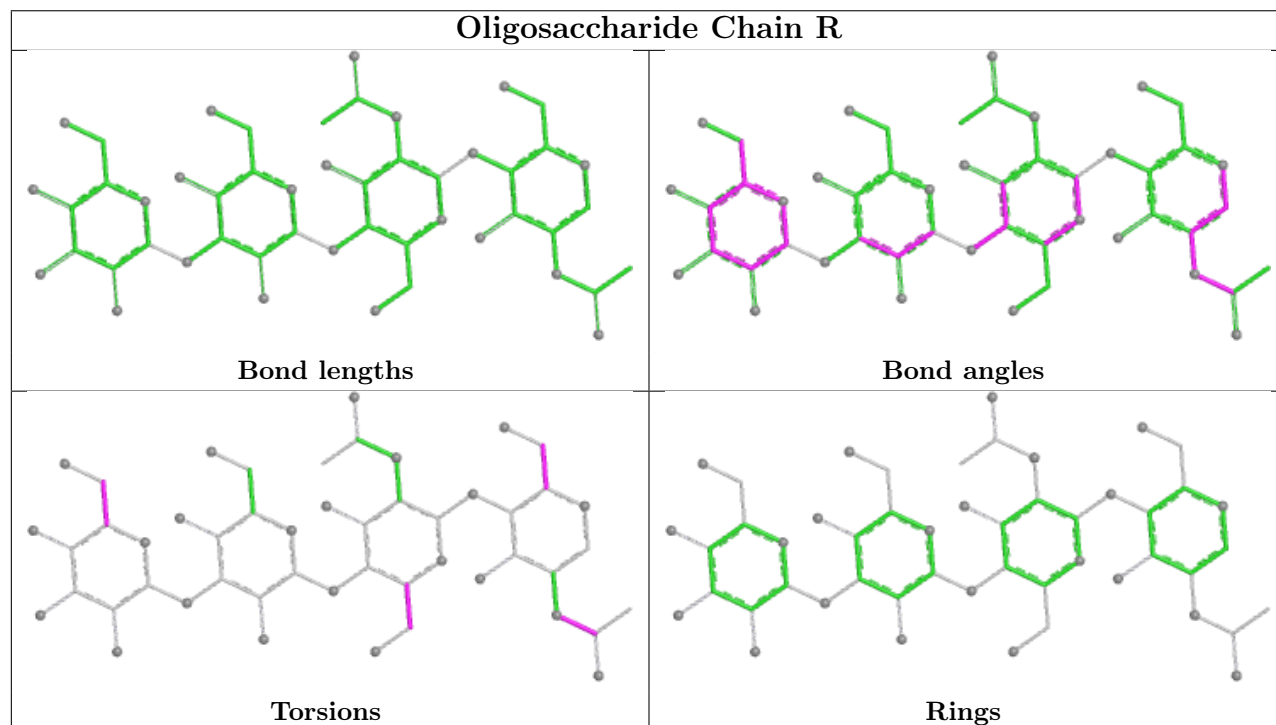
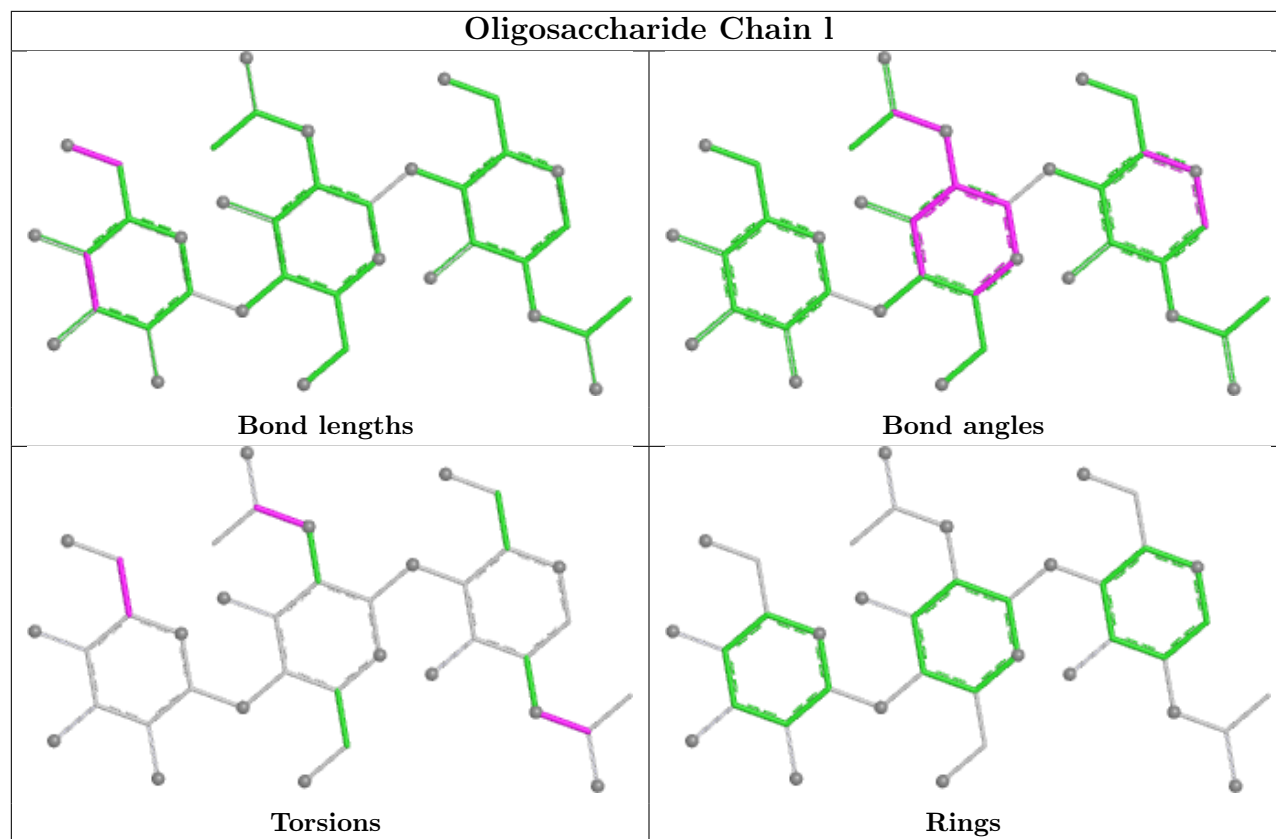


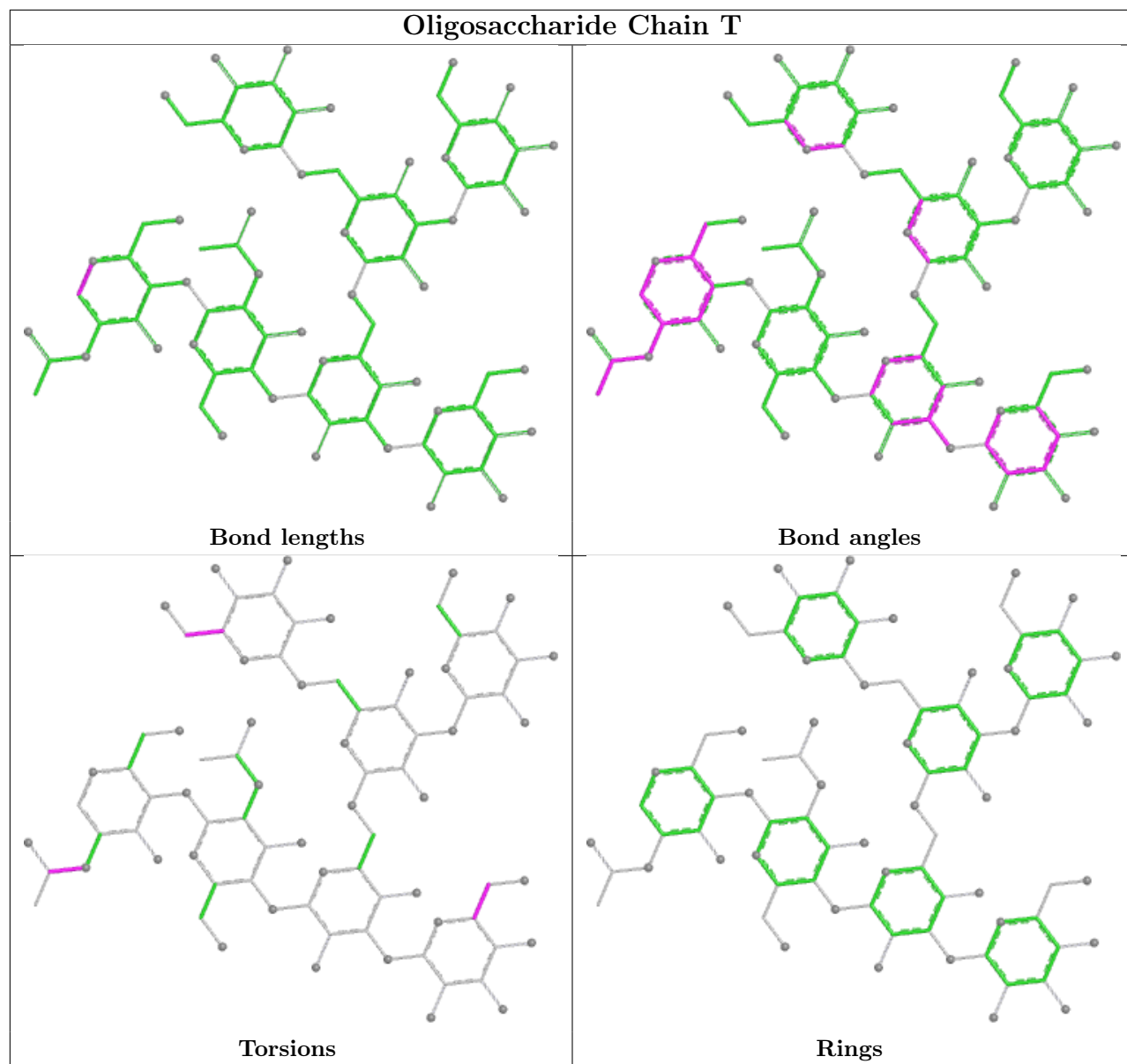


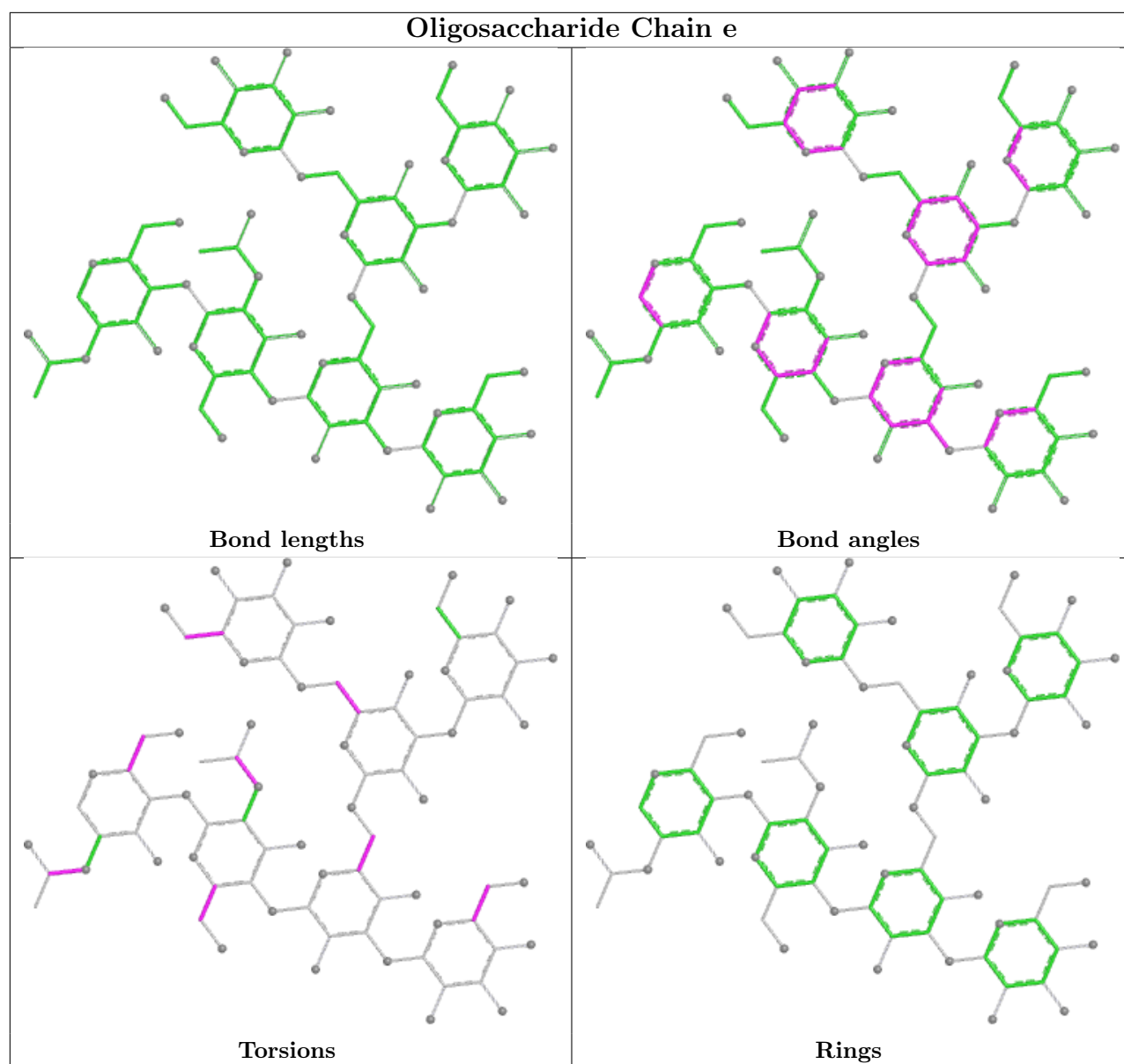












5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	2006	1	14,14,15	0.47	0	17,19,21	1.45	1 (5%)
8	NAG	E	2006	1	14,14,15	0.68	0	17,19,21	1.88	4 (23%)
8	NAG	F	2005	1	14,14,15	4.26	4 (28%)	17,19,21	1.96	4 (23%)
8	NAG	E	2008	1	14,14,15	0.52	0	17,19,21	0.94	0
8	NAG	E	2012	1	14,14,15	3.43	2 (14%)	17,19,21	1.50	3 (17%)
8	NAG	D	2014	1	14,14,15	0.52	0	17,19,21	0.91	0
8	NAG	D	2006	1	14,14,15	3.86	3 (21%)	17,19,21	2.07	4 (23%)
8	NAG	B	2005	1	14,14,15	0.58	0	17,19,21	1.00	2 (11%)
8	NAG	A	2014	1	14,14,15	0.64	0	17,19,21	1.08	0
8	NAG	A	2006	1	14,14,15	0.88	0	17,19,21	1.17	3 (17%)
8	NAG	D	2012	1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
8	NAG	E	2014	1	14,14,15	0.47	0	17,19,21	1.86	2 (11%)
8	NAG	F	2014	1	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
8	NAG	A	2018	1	14,14,15	0.70	0	17,19,21	1.55	2 (11%)
8	NAG	F	2006	1	14,14,15	4.11	4 (28%)	17,19,21	1.98	4 (23%)
8	NAG	D	2008	1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
8	NAG	C	2018	1	14,14,15	5.07	3 (21%)	17,19,21	2.19	4 (23%)
8	NAG	C	2005	1	14,14,15	0.54	0	17,19,21	1.70	4 (23%)
8	NAG	C	2012	1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
8	NAG	E	2005	1	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
8	NAG	B	2014	1	14,14,15	0.46	0	17,19,21	2.00	3 (17%)
8	NAG	B	2006	1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
8	NAG	A	2008	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
8	NAG	B	2018	1	14,14,15	0.80	1 (7%)	17,19,21	1.26	1 (5%)
8	NAG	B	2012	1	14,14,15	0.53	0	17,19,21	1.21	1 (5%)
8	NAG	F	2008	1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
8	NAG	F	2012	1	14,14,15	0.48	0	17,19,21	1.39	2 (11%)
8	NAG	D	2005	1	14,14,15	0.52	0	17,19,21	1.17	2 (11%)
8	NAG	C	2014	1	14,14,15	0.54	0	17,19,21	1.82	3 (17%)
8	NAG	A	2012	1	14,14,15	0.54	0	17,19,21	1.21	1 (5%)
8	NAG	F	2009	1	14,14,15	0.88	0	17,19,21	1.59	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2006	1	-	3/6/23/26	0/1/1/1
8	NAG	F	2005	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2008	1	-	2/6/23/26	0/1/1/1
8	NAG	D	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	B	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2012	1	-	5/6/23/26	0/1/1/1
8	NAG	E	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	F	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2018	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2012	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	E	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	B	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	B	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	B	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	F	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2012	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2009	1	1/1/5/7	5/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2018	NAG	O7-C7	14.52	1.55	1.23
8	F	2006	NAG	C8-C7	14.37	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	NAG	O7-C7	11.91	1.49	1.23
8	C	2018	NAG	C8-C7	11.45	1.74	1.50
8	E	2012	NAG	C8-C7	10.37	1.72	1.50

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2014	NAG	C1-O5-C5	6.36	120.71	112.19
8	C	2014	NAG	C1-O5-C5	5.97	120.19	112.19
8	F	2005	NAG	C1-O5-C5	5.46	119.51	112.19
8	D	2006	NAG	C8-C7-N2	-5.31	107.31	116.12
8	B	2014	NAG	C1-O5-C5	5.25	119.22	112.19

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	2006	NAG	C1
8	A	2012	NAG	C1
8	A	2018	NAG	C1
8	B	2006	NAG	C1
8	B	2012	NAG	C1

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2012	NAG	C8-C7-N2-C2
8	A	2012	NAG	O7-C7-N2-C2
8	A	2014	NAG	O7-C7-N2-C2
8	B	2005	NAG	C8-C7-N2-C2
8	B	2005	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	2006	NAG	1	0
8	F	2005	NAG	2	0
8	B	2005	NAG	3	0
8	F	2006	NAG	1	0
8	D	2008	NAG	1	0
8	C	2005	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	2005	NAG	1	0
8	F	2012	NAG	1	0
8	D	2005	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	529/534 (99%)	1.66	161 (30%) 1 1	67, 69, 71, 74	0
1	B	529/534 (99%)	1.21	72 (13%) 7 5	67, 69, 71, 74	0
1	C	529/534 (99%)	1.84	216 (40%) 0 0	67, 69, 71, 74	0
1	D	529/534 (99%)	1.57	131 (24%) 2 1	67, 69, 71, 73	0
1	E	529/534 (99%)	1.63	150 (28%) 1 1	68, 69, 71, 73	0
1	F	529/534 (99%)	2.67	363 (68%) 0 0	68, 69, 71, 73	0
All	All	3174/3204 (99%)	1.76	1093 (34%) 1 1	67, 69, 71, 74	0

The worst 5 of 1093 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	550	ALA	7.6
1	F	436	GLY	7.3
1	D	533	ALA	6.5
1	F	533	ALA	6.5
1	F	454	PRO	6.4

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

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

6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	MAN	Z	6	11/12	0.34	0.27	73,75,76,76	0
5	BMA	L	3	11/12	0.36	0.24	78,80,81,81	0
2	MAN	U	4	11/12	0.42	0.24	82,84,86,86	0
5	BMA	X	3	11/12	0.42	0.21	78,80,81,82	0
6	BMA	R	3	11/12	0.43	0.21	82,84,85,87	0
4	NAG	V	2	14/15	0.44	0.21	82,83,84,85	0
2	MAN	J	5	11/12	0.46	0.24	77,78,79,79	0
4	NAG	I	2	14/15	0.46	0.25	92,95,96,96	0
2	MAN	Y	5	11/12	0.46	0.21	77,78,78,78	0
6	MAN	R	4	11/12	0.46	0.19	88,88,89,89	0
2	MAN	O	4	11/12	0.47	0.22	70,73,74,75	0
2	MAN	Y	4	11/12	0.48	0.27	78,78,79,79	0
2	MAN	J	4	11/12	0.50	0.23	74,76,77,78	0
2	MAN	M	4	11/12	0.52	0.21	91,92,93,94	0
5	NAG	W	2	14/15	0.53	0.22	52,53,54,55	0
3	MAN	H	6	11/12	0.53	0.22	98,100,100,100	0
2	MAN	S	4	11/12	0.55	0.17	96,97,98,99	0
2	MAN	U	5	11/12	0.58	0.21	89,90,91,91	0
5	NAG	W	1	14/15	0.58	0.20	58,62,65,66	0
5	BMA	K	3	11/12	0.58	0.20	73,74,75,75	0
2	NAG	U	1	14/15	0.60	0.20	69,73,76,76	0
4	NAG	P	2	14/15	0.63	0.20	89,90,92,93	0
2	MAN	S	5	11/12	0.65	0.20	95,95,96,96	0
5	NAG	K	2	14/15	0.65	0.19	73,73,74,76	0
2	NAG	O	2	14/15	0.65	0.18	68,71,71,72	0
2	NAG	J	1	14/15	0.66	0.20	74,76,80,83	0
5	BMA	W	3	11/12	0.67	0.18	47,49,50,50	0
7	MAN	T	7	11/12	0.67	0.20	92,95,96,97	0
2	MAN	O	5	11/12	0.68	0.18	74,75,75,75	0
3	MAN	N	6	11/12	0.70	0.20	96,100,100,100	0
4	NAG	V	1	14/15	0.71	0.20	75,77,78,80	0
2	BMA	O	3	11/12	0.71	0.20	71,72,73,74	0
2	MAN	G	5	11/12	0.71	0.23	90,91,94,94	0
2	MAN	G	4	11/12	0.71	0.16	92,93,94,95	0
2	NAG	U	2	14/15	0.72	0.20	76,78,80,80	0
2	NAG	a	1	14/15	-	-	73,75,78,78	0
2	NAG	a	2	14/15	-	-	71,74,75,77	0
2	BMA	a	3	11/12	-	-	78,78,80,81	0
2	MAN	a	4	11/12	-	-	74,76,76,77	0
2	MAN	a	5	11/12	-	-	81,82,83,83	0
2	NAG	d	1	14/15	-	-	70,71,73,75	0
2	NAG	d	2	14/15	-	-	75,77,79,79	0
2	BMA	d	3	11/12	-	-	81,83,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	d	4	11/12	-	-	87,88,89,89	0
2	MAN	d	5	11/12	-	-	88,89,89,90	0
2	NAG	f	1	14/15	-	-	72,73,74,74	0
2	NAG	f	2	14/15	-	-	73,74,74,74	0
2	BMA	f	3	11/12	-	-	75,76,77,78	0
2	MAN	f	4	11/12	-	-	74,76,76,76	0
2	MAN	f	5	11/12	-	-	78,79,79,79	0
2	NAG	i	1	14/15	-	-	70,71,72,72	0
2	NAG	i	2	14/15	-	-	71,71,74,75	0
2	BMA	i	3	11/12	-	-	76,77,79,82	0
2	MAN	i	4	11/12	-	-	77,78,79,79	0
2	MAN	i	5	11/12	-	-	82,84,84,85	0
2	NAG	k	1	14/15	-	-	71,72,75,76	0
2	NAG	k	2	14/15	-	-	68,70,70,71	0
2	BMA	k	3	11/12	-	-	66,67,68,68	0
2	MAN	k	4	11/12	-	-	63,65,65,65	0
2	MAN	k	5	11/12	-	-	67,69,69,69	0
4	NAG	Q	1	14/15	0.72	0.17	70,71,73,74	0
4	NAG	Q	2	14/15	0.72	0.17	74,76,77,78	0
3	NAG	Z	2	14/15	0.73	0.21	67,68,69,71	0
2	NAG	O	1	14/15	0.73	0.19	74,77,81,84	0
6	NAG	R	2	14/15	0.75	0.19	73,75,76,79	0
7	MAN	T	6	11/12	0.75	0.15	86,87,88,90	0
5	NAG	K	1	14/15	0.75	0.16	64,69,71,72	0
3	MAN	Z	4	11/12	0.76	0.22	67,68,69,69	0
2	BMA	J	3	11/12	0.77	0.19	73,74,75,77	0
2	BMA	U	3	11/12	0.77	0.18	81,83,86,88	0
2	MAN	M	5	11/12	0.77	0.16	93,94,95,95	0
2	BMA	Y	3	11/12	0.78	0.17	75,76,77,77	0
2	NAG	J	2	14/15	0.78	0.18	71,73,75,75	0
3	BMA	Z	3	11/12	0.78	0.19	70,72,73,73	0
6	NAG	R	1	14/15	0.80	0.16	68,69,71,72	0
4	NAG	P	1	14/15	0.80	0.17	76,79,81,86	0
2	BMA	S	3	11/12	0.80	0.16	87,90,93,94	0
3	NAG	Z	1	14/15	0.82	0.18	64,68,70,71	0
3	NAG	j	1	14/15	-	-	78,81,83,83	0
3	NAG	j	2	14/15	-	-	82,83,85,85	0
3	BMA	j	3	11/12	-	-	80,82,82,83	0
3	MAN	j	4	11/12	-	-	76,78,79,79	0
3	MAN	j	5	11/12	-	-	75,76,77,77	0
3	MAN	j	6	11/12	-	-	80,80,81,82	0
5	NAG	X	2	14/15	0.82	0.18	68,71,75,76	0

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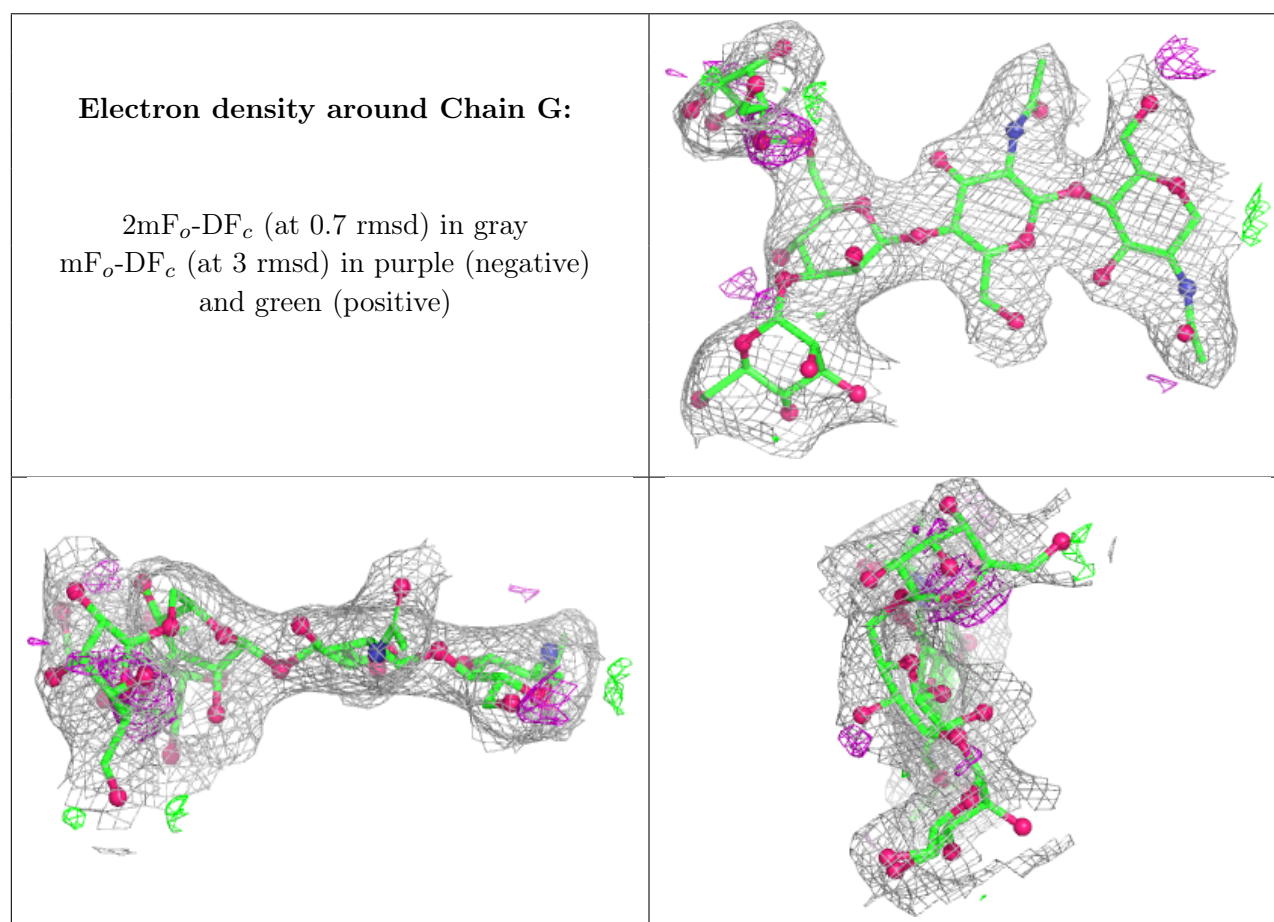
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	N	4	11/12	0.82	0.15	73,77,78,79	0
3	BMA	N	3	11/12	0.83	0.14	79,85,88,92	0
7	NAG	T	1	14/15	0.84	0.17	69,70,76,79	0
2	BMA	M	3	11/12	0.85	0.15	82,85,89,90	0
3	MAN	Z	5	11/12	0.85	0.16	63,64,65,65	0
5	NAG	X	1	14/15	0.86	0.13	62,64,67,68	0
2	BMA	G	3	11/12	0.86	0.14	80,84,88,89	0
4	NAG	b	1	14/15	-	-	68,69,70,72	0
4	NAG	b	2	14/15	-	-	73,74,75,76	0
4	NAG	g	1	14/15	-	-	65,67,67,67	0
4	NAG	g	2	14/15	-	-	64,65,66,66	0
4	NAG	I	1	14/15	0.87	0.14	71,76,80,87	0
7	BMA	T	3	11/12	0.88	0.14	77,81,85,88	0
2	NAG	Y	2	14/15	0.88	0.14	70,72,74,74	0
5	NAG	L	2	14/15	0.88	0.15	71,72,73,75	0
3	NAG	N	1	14/15	0.89	0.14	70,74,77,77	0
5	NAG	L	1	14/15	0.89	0.13	64,67,69,70	0
3	MAN	H	4	11/12	0.90	0.13	74,77,78,79	0
2	NAG	S	2	14/15	0.90	0.12	71,74,78,82	0
2	NAG	Y	1	14/15	0.90	0.12	68,69,69,71	0
7	MAN	T	4	11/12	0.90	0.13	72,76,80,83	0
3	NAG	H	1	14/15	0.90	0.14	67,72,78,80	0
3	BMA	H	3	11/12	0.90	0.11	80,86,89,93	0
5	NAG	c	1	14/15	-	-	72,73,75,76	0
5	NAG	c	2	14/15	-	-	75,76,76,78	0
5	BMA	c	3	11/12	-	-	80,80,80,81	0
5	NAG	h	1	14/15	-	-	63,66,69,69	0
5	NAG	h	2	14/15	-	-	65,65,66,66	0
5	BMA	h	3	11/12	-	-	65,66,66,66	0
5	NAG	l	1	14/15	-	-	75,76,77,77	0
5	NAG	l	2	14/15	-	-	77,78,79,81	0
5	BMA	l	3	11/12	-	-	81,82,82,83	0
2	NAG	S	1	14/15	0.91	0.12	67,69,71,72	0
3	NAG	N	2	14/15	0.92	0.15	78,79,80,82	0
7	NAG	T	2	14/15	0.93	0.13	72,75,77,79	0
2	NAG	M	1	14/15	0.93	0.12	67,68,70,71	0
3	NAG	H	2	14/15	0.93	0.14	79,82,86,86	0
2	NAG	G	1	14/15	0.93	0.11	63,65,68,68	0
3	MAN	N	5	11/12	0.93	0.11	68,70,71,73	0
3	MAN	H	5	11/12	0.94	0.10	67,72,73,75	0
2	NAG	M	2	14/15	0.94	0.10	72,74,76,79	0
2	NAG	G	2	14/15	0.95	0.11	70,72,73,77	0

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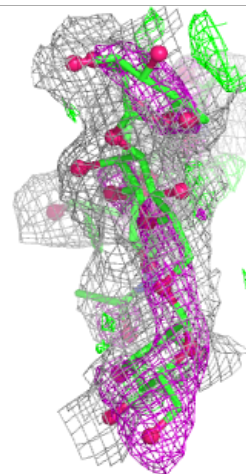
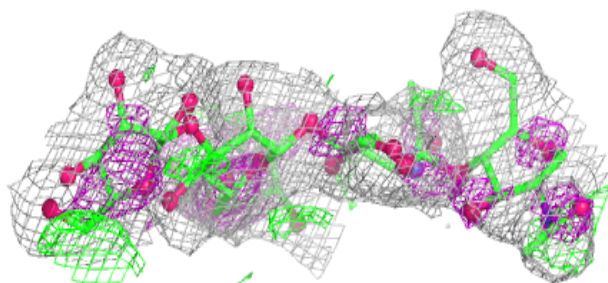
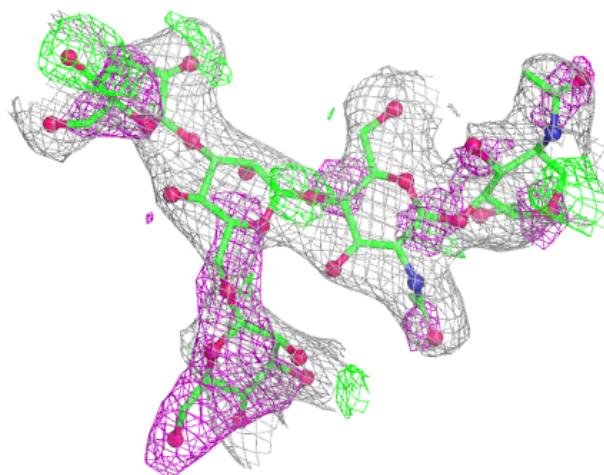
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	T	5	11/12	0.95	0.09	64,65,66,67	0
7	NAG	e	1	14/15	-	-	76,77,79,79	0
7	NAG	e	2	14/15	-	-	80,82,82,83	0
7	BMA	e	3	11/12	-	-	82,86,89,92	0
7	MAN	e	4	11/12	-	-	76,80,82,84	0
7	MAN	e	5	11/12	-	-	71,72,73,73	0
7	MAN	e	6	11/12	-	-	83,85,86,87	0
7	MAN	e	7	11/12	-	-	95,97,97,97	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.



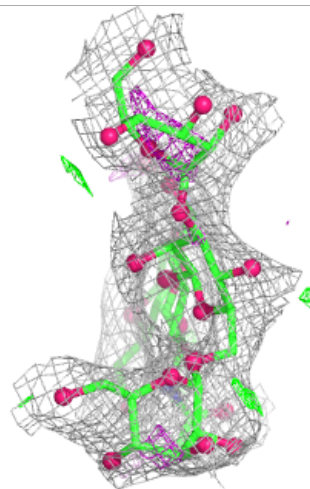
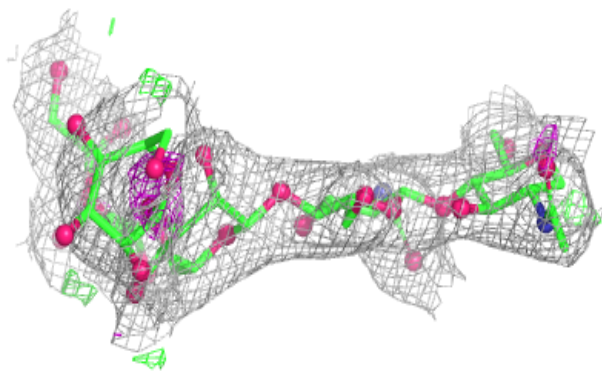
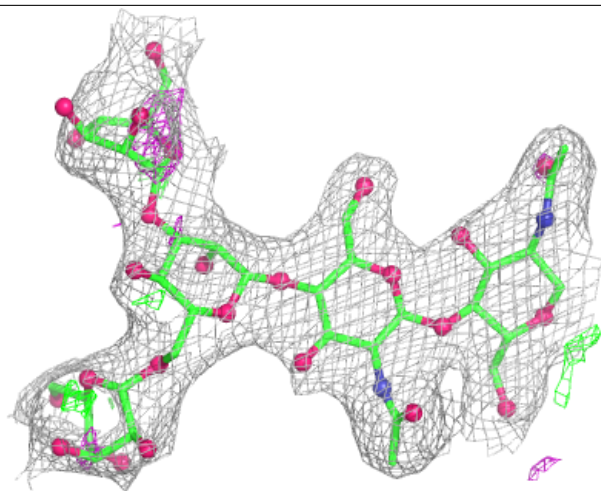
Electron density around Chain J:

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



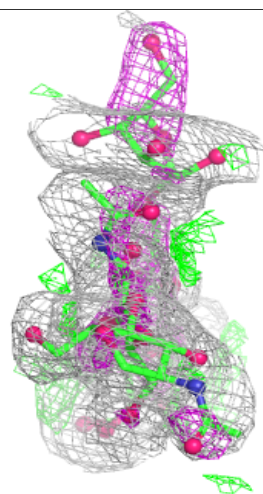
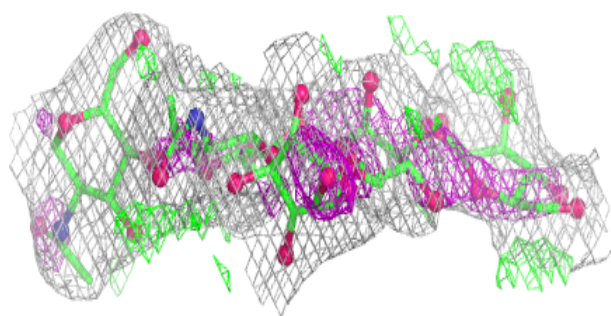
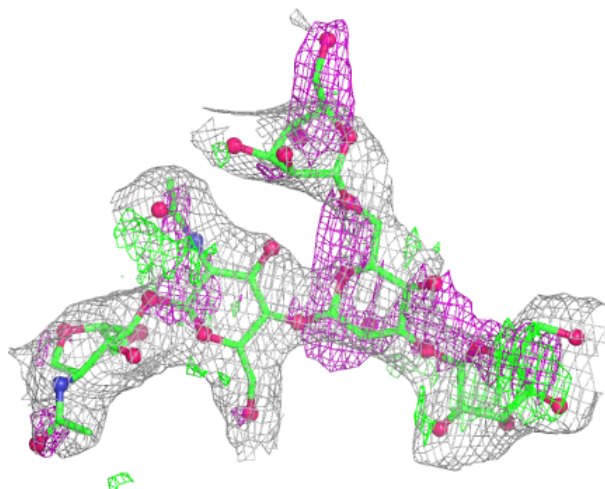
Electron density around Chain M:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



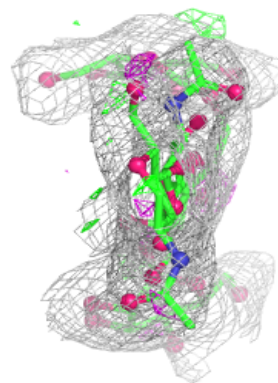
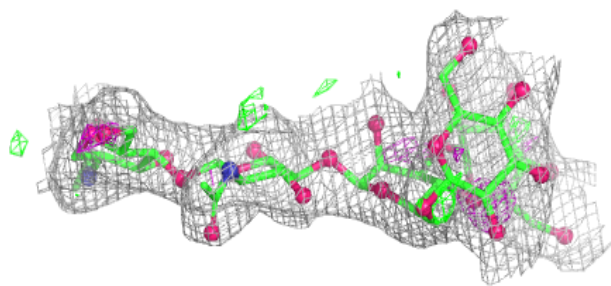
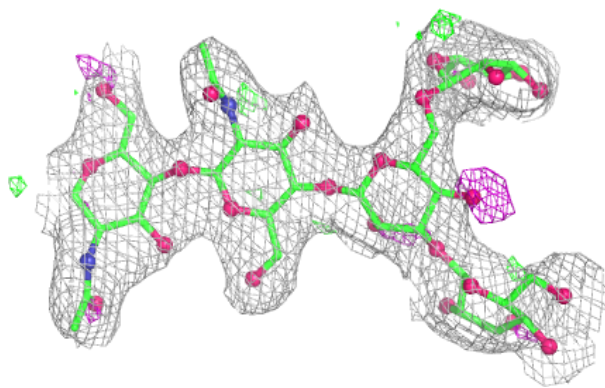
Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

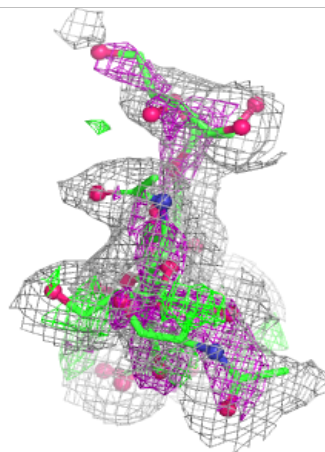
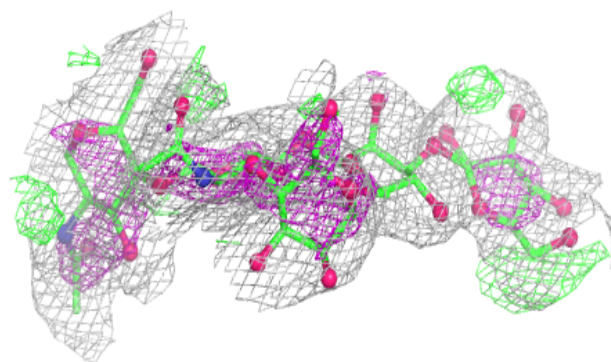
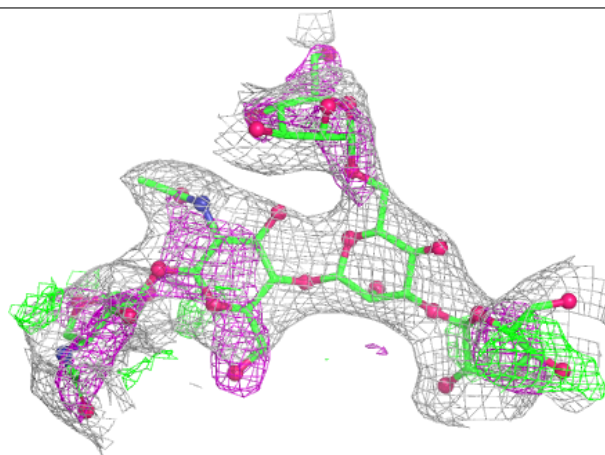


Electron density around Chain S:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

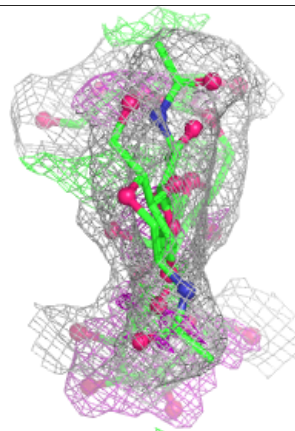
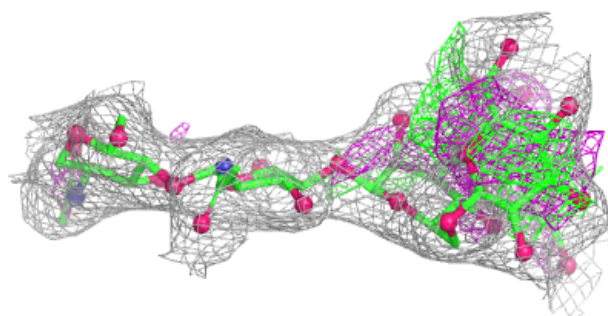
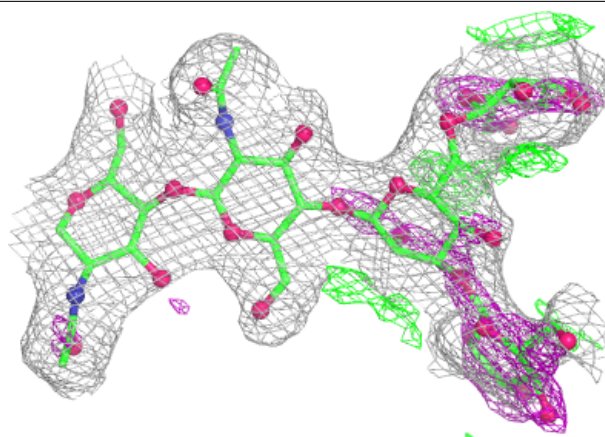
**Electron density around Chain U:**

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and green (positive)

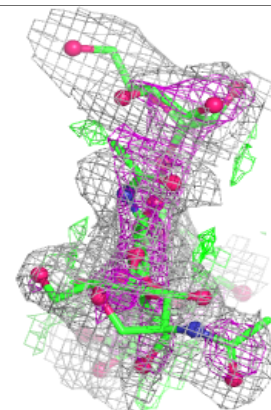
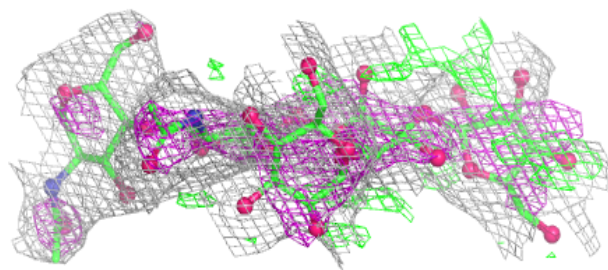
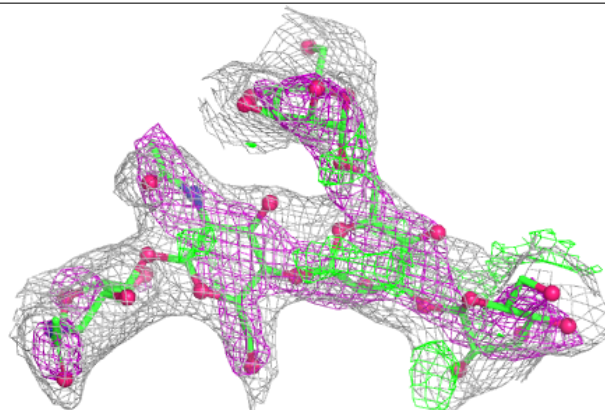


Electron density around Chain Y:

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and green (positive)

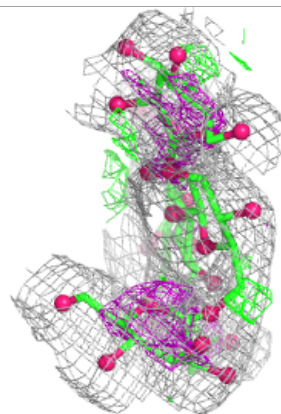
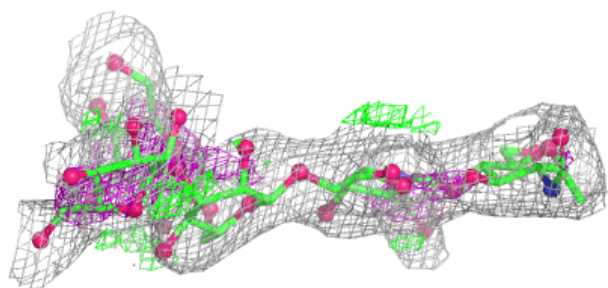
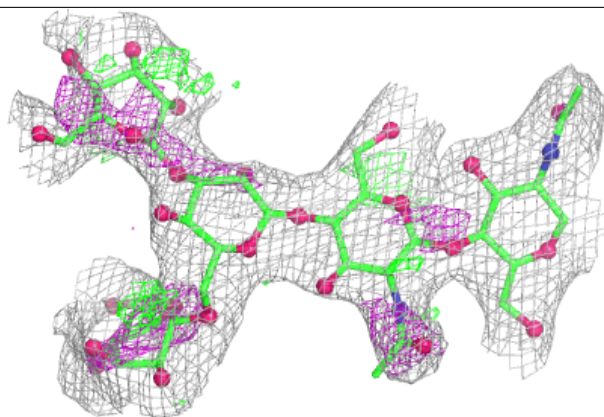
**Electron density around Chain a:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

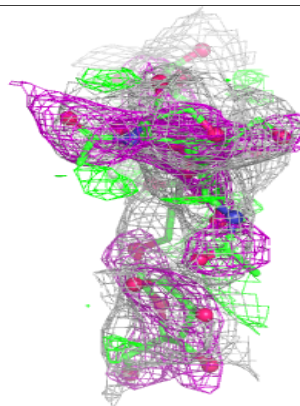
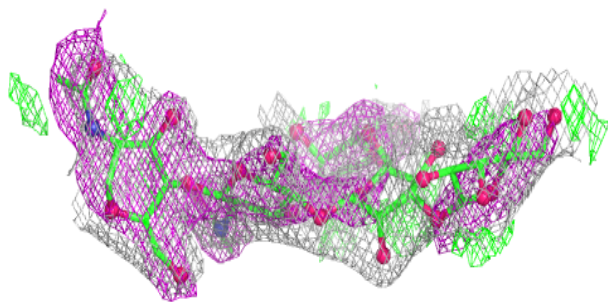
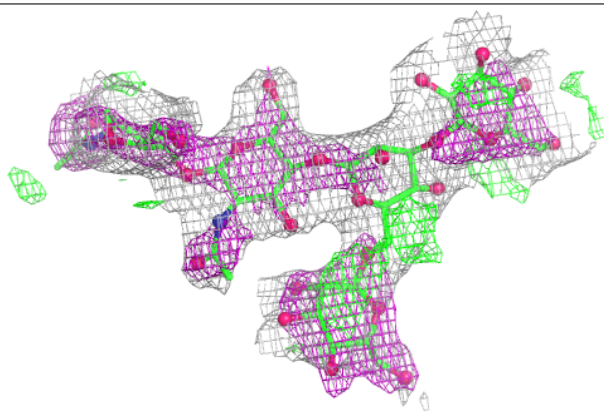


Electron density around Chain d:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

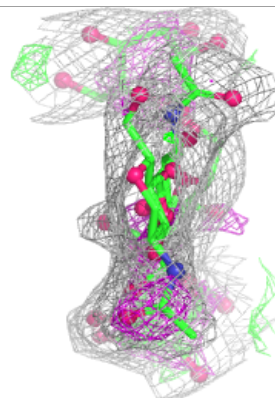
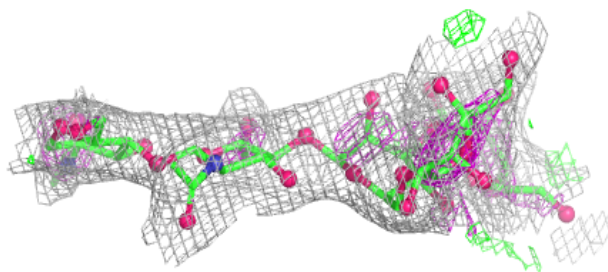
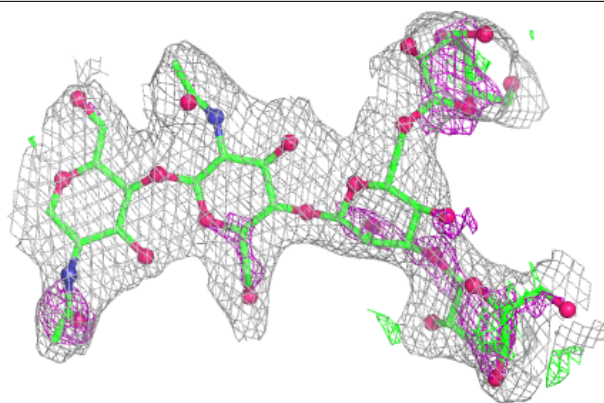
**Electron density around Chain f:**

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



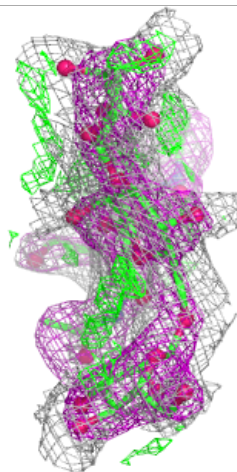
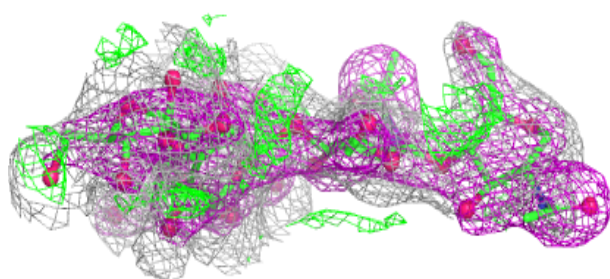
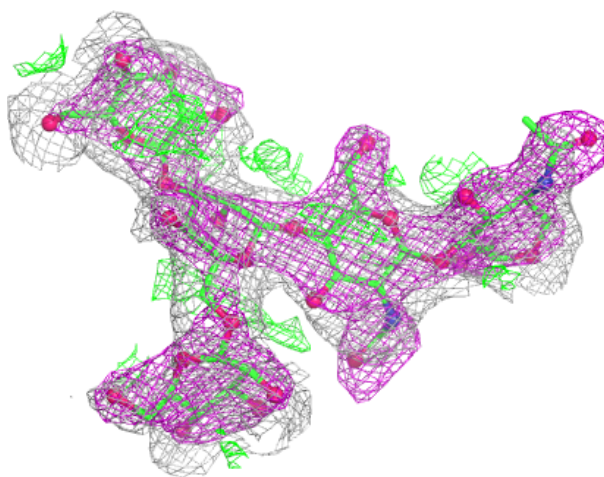
Electron density around Chain i:

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



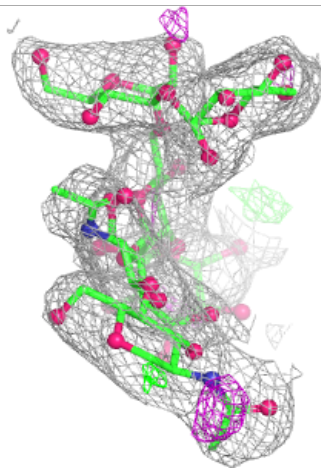
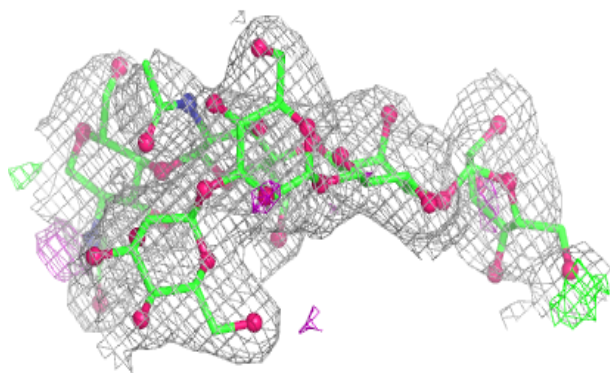
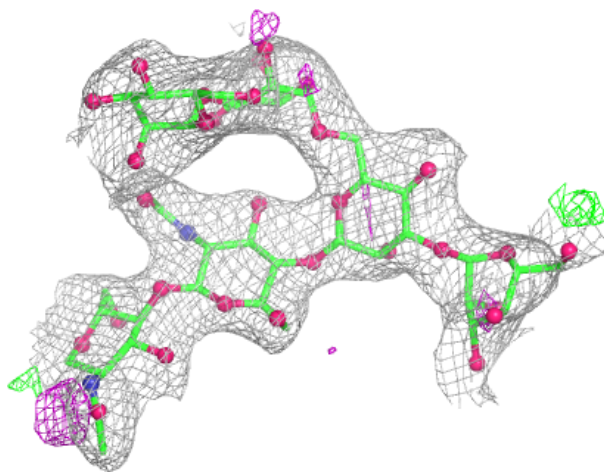
Electron density around Chain k:

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



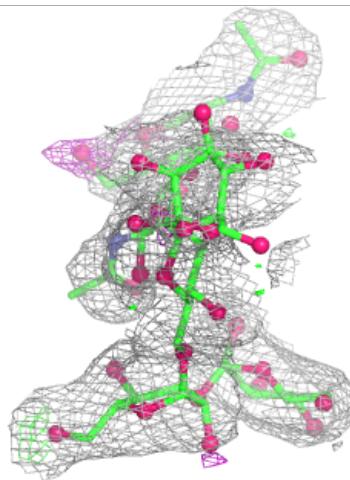
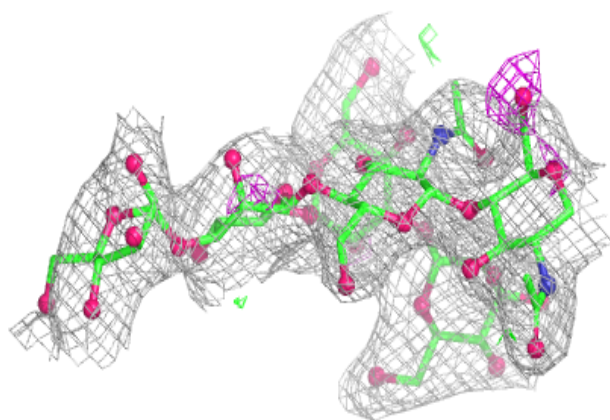
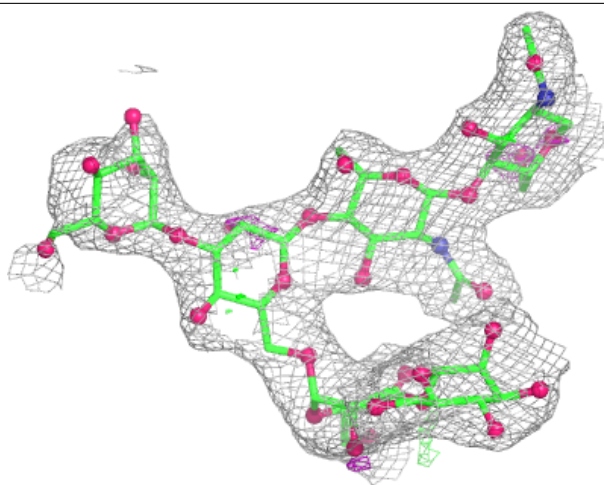
Electron density around Chain H:

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



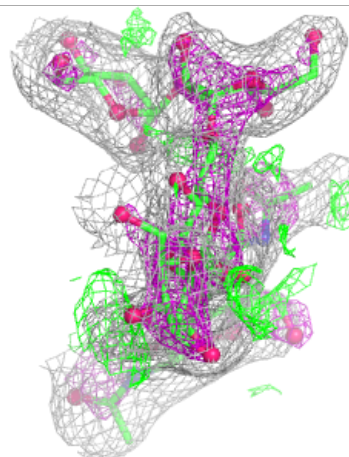
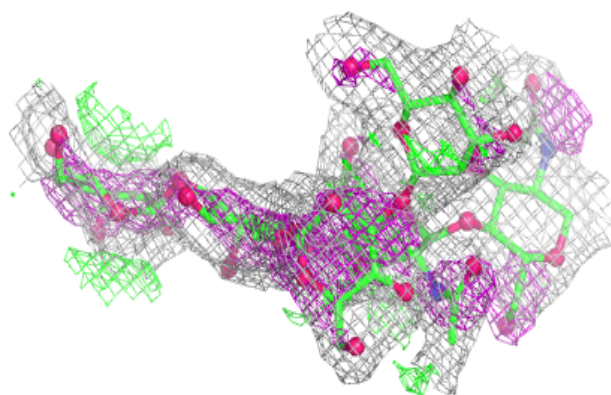
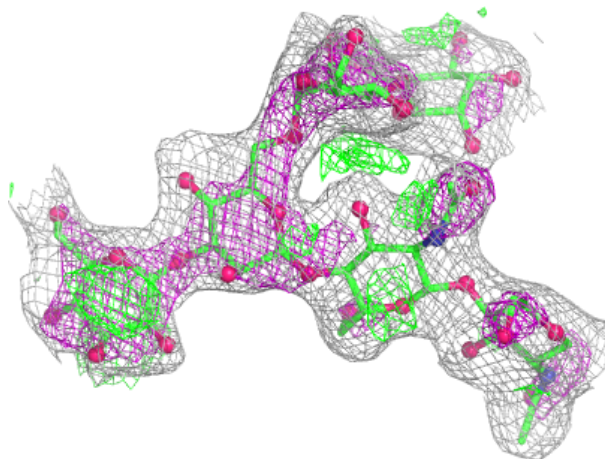
Electron density around Chain N:

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



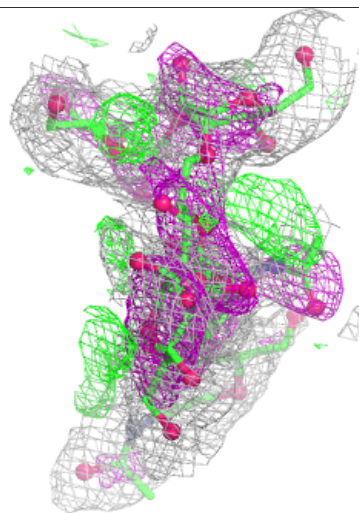
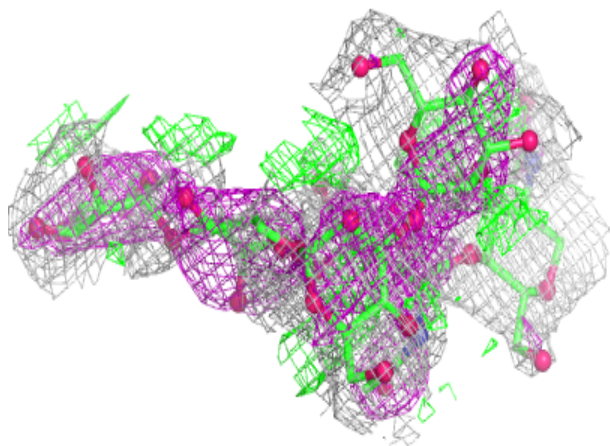
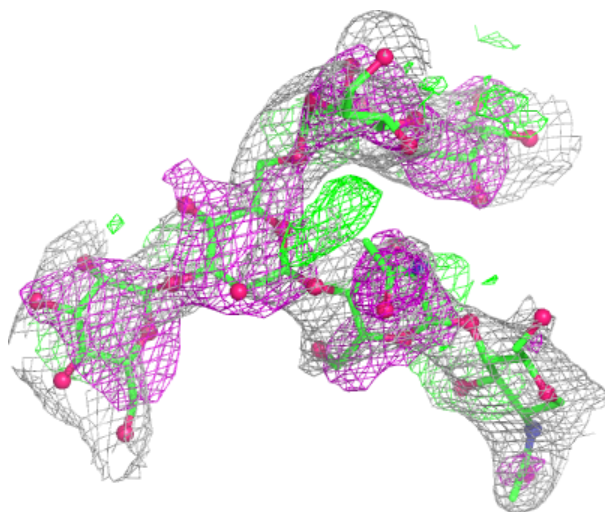
Electron density around Chain Z:

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



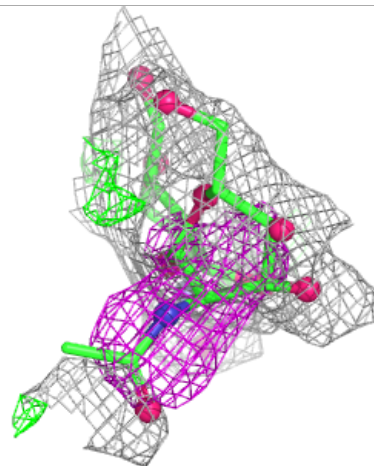
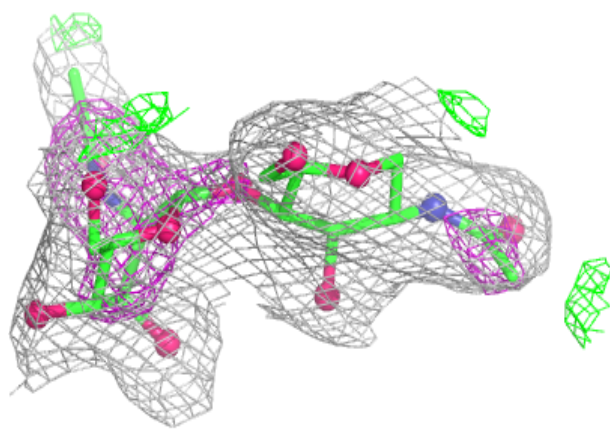
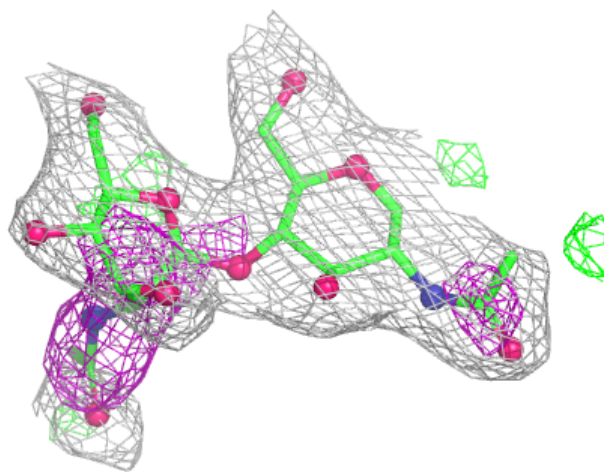
Electron density around Chain j:

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



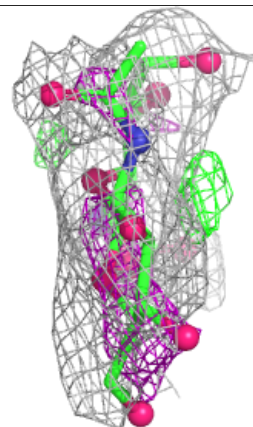
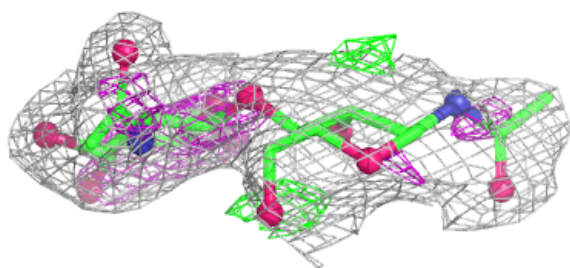
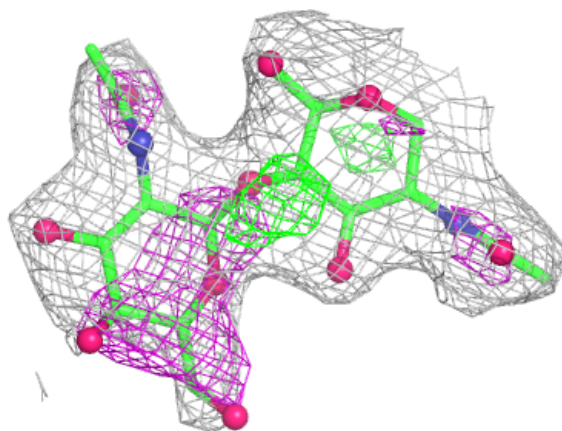
Electron density around Chain I:

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



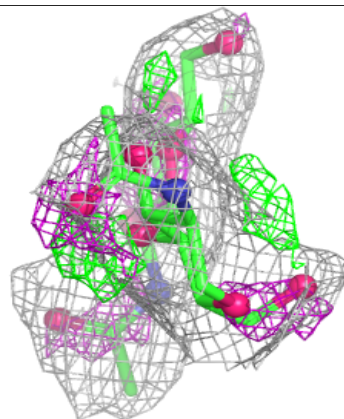
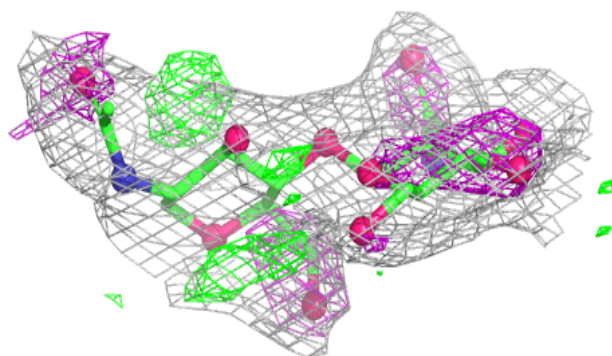
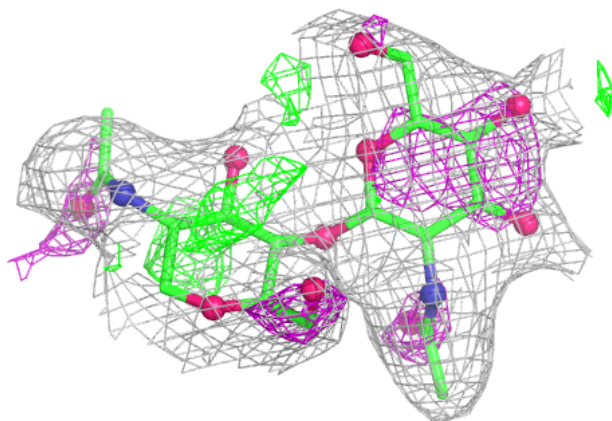
Electron density around Chain P:

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

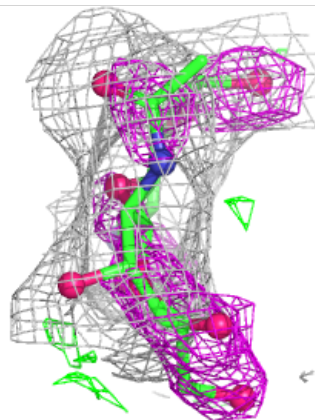
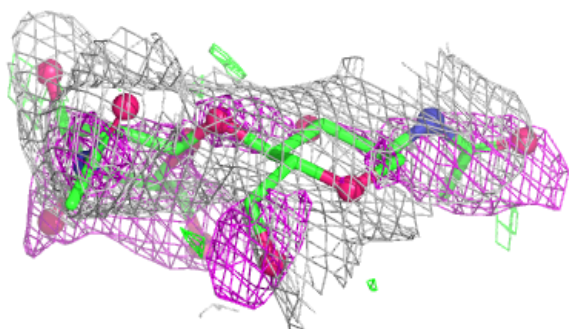
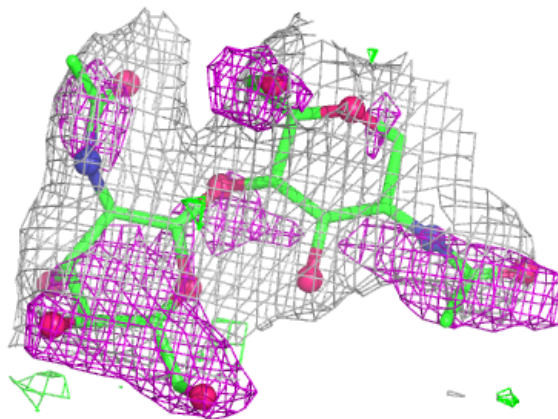


Electron density around Chain Q:

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

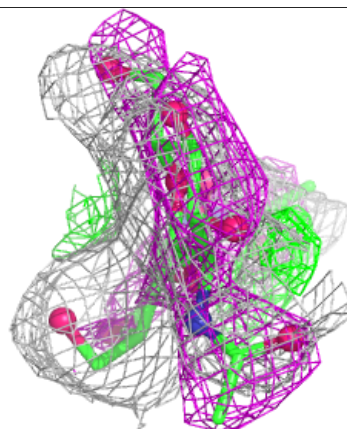
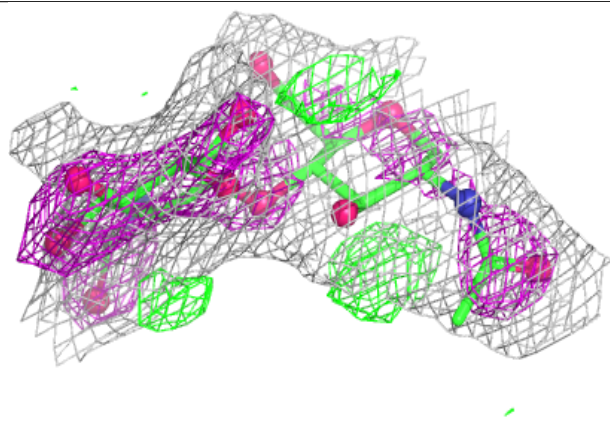
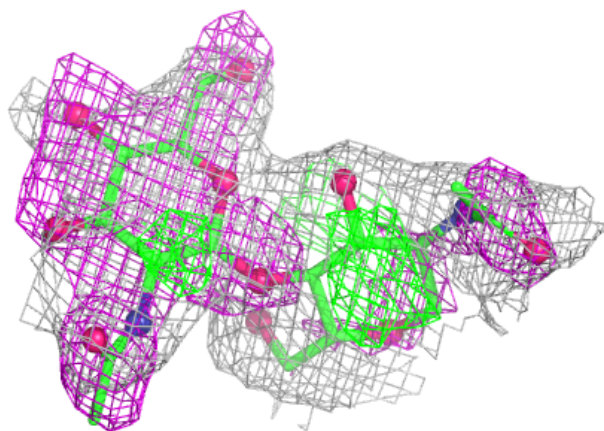
**Electron density around Chain V:**

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



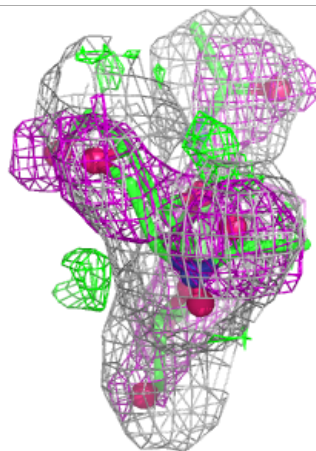
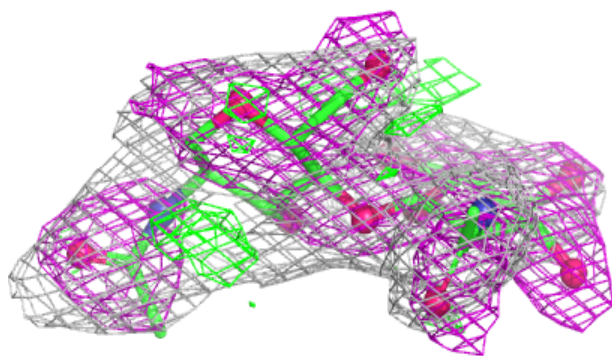
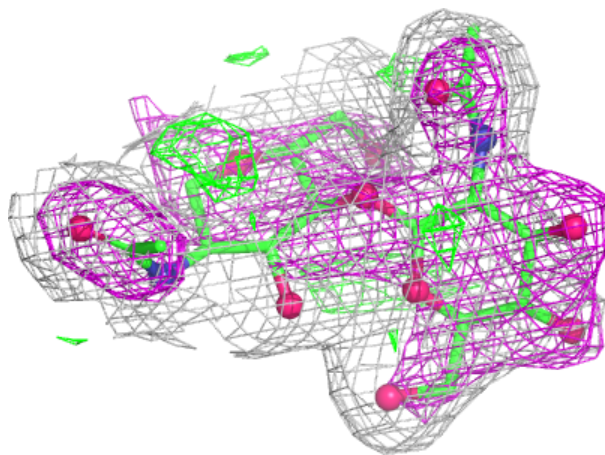
Electron density around Chain b:

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



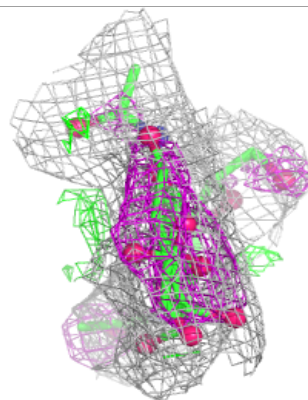
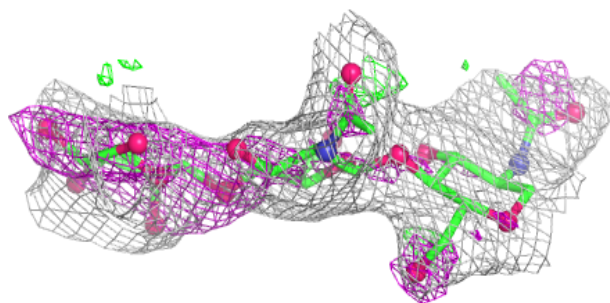
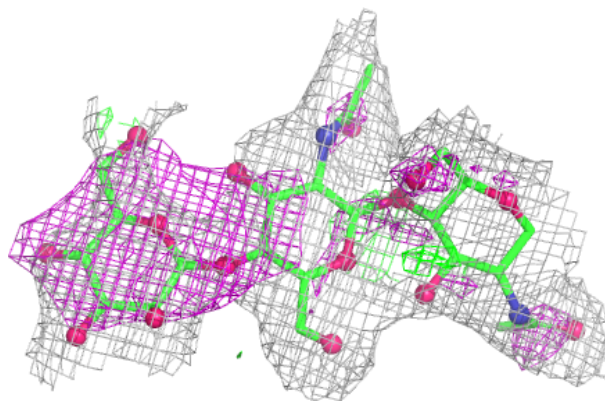
Electron density around Chain g:

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

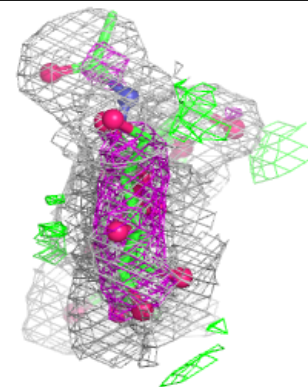
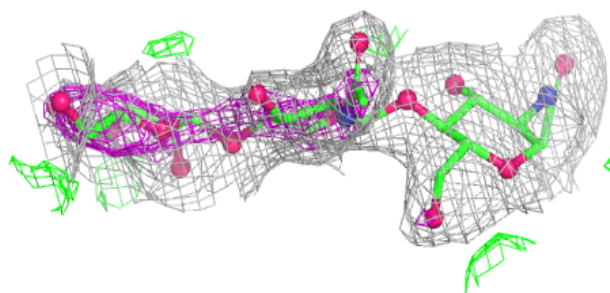
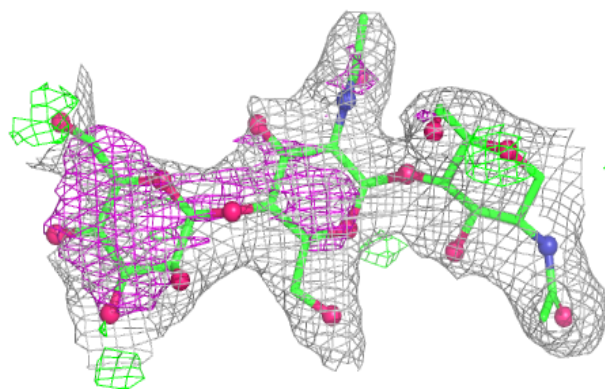


Electron density around Chain K:

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

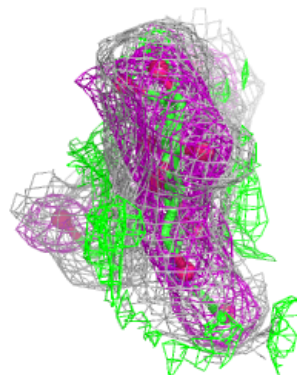
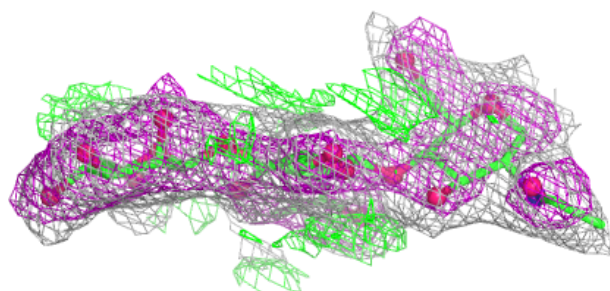
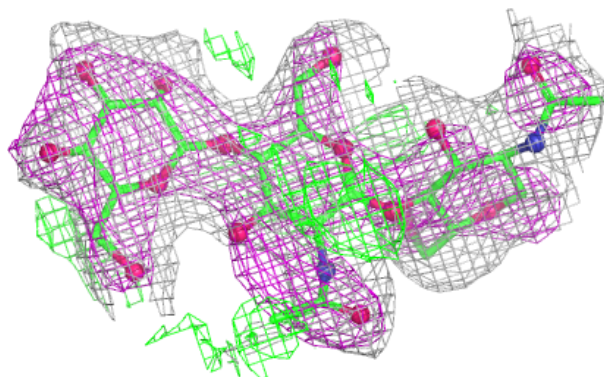
**Electron density around Chain L:**

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

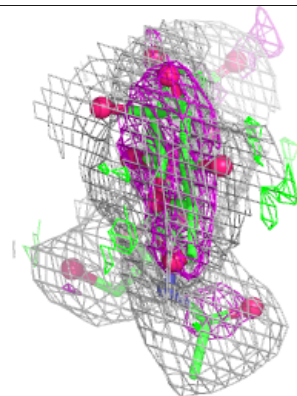
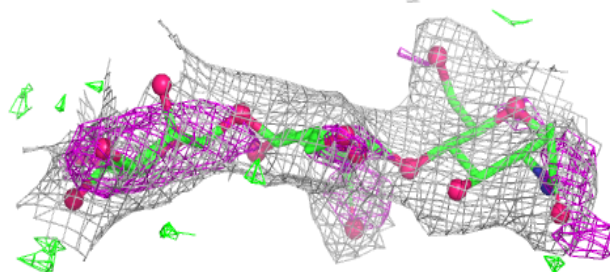
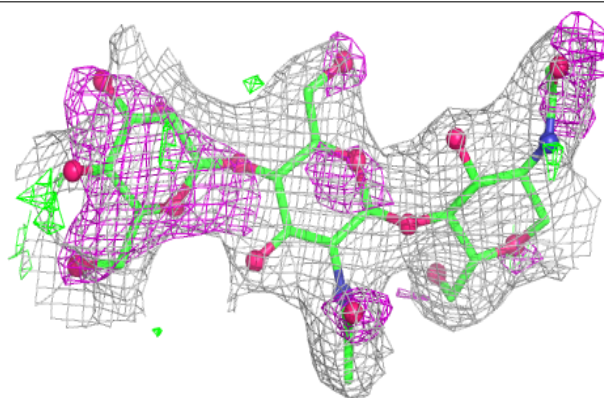


Electron density around Chain W:

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

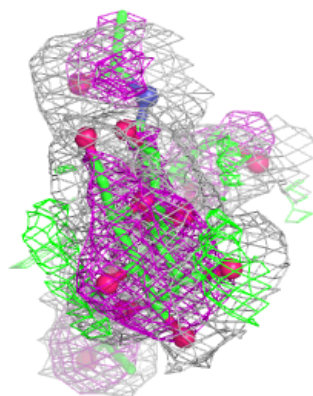
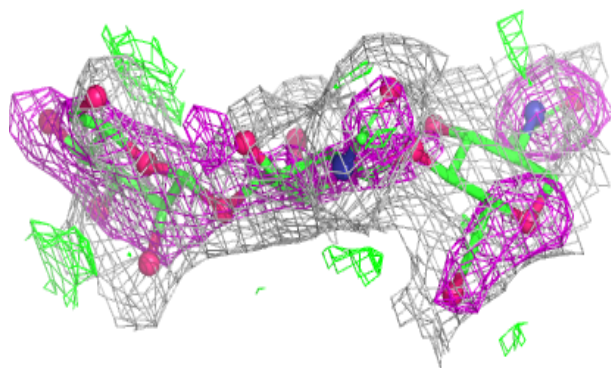
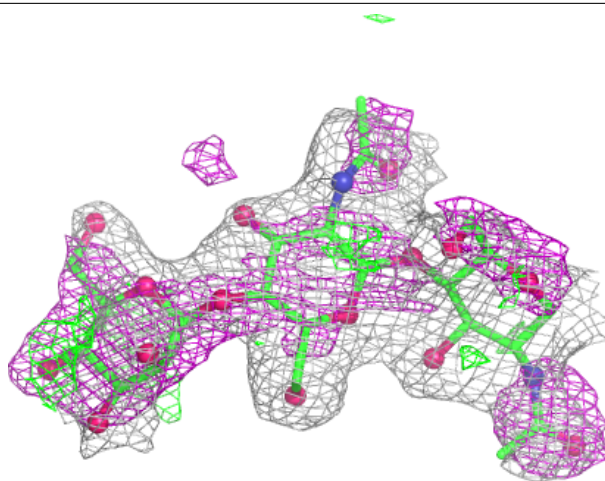
**Electron density around Chain X:**

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



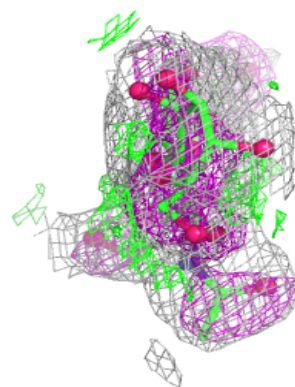
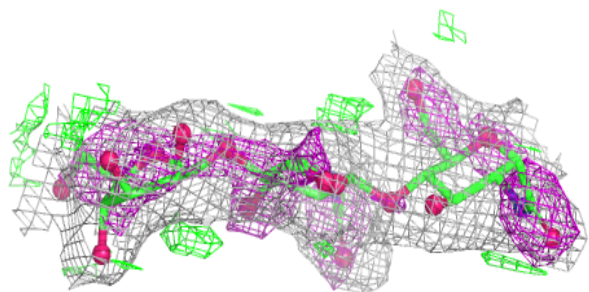
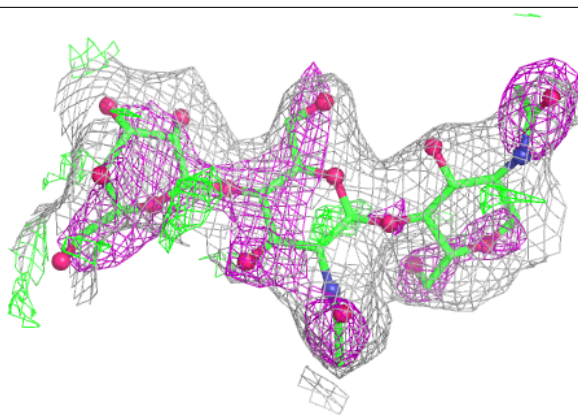
Electron density around Chain c:

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

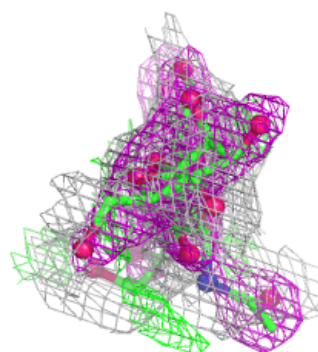
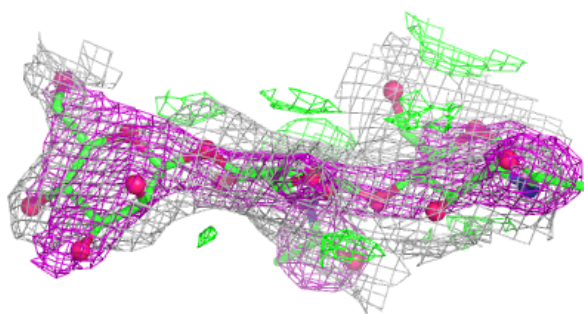
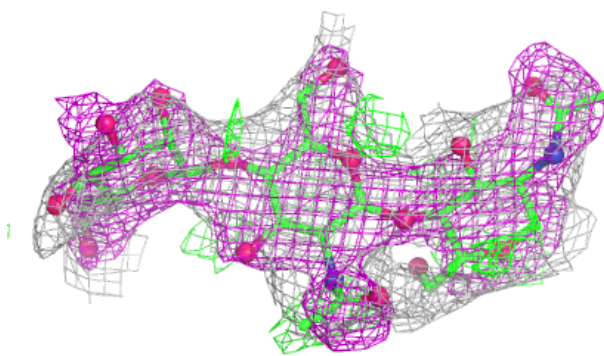


Electron density around Chain h:

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

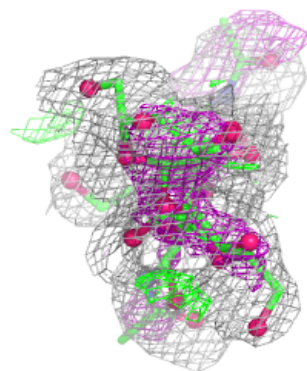
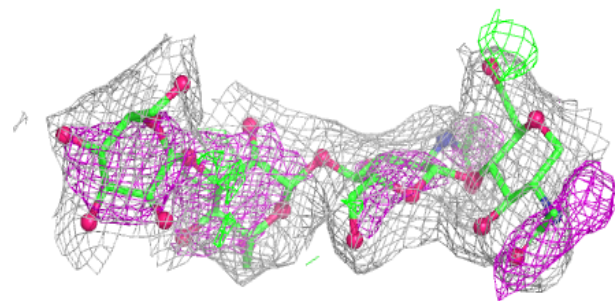
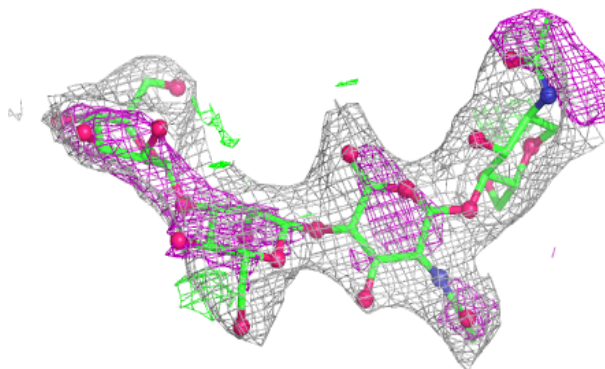
**Electron density around Chain l:**

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



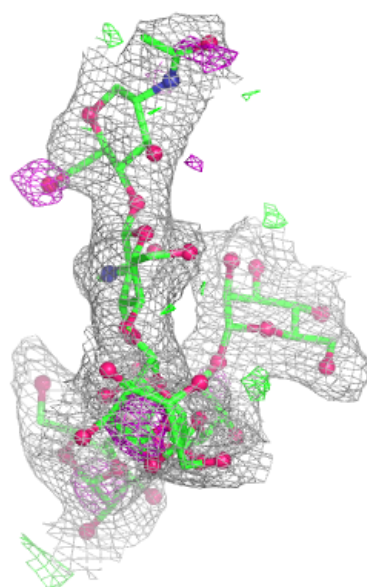
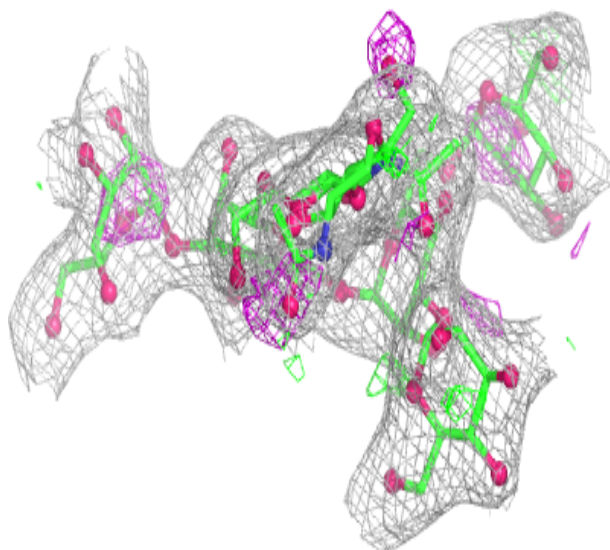
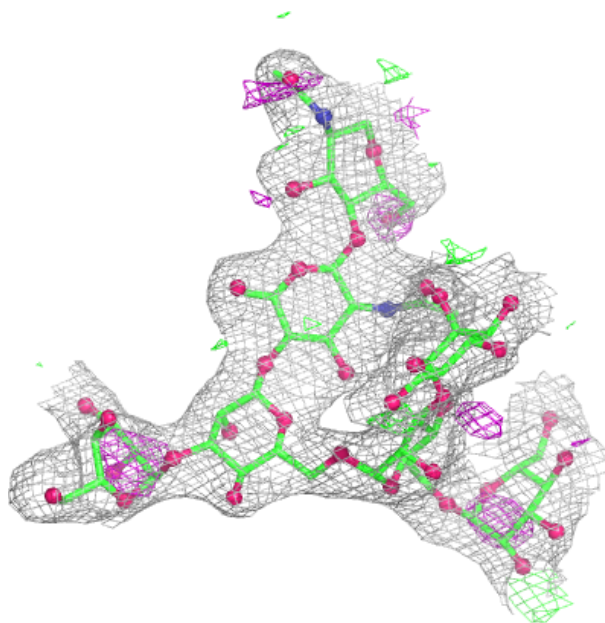
Electron density around Chain R:

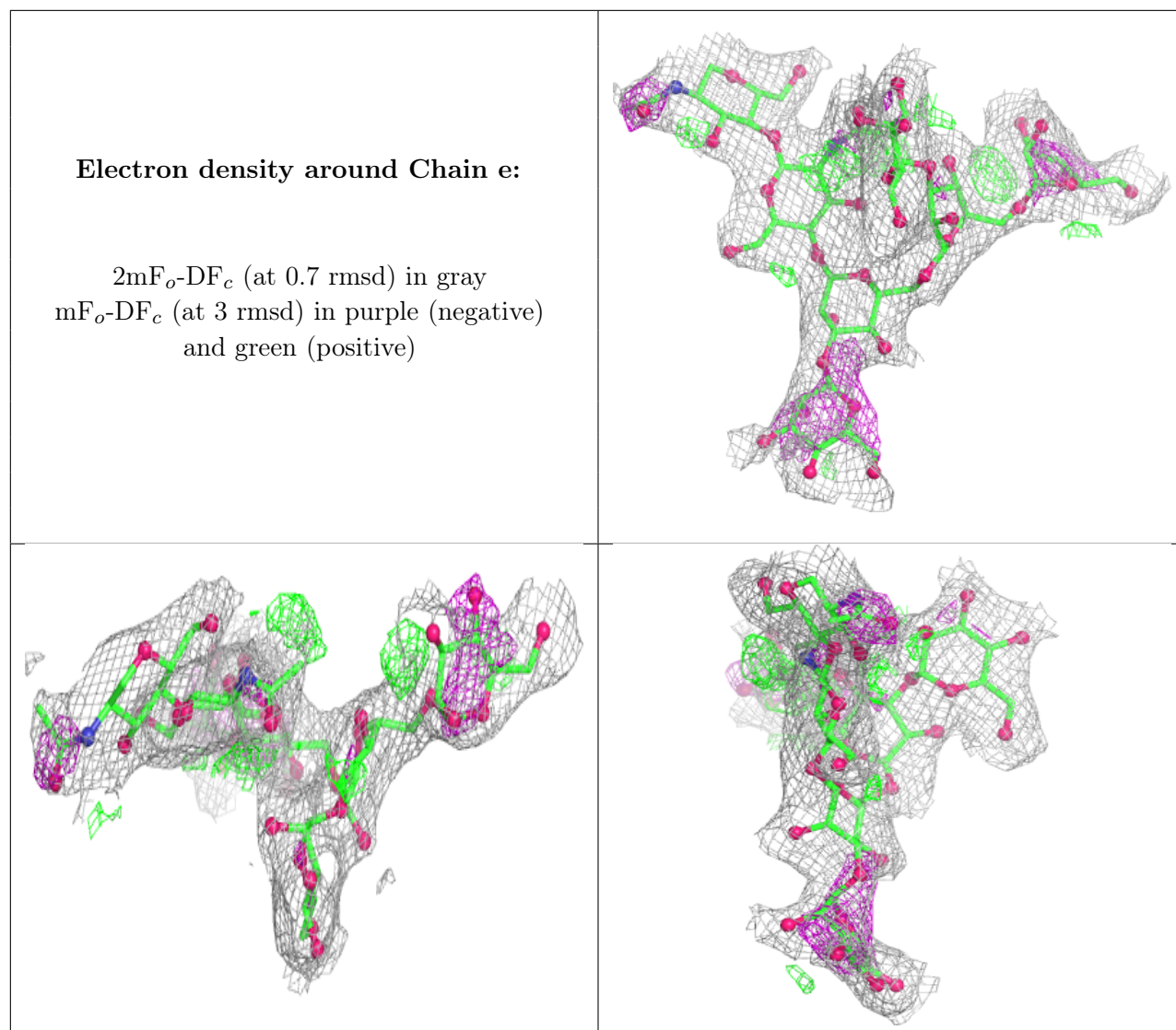
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	NAG	E	2005	14/15	0.29	0.23	70,71,71,71	0
8	NAG	E	2012	14/15	0.35	0.23	73,74,77,77	0
8	NAG	F	2012	14/15	0.35	0.22	72,73,75,75	0
8	NAG	F	2006	14/15	0.37	0.23	67,68,70,70	0
8	NAG	C	2018	14/15	0.52	0.19	74,76,77,78	0
8	NAG	E	2008	14/15	0.53	0.22	72,72,73,73	0
8	NAG	A	2018	14/15	0.53	0.20	78,80,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	D	2014	14/15	0.54	0.21	65,66,67,67	0
8	NAG	E	2006	14/15	0.55	0.22	73,74,75,76	0
8	NAG	F	2008	14/15	0.56	0.23	71,71,72,72	0
8	NAG	B	2014	14/15	0.56	0.22	67,70,71,71	0
8	NAG	B	2018	14/15	0.60	0.18	80,83,83,83	0
8	NAG	F	2005	14/15	0.61	0.18	67,70,71,72	0
8	NAG	F	2009	14/15	0.61	0.19	66,69,69,69	0
8	NAG	C	2006	14/15	0.61	0.19	74,76,77,78	0
8	NAG	D	2006	14/15	0.63	0.18	65,68,70,71	0
8	NAG	A	2006	14/15	0.64	0.19	71,73,74,74	0
8	NAG	C	2012	14/15	0.69	0.18	75,77,79,80	0
8	NAG	A	2012	14/15	0.71	0.18	76,79,80,81	0
8	NAG	D	2012	14/15	0.72	0.16	73,74,76,77	0
8	NAG	D	2008	14/15	0.73	0.19	70,71,73,73	0
8	NAG	D	2005	14/15	0.73	0.18	71,72,74,75	0
8	NAG	F	2014	14/15	0.74	0.16	59,62,63,64	0
8	NAG	B	2006	14/15	0.76	0.14	74,76,78,79	0
8	NAG	A	2014	14/15	0.79	0.16	67,67,71,72	0
8	NAG	B	2012	14/15	0.79	0.15	74,75,79,79	0
8	NAG	B	2005	14/15	0.83	0.14	64,67,69,70	0
8	NAG	C	2005	14/15	0.83	0.16	64,68,70,70	0
8	NAG	E	2014	14/15	0.84	0.13	52,56,57,58	0
8	NAG	A	2008	14/15	0.86	0.15	68,69,70,70	0
8	NAG	C	2014	14/15	0.88	0.12	53,55,57,58	0
9	CU1	F	1001	1/1	0.88	0.19	90,90,90,90	0
9	CU1	D	1004	1/1	0.91	0.19	100,100,100,100	0
9	CU1	F	1004	1/1	0.94	0.17	100,100,100,100	0
9	CU1	F	1003	1/1	0.95	0.14	91,91,91,91	0
9	CU1	A	1004	1/1	0.95	0.12	100,100,100,100	0
9	CU1	E	1003	1/1	0.96	0.14	99,99,99,99	0
9	CU1	E	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	C	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	F	1002	1/1	0.96	0.10	96,96,96,96	0
9	CU1	C	1001	1/1	0.96	0.07	85,85,85,85	0
9	CU1	E	1001	1/1	0.96	0.14	88,88,88,88	0
9	CU1	D	1003	1/1	0.97	0.07	89,89,89,89	0
9	CU1	B	1004	1/1	0.97	0.07	100,100,100,100	0
9	CU1	D	1001	1/1	0.97	0.05	86,86,86,86	0
9	CU1	E	1002	1/1	0.97	0.16	93,93,93,93	0
9	CU1	D	1002	1/1	0.97	0.07	87,87,87,87	0
9	CU1	C	1003	1/1	0.98	0.05	83,83,83,83	0
9	CU1	B	1002	1/1	0.98	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CU1	B	1003	1/1	0.99	0.09	87,87,87,87	0
9	CU1	A	1003	1/1	0.99	0.10	89,89,89,89	0
9	CU1	A	1001	1/1	0.99	0.03	82,82,82,82	0
9	CU1	C	1002	1/1	0.99	0.04	85,85,85,85	0
9	CU1	B	1001	1/1	0.99	0.05	87,87,87,87	0
9	CU1	A	1002	1/1	0.99	0.09	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.