



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:32 PM UTC

PDB ID : 5WDU / pdb_00005wdu
Title : HIV-1 Env BG505 SOSIP.664 H72C-H564C trimer in complex with bNAbs
PGT122 Fab, 35O22 Fab and NIH45-46 scFv
Authors : Julien, J.-P.; Torrents de la Pena, A.; Sanders, R.W.; Wilson, I.A.
Deposited on : 2017-07-06
Resolution : 7.00 Å(reported)

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

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

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

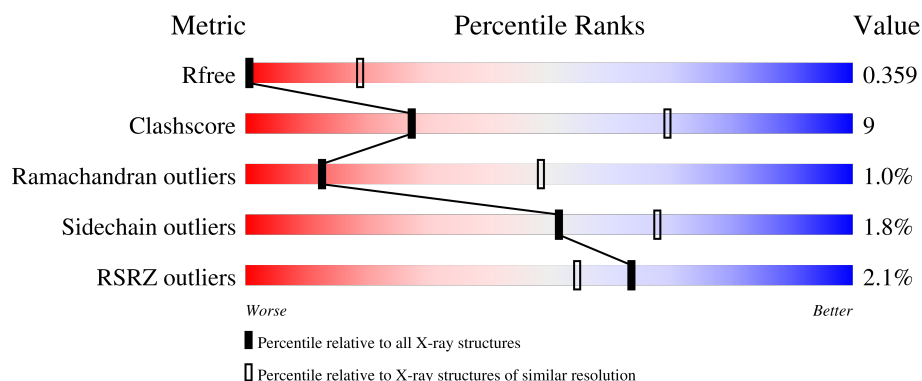
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 Å.

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



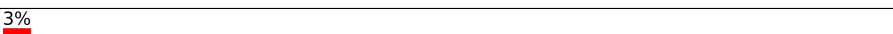
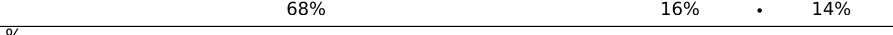
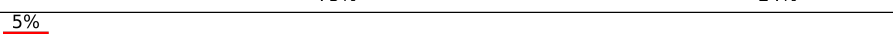
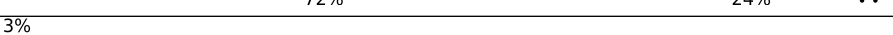
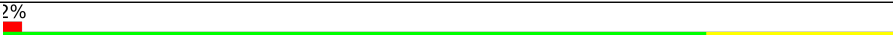
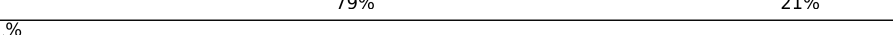
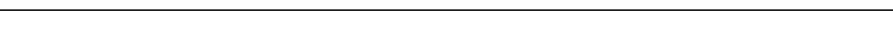
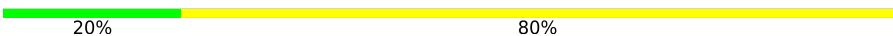
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	F	471	2% 68% 26% • 5%
1	G	471	4% 69% 25% • 5%
1	Q	471	% 68% 25% • 5%
2	D	250	2% 74% 15% • 11%
2	O	250	% 70% 17% • 11%

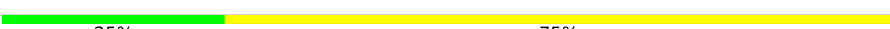
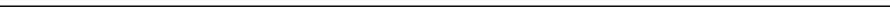
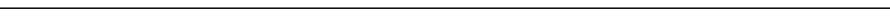
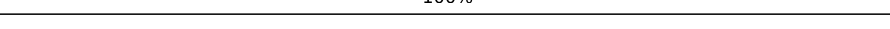
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Mol	Chain	Length	Quality of chain
2	W	250	
3	A	147	
3	J	147	
3	R	147	
4	B	210	
4	K	210	
4	S	210	
5	C	232	
5	L	232	
5	T	232	
6	H	242	
6	M	242	
6	U	242	
7	I	213	
7	N	213	
7	V	213	
8	E	5	
8	X	5	
8	c	5	
8	e	5	
8	g	5	
8	l	5	
8	n	5	
8	p	5	
8	u	5	

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Mol	Chain	Length	Quality of chain
9	P	3	
9	f	3	
9	o	3	
10	Y	4	
10	h	4	
10	q	4	
11	Z	7	
11	i	7	
11	r	7	
12	a	6	
12	j	6	
12	s	6	
13	b	2	
13	k	2	
13	t	2	
14	d	8	
14	m	8	
14	v	8	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 41285 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	449	Total	C	N	O	S	0	0	0
			3535	2218	624	664	29			
1	F	449	Total	C	N	O	S	0	0	0
			3535	2218	624	664	29			
1	Q	449	Total	C	N	O	S	0	0	0
			3535	2218	624	664	29			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	72	CYS	HIS	conflict	UNP Q2N0S6
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
F	72	CYS	HIS	conflict	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	460	ALA	SER	conflict	UNP Q2N0S6
F	461	ASN	THR	conflict	UNP Q2N0S6
F	463	THR	SER	conflict	UNP Q2N0S6
F	464	SER	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
Q	72	CYS	HIS	conflict	UNP Q2N0S6
Q	332	ASN	THR	conflict	UNP Q2N0S6
Q	460	ALA	SER	conflict	UNP Q2N0S6
Q	461	ASN	THR	conflict	UNP Q2N0S6
Q	463	THR	SER	conflict	UNP Q2N0S6
Q	464	SER	THR	conflict	UNP Q2N0S6
Q	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called bnAb NIH45-46 scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	223	Total	C	N	O	S	0	0	0
			1761	1107	316	328	10			
2	O	222	Total	C	N	O	S	0	0	0
			1753	1102	315	326	10			
2	W	223	Total	C	N	O	S	0	0	0
			1761	1107	316	328	10			

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
3	J	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			
3	R	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	CYS	THR	conflict	UNP Q2N0S8
J	605	CYS	THR	conflict	UNP Q2N0S8
R	605	CYS	THR	conflict	UNP Q2N0S8

- Molecule 4 is a protein called bnAb PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			
4	K	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			
4	S	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 5 is a protein called bnAb PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			
5	L	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			
5	T	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

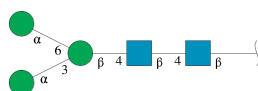
- Molecule 6 is a protein called bnAb 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			
6	M	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			
6	U	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 7 is a protein called bnAb 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	207	Total	C	N	O	S	0	0	0
			1574	989	258	319	8			
7	N	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			
7	V	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 8 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.



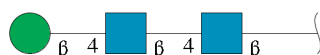
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	X	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	c	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	e	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	g	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	l	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	n	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	p	5	Total	C	N	O	0	0	0
			61	34	2	25			
8	u	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 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.



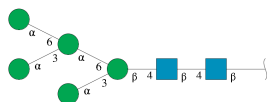
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	f	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	o	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called 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.



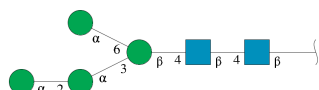
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
10	h	4	Total	C	N	O	0	0	0
			50	28	2	20			
10	q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 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.



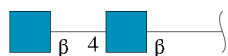
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			
11	i	7	Total	C	N	O	0	0	0
			83	46	2	35			
11	r	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



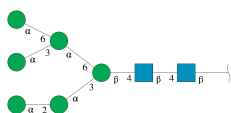
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	a	6	Total	C	N	O	0	0	0
			72	40	2	30			
12	j	6	Total	C	N	O	0	0	0
			72	40	2	30			
12	s	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



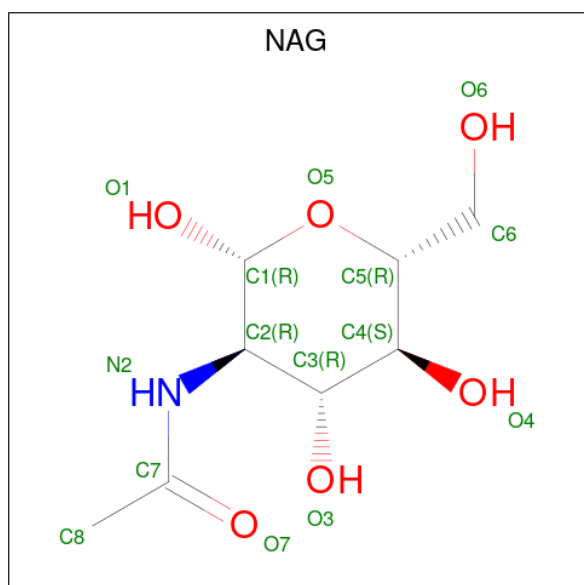
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
13	k	2	Total	C	N	O	0	0	0
			28	16	2	10			
13	t	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
14	d	8	Total	C	N	O	0	0	0
			94	52	2	40			
14	m	8	Total	C	N	O	0	0	0
			94	52	2	40			
14	v	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

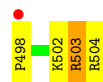
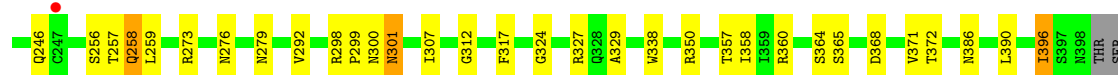
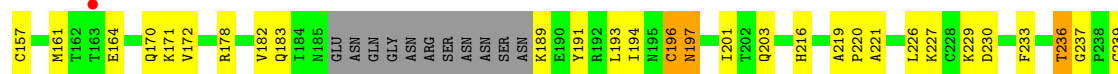
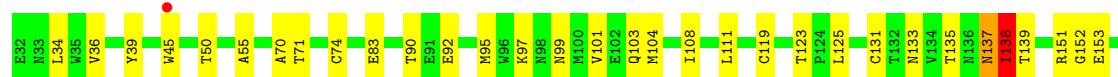
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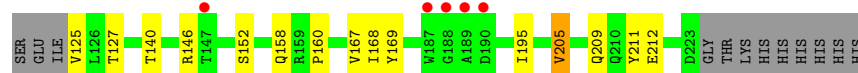
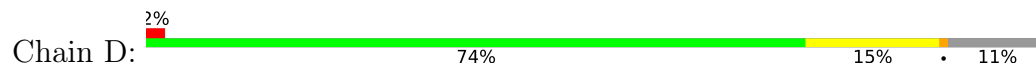
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	N	O	0	0
			14	8	1	5		
15	A	1	Total	C	N	O	0	0
			14	8	1	5		
15	J	1	Total	C	N	O	0	0
			14	8	1	5		
15	J	1	Total	C	N	O	0	0
			14	8	1	5		
15	J	1	Total	C	N	O	0	0
			14	8	1	5		
15	R	1	Total	C	N	O	0	0
			14	8	1	5		
15	R	1	Total	C	N	O	0	0
			14	8	1	5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



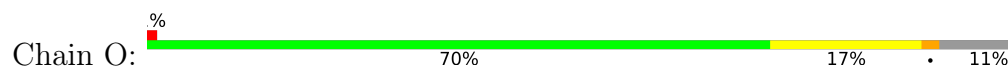
- Molecule 1: Envelope glycoprotein gp160



- Molecule 2: bnAb NIH45-46 scFv



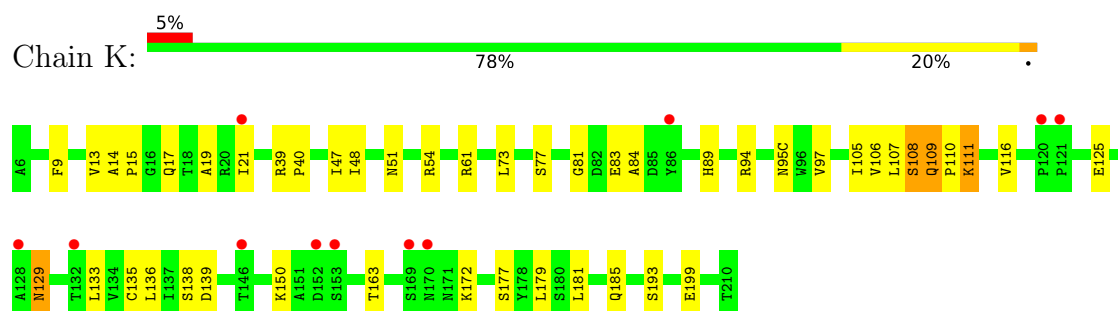
- Molecule 2: bnAb NIH45-46 scFv



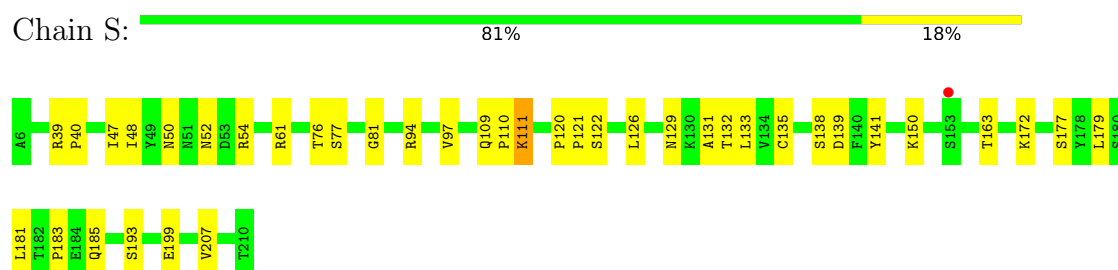
- Molecule 2: bnAb NIH45-46 scFv



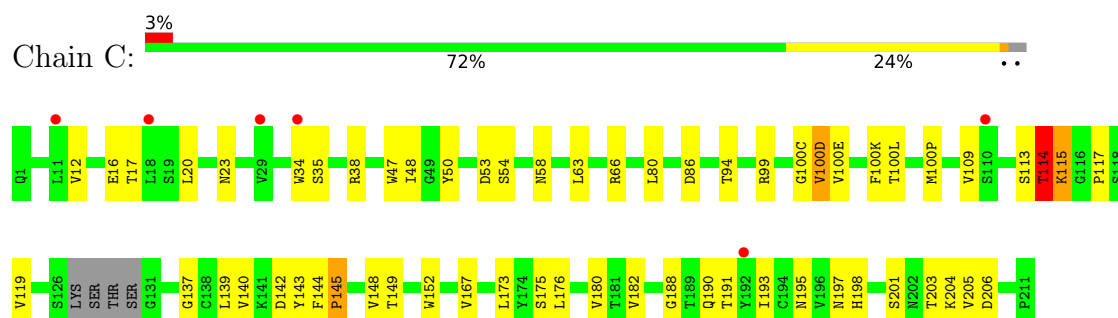
- Molecule 4: bnAb PGT122 Fab light chain



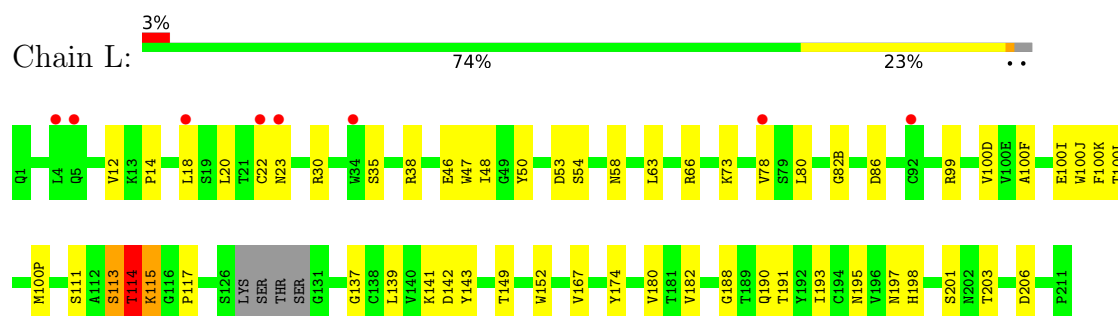
- Molecule 4: bnAb PGT122 Fab light chain



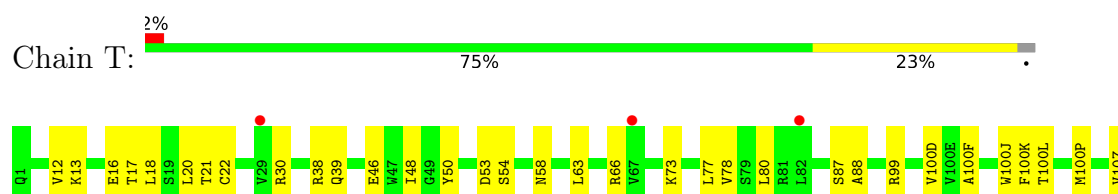
- Molecule 5: bnAb PGT122 Fab heavy chain



- Molecule 5: bnAb PGT122 Fab heavy chain

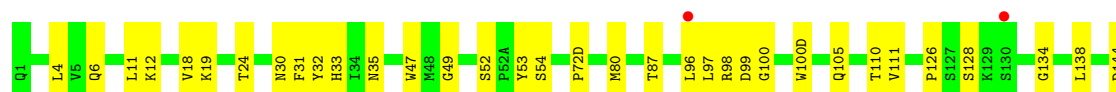
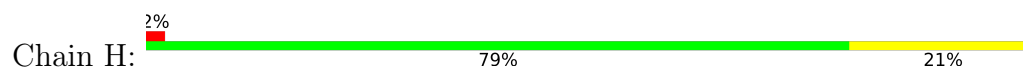


- Molecule 5: bnAb PGT122 Fab heavy chain

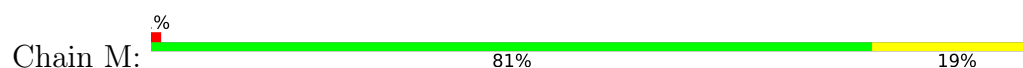




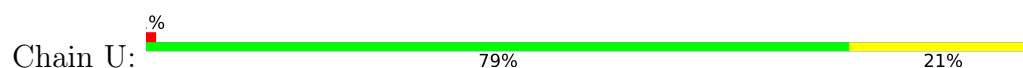
- Molecule 6: bnAb 35O22 Fab heavy chain



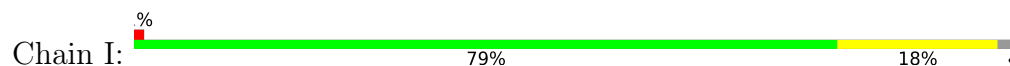
- Molecule 6: bnAb 35O22 Fab heavy chain



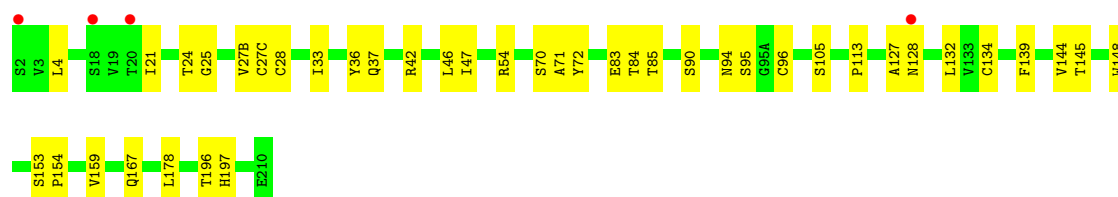
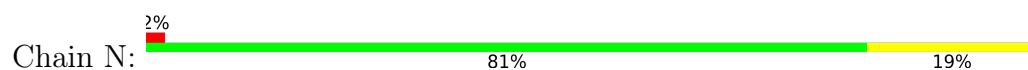
- Molecule 6: bnAb 35O22 Fab heavy chain



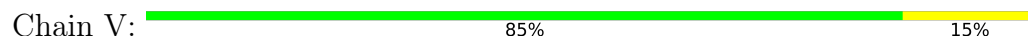
- Molecule 7: bnAb 35O22 Fab light chain



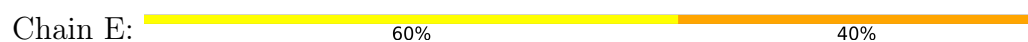
- Molecule 7: bnAb 35O22 Fab light chain



- Molecule 7: bnAb 35O22 Fab light chain



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



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



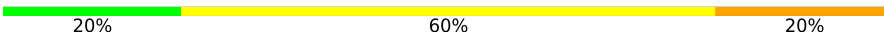
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 8: 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: 

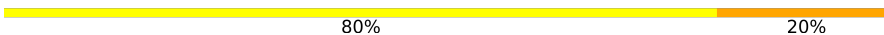


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 

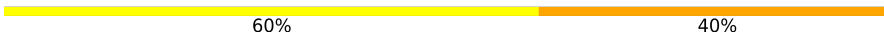


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 



- Molecule 8: 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: 



- Molecule 8: 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: 



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

Chain P: 



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

Chain f:  33% 67%

NAG1
NAG2
BMA3

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

Chain o:  33% 67%

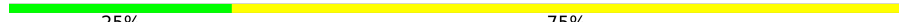
NAG1
NAG2
BMA3

- Molecule 10: 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:  75% 25%

NAG1
NAG2
BMA3
MAN4

- Molecule 10: 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 h:  25% 75%

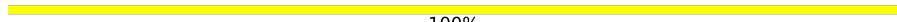
NAG1
NAG2
BMA3
MAN4

- Molecule 10: 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 q:  75% 25%

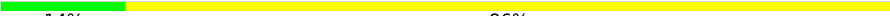
NAG1
NAG2
BMA3
MAN4

- Molecule 11: 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 Z:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 11: 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 i:  14% 86%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 11: 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 r:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

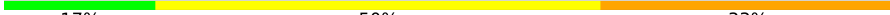
NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  17% 67% 17%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  17% 50% 33%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

NAG1
NAG2

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

MAG1
MAG2

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  100%

MAG1
MAG2

- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 d:  88% 12%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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:  12% 62% 25%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 v:  88% 12%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	361.81Å 215.85Å 176.61Å 90.00° 114.03° 90.00°	Depositor
Resolution (Å)	39.71 – 7.00 39.71 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.71-7.00) 99.3 (39.71-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 7.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.301 , 0.363 0.299 , 0.359	Depositor DCC
R_{free} test set	978 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	277.9	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 777.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	41285	wwPDB-VP
Average B, all atoms (Å ²)	458.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: BMA, NAG, MAN, PCA

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	F	0.17	0/3608	0.57	2/4898 (0.0%)
1	G	0.19	0/3608	0.58	2/4898 (0.0%)
1	Q	0.17	0/3608	0.56	2/4898 (0.0%)
2	D	0.12	0/1800	0.41	0/2439
2	O	0.12	0/1799	0.40	0/2436
2	W	0.13	0/1800	0.42	0/2439
3	A	0.15	0/1019	0.49	0/1382
3	J	0.15	0/1019	0.51	0/1382
3	R	0.16	0/1019	0.48	0/1382
4	B	0.24	0/1632	0.56	2/2236 (0.1%)
4	K	0.18	0/1632	0.55	1/2236 (0.0%)
4	S	0.17	0/1632	0.47	0/2236
5	C	0.31	1/1789 (0.1%)	0.66	4/2443 (0.2%)
5	L	0.18	0/1789	0.50	1/2443 (0.0%)
5	T	0.13	0/1789	0.46	0/2443
6	H	0.14	0/1880	0.47	0/2560
6	M	0.15	0/1880	0.46	0/2560
6	U	0.13	0/1880	0.45	0/2560
7	I	0.15	0/1617	0.46	0/2211
7	N	0.14	0/1659	0.46	0/2269
7	V	0.14	0/1659	0.45	0/2269
All	All	0.17	1/40118 (0.0%)	0.51	14/54620 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	145	PRO	C-N	-5.68	1.25	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	113	SER	N-CA-C	8.56	120.69	111.36
5	C	114	THR	CA-C-N	6.63	130.13	120.71
5	C	114	THR	C-N-CA	6.63	130.13	120.71
5	C	114	THR	N-CA-C	6.43	117.92	108.14
1	F	196	CYS	CA-C-N	5.49	132.01	121.54

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	F	3535	0	3468	98	0
1	G	3535	0	3468	96	0
1	Q	3535	0	3468	90	0
2	D	1761	0	1682	26	0
2	O	1753	0	1675	34	0
2	W	1761	0	1682	31	0
3	A	1001	0	975	24	0
3	J	1001	0	975	21	0
3	R	1001	0	975	27	0
4	B	1589	0	1530	31	0
4	K	1589	0	1530	40	0
4	S	1589	0	1530	26	0
5	C	1742	0	1716	39	0
5	L	1742	0	1716	35	0
5	T	1742	0	1716	31	0
6	H	1832	0	1806	40	0
6	M	1832	0	1806	30	0
6	U	1832	0	1806	32	0
7	I	1574	0	1502	21	0
7	N	1615	0	1542	25	0
7	V	1615	0	1542	17	0
8	E	61	0	52	7	0
8	X	61	0	52	0	0
8	c	61	0	52	0	0
8	e	61	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	g	61	0	52	1	0
8	l	61	0	52	0	0
8	n	61	0	52	1	0
8	p	61	0	52	2	0
8	u	61	0	52	0	0
9	P	39	0	34	4	0
9	f	39	0	34	4	0
9	o	39	0	34	3	0
10	Y	50	0	43	0	0
10	h	50	0	43	1	0
10	q	50	0	43	0	0
11	Z	83	0	69	0	0
11	i	83	0	70	0	0
11	r	83	0	70	0	0
12	a	72	0	61	0	0
12	j	72	0	61	1	0
12	s	72	0	61	1	0
13	b	28	0	25	1	0
13	k	28	0	25	0	0
13	t	28	0	25	0	0
14	d	94	0	79	2	0
14	m	94	0	79	2	0
14	v	94	0	77	4	0
15	A	42	0	39	1	0
15	F	112	0	104	11	0
15	G	112	0	104	10	0
15	J	42	0	39	2	0
15	Q	112	0	104	10	0
15	R	42	0	39	2	0
All	All	41285	0	39940	740	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 740 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:K:14:ALA:HB2	4:K:107:LEU:HD22	1.23	1.18
4:K:14:ALA:CB	4:K:107:LEU:HD22	1.78	1.11
4:K:14:ALA:HA	4:K:107:LEU:HB2	1.32	1.04
5:C:114:THR:HG21	5:C:145:PRO:HD3	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:SER:HB3	15:F:653:NAG:H82	1.50	0.91

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	F	443/471 (94%)	392 (88%)	43 (10%)	8 (2%)	6	34
1	G	443/471 (94%)	392 (88%)	43 (10%)	8 (2%)	6	34
1	Q	443/471 (94%)	391 (88%)	44 (10%)	8 (2%)	6	34
2	D	219/250 (88%)	209 (95%)	8 (4%)	2 (1%)	14	51
2	O	218/250 (87%)	208 (95%)	9 (4%)	1 (0%)	24	63
2	W	219/250 (88%)	209 (95%)	8 (4%)	2 (1%)	14	51
3	A	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	7	38
3	J	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	7	38
3	R	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	7	38
4	B	208/210 (99%)	193 (93%)	13 (6%)	2 (1%)	12	48
4	K	208/210 (99%)	193 (93%)	13 (6%)	2 (1%)	12	48
4	S	208/210 (99%)	192 (92%)	15 (7%)	1 (0%)	24	63
5	C	224/232 (97%)	210 (94%)	10 (4%)	4 (2%)	6	34
5	L	224/232 (97%)	210 (94%)	11 (5%)	3 (1%)	9	42
5	T	224/232 (97%)	210 (94%)	13 (6%)	1 (0%)	30	67
6	H	240/242 (99%)	227 (95%)	13 (5%)	0	100	100
6	M	240/242 (99%)	228 (95%)	12 (5%)	0	100	100
6	U	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	30	67
7	I	203/213 (95%)	188 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
7	V	211/213 (99%)	196 (93%)	15 (7%)	0	100	100
All	All	4992/5295 (94%)	4592 (92%)	351 (7%)	49 (1%)	12	48

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	138	ILE
1	G	197	ASN
1	F	138	ILE
1	F	197	ASN
1	Q	138	ILE

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	F	400/419 (96%)	389 (97%)	11 (3%)	38	59
1	G	400/419 (96%)	389 (97%)	11 (3%)	38	59
1	Q	400/419 (96%)	389 (97%)	11 (3%)	38	59
2	D	184/198 (93%)	179 (97%)	5 (3%)	39	61
2	O	184/198 (93%)	178 (97%)	6 (3%)	33	55
2	W	184/198 (93%)	178 (97%)	6 (3%)	33	55
3	A	108/127 (85%)	104 (96%)	4 (4%)	30	51
3	J	108/127 (85%)	105 (97%)	3 (3%)	38	59
3	R	108/127 (85%)	104 (96%)	4 (4%)	30	51
4	B	178/178 (100%)	176 (99%)	2 (1%)	65	76
4	K	178/178 (100%)	174 (98%)	4 (2%)	45	64
4	S	178/178 (100%)	176 (99%)	2 (1%)	65	76
5	C	198/202 (98%)	195 (98%)	3 (2%)	57	72
5	L	198/202 (98%)	195 (98%)	3 (2%)	57	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	198/202 (98%)	196 (99%)	2 (1%)	68	78
6	H	205/205 (100%)	205 (100%)	0	100	100
6	M	205/205 (100%)	205 (100%)	0	100	100
6	U	205/205 (100%)	205 (100%)	0	100	100
7	I	182/186 (98%)	181 (100%)	1 (0%)	81	83
7	N	186/186 (100%)	185 (100%)	1 (0%)	81	83
7	V	186/186 (100%)	185 (100%)	1 (0%)	81	83
All	All	4373/4545 (96%)	4293 (98%)	80 (2%)	51	68

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	114	THR
3	R	536	THR
7	I	96	CYS
4	K	111	LYS
4	S	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	616	ASN
6	U	105	GLN
4	S	37	GLN
5	T	153	ASN
3	A	616	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
2	PCA	W	1	2	7,8,9	1.93	1 (14%)	9,10,12	2.18	5 (55%)
2	PCA	D	1	2	7,8,9	1.93	1 (14%)	9,10,12	2.15	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
2	PCA	W	1	2	-	0/0/11/13	0/1/1/1
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	PCA	CD-N	4.99	1.46	1.34
2	W	1	PCA	CD-N	4.98	1.46	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	1	PCA	OE-CD-CG	-3.00	121.37	126.72
2	D	1	PCA	OE-CD-CG	-3.00	121.37	126.72
2	W	1	PCA	CA-N-CD	-2.87	103.74	113.58
2	D	1	PCA	CA-N-CD	-2.84	103.87	113.58
2	W	1	PCA	CB-CA-N	2.70	110.68	103.24

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 ⓘ

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
8	NAG	E	1	8,1	14,14,15	1.88	2 (14%)	17,19,21	1.46	3 (17%)
8	NAG	E	2	8	14,14,15	2.22	2 (14%)	17,19,21	1.83	3 (17%)
8	BMA	E	3	8	11,11,12	2.76	6 (54%)	15,15,17	2.01	5 (33%)
8	MAN	E	4	8	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
8	MAN	E	5	8	11,11,12	1.66	3 (27%)	15,15,17	2.96	9 (60%)
9	NAG	P	1	9,1	14,14,15	0.96	1 (7%)	17,19,21	0.78	1 (5%)
9	NAG	P	2	9	14,14,15	0.99	1 (7%)	17,19,21	0.65	0
9	BMA	P	3	9	11,11,12	0.72	0	15,15,17	0.74	0
8	NAG	X	1	8,1	14,14,15	2.08	2 (14%)	17,19,21	1.77	3 (17%)
8	NAG	X	2	8	14,14,15	0.68	1 (7%)	17,19,21	0.54	0
8	BMA	X	3	8	11,11,12	0.59	0	15,15,17	0.75	0
8	MAN	X	4	8	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
8	MAN	X	5	8	11,11,12	0.69	0	15,15,17	0.94	2 (13%)
10	NAG	Y	1	10,1	14,14,15	0.37	0	17,19,21	0.60	0
10	NAG	Y	2	10	14,14,15	0.39	0	17,19,21	0.43	0
10	BMA	Y	3	10	11,11,12	0.62	0	15,15,17	0.70	0
10	MAN	Y	4	10	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
11	NAG	Z	1	1,11	14,14,15	1.86	2 (14%)	17,19,21	1.56	3 (17%)
11	NAG	Z	2	11	14,14,15	2.19	2 (14%)	17,19,21	1.88	4 (23%)
11	BMA	Z	3	11	11,11,12	2.40	5 (45%)	15,15,17	2.18	4 (26%)
11	MAN	Z	4	11	11,11,12	1.45	1 (9%)	15,15,17	2.84	7 (46%)
11	MAN	Z	5	11	11,11,12	1.46	2 (18%)	15,15,17	2.64	6 (40%)
11	MAN	Z	6	11	11,11,12	1.34	2 (18%)	15,15,17	3.08	8 (53%)
11	MAN	Z	7	11	11,11,12	2.35	2 (18%)	15,15,17	3.30	6 (40%)
12	NAG	a	1	12,1	14,14,15	0.65	1 (7%)	17,19,21	0.45	0
12	NAG	a	2	12	14,14,15	1.81	2 (14%)	17,19,21	1.74	3 (17%)
12	BMA	a	3	12	11,11,12	1.47	3 (27%)	15,15,17	1.13	2 (13%)
12	MAN	a	4	12	11,11,12	1.51	3 (27%)	15,15,17	1.80	2 (13%)
12	MAN	a	5	12	11,11,12	1.34	2 (18%)	15,15,17	1.31	3 (20%)
12	MAN	a	6	12	11,11,12	1.17	1 (9%)	15,15,17	1.75	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	b	1	13,1	14,14,15	0.22	0	17,19,21	0.48	0
13	NAG	b	2	13	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	c	1	8,1	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	c	2	8	14,14,15	0.20	0	17,19,21	0.48	0
8	BMA	c	3	8	11,11,12	0.49	0	15,15,17	0.70	0
8	MAN	c	4	8	11,11,12	0.63	0	15,15,17	1.04	2 (13%)
8	MAN	c	5	8	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
14	NAG	d	1	14,1	14,14,15	0.42	0	17,19,21	1.55	2 (11%)
14	NAG	d	2	14	14,14,15	0.22	0	17,19,21	0.47	0
14	BMA	d	3	14	11,11,12	0.96	1 (9%)	15,15,17	0.94	1 (6%)
14	MAN	d	4	14	11,11,12	1.06	0	15,15,17	2.27	5 (33%)
14	MAN	d	5	14	11,11,12	0.76	0	15,15,17	1.15	2 (13%)
14	MAN	d	6	14	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
14	MAN	d	7	14	11,11,12	0.75	0	15,15,17	1.23	2 (13%)
14	MAN	d	8	14	11,11,12	0.74	0	15,15,17	1.08	2 (13%)
8	NAG	e	1	8,1	14,14,15	2.64	2 (14%)	17,19,21	1.43	3 (17%)
8	NAG	e	2	8	14,14,15	1.72	2 (14%)	17,19,21	2.13	2 (11%)
8	BMA	e	3	8	11,11,12	2.12	5 (45%)	15,15,17	1.92	5 (33%)
8	MAN	e	4	8	11,11,12	1.19	1 (9%)	15,15,17	1.54	3 (20%)
8	MAN	e	5	8	11,11,12	1.56	4 (36%)	15,15,17	2.17	6 (40%)
9	NAG	f	1	9,1	14,14,15	0.98	1 (7%)	17,19,21	0.77	1 (5%)
9	NAG	f	2	9	14,14,15	1.02	1 (7%)	17,19,21	0.67	0
9	BMA	f	3	9	11,11,12	0.73	0	15,15,17	0.75	0
8	NAG	g	1	8,1	14,14,15	2.06	2 (14%)	17,19,21	1.62	3 (17%)
8	NAG	g	2	8	14,14,15	0.66	1 (7%)	17,19,21	0.56	0
8	BMA	g	3	8	11,11,12	0.59	0	15,15,17	0.73	0
8	MAN	g	4	8	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
8	MAN	g	5	8	11,11,12	0.66	0	15,15,17	0.94	2 (13%)
10	NAG	h	1	10,1	14,14,15	0.67	1 (7%)	17,19,21	0.80	0
10	NAG	h	2	10	14,14,15	0.22	0	17,19,21	0.45	0
10	BMA	h	3	10	11,11,12	0.61	0	15,15,17	0.74	0
10	MAN	h	4	10	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
11	NAG	i	1	1,11	14,14,15	1.86	2 (14%)	17,19,21	1.66	3 (17%)
11	NAG	i	2	11	14,14,15	2.27	2 (14%)	17,19,21	1.88	4 (23%)
11	BMA	i	3	11	11,11,12	0.22	0	15,15,17	0.61	0
11	MAN	i	4	11	11,11,12	0.87	1 (9%)	15,15,17	1.58	1 (6%)
11	MAN	i	5	11	11,11,12	1.46	2 (18%)	15,15,17	2.59	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	i	6	11	11,11,12	1.40	2 (18%)	15,15,17	2.83	7 (46%)
11	MAN	i	7	11	11,11,12	1.03	1 (9%)	15,15,17	2.49	5 (33%)
12	NAG	j	1	12,1	14,14,15	0.16	0	17,19,21	0.58	0
12	NAG	j	2	12	14,14,15	1.17	1 (7%)	17,19,21	1.94	5 (29%)
12	BMA	j	3	12	11,11,12	1.66	3 (27%)	15,15,17	1.22	2 (13%)
12	MAN	j	4	12	11,11,12	1.50	3 (27%)	15,15,17	1.87	2 (13%)
12	MAN	j	5	12	11,11,12	1.27	1 (9%)	15,15,17	1.35	3 (20%)
12	MAN	j	6	12	11,11,12	1.21	2 (18%)	15,15,17	1.81	2 (13%)
13	NAG	k	1	13,1	14,14,15	0.19	0	17,19,21	0.49	0
13	NAG	k	2	13	14,14,15	0.26	0	17,19,21	0.44	0
8	NAG	l	1	8,1	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	l	2	8	14,14,15	0.21	0	17,19,21	0.47	0
8	BMA	l	3	8	11,11,12	0.50	0	15,15,17	0.68	0
8	MAN	l	4	8	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
8	MAN	l	5	8	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
14	NAG	m	1	14,1	14,14,15	0.43	0	17,19,21	1.56	2 (11%)
14	NAG	m	2	14	14,14,15	0.24	0	17,19,21	0.46	0
14	BMA	m	3	14	11,11,12	0.91	1 (9%)	15,15,17	0.95	1 (6%)
14	MAN	m	4	14	11,11,12	1.08	1 (9%)	15,15,17	2.34	5 (33%)
14	MAN	m	5	14	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
14	MAN	m	6	14	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
14	MAN	m	7	14	11,11,12	0.77	1 (9%)	15,15,17	1.25	2 (13%)
14	MAN	m	8	14	11,11,12	0.75	0	15,15,17	1.06	2 (13%)
8	NAG	n	1	8,1	14,14,15	1.87	2 (14%)	17,19,21	1.47	3 (17%)
8	NAG	n	2	8	14,14,15	2.57	2 (14%)	17,19,21	1.84	4 (23%)
8	BMA	n	3	8	11,11,12	3.26	6 (54%)	15,15,17	1.75	5 (33%)
8	MAN	n	4	8	11,11,12	0.63	0	15,15,17	1.16	2 (13%)
8	MAN	n	5	8	11,11,12	1.75	4 (36%)	15,15,17	2.99	10 (66%)
9	NAG	o	1	9,1	14,14,15	0.89	1 (7%)	17,19,21	0.81	1 (5%)
9	NAG	o	2	9	14,14,15	0.99	1 (7%)	17,19,21	0.66	0
9	BMA	o	3	9	11,11,12	0.73	0	15,15,17	0.75	0
8	NAG	p	1	8,1	14,14,15	2.09	2 (14%)	17,19,21	1.63	3 (17%)
8	NAG	p	2	8	14,14,15	0.64	1 (7%)	17,19,21	0.56	0
8	BMA	p	3	8	11,11,12	0.58	0	15,15,17	0.74	0
8	MAN	p	4	8	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
8	MAN	p	5	8	11,11,12	0.67	0	15,15,17	0.93	2 (13%)
10	NAG	q	1	10,1	14,14,15	0.48	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	q	2	10	14,14,15	0.29	0	17,19,21	0.53	0
10	BMA	q	3	10	11,11,12	0.63	0	15,15,17	0.73	0
10	MAN	q	4	10	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
11	NAG	r	1	1,11	14,14,15	1.88	2 (14%)	17,19,21	1.69	3 (17%)
11	NAG	r	2	11	14,14,15	2.21	2 (14%)	17,19,21	1.87	4 (23%)
11	BMA	r	3	11	11,11,12	2.17	4 (36%)	15,15,17	2.10	3 (20%)
11	MAN	r	4	11	11,11,12	1.89	4 (36%)	15,15,17	2.90	8 (53%)
11	MAN	r	5	11	11,11,12	1.36	2 (18%)	15,15,17	2.57	6 (40%)
11	MAN	r	6	11	11,11,12	2.15	5 (45%)	15,15,17	3.46	8 (53%)
11	MAN	r	7	11	11,11,12	1.86	3 (27%)	15,15,17	1.57	4 (26%)
12	NAG	s	1	12,1	14,14,15	0.37	0	17,19,21	0.49	0
12	NAG	s	2	12	14,14,15	1.72	1 (7%)	17,19,21	1.81	3 (17%)
12	BMA	s	3	12	11,11,12	1.45	3 (27%)	15,15,17	1.07	2 (13%)
12	MAN	s	4	12	11,11,12	2.77	4 (36%)	15,15,17	1.87	5 (33%)
12	MAN	s	5	12	11,11,12	1.41	2 (18%)	15,15,17	2.31	6 (40%)
12	MAN	s	6	12	11,11,12	1.19	1 (9%)	15,15,17	1.73	2 (13%)
13	NAG	t	1	13,1	14,14,15	0.20	0	17,19,21	0.50	0
13	NAG	t	2	13	14,14,15	0.23	0	17,19,21	0.44	0
8	NAG	u	1	8,1	14,14,15	0.27	0	17,19,21	0.43	0
8	NAG	u	2	8	14,14,15	0.22	0	17,19,21	0.47	0
8	BMA	u	3	8	11,11,12	0.52	0	15,15,17	0.70	0
8	MAN	u	4	8	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
8	MAN	u	5	8	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
14	NAG	v	1	14,1	14,14,15	0.57	0	17,19,21	1.55	2 (11%)
14	NAG	v	2	14	14,14,15	0.27	0	17,19,21	0.49	0
14	BMA	v	3	14	11,11,12	0.77	0	15,15,17	1.00	1 (6%)
14	MAN	v	4	14	11,11,12	0.72	1 (9%)	15,15,17	1.21	2 (13%)
14	MAN	v	5	14	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
14	MAN	v	6	14	11,11,12	0.90	0	15,15,17	1.03	1 (6%)
14	MAN	v	7	14	11,11,12	2.36	5 (45%)	15,15,17	3.51	7 (46%)
14	MAN	v	8	14	11,11,12	0.76	1 (9%)	15,15,17	1.08	2 (13%)

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	E	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	E	2	8	-	0/6/23/26	0/1/1/1
8	BMA	E	3	8	-	1/2/19/22	0/1/1/1
8	MAN	E	4	8	-	0/2/19/22	0/1/1/1
8	MAN	E	5	8	-	0/2/19/22	0/1/1/1
9	NAG	P	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	P	2	9	-	0/6/23/26	0/1/1/1
9	BMA	P	3	9	-	1/2/19/22	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	1/2/19/22	0/1/1/1
8	MAN	X	5	8	-	0/2/19/22	0/1/1/1
10	NAG	Y	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	1/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	1/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
11	NAG	Z	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Z	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Z	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	6	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	7	11	-	0/2/19/22	0/1/1/1
12	NAG	a	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	a	2	12	-	1/6/23/26	0/1/1/1
12	BMA	a	3	12	-	0/2/19/22	0/1/1/1
12	MAN	a	4	12	-	2/2/19/22	0/1/1/1
12	MAN	a	5	12	-	2/2/19/22	0/1/1/1
12	MAN	a	6	12	-	1/2/19/22	0/1/1/1
13	NAG	b	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	b	2	13	-	0/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
8	MAN	c	4	8	-	0/2/19/22	0/1/1/1
8	MAN	c	5	8	-	0/2/19/22	0/1/1/1
14	NAG	d	1	14,1	-	6/6/23/26	0/1/1/1
14	NAG	d	2	14	-	2/6/23/26	0/1/1/1
14	BMA	d	3	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	d	4	14	-	2/2/19/22	0/1/1/1
14	MAN	d	5	14	-	2/2/19/22	0/1/1/1
14	MAN	d	6	14	-	0/2/19/22	0/1/1/1
14	MAN	d	7	14	-	0/2/19/22	0/1/1/1
14	MAN	d	8	14	-	0/2/19/22	0/1/1/1
8	NAG	e	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
8	MAN	e	4	8	-	1/2/19/22	0/1/1/1
8	MAN	e	5	8	-	0/2/19/22	0/1/1/1
9	NAG	f	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
9	BMA	f	3	9	-	1/2/19/22	0/1/1/1
8	NAG	g	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	BMA	g	3	8	-	2/2/19/22	0/1/1/1
8	MAN	g	4	8	-	1/2/19/22	0/1/1/1
8	MAN	g	5	8	-	0/2/19/22	0/1/1/1
10	NAG	h	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	h	2	10	-	1/6/23/26	0/1/1/1
10	BMA	h	3	10	-	1/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1
11	NAG	i	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	i	2	11	-	2/6/23/26	0/1/1/1
11	BMA	i	3	11	-	0/2/19/22	0/1/1/1
11	MAN	i	4	11	-	0/2/19/22	0/1/1/1
11	MAN	i	5	11	-	0/2/19/22	0/1/1/1
11	MAN	i	6	11	-	0/2/19/22	0/1/1/1
11	MAN	i	7	11	-	1/2/19/22	0/1/1/1
12	NAG	j	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	j	2	12	-	1/6/23/26	0/1/1/1
12	BMA	j	3	12	-	0/2/19/22	0/1/1/1
12	MAN	j	4	12	-	2/2/19/22	0/1/1/1
12	MAN	j	5	12	-	2/2/19/22	0/1/1/1
12	MAN	j	6	12	-	1/2/19/22	0/1/1/1
13	NAG	k	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	k	2	13	-	0/6/23/26	0/1/1/1
8	NAG	l	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
8	MAN	l	4	8	-	0/2/19/22	0/1/1/1
8	MAN	l	5	8	-	0/2/19/22	0/1/1/1
14	NAG	m	1	14,1	-	5/6/23/26	0/1/1/1
14	NAG	m	2	14	-	1/6/23/26	0/1/1/1
14	BMA	m	3	14	-	0/2/19/22	0/1/1/1
14	MAN	m	4	14	-	2/2/19/22	0/1/1/1
14	MAN	m	5	14	-	2/2/19/22	0/1/1/1
14	MAN	m	6	14	-	0/2/19/22	0/1/1/1
14	MAN	m	7	14	-	0/2/19/22	0/1/1/1
14	MAN	m	8	14	-	0/2/19/22	0/1/1/1
8	NAG	n	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	n	2	8	-	2/6/23/26	0/1/1/1
8	BMA	n	3	8	-	1/2/19/22	0/1/1/1
8	MAN	n	4	8	-	0/2/19/22	0/1/1/1
8	MAN	n	5	8	-	0/2/19/22	0/1/1/1
9	NAG	o	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	o	2	9	-	0/6/23/26	0/1/1/1
9	BMA	o	3	9	-	1/2/19/22	0/1/1/1
8	NAG	p	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	BMA	p	3	8	-	2/2/19/22	0/1/1/1
8	MAN	p	4	8	-	1/2/19/22	0/1/1/1
8	MAN	p	5	8	-	0/2/19/22	0/1/1/1
10	NAG	q	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	2/6/23/26	0/1/1/1
10	BMA	q	3	10	-	1/2/19/22	0/1/1/1
10	MAN	q	4	10	-	0/2/19/22	0/1/1/1
11	NAG	r	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	r	2	11	-	2/6/23/26	0/1/1/1
11	BMA	r	3	11	-	0/2/19/22	0/1/1/1
11	MAN	r	4	11	-	0/2/19/22	0/1/1/1
11	MAN	r	5	11	-	0/2/19/22	0/1/1/1
11	MAN	r	6	11	-	1/2/19/22	0/1/1/1
11	MAN	r	7	11	-	0/2/19/22	0/1/1/1
12	NAG	s	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	s	2	12	-	1/6/23/26	0/1/1/1
12	BMA	s	3	12	-	0/2/19/22	0/1/1/1
12	MAN	s	4	12	-	0/2/19/22	0/1/1/1
12	MAN	s	5	12	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	s	6	12	-	1/2/19/22	0/1/1/1
13	NAG	t	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	t	2	13	-	0/6/23/26	0/1/1/1
8	NAG	u	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	u	2	8	-	0/6/23/26	0/1/1/1
8	BMA	u	3	8	-	0/2/19/22	0/1/1/1
8	MAN	u	4	8	-	0/2/19/22	0/1/1/1
8	MAN	u	5	8	-	0/2/19/22	0/1/1/1
14	NAG	v	1	14,1	-	4/6/23/26	0/1/1/1
14	NAG	v	2	14	-	2/6/23/26	0/1/1/1
14	BMA	v	3	14	-	0/2/19/22	0/1/1/1
14	MAN	v	4	14	-	2/2/19/22	0/1/1/1
14	MAN	v	5	14	-	2/2/19/22	0/1/1/1
14	MAN	v	6	14	-	0/2/19/22	0/1/1/1
14	MAN	v	7	14	-	0/2/19/22	0/1/1/1
14	MAN	v	8	14	-	0/2/19/22	0/1/1/1

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	1	NAG	O5-C1	-9.23	1.28	1.43
8	n	2	NAG	O5-C1	-8.82	1.28	1.43
11	i	2	NAG	O5-C1	-7.77	1.30	1.43
11	r	2	NAG	O5-C1	-7.61	1.30	1.43
11	Z	2	NAG	O5-C1	-7.47	1.31	1.43

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	2	NAG	C1-O5-C5	7.95	122.84	112.19
11	Z	6	MAN	O3-C3-C4	-7.72	92.17	110.38
14	v	7	MAN	C1-O5-C5	7.30	121.97	112.19
14	v	7	MAN	O5-C5-C6	-7.21	93.63	107.66
8	n	5	MAN	O3-C3-C4	-6.71	94.55	110.38

There are no chirality outliers.

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	X	3	BMA	C4-C5-C6-O6
8	g	3	BMA	C4-C5-C6-O6

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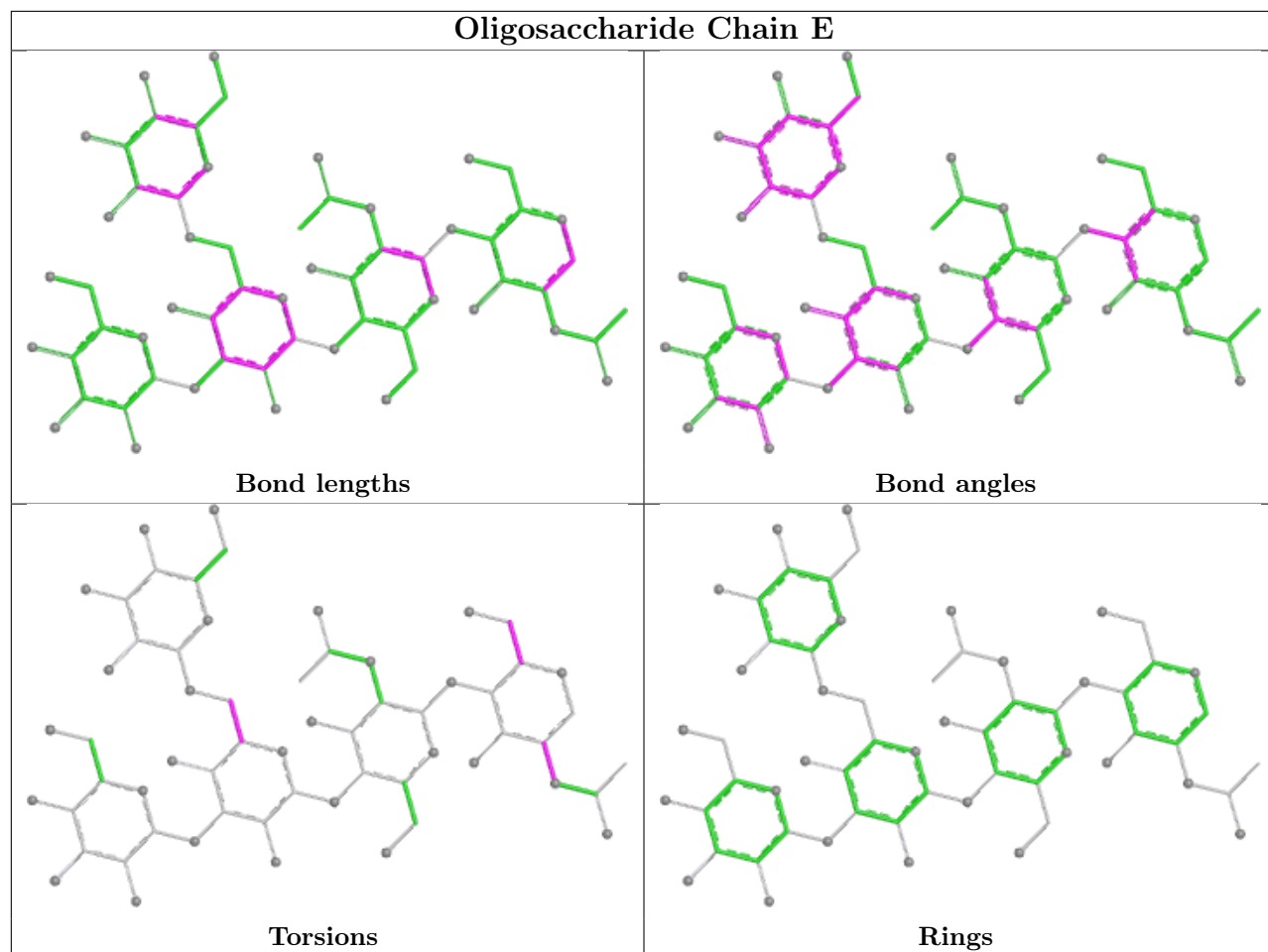
Mol	Chain	Res	Type	Atoms
8	p	3	BMA	C4-C5-C6-O6
12	j	1	NAG	C4-C5-C6-O6
11	i	7	MAN	O5-C5-C6-O6

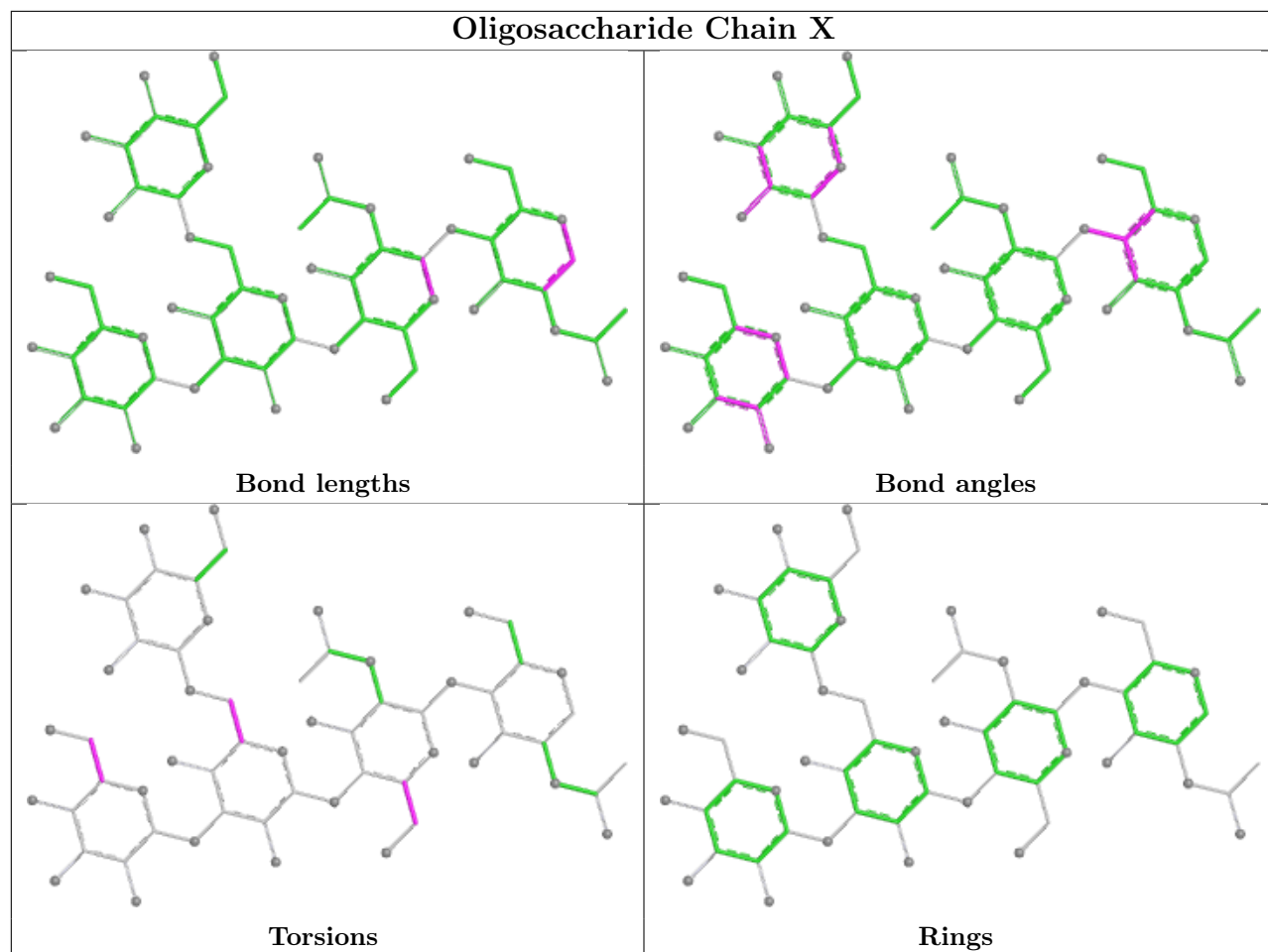
There are no ring outliers.

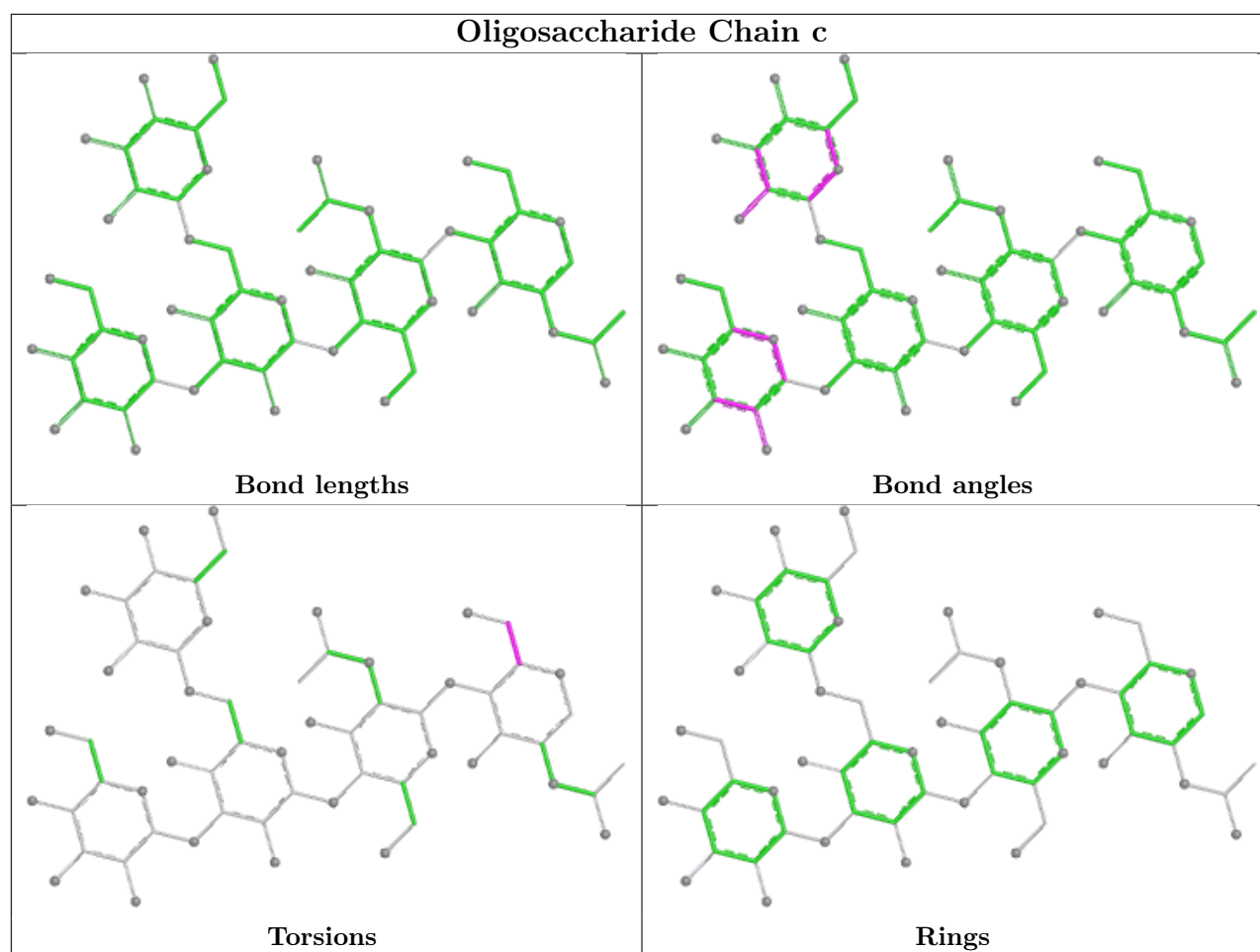
27 monomers are involved in 37 short contacts:

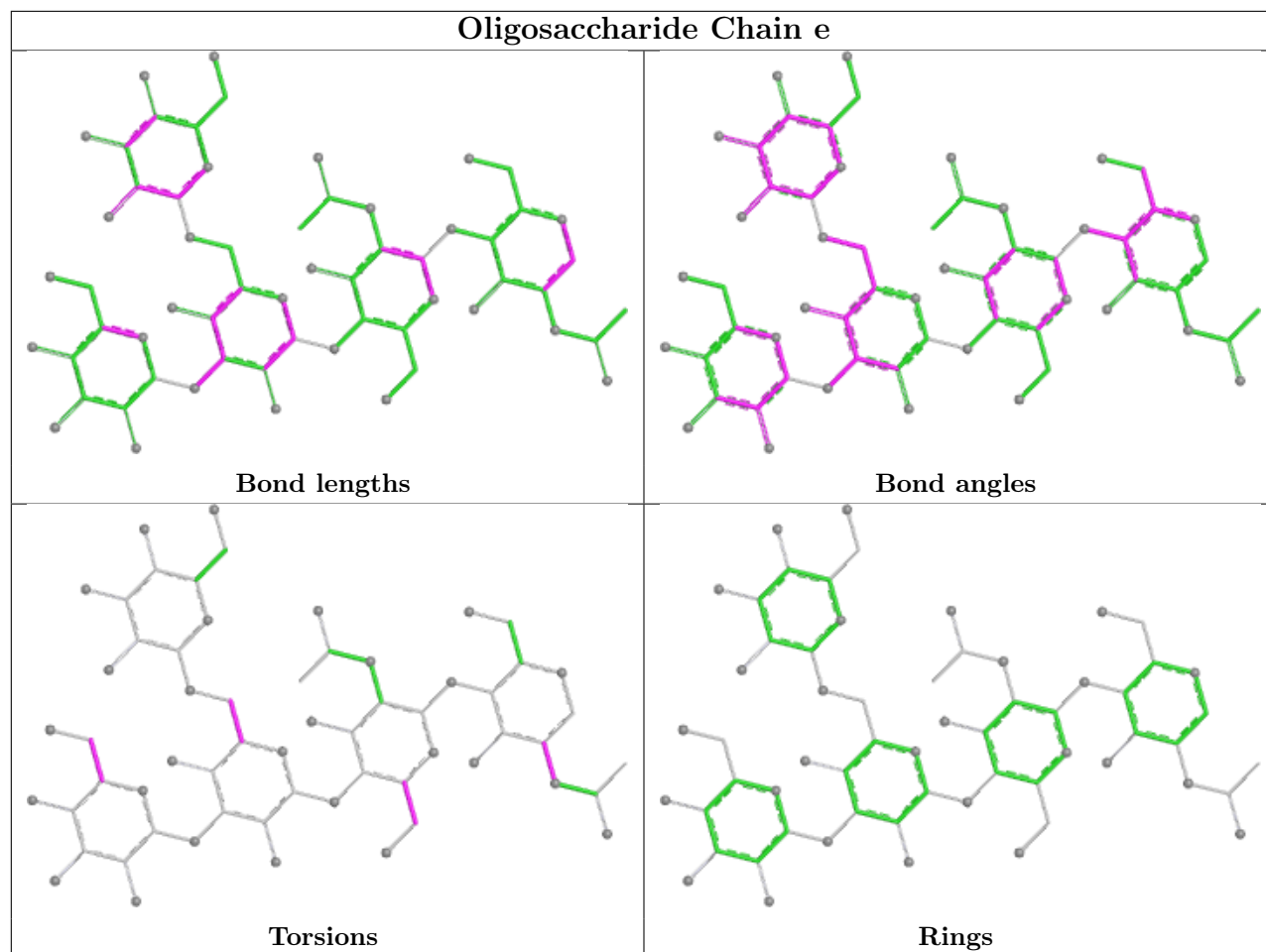
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	e	1	NAG	2	0
8	p	3	BMA	1	0
13	b	2	NAG	1	0
14	v	1	NAG	3	0
9	f	2	NAG	1	0
13	b	1	NAG	1	0
8	E	1	NAG	2	0
9	o	1	NAG	3	0
8	E	2	NAG	5	0
9	P	2	NAG	2	0
14	d	2	NAG	1	0
14	m	5	MAN	1	0
8	p	1	NAG	1	0
12	s	4	MAN	1	0
14	d	1	NAG	1	0
12	j	5	MAN	1	0
10	h	2	NAG	1	0
9	o	2	NAG	1	0
9	f	1	NAG	4	0
8	e	2	NAG	3	0
8	g	1	NAG	1	0
14	v	2	NAG	3	0
9	P	1	NAG	3	0
8	n	2	NAG	1	0
12	s	5	MAN	1	0
8	p	5	MAN	1	0
14	m	1	NAG	1	0

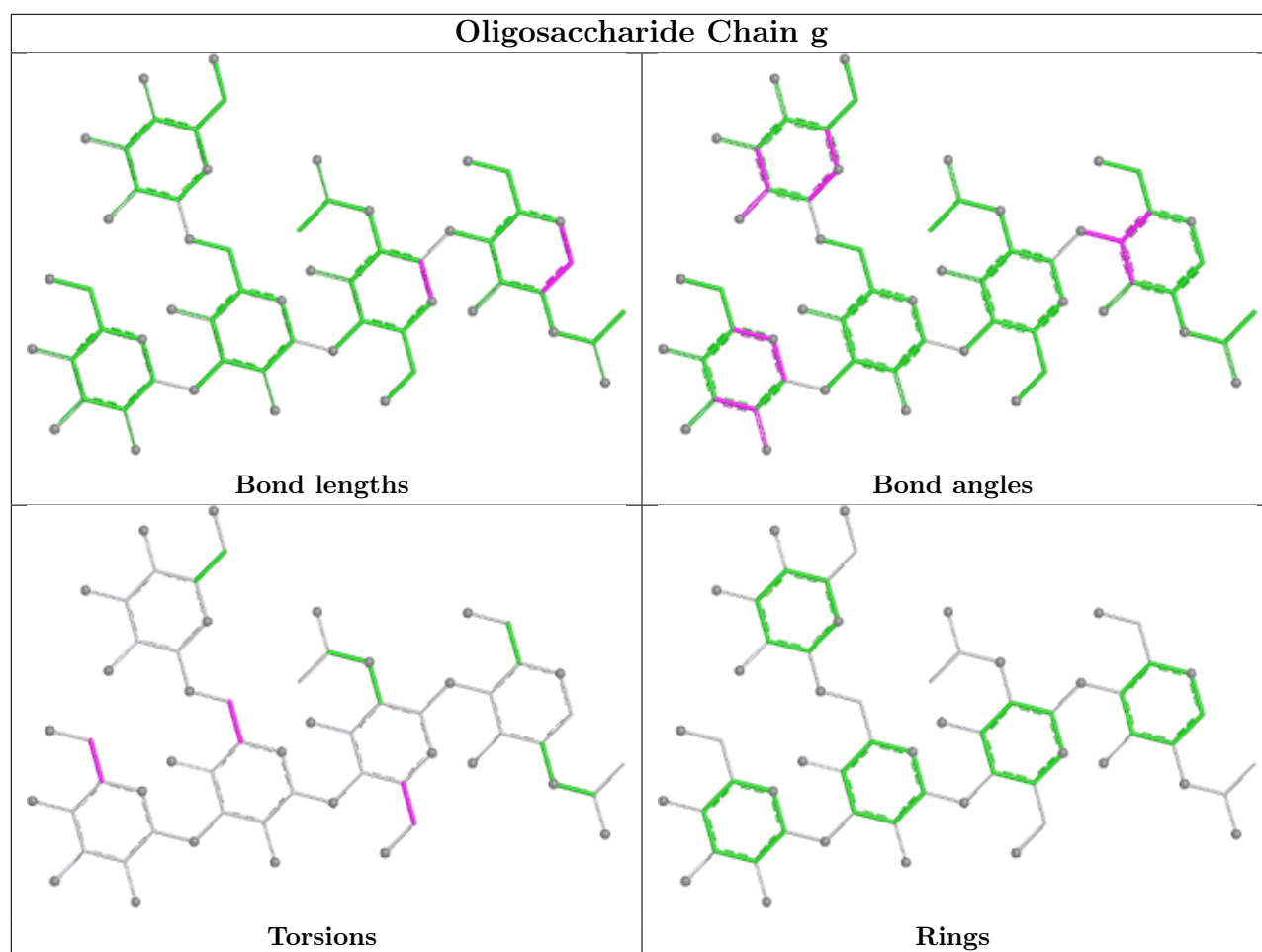
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

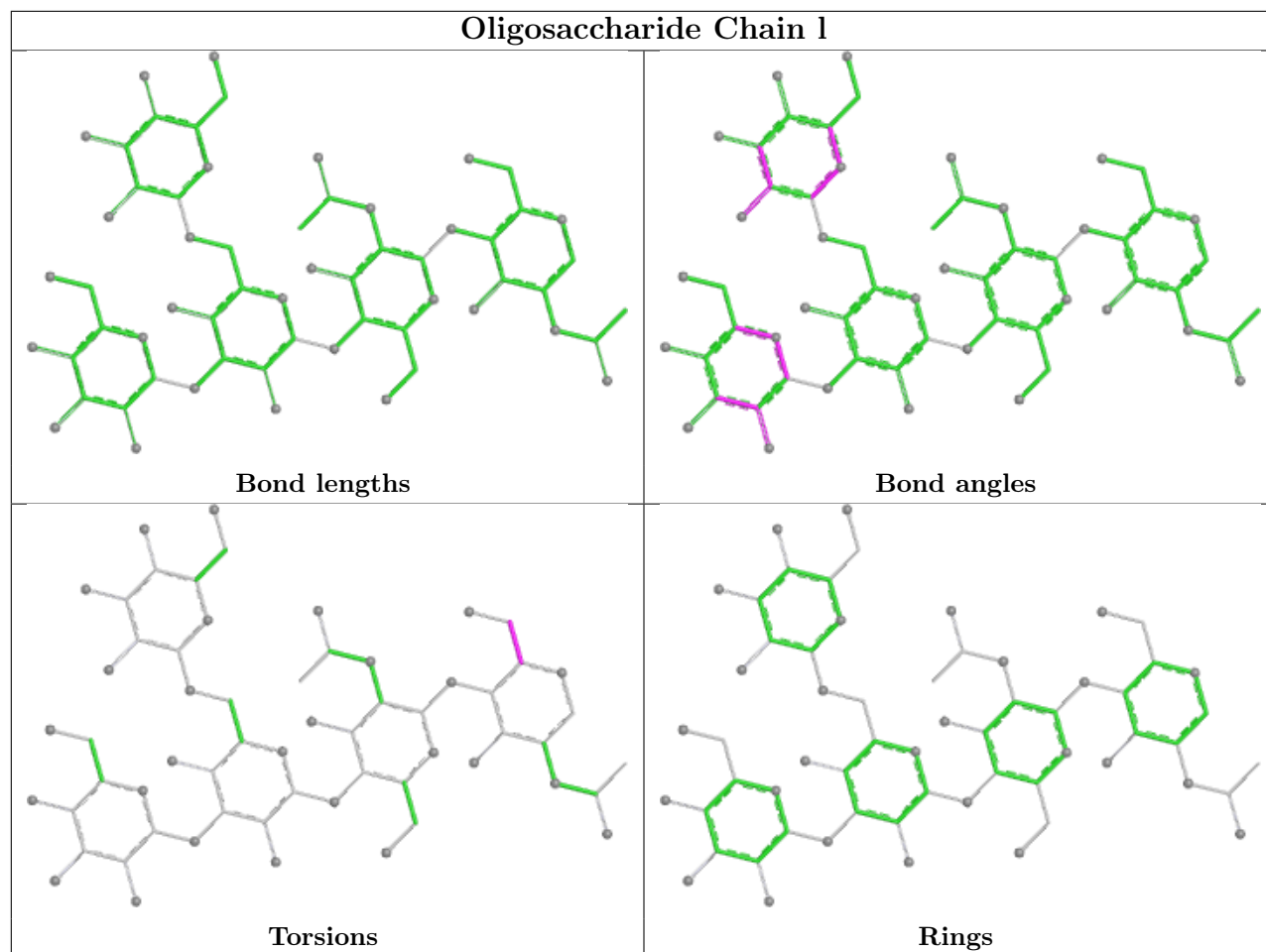


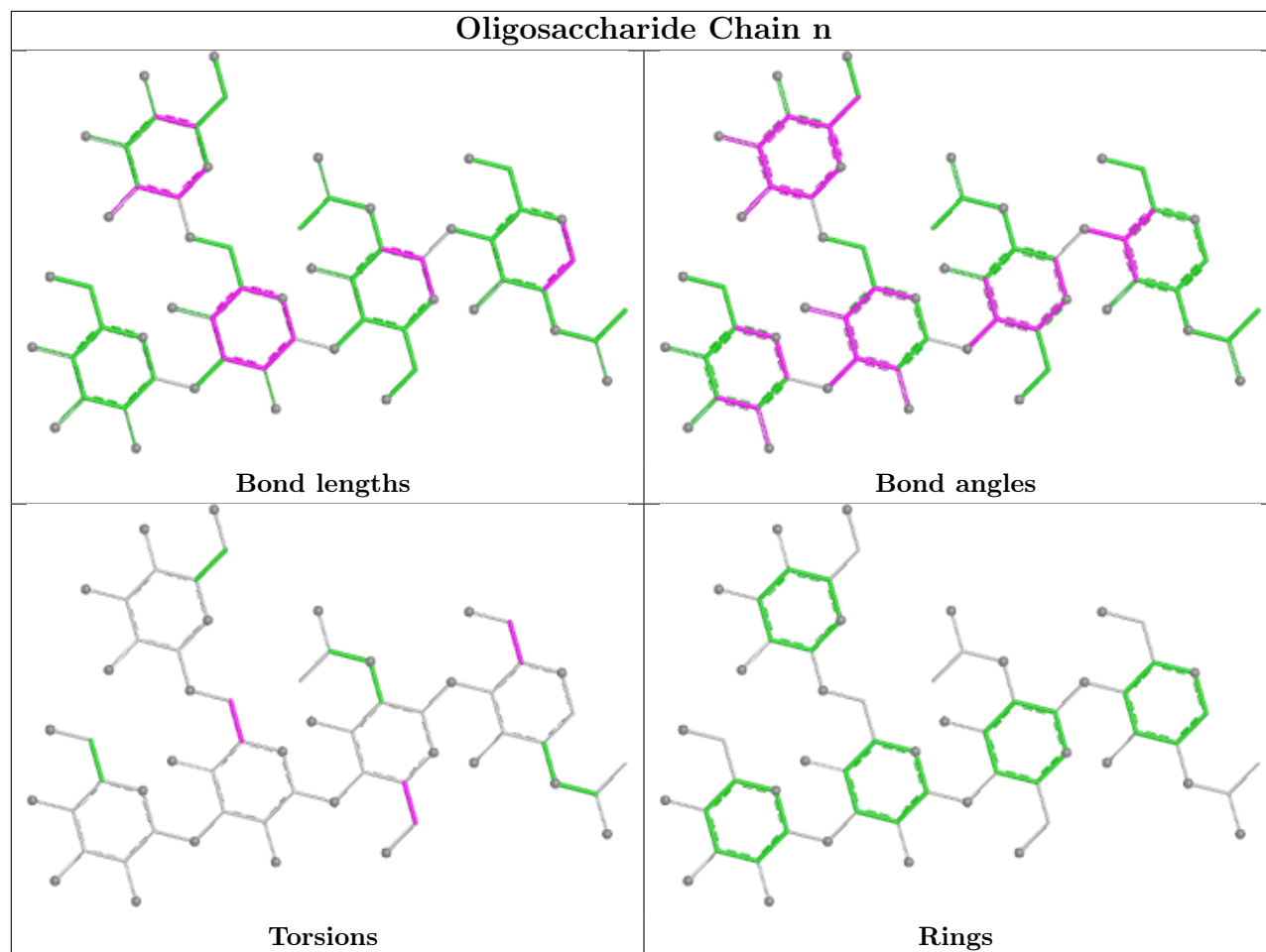


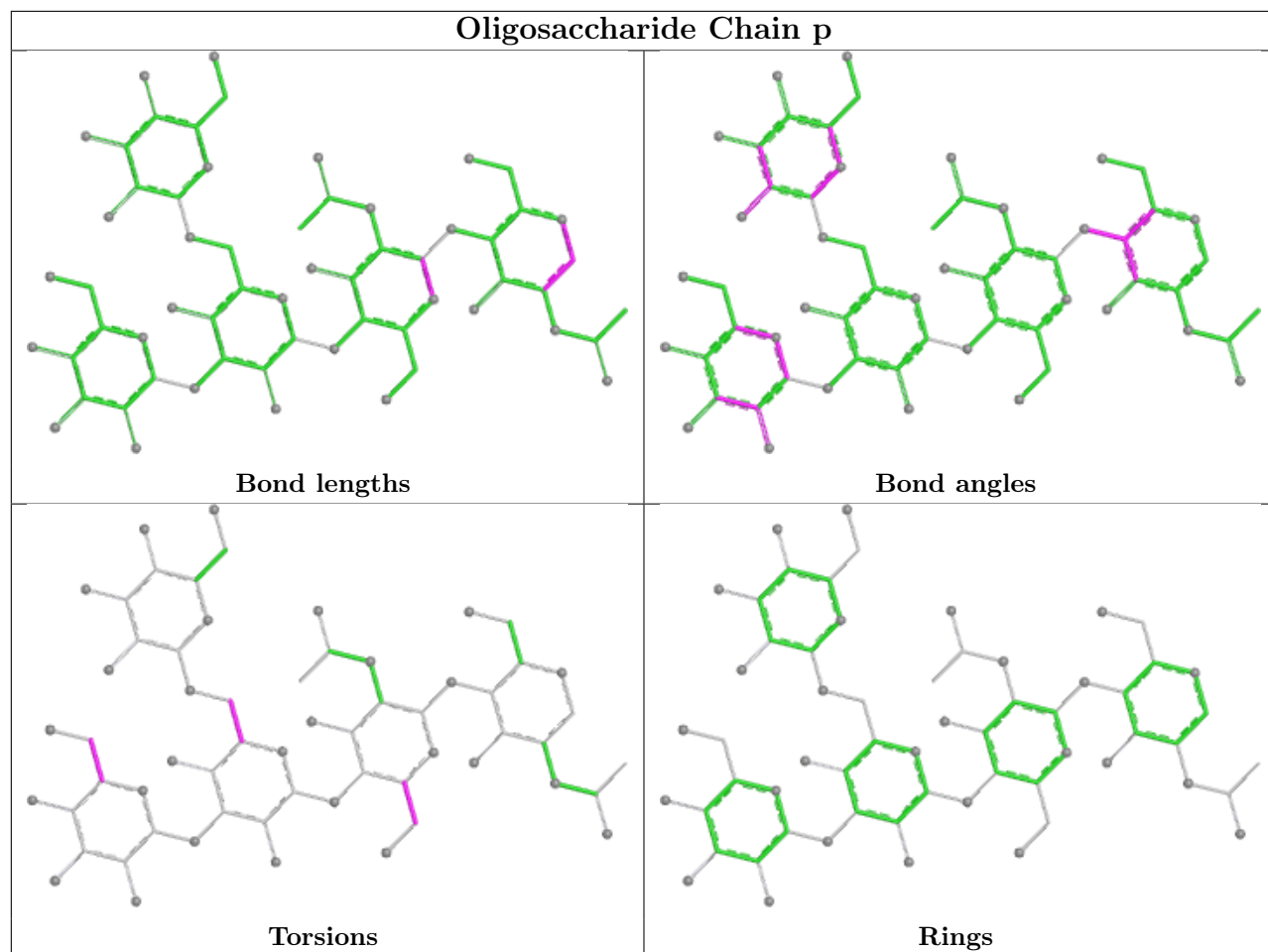


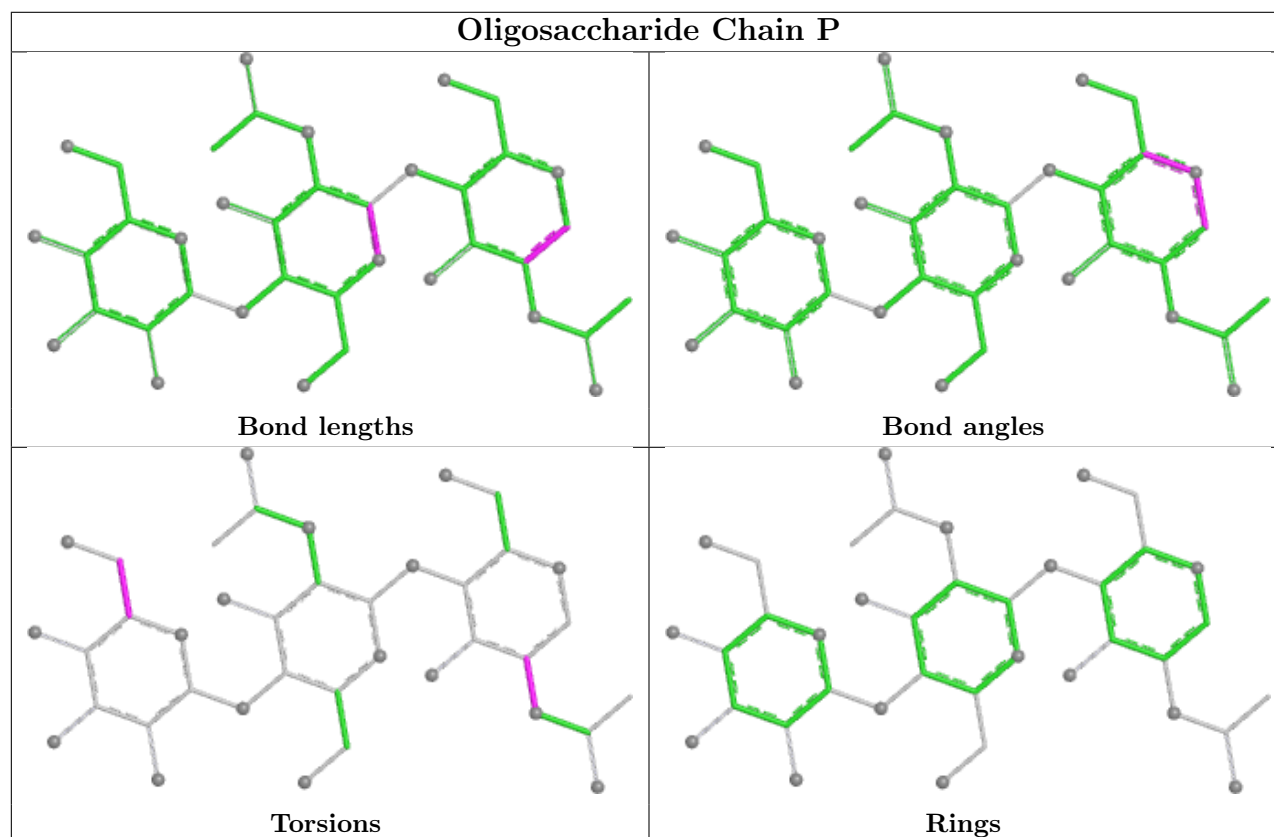
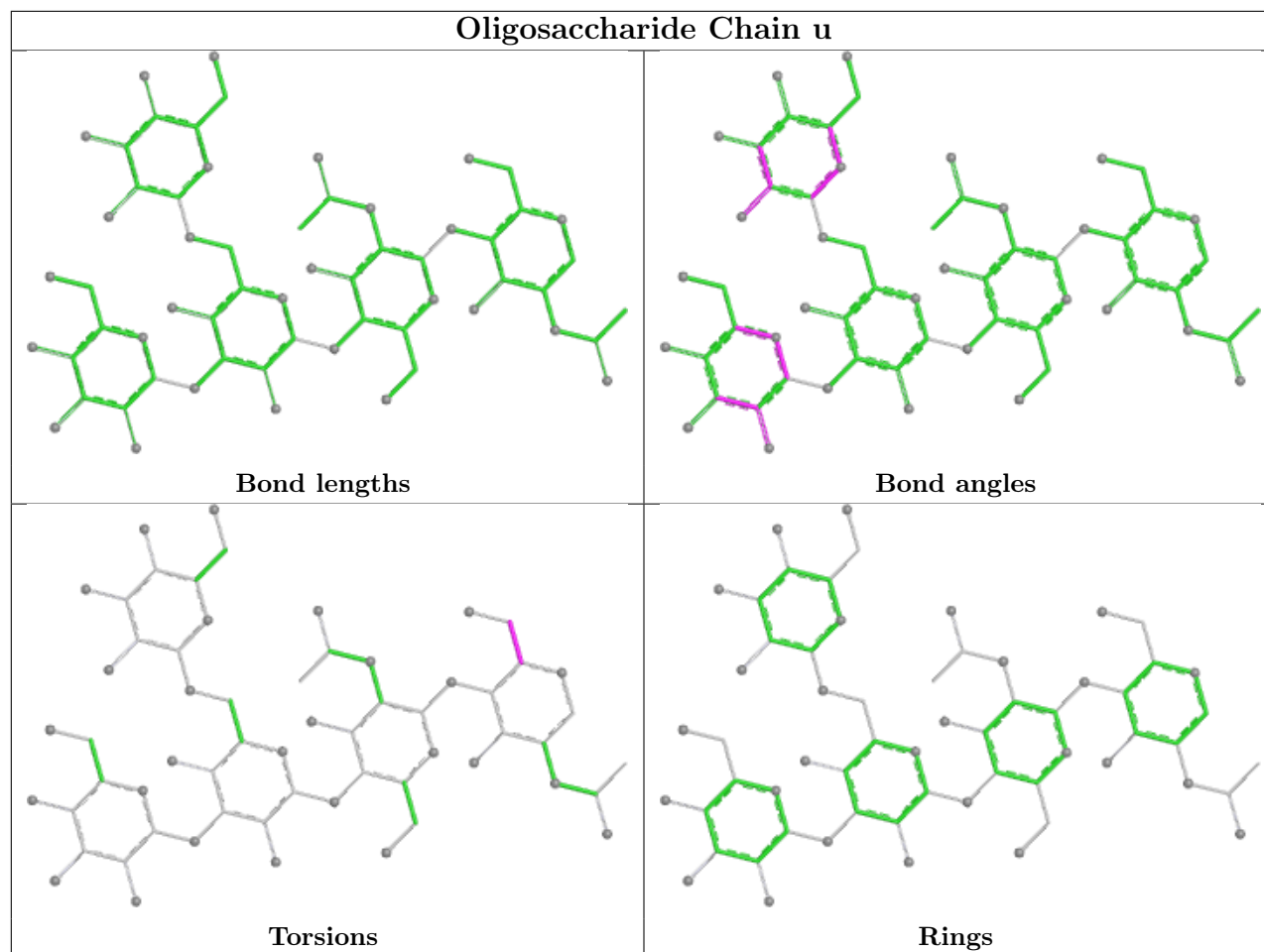


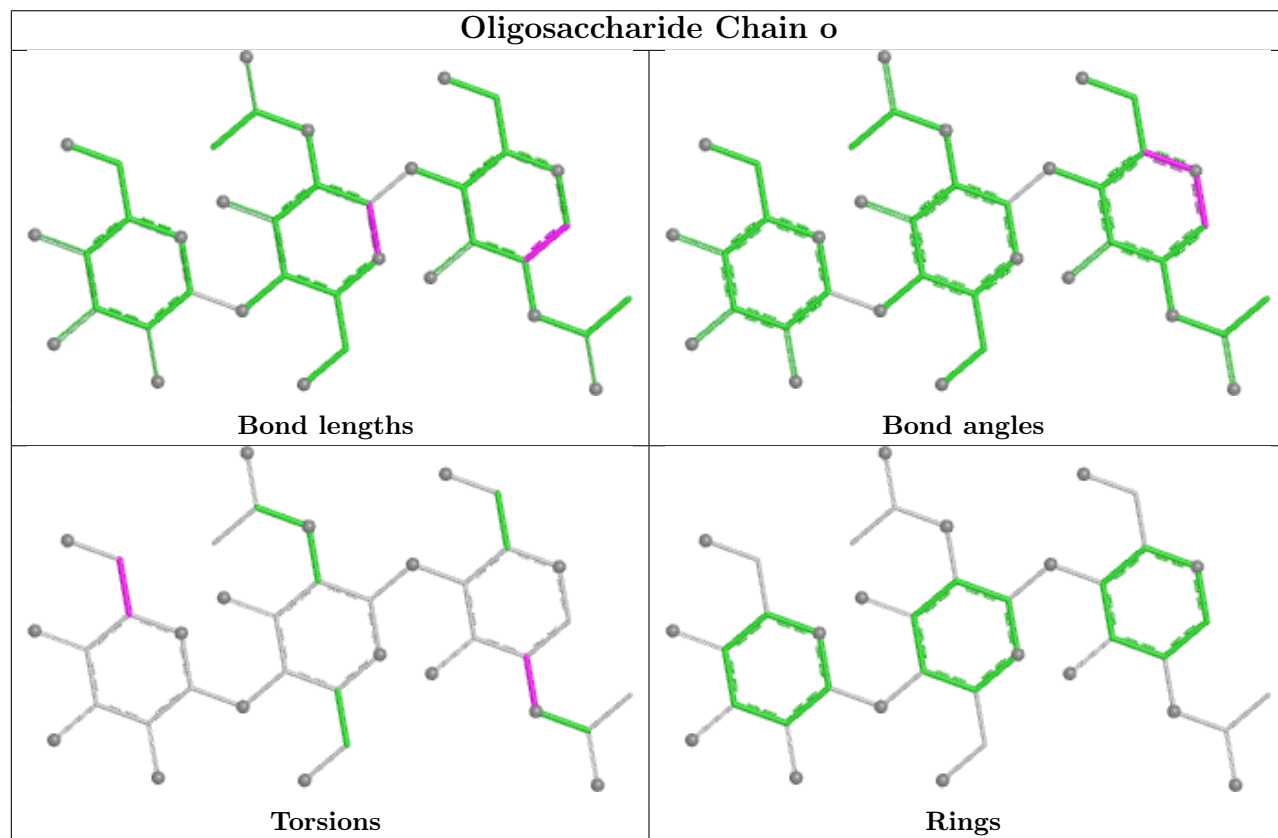
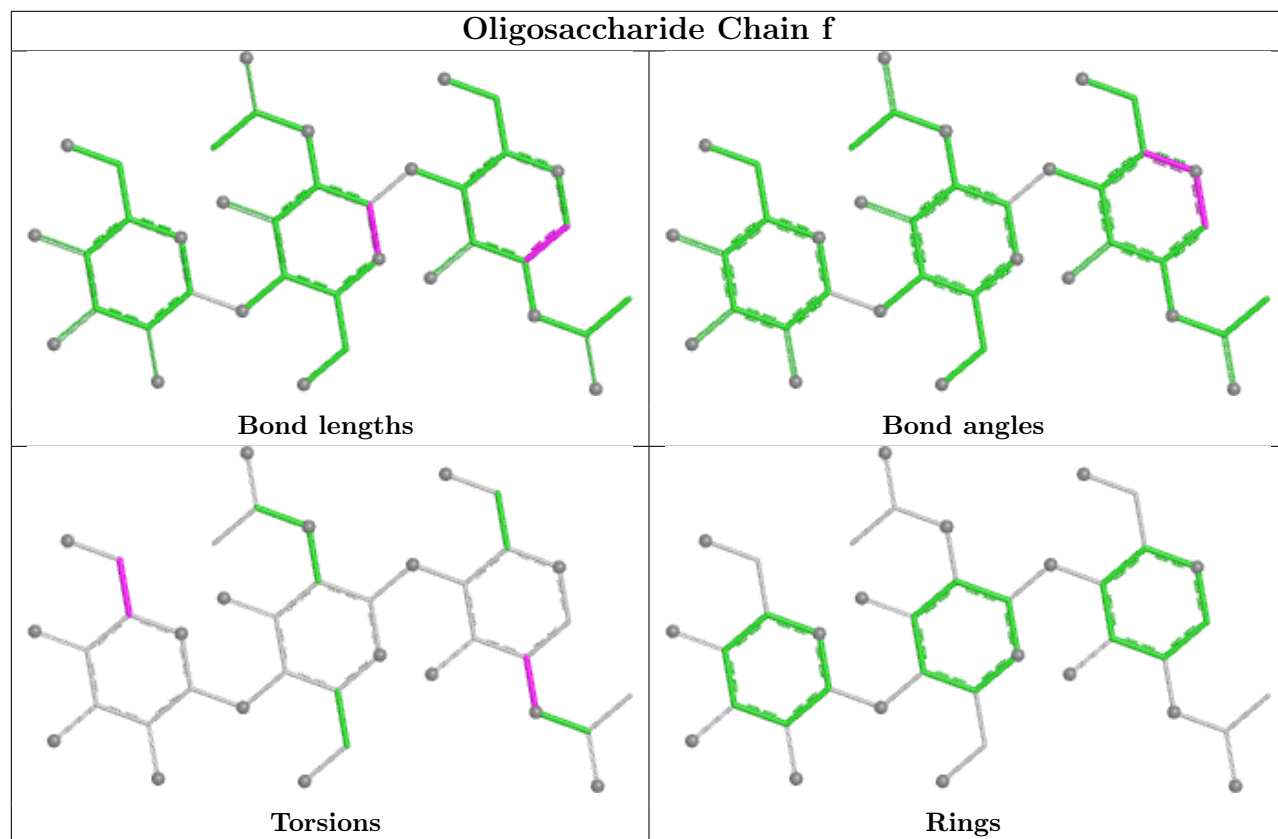


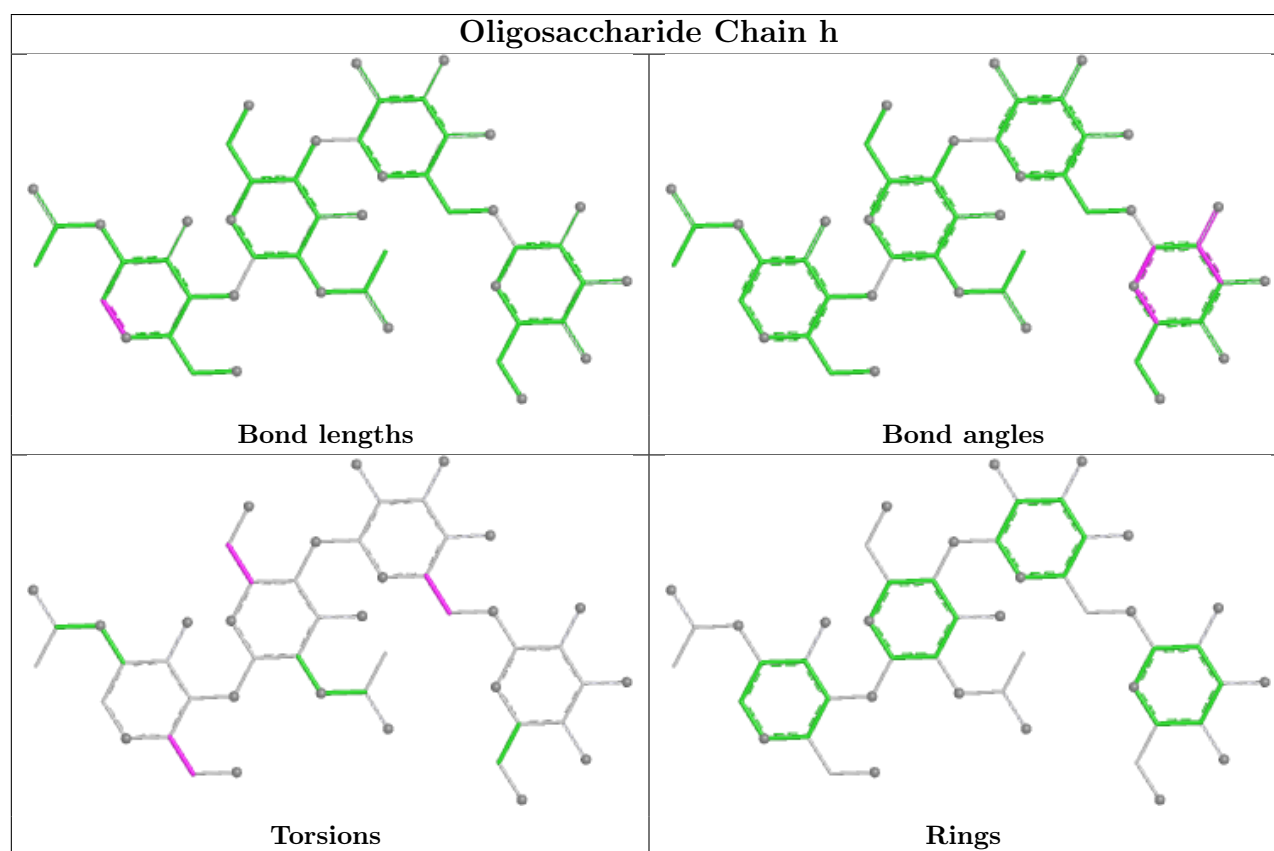
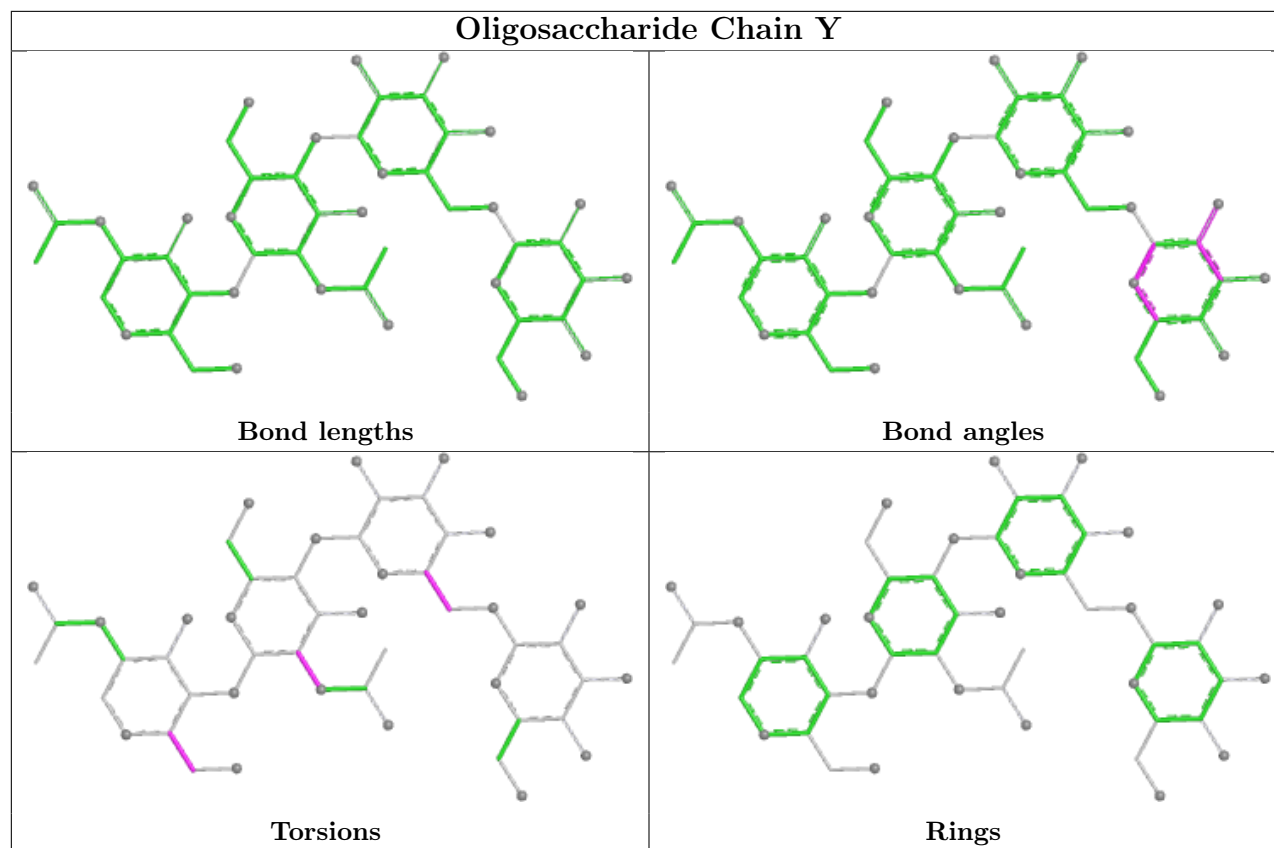


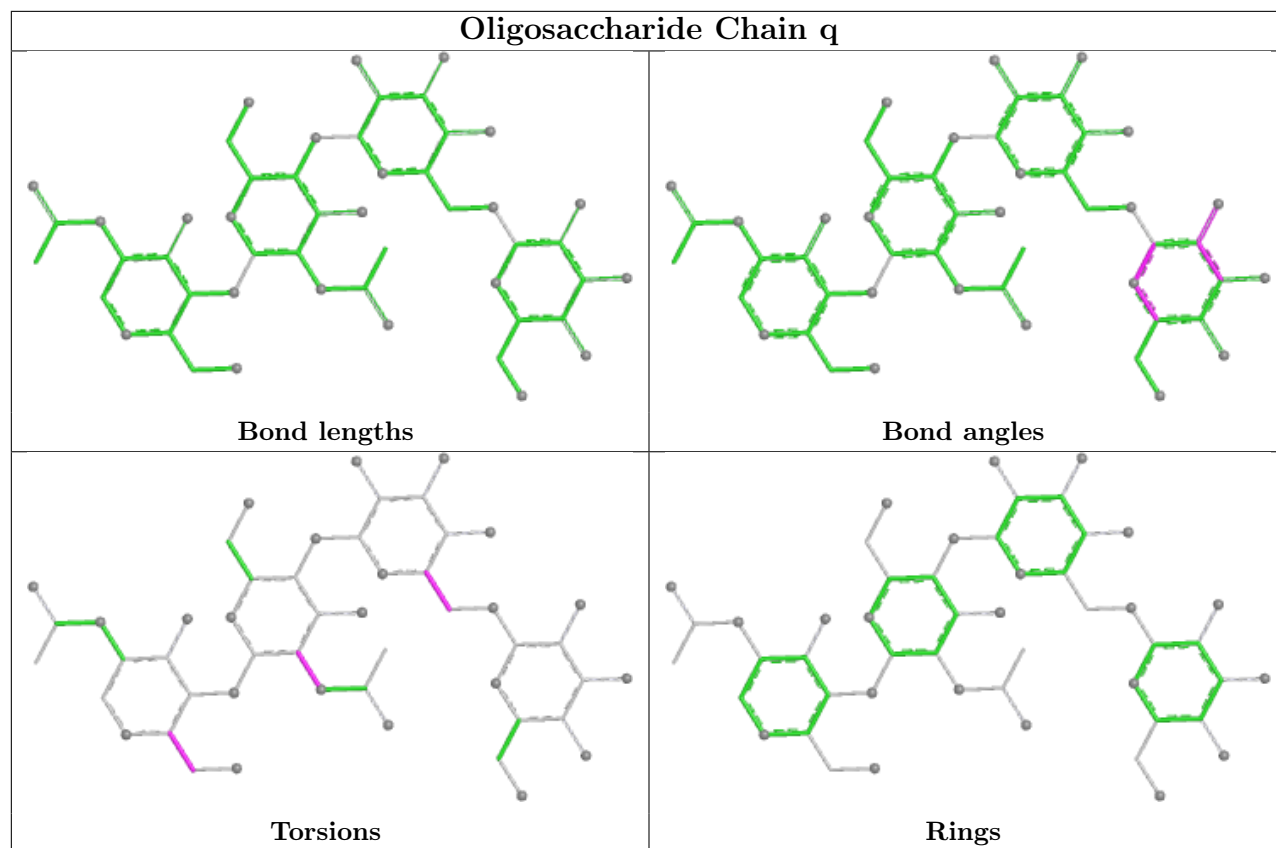


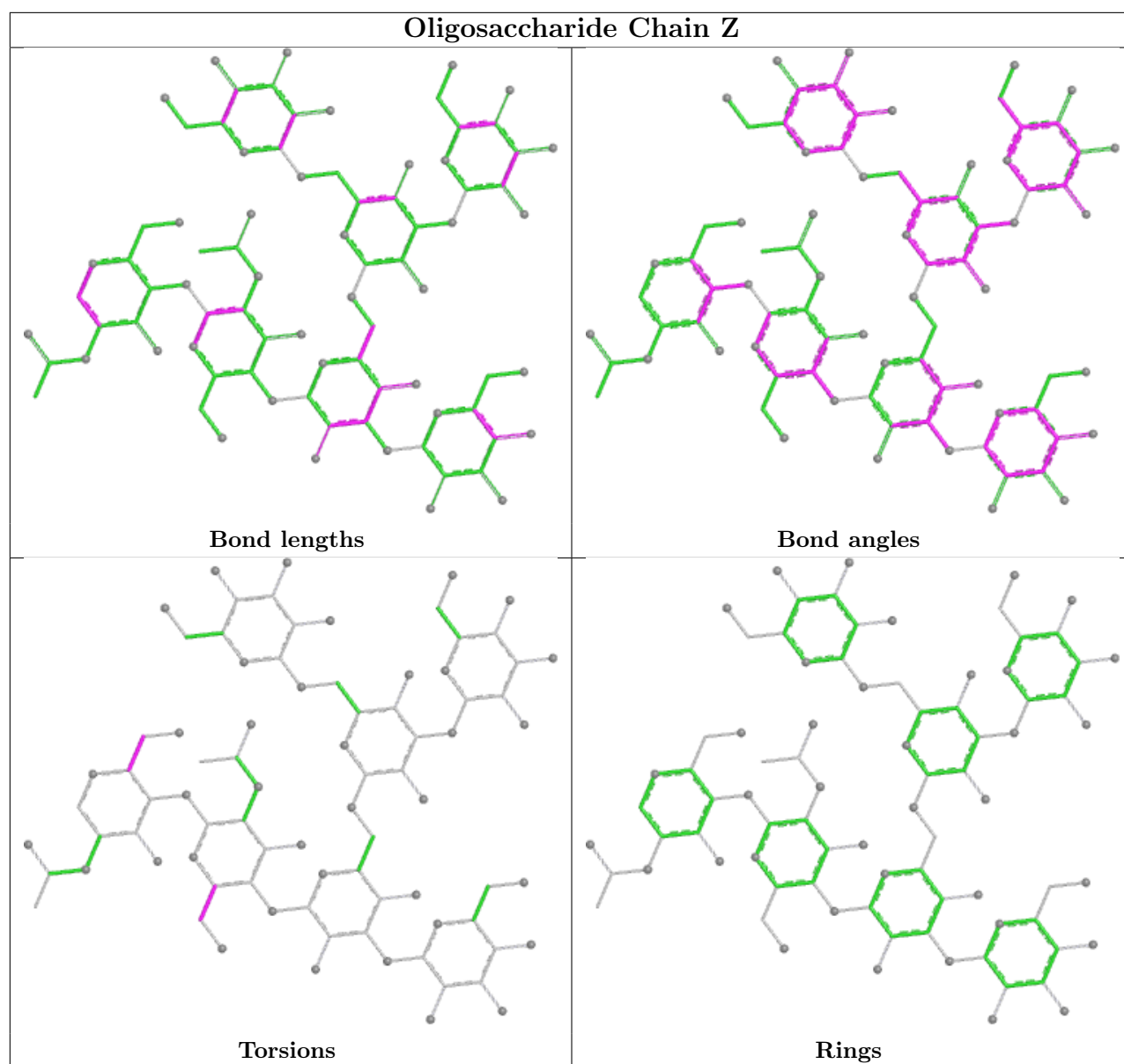


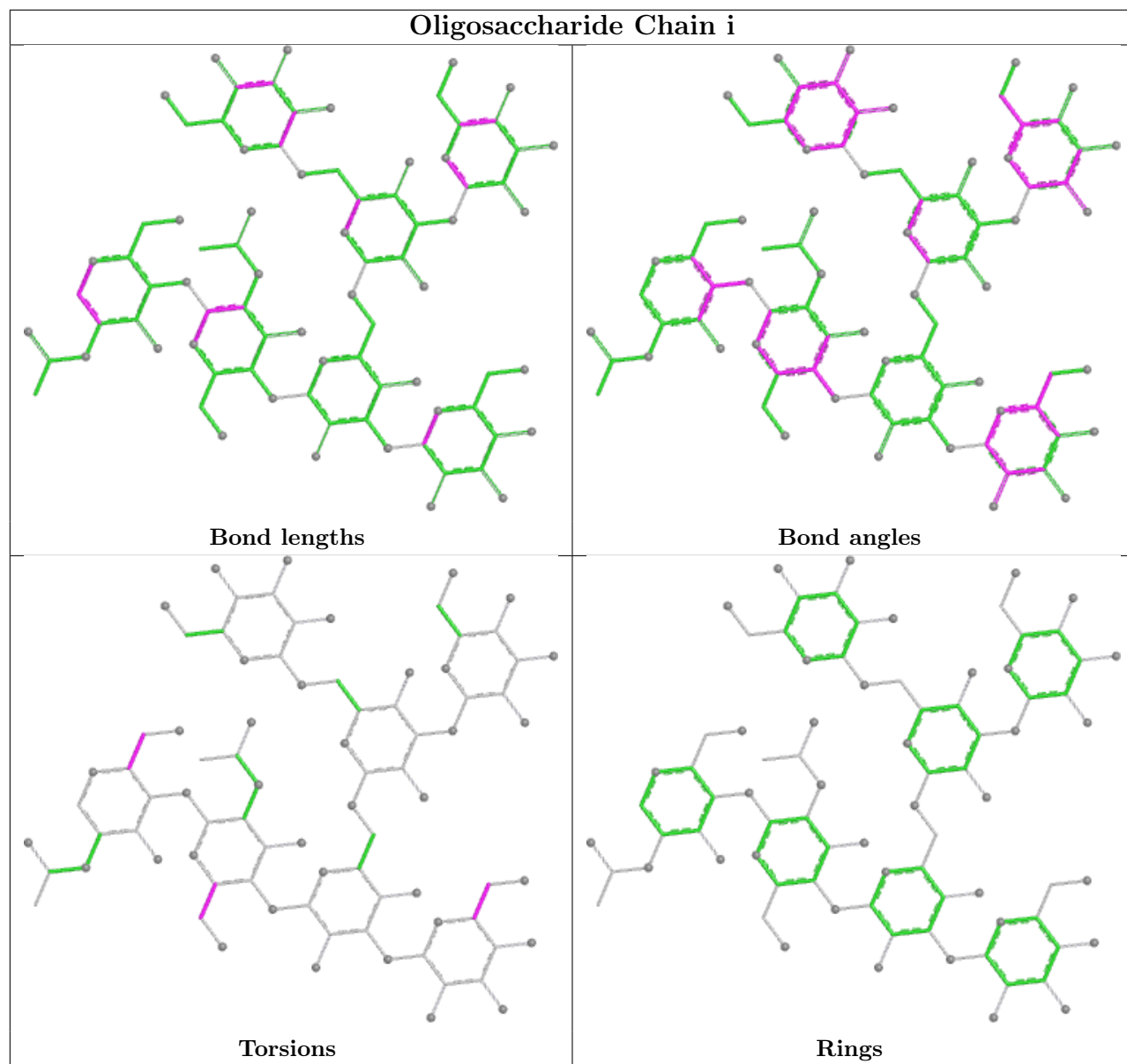


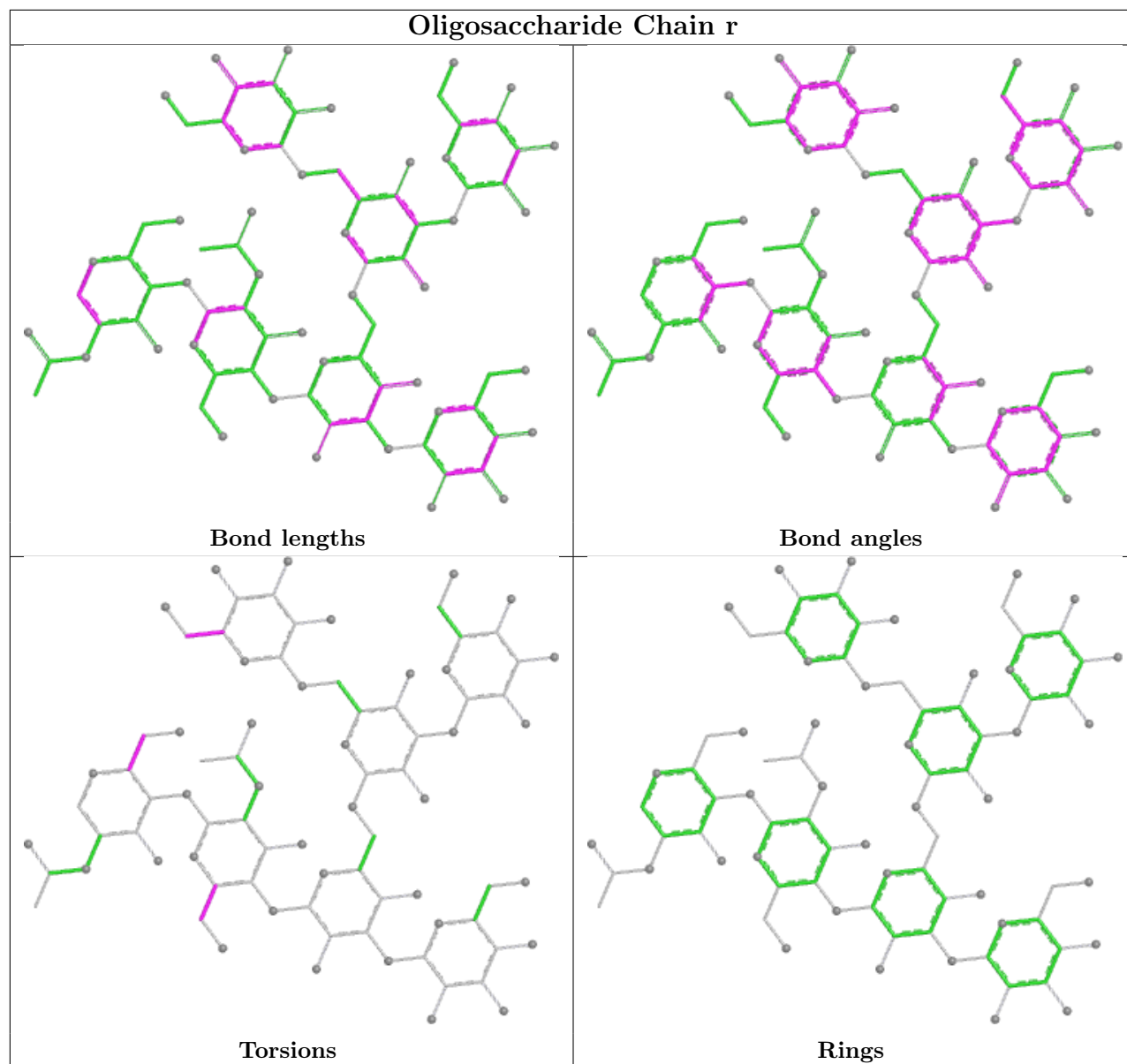


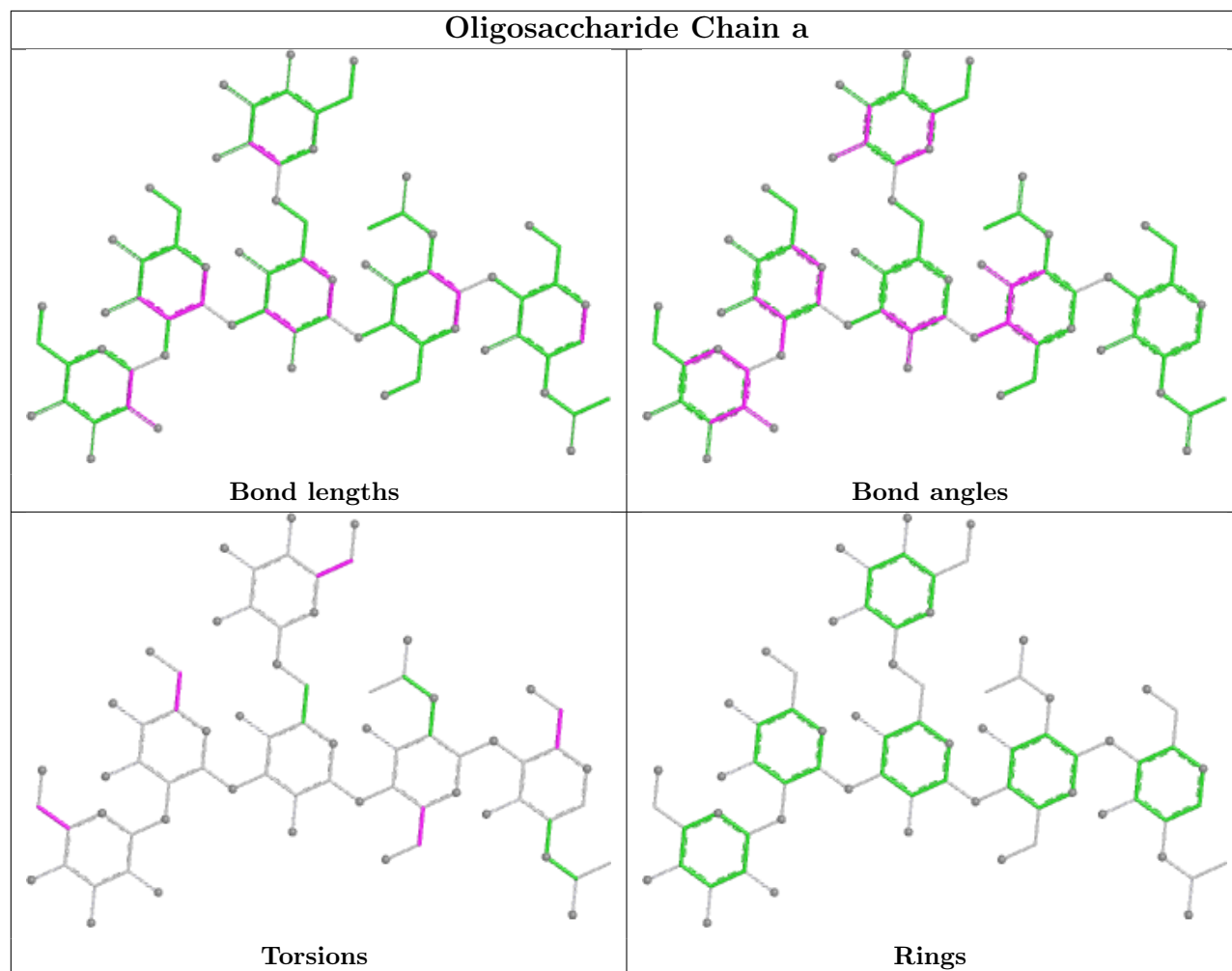


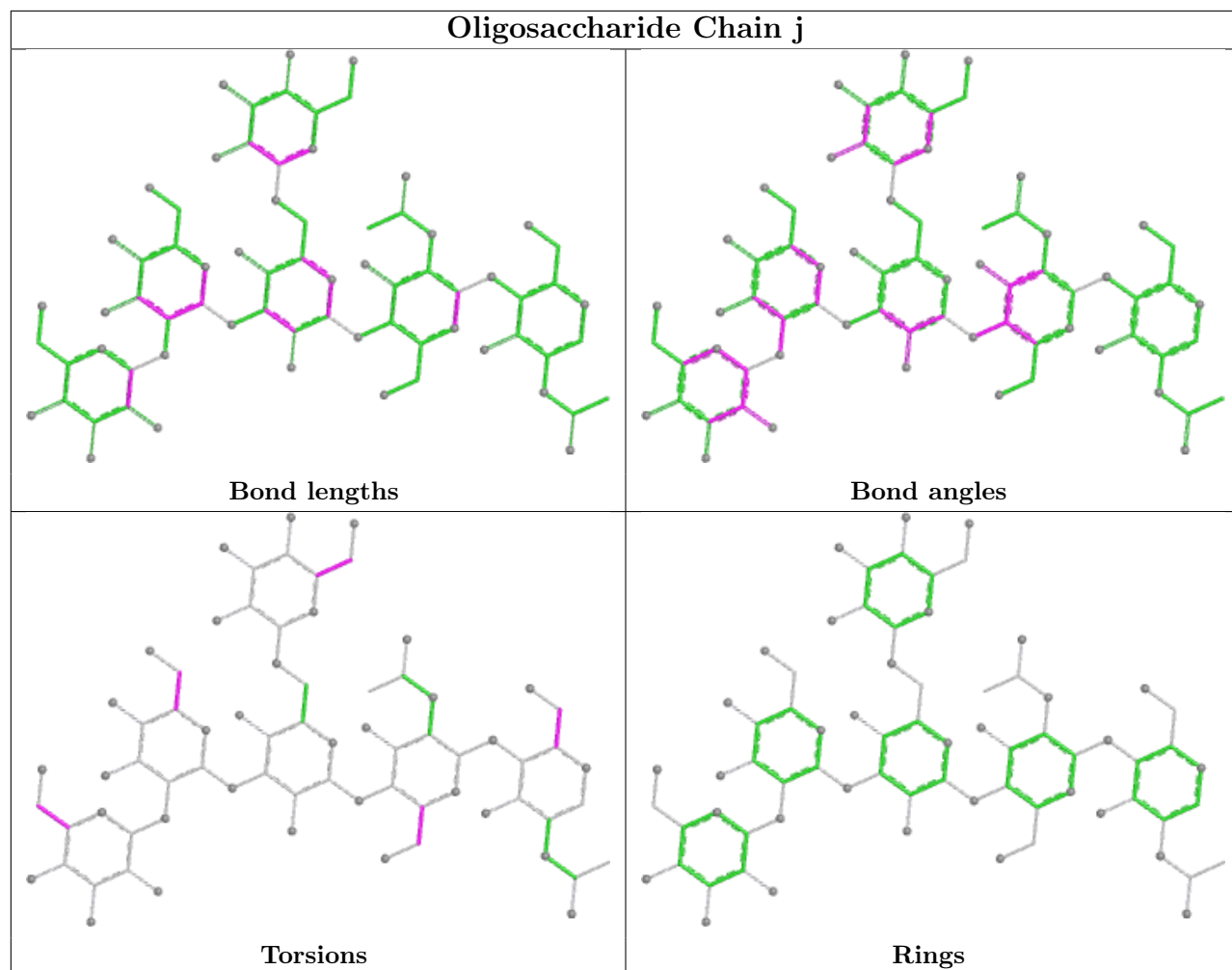


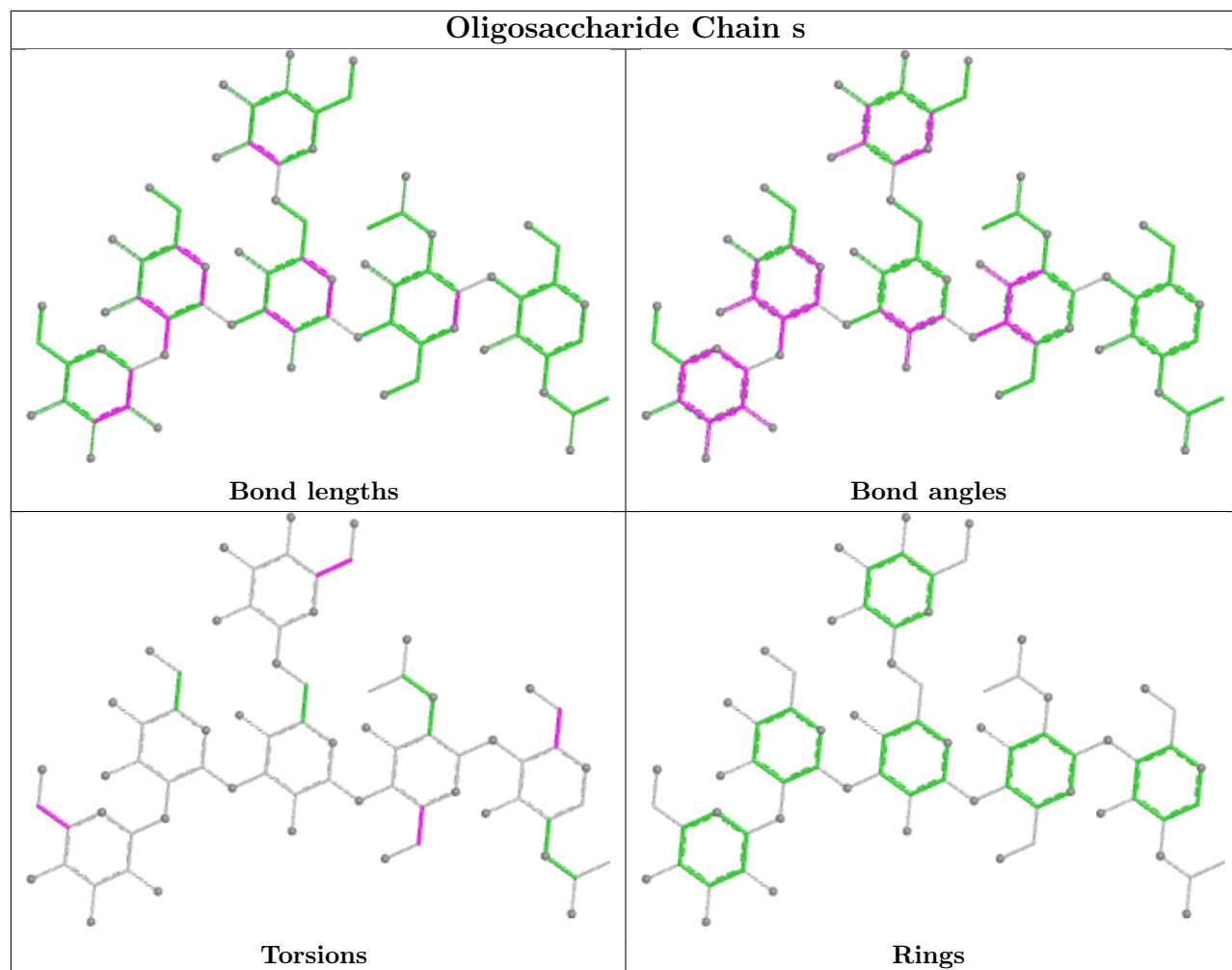


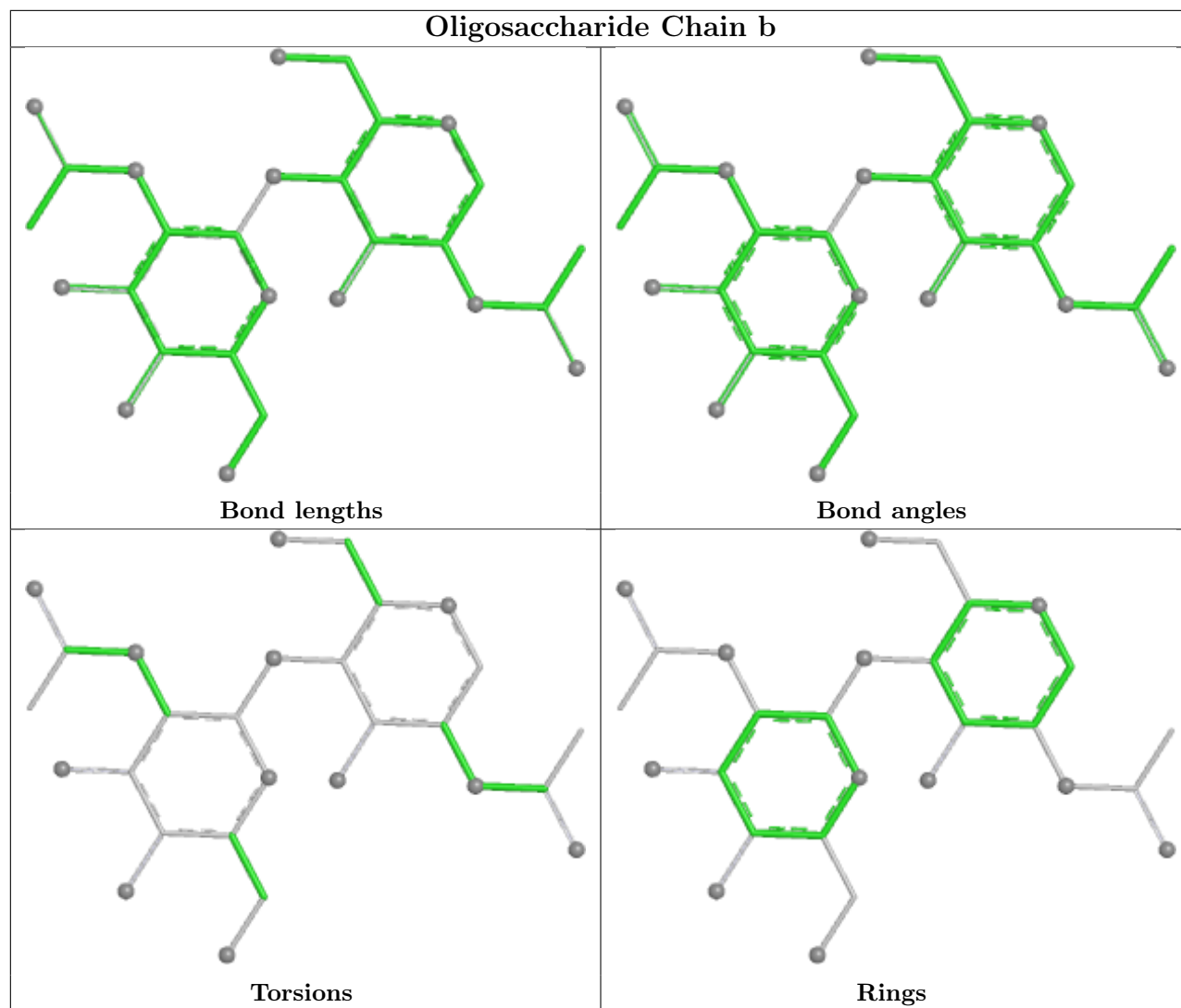


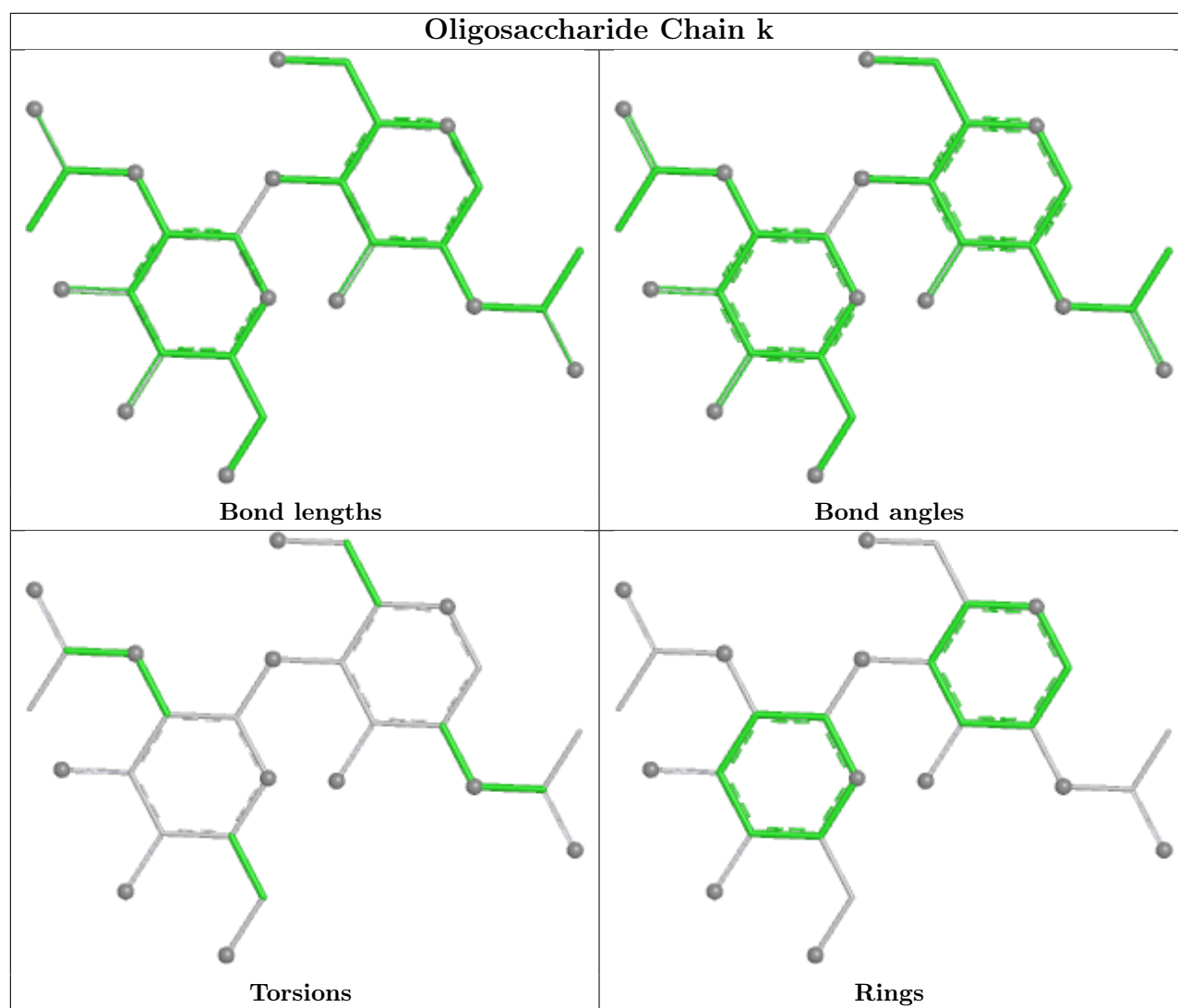


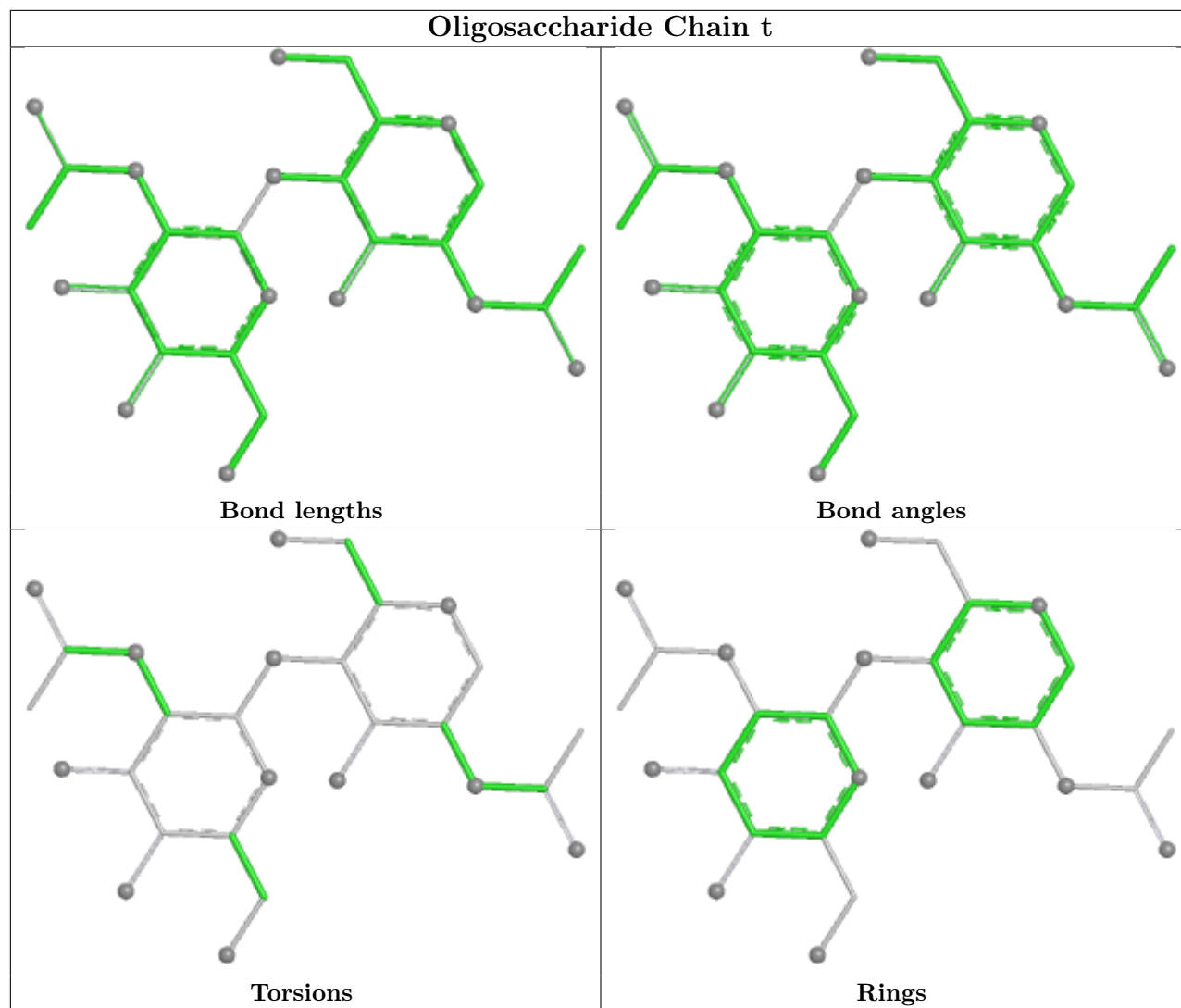


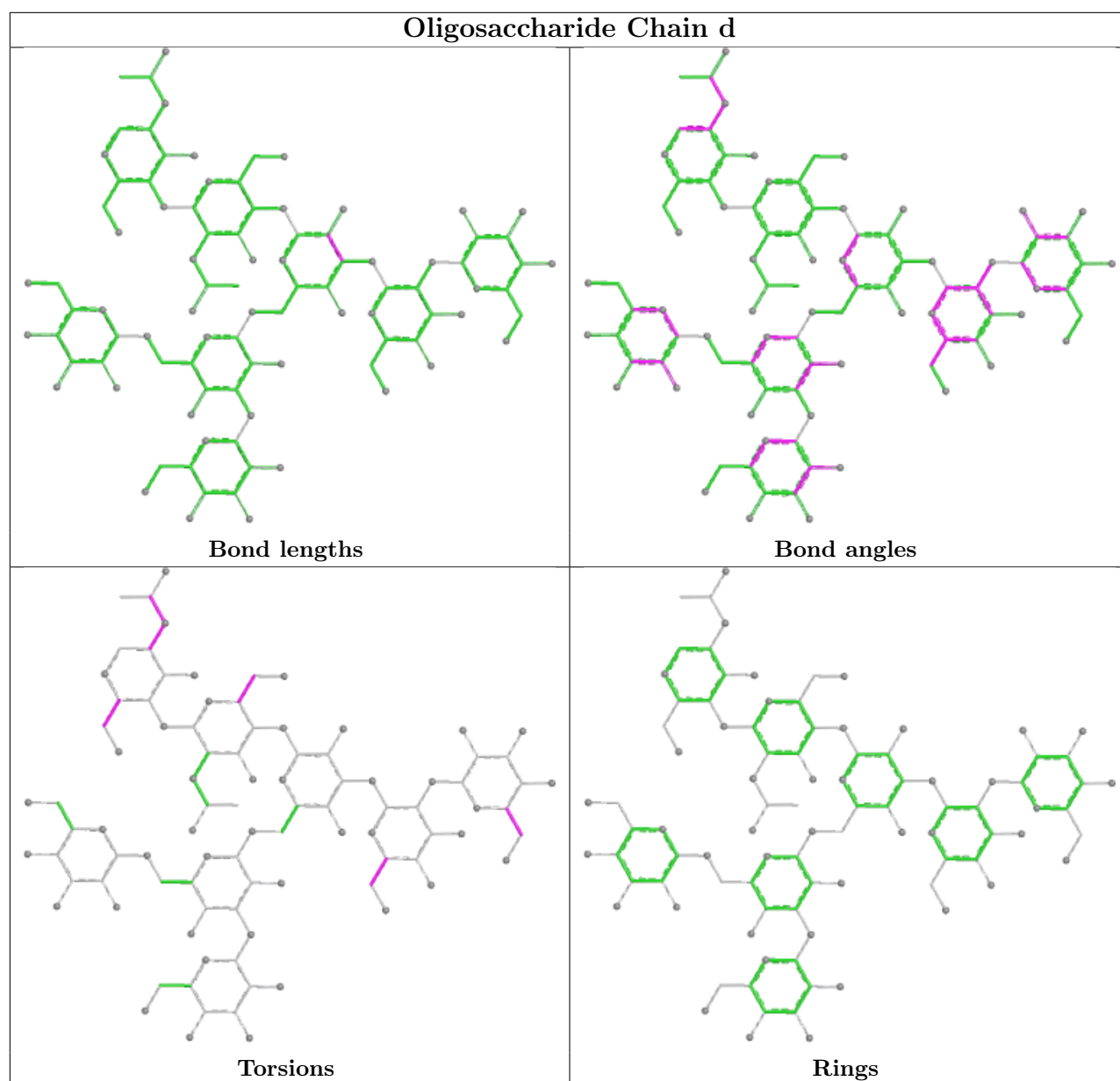


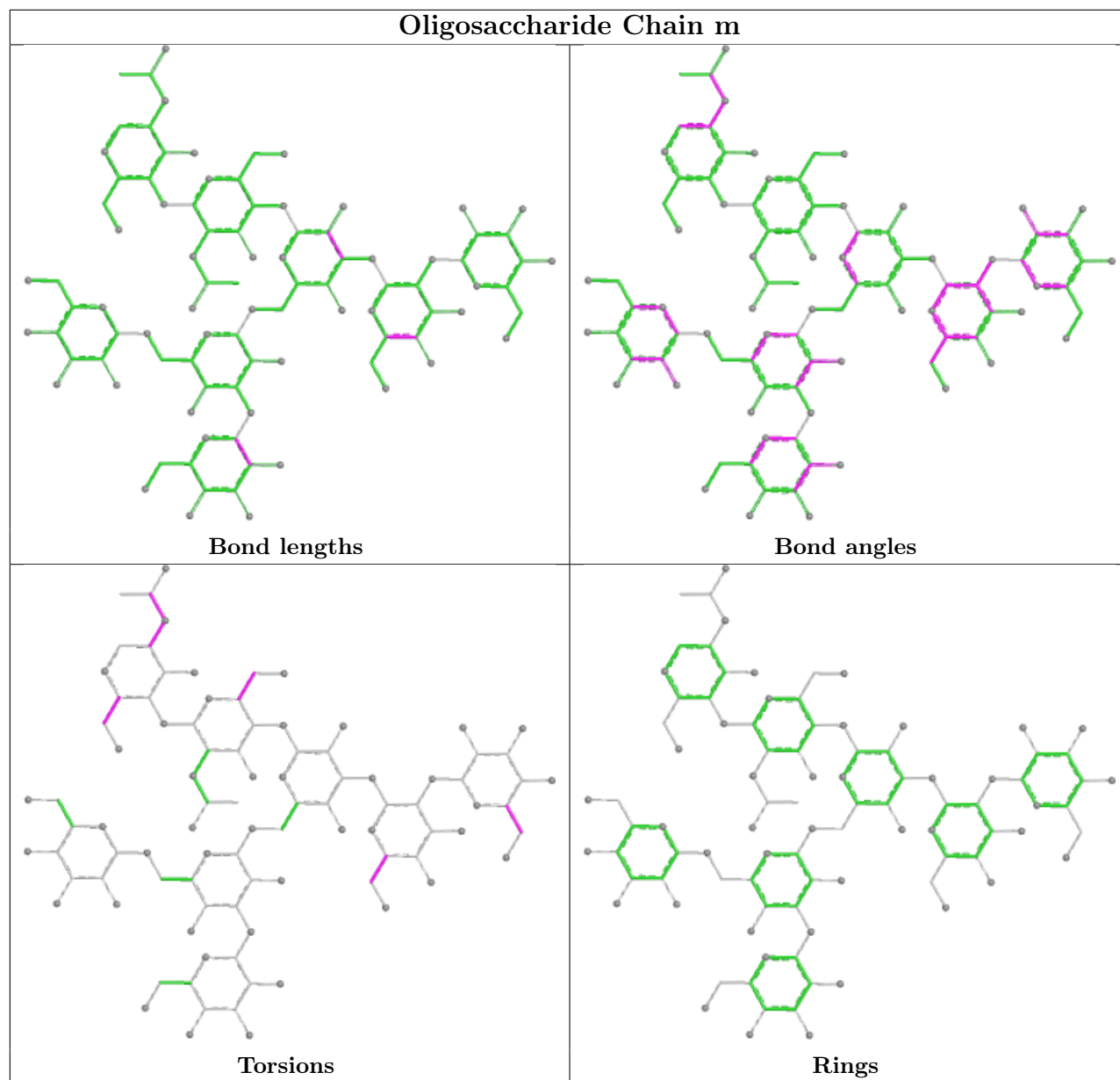


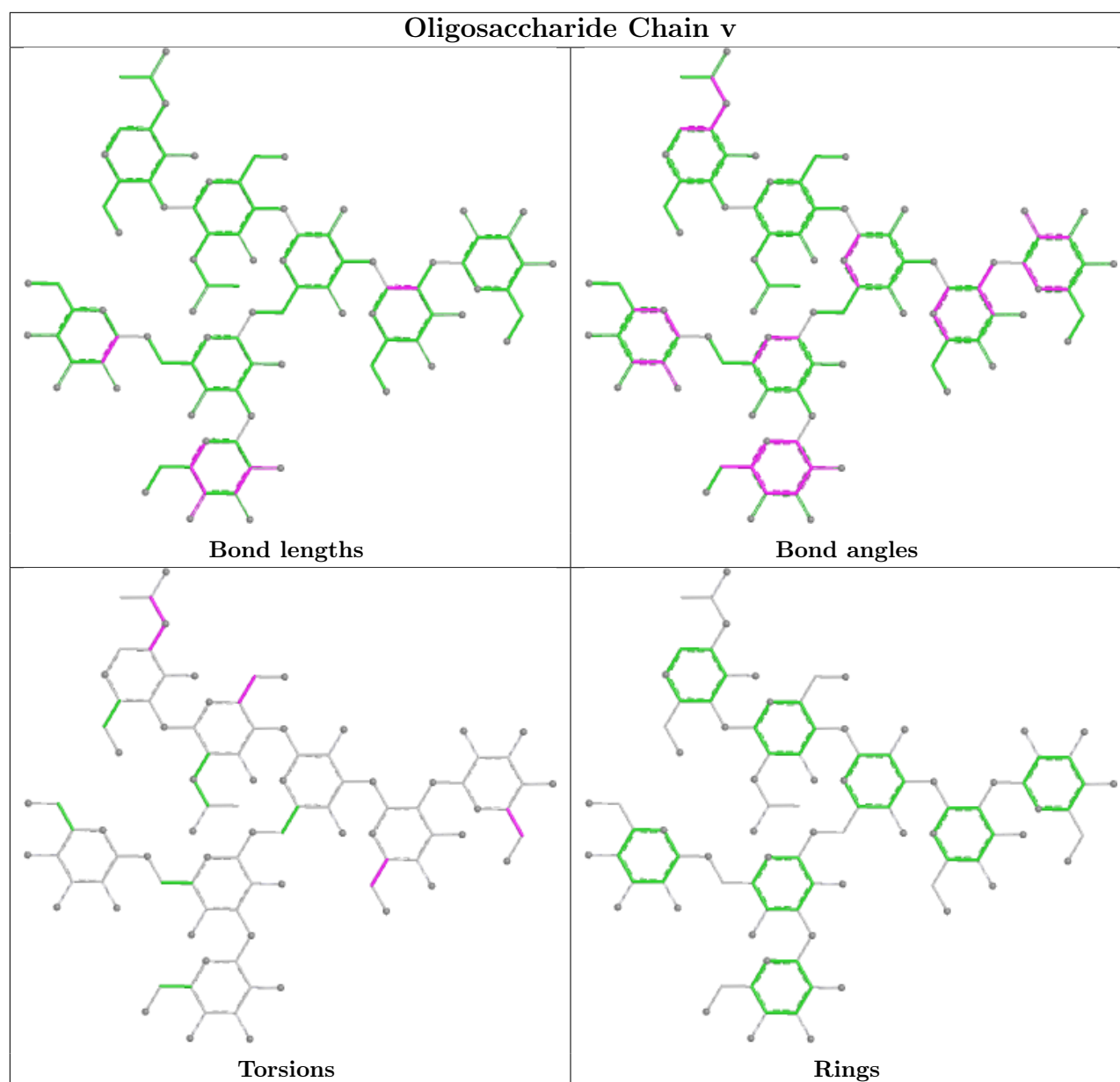












5.6 Ligand geometry [i](#)

33 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
15	NAG	F	652	1	14,14,15	0.19	0	17,19,21	0.37	0
15	NAG	G	651	1	14,14,15	0.34	0	17,19,21	0.53	0
15	NAG	Q	606	1	14,14,15	0.44	0	17,19,21	0.57	0
15	NAG	G	652	1	14,14,15	0.18	0	17,19,21	0.35	0
15	NAG	F	651	1	14,14,15	0.23	0	17,19,21	0.38	0
15	NAG	Q	653	1	14,14,15	1.06	1 (7%)	17,19,21	0.76	1 (5%)
15	NAG	G	653	1	14,14,15	0.49	0	17,19,21	0.48	0
15	NAG	G	606	1	14,14,15	0.46	0	17,19,21	0.57	0
15	NAG	Q	652	1	14,14,15	0.18	0	17,19,21	0.37	0
15	NAG	A	702	3	14,14,15	0.64	1 (7%)	17,19,21	0.53	0
15	NAG	G	650	1	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
15	NAG	Q	651	1	14,14,15	2.00	1 (7%)	17,19,21	2.08	6 (35%)
15	NAG	F	649	1	14,14,15	1.62	3 (21%)	17,19,21	2.36	8 (47%)
15	NAG	R	702	3	14,14,15	0.75	1 (7%)	17,19,21	0.59	0
15	NAG	J	703	3	14,14,15	0.68	1 (7%)	17,19,21	0.81	0
15	NAG	Q	615	1	14,14,15	0.19	0	17,19,21	0.50	0
15	NAG	Q	650	1	14,14,15	0.26	0	17,19,21	0.56	0
15	NAG	F	606	1	14,14,15	0.45	0	17,19,21	0.57	0
15	NAG	G	649	1	14,14,15	1.73	2 (14%)	17,19,21	2.30	8 (47%)
15	NAG	Q	649	1	14,14,15	0.35	0	17,19,21	0.75	1 (5%)
15	NAG	A	701	3	14,14,15	0.64	1 (7%)	17,19,21	0.56	0
15	NAG	J	701	3	14,14,15	0.63	1 (7%)	17,19,21	0.59	0
15	NAG	F	633	1	14,14,15	0.23	0	17,19,21	0.41	0
15	NAG	F	653	1	14,14,15	0.81	1 (7%)	17,19,21	0.59	0
15	NAG	A	703	3	14,14,15	0.62	0	17,19,21	0.79	0
15	NAG	G	633	1	14,14,15	0.25	0	17,19,21	0.40	0
15	NAG	R	701	3	14,14,15	0.78	1 (7%)	17,19,21	0.54	0
15	NAG	Q	633	1	14,14,15	0.21	0	17,19,21	0.42	0
15	NAG	J	702	3	14,14,15	0.88	1 (7%)	17,19,21	0.57	0
15	NAG	R	703	3	14,14,15	0.66	0	17,19,21	0.77	0
15	NAG	F	615	1	14,14,15	0.17	0	17,19,21	0.50	0
15	NAG	F	650	1	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
15	NAG	G	615	1	14,14,15	0.99	1 (7%)	17,19,21	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	F	652	1	-	4/6/23/26	0/1/1/1
15	NAG	G	651	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	606	1	-	2/6/23/26	0/1/1/1
15	NAG	G	652	1	-	4/6/23/26	0/1/1/1
15	NAG	F	651	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	653	1	-	0/6/23/26	0/1/1/1
15	NAG	G	653	1	-	3/6/23/26	0/1/1/1
15	NAG	G	606	1	-	2/6/23/26	0/1/1/1
15	NAG	Q	652	1	-	4/6/23/26	0/1/1/1
15	NAG	A	702	3	-	0/6/23/26	0/1/1/1
15	NAG	G	650	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	651	1	-	0/6/23/26	0/1/1/1
15	NAG	F	649	1	-	1/6/23/26	0/1/1/1
15	NAG	R	702	3	-	0/6/23/26	0/1/1/1
15	NAG	J	703	3	-	0/6/23/26	0/1/1/1
15	NAG	Q	615	1	-	4/6/23/26	0/1/1/1
15	NAG	Q	650	1	-	0/6/23/26	0/1/1/1
15	NAG	F	606	1	-	2/6/23/26	0/1/1/1
15	NAG	G	649	1	-	1/6/23/26	0/1/1/1
15	NAG	Q	649	1	-	0/6/23/26	0/1/1/1
15	NAG	A	701	3	-	1/6/23/26	0/1/1/1
15	NAG	J	701	3	-	2/6/23/26	0/1/1/1
15	NAG	F	633	1	-	0/6/23/26	0/1/1/1
15	NAG	F	653	1	-	0/6/23/26	0/1/1/1
15	NAG	A	703	3	-	0/6/23/26	0/1/1/1
15	NAG	G	633	1	-	0/6/23/26	0/1/1/1
15	NAG	R	701	3	-	2/6/23/26	0/1/1/1
15	NAG	Q	633	1	-	0/6/23/26	0/1/1/1
15	NAG	J	702	3	-	0/6/23/26	0/1/1/1
15	NAG	R	703	3	-	0/6/23/26	0/1/1/1
15	NAG	F	615	1	-	4/6/23/26	0/1/1/1
15	NAG	F	650	1	-	0/6/23/26	0/1/1/1
15	NAG	G	615	1	-	3/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	651	NAG	O5-C1	-6.83	1.32	1.43
15	G	649	NAG	O5-C1	-5.25	1.34	1.43
15	F	649	NAG	O5-C1	-4.58	1.36	1.43
15	Q	653	NAG	O5-C1	-3.40	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	615	NAG	C1-C2	3.06	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	649	NAG	C3-C4-C5	4.66	118.67	110.23
15	G	649	NAG	C3-C4-C5	4.37	118.16	110.23
15	G	649	NAG	O4-C4-C5	4.10	119.41	109.32
15	Q	651	NAG	O4-C4-C5	4.06	119.31	109.32
15	F	649	NAG	O4-C4-C5	4.03	119.25	109.32

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	615	NAG	O5-C5-C6-O6
15	Q	615	NAG	O5-C5-C6-O6
15	G	653	NAG	C4-C5-C6-O6
15	G	615	NAG	O5-C5-C6-O6
15	G	615	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	606	NAG	3	0
15	Q	653	NAG	6	0
15	G	653	NAG	3	0
15	G	606	NAG	3	0
15	G	650	NAG	1	0
15	J	703	NAG	2	0
15	Q	615	NAG	1	0
15	Q	650	NAG	1	0
15	F	606	NAG	3	0
15	F	653	NAG	6	0
15	A	703	NAG	1	0
15	R	703	NAG	2	0
15	F	615	NAG	2	0
15	F	650	NAG	1	0
15	G	615	NAG	4	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	F	449/471 (95%)	-0.17	11 (2%) 59 52	261, 419, 512, 568	0
1	G	449/471 (95%)	-0.14	18 (4%) 42 41	251, 420, 504, 599	0
1	Q	449/471 (95%)	-0.19	4 (0%) 81 70	240, 430, 527, 617	0
2	D	222/250 (88%)	-0.33	5 (2%) 61 53	303, 478, 541, 600	0
2	O	222/250 (88%)	-0.07	2 (0%) 81 70	285, 453, 530, 563	0
2	W	222/250 (88%)	-0.27	1 (0%) 87 78	292, 497, 603, 637	0
3	A	126/147 (85%)	-0.07	3 (2%) 59 52	241, 374, 496, 610	0
3	J	126/147 (85%)	-0.04	5 (3%) 42 41	245, 378, 467, 584	0
3	R	126/147 (85%)	-0.23	2 (1%) 70 59	209, 367, 476, 681	0
4	B	210/210 (100%)	-0.01	6 (2%) 53 47	274, 470, 717, 766	0
4	K	210/210 (100%)	0.10	11 (5%) 33 35	308, 556, 766, 872	0
4	S	210/210 (100%)	-0.23	1 (0%) 87 78	316, 507, 686, 716	0
5	C	228/232 (98%)	-0.08	6 (2%) 57 49	328, 474, 737, 788	0
5	L	228/232 (98%)	0.04	8 (3%) 47 43	311, 467, 818, 919	0
5	T	228/232 (98%)	-0.13	4 (1%) 67 58	367, 548, 770, 828	0
6	H	242/242 (100%)	-0.08	5 (2%) 63 54	214, 360, 510, 653	0
6	M	242/242 (100%)	-0.11	2 (0%) 82 72	272, 501, 677, 748	0
6	U	242/242 (100%)	-0.17	3 (1%) 76 65	214, 438, 635, 673	0
7	I	207/213 (97%)	-0.17	3 (1%) 73 62	139, 326, 450, 512	0
7	N	213/213 (100%)	-0.04	4 (1%) 66 56	209, 470, 714, 764	0
7	V	213/213 (100%)	-0.27	0 100 100	175, 400, 572, 618	0
All	All	5064/5295 (95%)	-0.13	104 (2%) 63 54	139, 441, 705, 919	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	23	ASN	7.1
5	L	92	CYS	6.9
1	G	219	ALA	6.4
4	K	121	PRO	5.3
2	D	187	TRP	4.9

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
2	PCA	W	1	8/9	0.17	0.13	355,368,480,481	0
2	PCA	D	1	8/9	0.56	0.08	434,443,508,513	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
8	NAG	E	1	14/15	-	-	366,367,368,369	0
8	NAG	E	2	14/15	-	-	430,433,437,437	0
8	BMA	E	3	11/12	-	-	434,435,439,440	0
8	MAN	E	4	11/12	-	-	400,402,404,404	0
8	MAN	E	5	11/12	-	-	482,484,485,485	0
8	MAN	X	5	11/12	0.37	0.08	510,528,545,546	0
8	MAN	X	4	11/12	0.50	0.09	521,546,562,562	0
11	MAN	Z	7	11/12	0.59	0.08	488,488,488,488	0
11	NAG	Z	2	14/15	0.64	0.10	470,472,474,476	0
11	MAN	Z	4	11/12	0.67	0.09	613,615,616,616	0
8	NAG	c	1	14/15	-	-	348,350,351,353	0
8	NAG	c	2	14/15	-	-	410,416,420,420	0
8	BMA	c	3	11/12	-	-	512,514,518,519	0
8	MAN	c	4	11/12	-	-	502,506,510,511	0
8	MAN	c	5	11/12	-	-	540,543,547,549	0
8	NAG	e	1	14/15	-	-	444,448,454,455	0
8	NAG	e	2	14/15	-	-	499,504,507,509	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	BMA	e	3	11/12	-	-	558,559,560,562	0
8	MAN	e	4	11/12	-	-	508,509,512,512	0
8	MAN	e	5	11/12	-	-	555,558,560,561	0
8	NAG	g	1	14/15	-	-	414,418,440,441	0
8	NAG	g	2	14/15	-	-	531,555,576,580	0
8	BMA	g	3	11/12	-	-	626,642,653,670	0
8	MAN	g	4	11/12	-	-	637,667,676,683	0
8	MAN	g	5	11/12	-	-	526,544,561,562	0
8	NAG	l	1	14/15	-	-	477,479,481,483	0
8	NAG	l	2	14/15	-	-	461,463,465,465	0
8	BMA	l	3	11/12	-	-	537,539,542,542	0
8	MAN	l	4	11/12	-	-	512,515,515,517	0
8	MAN	l	5	11/12	-	-	622,623,625,625	0
8	NAG	n	1	14/15	-	-	426,428,429,430	0
8	NAG	n	2	14/15	-	-	492,493,494,495	0
8	BMA	n	3	11/12	-	-	470,471,471,471	0
8	MAN	n	4	11/12	-	-	422,422,423,424	0
8	MAN	n	5	11/12	-	-	457,458,458,459	0
8	NAG	p	1	14/15	-	-	364,371,393,395	0
8	NAG	p	2	14/15	-	-	465,488,513,516	0
8	BMA	p	3	11/12	-	-	527,544,557,575	0
8	MAN	p	4	11/12	-	-	563,590,602,606	0
8	MAN	p	5	11/12	-	-	546,563,582,583	0
8	NAG	u	1	14/15	-	-	345,347,349,350	0
8	NAG	u	2	14/15	-	-	352,353,354,354	0
8	BMA	u	3	11/12	-	-	480,480,481,481	0
8	MAN	u	4	11/12	-	-	558,559,560,561	0
8	MAN	u	5	11/12	-	-	435,435,438,438	0
9	NAG	P	1	14/15	-	-	529,532,535,535	0
9	NAG	P	2	14/15	-	-	511,513,515,517	0
9	BMA	P	3	11/12	-	-	536,538,539,539	0
9	NAG	f	1	14/15	-	-	473,478,482,482	0
9	NAG	f	2	14/15	-	-	485,488,490,491	0
9	BMA	f	3	11/12	-	-	435,438,442,444	0
9	NAG	o	1	14/15	-	-	542,543,544,545	0
9	NAG	o	2	14/15	-	-	620,622,625,626	0
9	BMA	o	3	11/12	-	-	641,642,644,644	0
11	BMA	Z	3	11/12	0.67	0.06	541,543,545,545	0
11	MAN	Z	5	11/12	0.74	0.09	582,584,585,586	0
10	NAG	Y	2	14/15	0.74	0.07	426,430,433,434	0
8	NAG	X	2	14/15	0.76	0.11	418,443,465,472	0
10	NAG	h	1	14/15	-	-	345,348,350,351	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	h	2	14/15	-	-	419,421,424,425	0
10	BMA	h	3	11/12	-	-	437,440,442,443	0
10	MAN	h	4	11/12	-	-	519,522,525,526	0
10	NAG	q	1	14/15	-	-	404,407,410,412	0
10	NAG	q	2	14/15	-	-	485,487,489,489	0
10	BMA	q	3	11/12	-	-	489,490,491,492	0
10	MAN	q	4	11/12	-	-	526,527,528,529	0
10	MAN	Y	4	11/12	0.80	0.09	580,581,582,583	0
8	BMA	X	3	11/12	0.80	0.05	526,543,558,577	0
11	MAN	Z	6	11/12	0.84	0.10	708,709,711,711	0
10	BMA	Y	3	11/12	0.88	0.06	467,469,470,471	0
11	NAG	Z	1	14/15	0.93	0.10	401,403,404,404	0
10	NAG	Y	1	14/15	0.95	0.14	401,402,404,405	0
8	NAG	X	1	14/15	0.96	0.06	395,399,426,427	0
11	NAG	i	1	14/15	-	-	417,419,420,421	0
11	NAG	i	2	14/15	-	-	501,506,509,511	0
11	BMA	i	3	11/12	-	-	485,487,490,492	0
11	MAN	i	4	11/12	-	-	489,492,496,496	0
11	MAN	i	5	11/12	-	-	507,509,513,514	0
11	MAN	i	6	11/12	-	-	438,440,445,447	0
11	MAN	i	7	11/12	-	-	448,448,448,448	0
11	NAG	r	1	14/15	-	-	388,390,392,393	0
11	NAG	r	2	14/15	-	-	509,510,511,511	0
11	BMA	r	3	11/12	-	-	549,550,550,551	0
11	MAN	r	4	11/12	-	-	576,577,579,579	0
11	MAN	r	5	11/12	-	-	605,605,606,607	0
11	MAN	r	6	11/12	-	-	454,455,456,457	0
11	MAN	r	7	11/12	-	-	620,620,620,620	0
12	NAG	a	1	14/15	-	-	324,331,339,351	0
12	NAG	a	2	14/15	-	-	366,377,383,390	0
12	BMA	a	3	11/12	-	-	418,427,431,437	0
12	MAN	a	4	11/12	-	-	479,498,500,501	0
12	MAN	a	5	11/12	-	-	502,517,520,521	0
12	MAN	a	6	11/12	-	-	408,413,418,418	0
12	NAG	j	1	14/15	-	-	433,439,447,461	0
12	NAG	j	2	14/15	-	-	366,376,381,387	0
12	BMA	j	3	11/12	-	-	407,417,420,424	0
12	MAN	j	4	11/12	-	-	469,484,487,488	0
12	MAN	j	5	11/12	-	-	453,467,469,470	0
12	MAN	j	6	11/12	-	-	507,511,517,517	0
12	NAG	s	1	14/15	-	-	420,425,434,447	0
12	NAG	s	2	14/15	-	-	434,446,451,458	0

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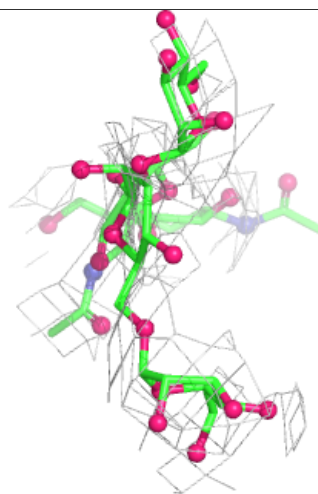
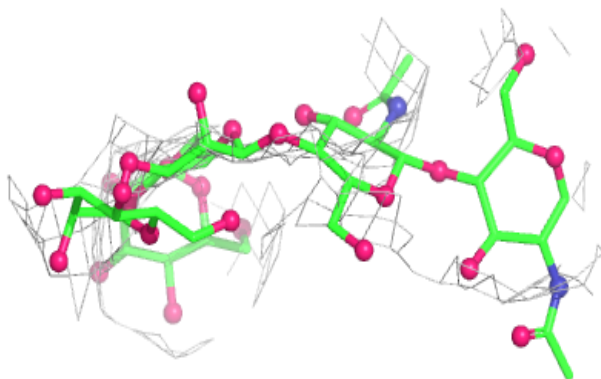
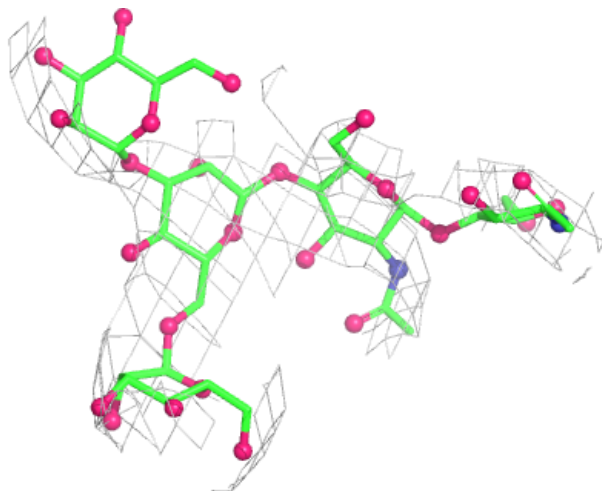
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	BMA	s	3	11/12	-	-	508,516,520,524	0
12	MAN	s	4	11/12	-	-	567,567,567,567	0
12	MAN	s	5	11/12	-	-	589,589,589,589	0
12	MAN	s	6	11/12	-	-	440,445,450,450	0
13	NAG	b	1	14/15	-	-	374,378,381,382	0
13	NAG	b	2	14/15	-	-	398,401,404,406	0
13	NAG	k	1	14/15	-	-	367,370,375,376	0
13	NAG	k	2	14/15	-	-	416,421,426,426	0
13	NAG	t	1	14/15	-	-	446,447,448,449	0
13	NAG	t	2	14/15	-	-	521,522,522,523	0
14	NAG	d	1	14/15	-	-	456,462,468,471	0
14	NAG	d	2	14/15	-	-	452,460,471,473	0
14	BMA	d	3	11/12	-	-	471,476,486,491	0
14	MAN	d	4	11/12	-	-	410,421,430,432	0
14	MAN	d	5	11/12	-	-	392,395,397,399	0
14	MAN	d	6	11/12	-	-	465,467,473,475	0
14	MAN	d	7	11/12	-	-	499,503,504,506	0
14	MAN	d	8	11/12	-	-	390,393,399,407	0
14	NAG	m	1	14/15	-	-	426,430,436,438	0
14	NAG	m	2	14/15	-	-	427,437,446,456	0
14	BMA	m	3	11/12	-	-	470,474,482,483	0
14	MAN	m	4	11/12	-	-	400,403,419,420	0
14	MAN	m	5	11/12	-	-	384,389,393,393	0
14	MAN	m	6	11/12	-	-	469,477,482,485	0
14	MAN	m	7	11/12	-	-	425,428,432,433	0
14	MAN	m	8	11/12	-	-	506,514,524,533	0
14	NAG	v	1	14/15	-	-	374,381,388,390	0
14	NAG	v	2	14/15	-	-	432,437,446,450	0
14	BMA	v	3	11/12	-	-	445,449,459,463	0
14	MAN	v	4	11/12	-	-	452,458,471,472	0
14	MAN	v	5	11/12	-	-	454,458,461,462	0
14	MAN	v	6	11/12	-	-	481,485,491,492	0
14	MAN	v	7	11/12	-	-	455,460,462,463	0
14	MAN	v	8	11/12	-	-	480,486,493,502	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.

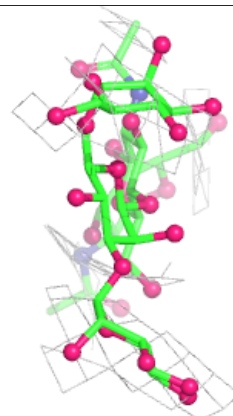
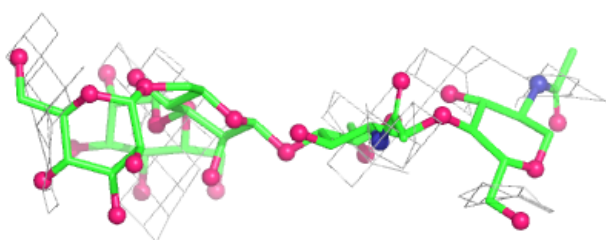
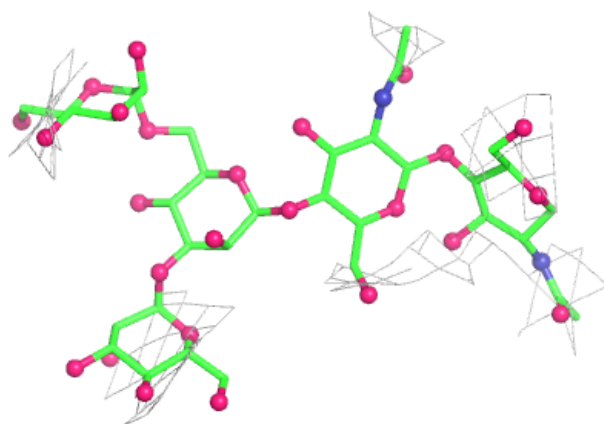
Electron density around Chain E:

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



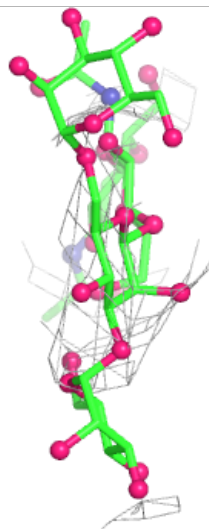
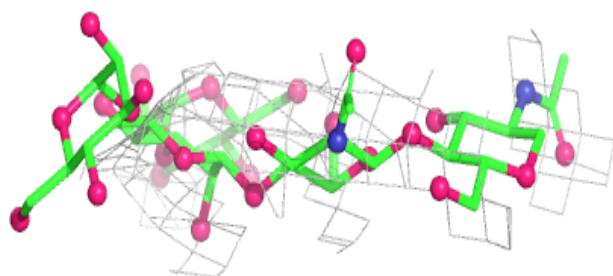
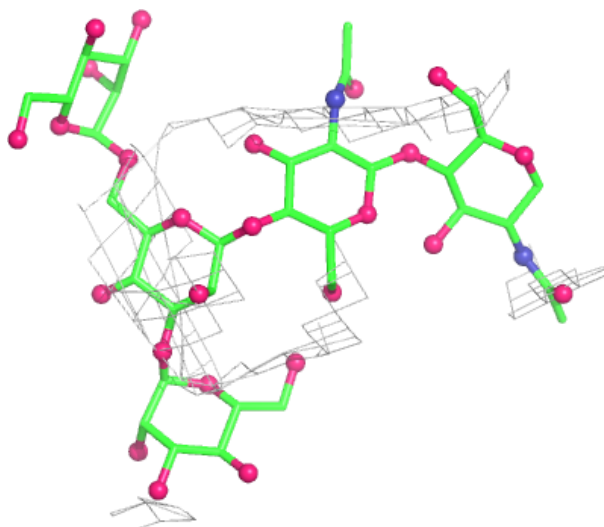
Electron density around Chain X:

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



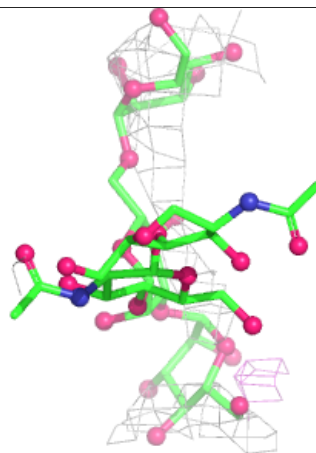
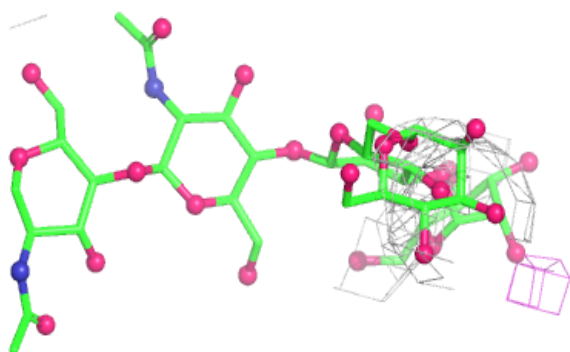
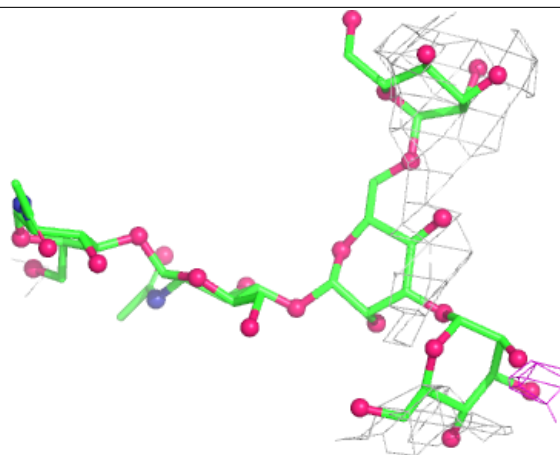
Electron density around Chain c:

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



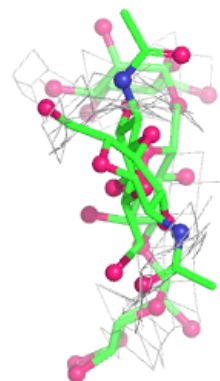
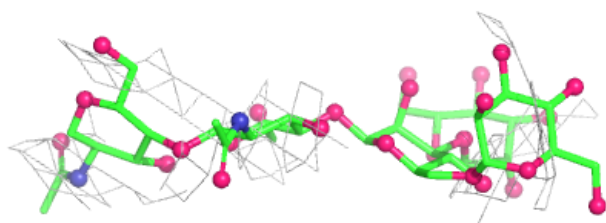
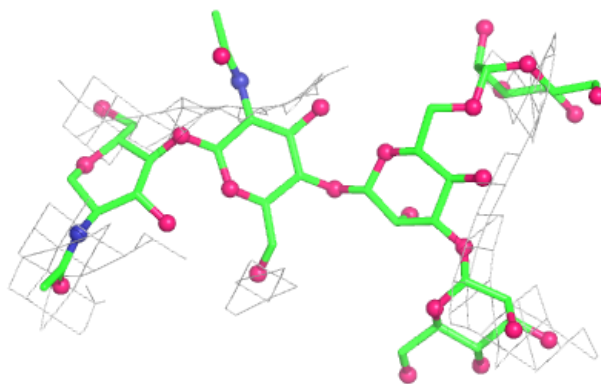
Electron density around Chain e:

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



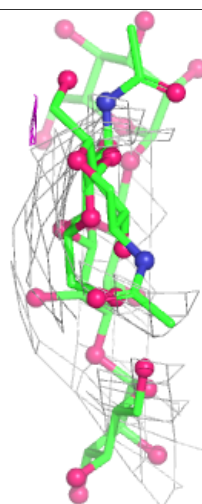
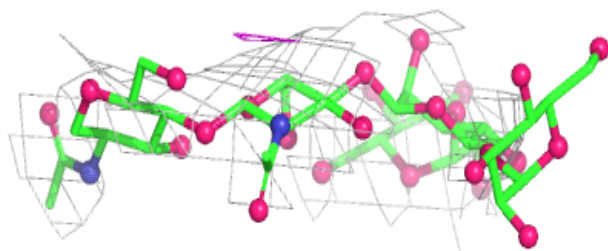
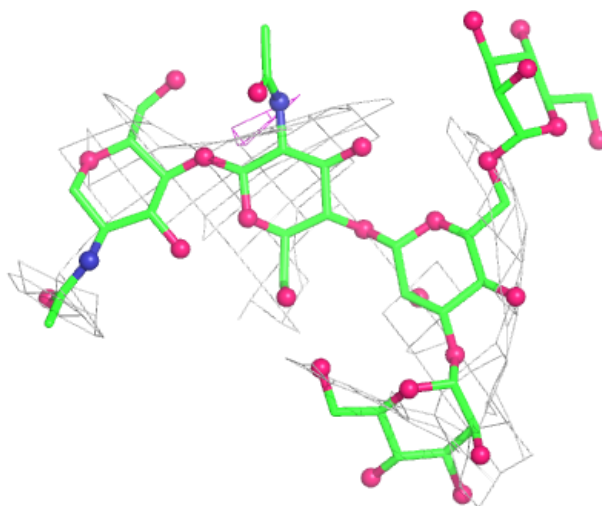
Electron density around Chain g:

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



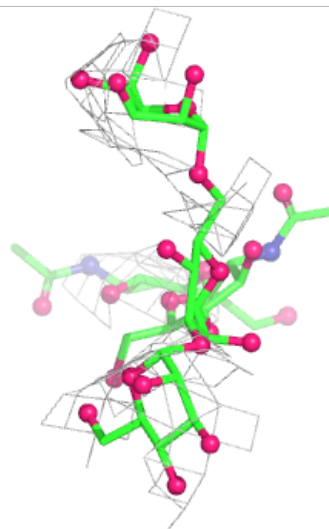
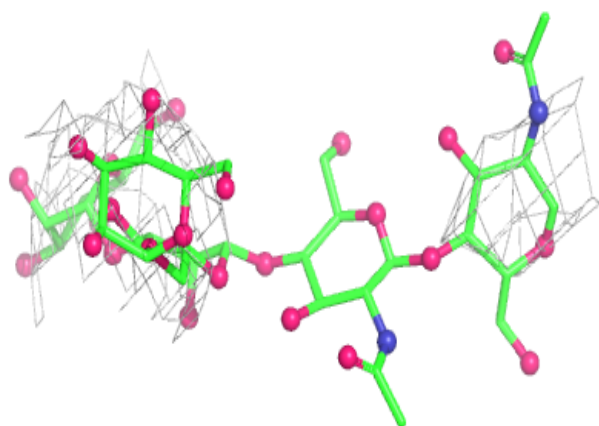
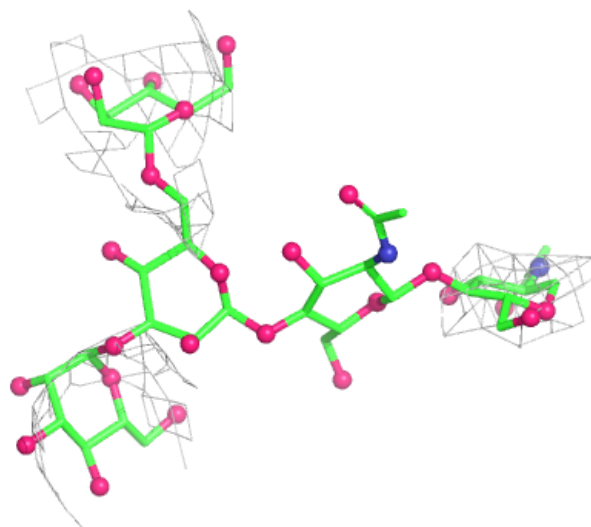
Electron density around Chain 1:

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



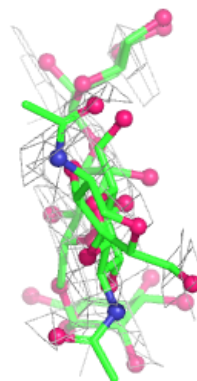
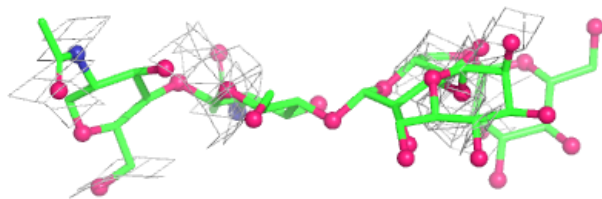
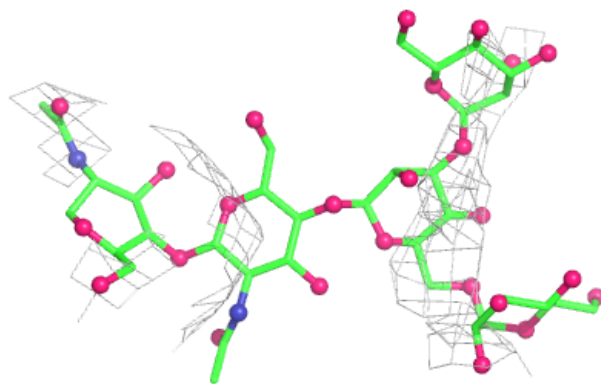
Electron density around Chain n:

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



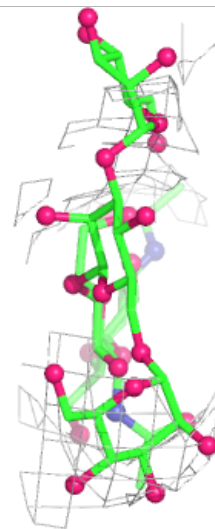
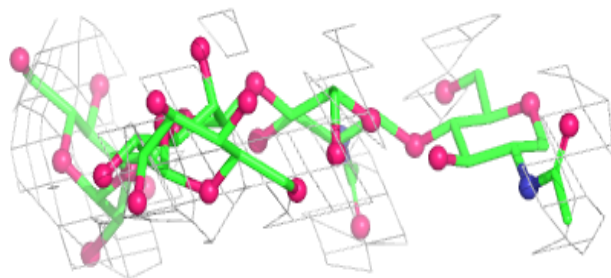
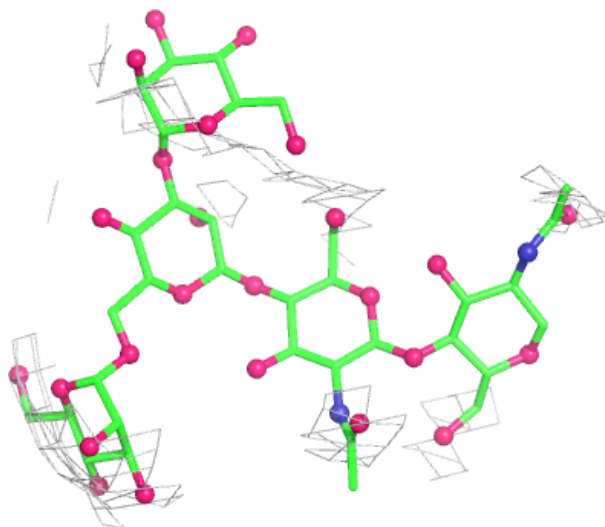
Electron density around Chain p:

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



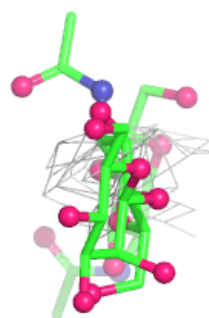
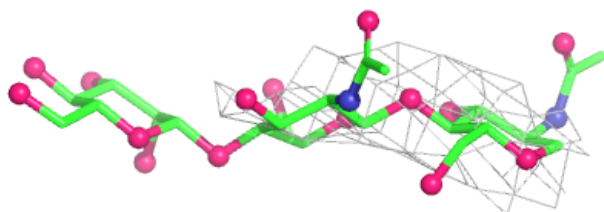
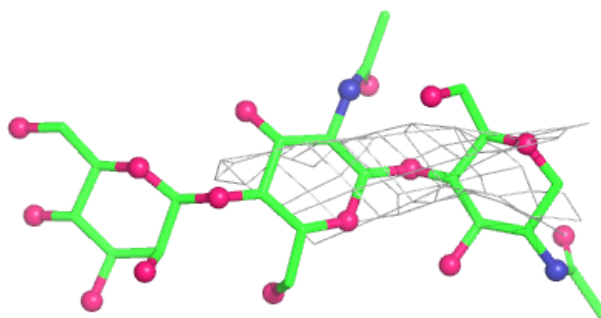
Electron density around Chain u:

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

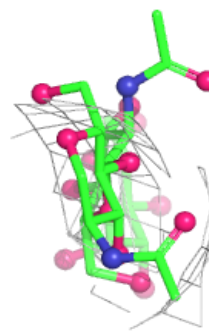
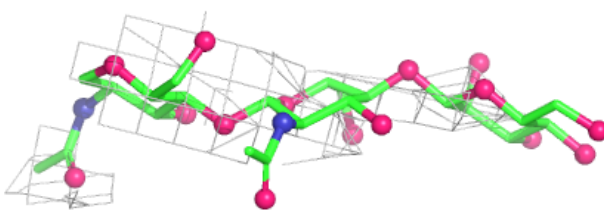
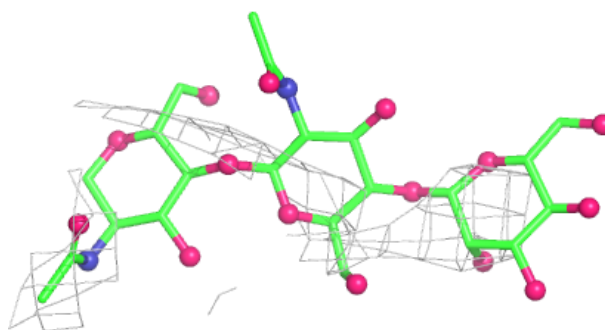


Electron density around Chain P:

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

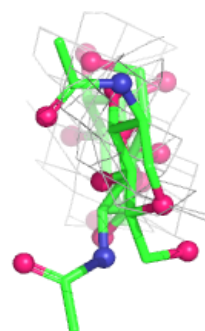
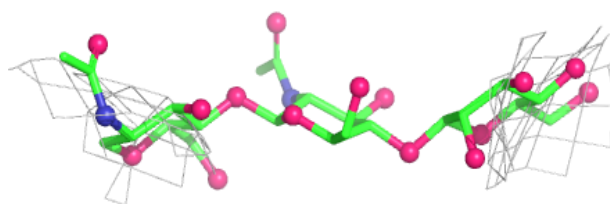
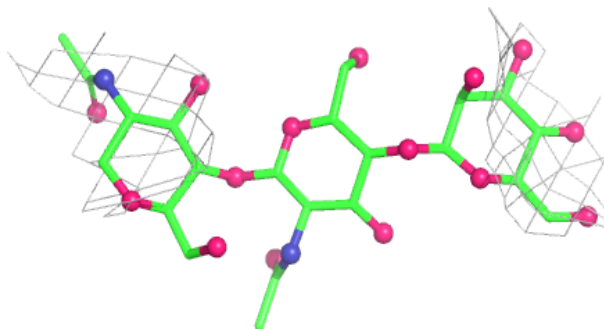
**Electron density around Chain f:**

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

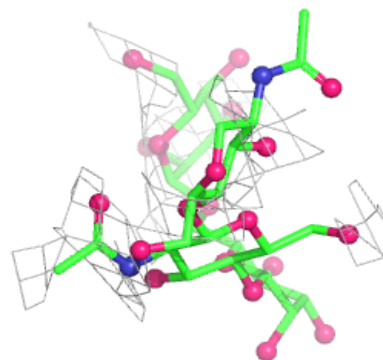
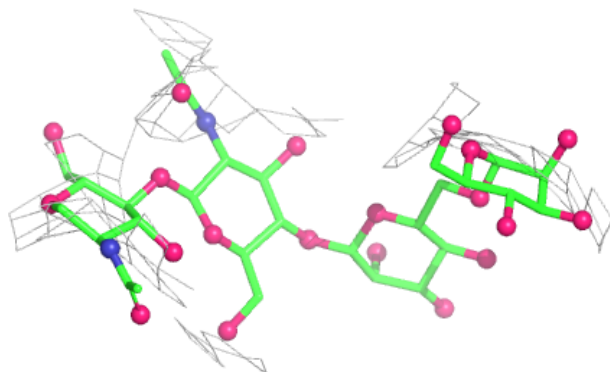
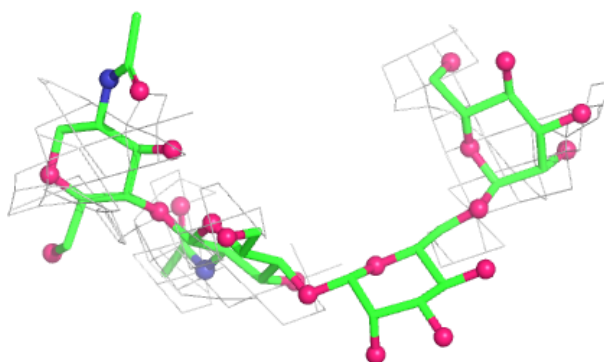


Electron density around Chain o:

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

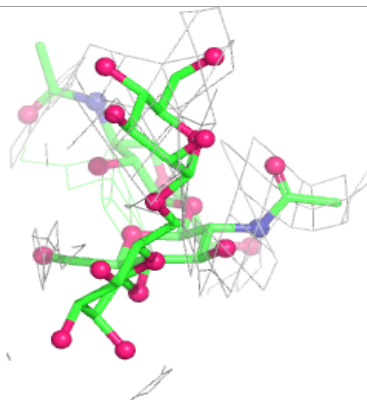
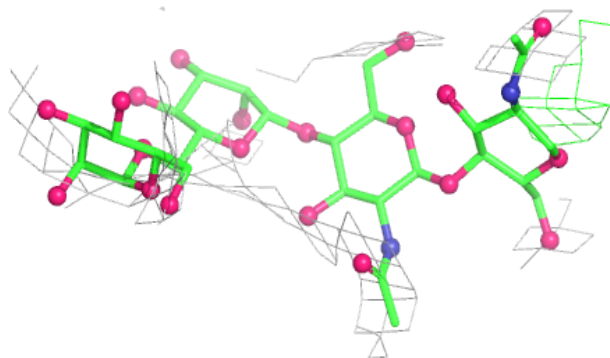
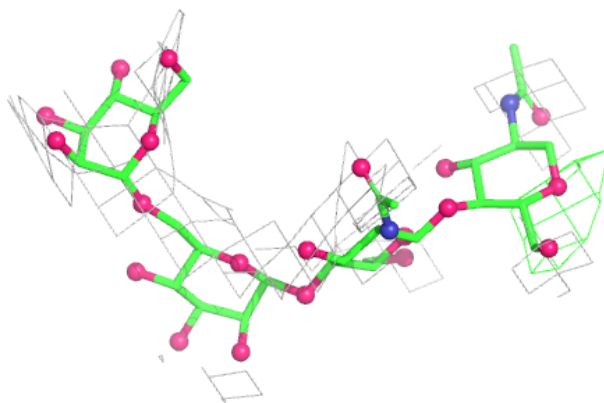
**Electron density around Chain Y:**

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

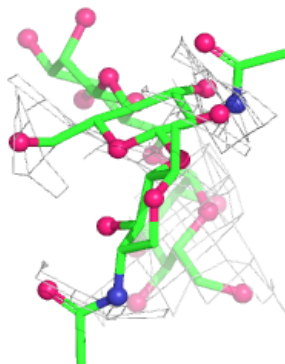
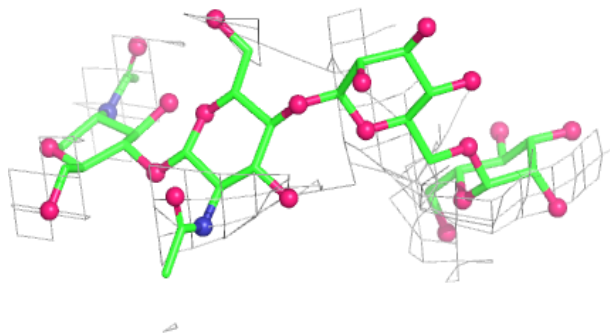
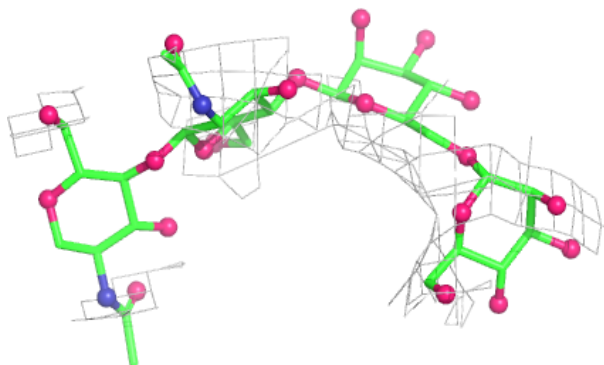


Electron density around Chain h:

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

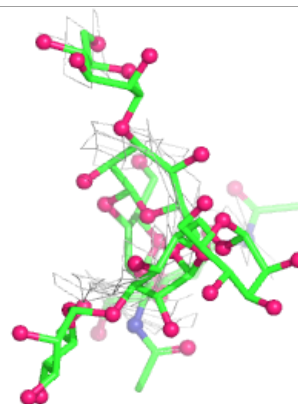
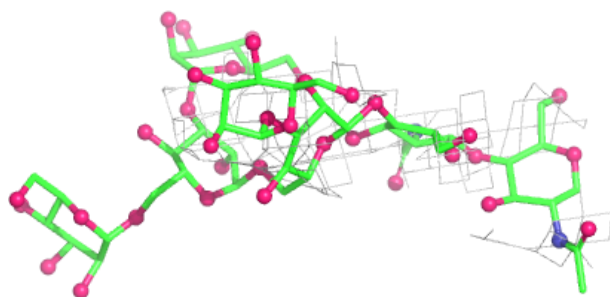
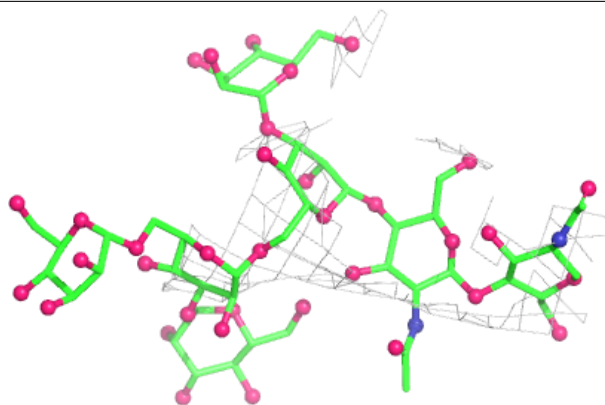
**Electron density around Chain q:**

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

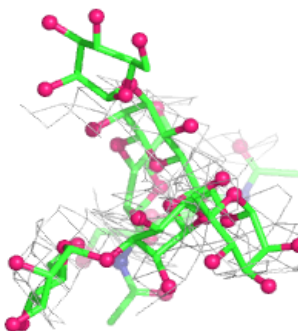
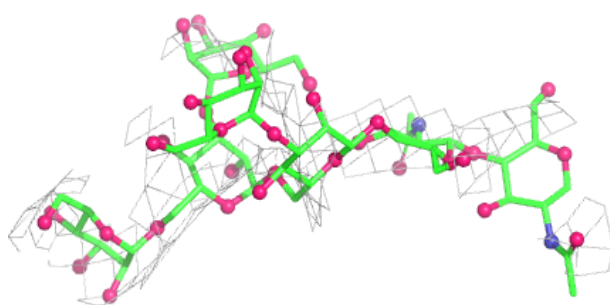
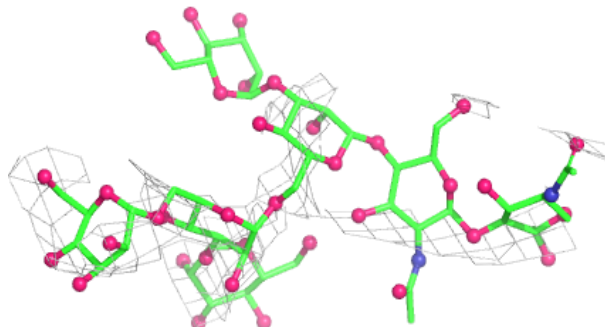


Electron density around Chain Z:

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

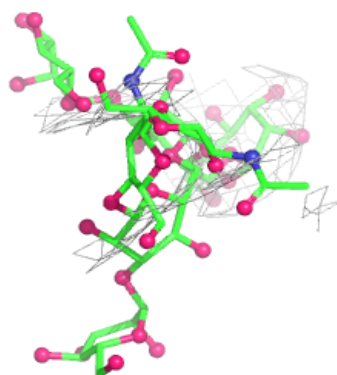
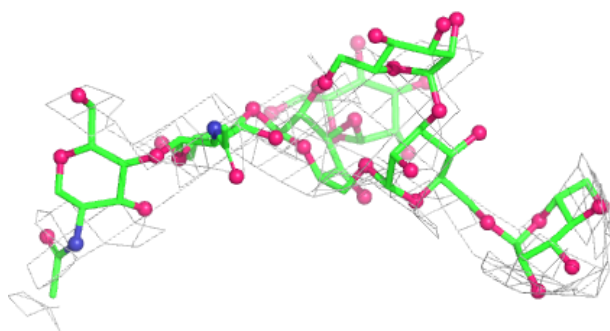
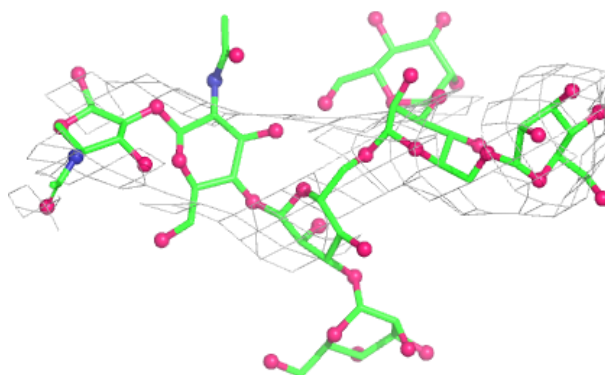
**Electron density around Chain i:**

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

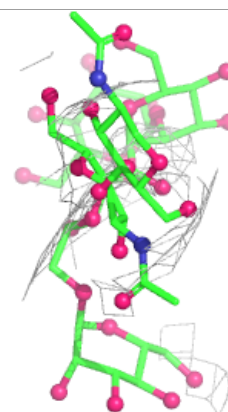
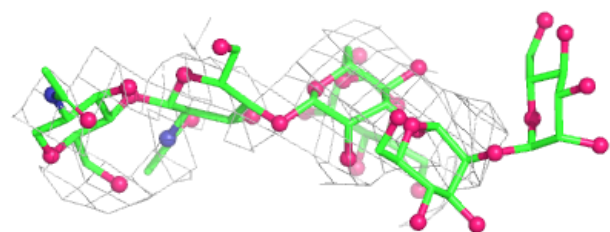
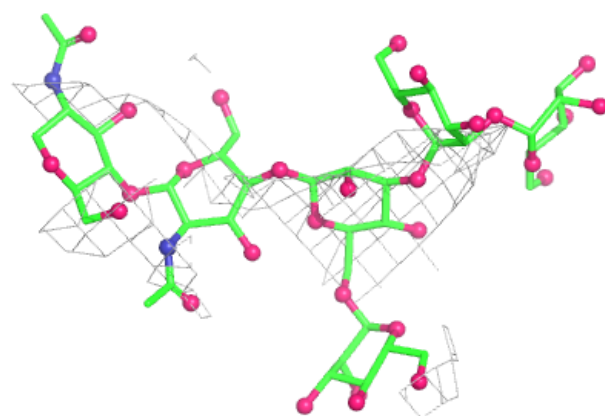


Electron density around Chain r:

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

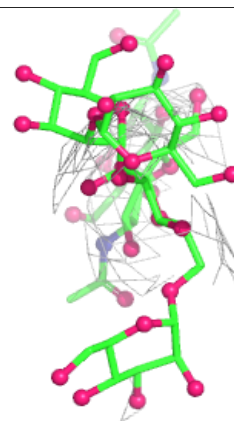
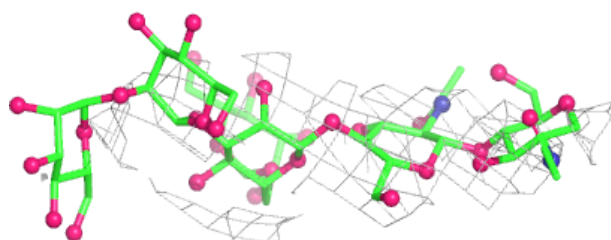
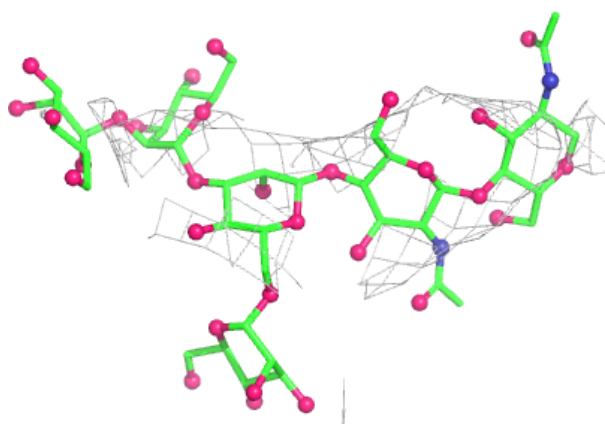
**Electron density around Chain a:**

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



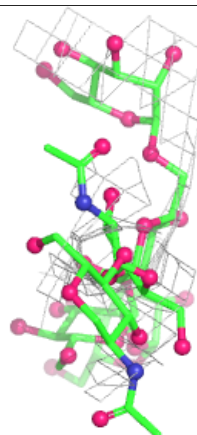
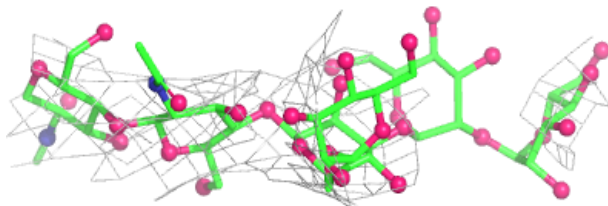
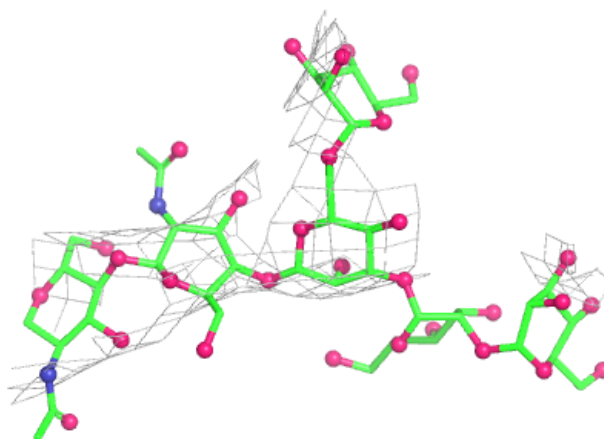
Electron density around Chain j:

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



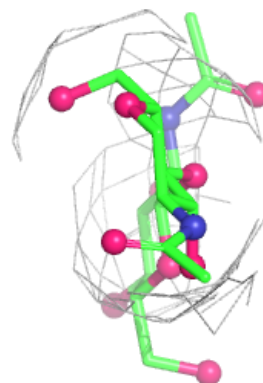
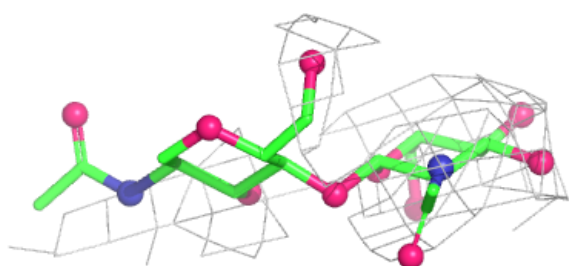
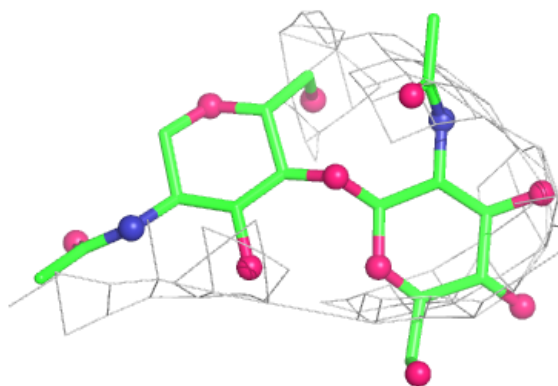
Electron density around Chain s:

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

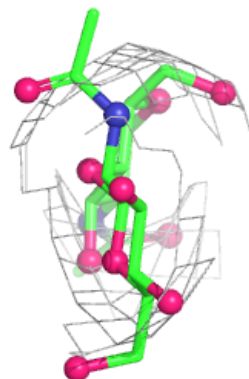
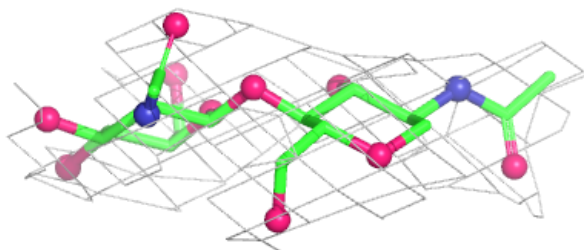
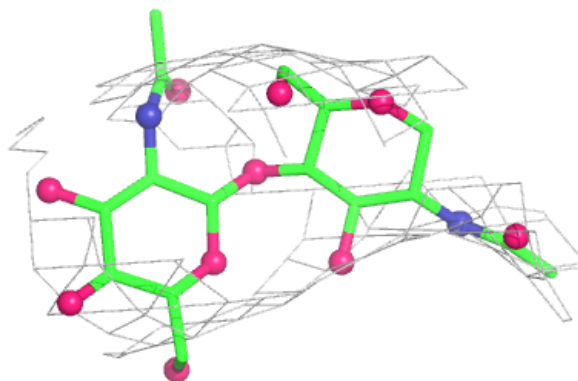


Electron density around Chain b:

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

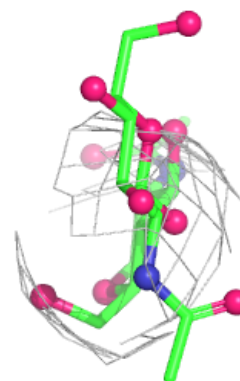
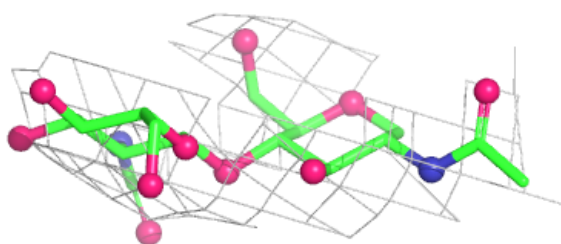
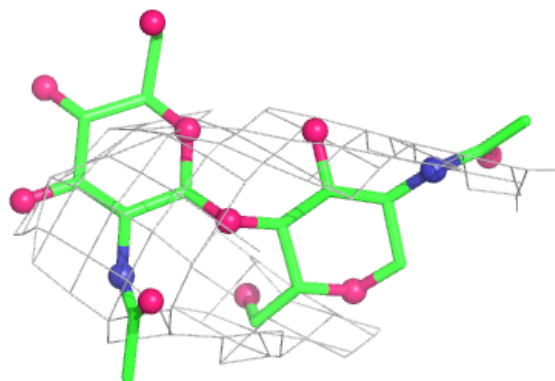
**Electron density around Chain k:**

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

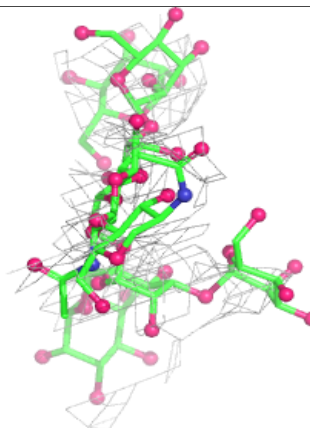
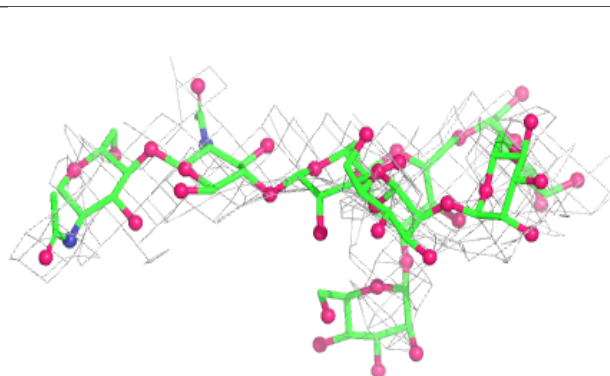
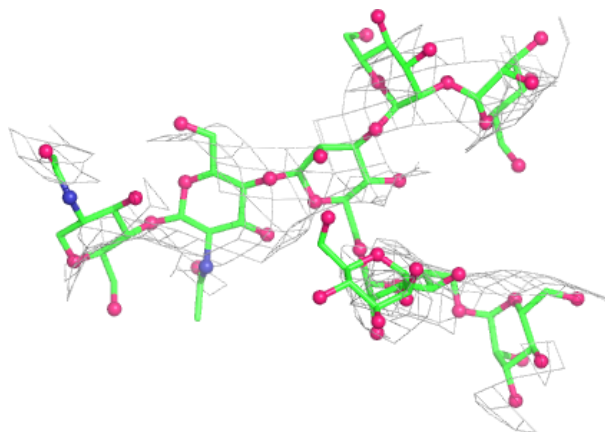


Electron density around Chain t:

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

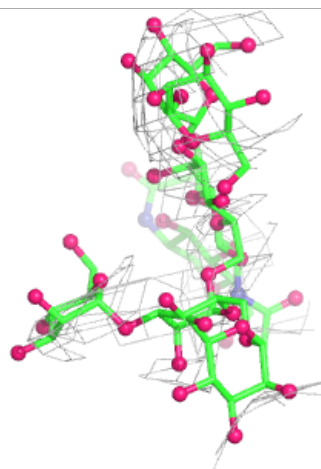
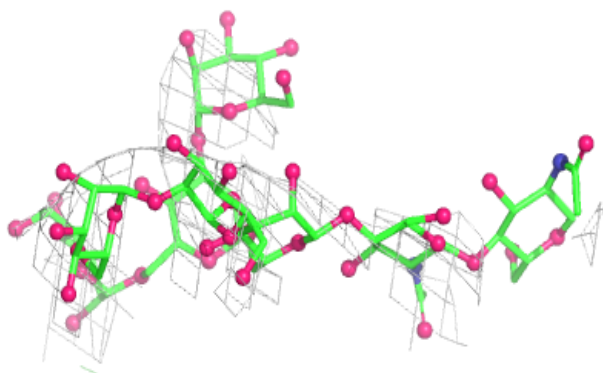
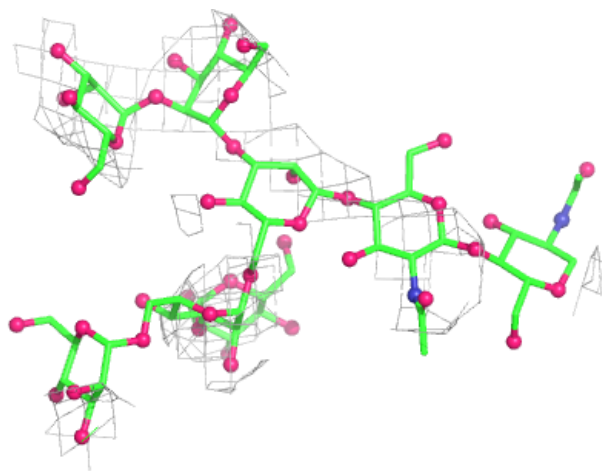
**Electron density around Chain d:**

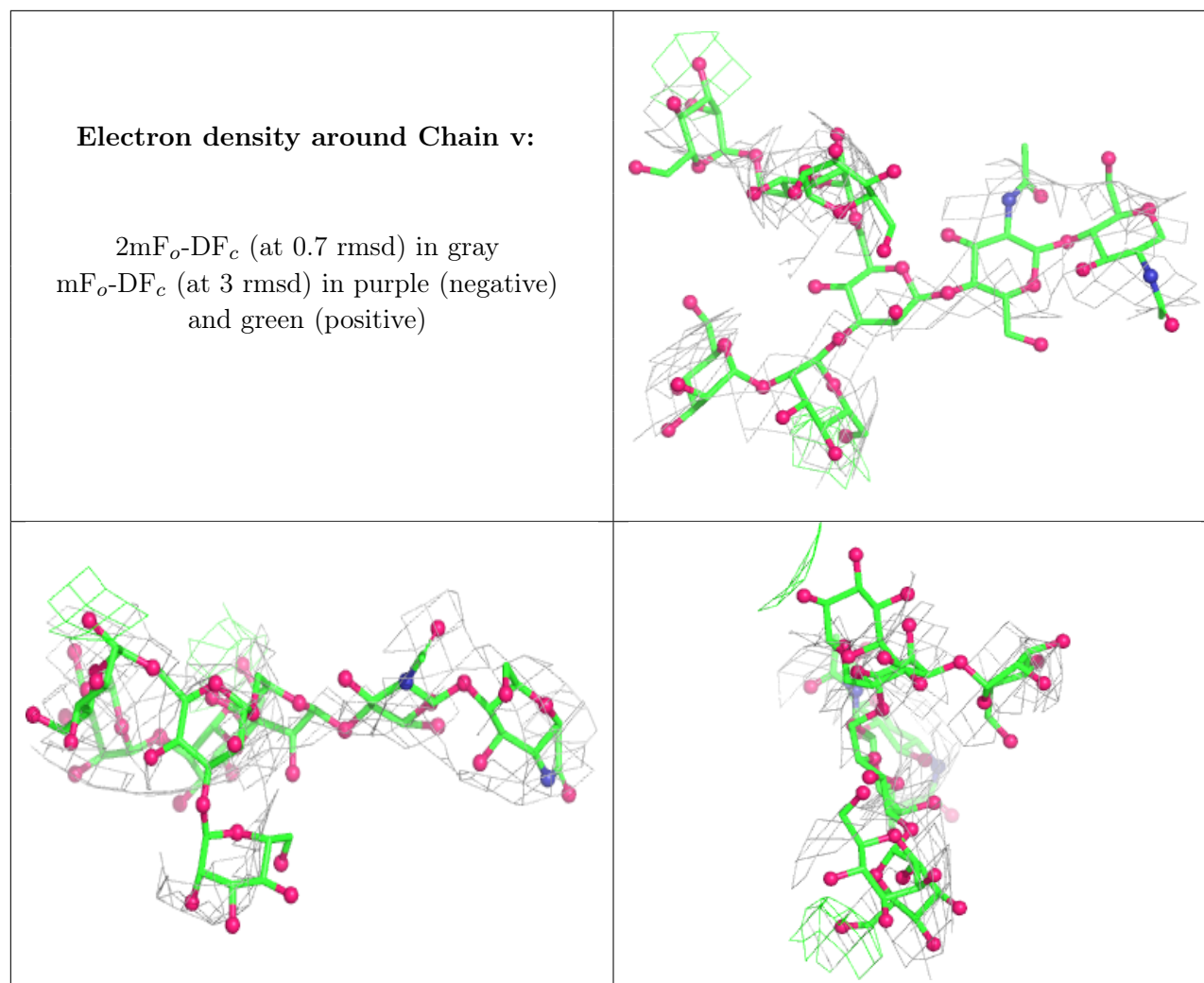
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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
15	NAG	J	702	14/15	0.49	0.08	480,482,485,487	0
15	NAG	F	606	14/15	0.50	0.11	460,464,467,468	0
15	NAG	F	653	14/15	0.53	0.09	399,399,399,399	0
15	NAG	G	651	14/15	0.53	0.21	448,451,453,454	0
15	NAG	J	703	14/15	0.56	0.24	511,511,511,511	0
15	NAG	G	653	14/15	0.57	0.09	431,431,431,431	0
15	NAG	F	651	14/15	0.59	0.15	425,429,432,434	0
15	NAG	G	606	14/15	0.60	0.07	449,452,455,456	0
15	NAG	Q	652	14/15	0.61	0.11	410,411,411,411	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	NAG	F	633	14/15	0.63	0.14	511,516,521,523	0
15	NAG	G	633	14/15	0.63	0.10	475,477,480,480	0
15	NAG	Q	606	14/15	0.72	0.10	474,477,479,480	0
15	NAG	Q	651	14/15	0.73	0.17	446,448,449,449	0
15	NAG	G	615	14/15	0.73	0.06	429,431,432,434	0
15	NAG	G	649	14/15	0.75	0.07	491,493,495,496	0
15	NAG	Q	615	14/15	0.76	0.07	499,500,501,502	0
15	NAG	Q	633	14/15	0.78	0.09	517,518,519,519	0
15	NAG	Q	649	14/15	0.79	0.12	505,508,510,511	0
15	NAG	A	703	14/15	0.79	0.12	461,461,461,461	0
15	NAG	Q	653	14/15	0.81	0.10	441,441,441,441	0
15	NAG	F	615	14/15	0.81	0.06	506,511,514,515	0
15	NAG	R	702	14/15	0.81	0.07	479,481,484,484	0
15	NAG	R	703	14/15	0.81	0.08	390,390,390,390	0
15	NAG	A	702	14/15	0.84	0.08	410,413,414,415	0
15	NAG	F	649	14/15	0.84	0.06	468,470,474,474	0
15	NAG	Q	650	14/15	0.85	0.10	351,352,354,354	0
15	NAG	F	652	14/15	0.85	0.17	405,407,410,411	0
15	NAG	G	652	14/15	0.86	0.10	302,308,311,311	0
15	NAG	R	701	14/15	0.86	0.11	448,450,452,452	0
15	NAG	J	701	14/15	0.87	0.07	503,510,514,514	0
15	NAG	F	650	14/15	0.89	0.07	345,348,352,354	0
15	NAG	G	650	14/15	0.89	0.14	347,349,352,353	0
15	NAG	A	701	14/15	0.90	0.07	406,407,409,409	0

6.5 Other polymers

There are no such residues in this entry.