



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:25 AM UTC

PDB ID : 3WHE / pdb_00003whe
Title : A new conserved neutralizing epitope at the globular head of hemagglutinin in H3N2 influenza viruses
Authors : Fujii, Y.; Sumida, T.; Shirouzu, M.; Yokoyama, S.
Deposited on : 2013-08-25
Resolution : 4.00 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

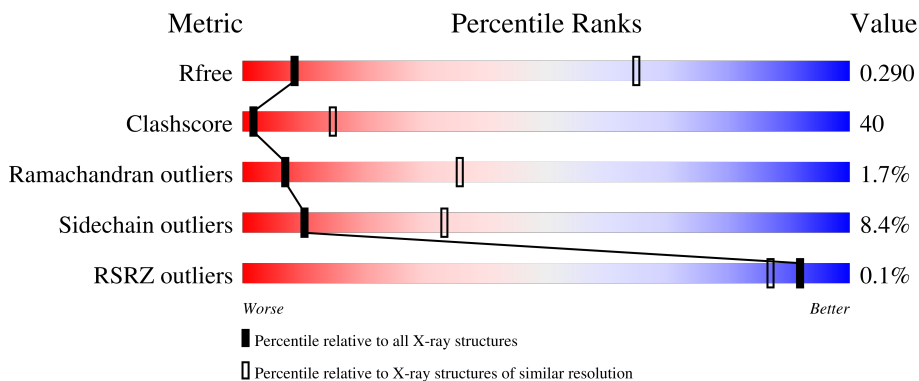
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	493	48% 47% 5%
1	B	493	45% 49% 5%
1	C	493	45% 50% 5%
1	D	493	47% 48% 5%
1	E	493	45% 50% 5%




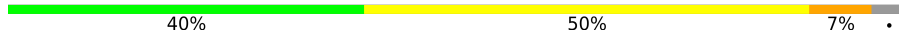
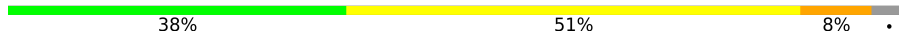
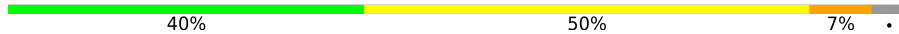
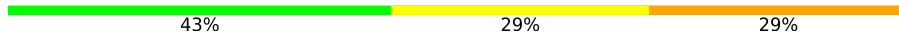
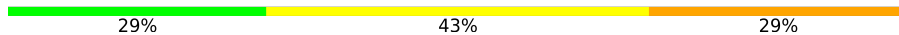
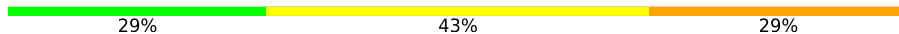
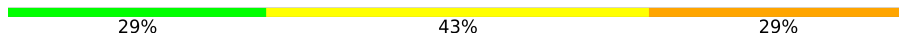
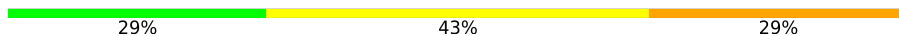
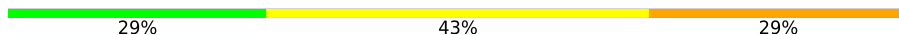
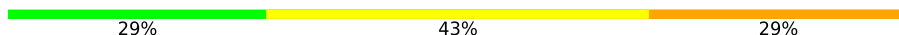
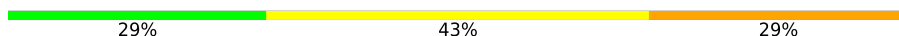
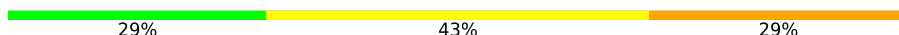
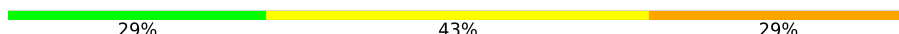
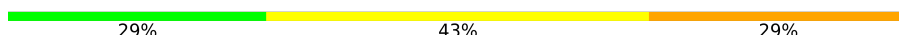
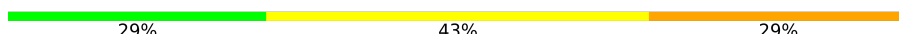

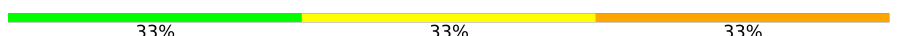

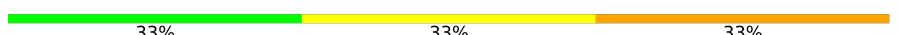


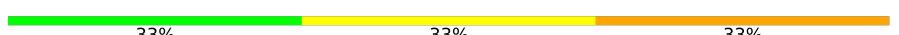
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Mol	Chain	Length	Quality of chain		
1	F	493	45%	49%	5%
1	G	493	47%	48%	5%
1	H	493	45%	49%	5%
1	I	493	45%	51%	5%
1	J	493	46%	49%	5%
1	K	493	46%	49%	5%
1	L	493	46%	49%	5%
2	1	226	30%	58%	12%
2	3	226	32%	57%	12%
2	5	226	32%	55%	12%
2	7	226	30%	58%	12%
2	9	226	31%	58%	12%
2	M	226	28%	59%	13%
2	O	226	30%	58%	12%
2	Q	226	29%	59%	12%
2	S	226	31%	57%	12%
2	U	226	31%	56%	12%
2	W	226	32%	55%	13%
2	Y	226	29%	58%	12%
3	0	220	38%	51%	7%
3	2	220	40%	49%	8%
3	4	220	39%	50%	8%
3	6	220	39%	50%	8%
3	8	220	40%	49%	7%
3	N	220	35%	54%	8%

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Mol	Chain	Length	Quality of chain
3	P	220	
3	R	220	
3	T	220	
3	V	220	
3	X	220	
3	Z	220	
4	BA	7	
4	EA	7	
4	HA	7	
4	a	7	
4	d	7	
4	g	7	
4	j	7	
4	m	7	
4	p	7	
4	s	7	
4	v	7	
4	y	7	
5	CA	6	
5	FA	6	
5	IA	6	
5	b	6	
5	e	6	
5	h	6	
5	k	6	

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Mol	Chain	Length	Quality of chain
5	n	6	
5	q	6	
5	t	6	
5	w	6	
5	z	6	
6	AA	3	
6	DA	3	
6	GA	3	
6	JA	3	
6	c	3	
6	f	3	
6	i	3	
6	l	3	
6	o	3	
6	r	3	
6	u	3	
6	x	3	

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
4	NAG	EA	2	-	-	X	-
5	NAG	h	2	-	-	X	-
5	NAG	k	2	-	-	X	-
5	NAG	q	2	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 88152 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	3878	2418	684	757	19	0	0	0
1	B	493	3878	2418	684	757	19	0	0	0
1	C	493	3878	2418	684	757	19	0	0	0
1	D	493	3878	2418	684	757	19	0	0	0
1	E	493	3878	2418	684	757	19	0	0	0
1	F	493	3878	2418	684	757	19	0	0	0
1	G	493	3878	2418	684	757	19	0	0	0
1	H	493	3878	2418	684	757	19	0	0	0
1	I	493	3878	2418	684	757	19	0	0	0
1	J	493	3878	2418	684	757	19	0	0	0
1	K	493	3878	2418	684	757	19	0	0	0
1	L	493	3878	2418	684	757	19	0	0	0

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	226	1697	1072	284	331	10	0	0	0
2	O	226	1697	1072	284	331	10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	S	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	U	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	W	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	Y	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	1	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	3	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	5	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	7	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	9	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

- Molecule 3 is a protein called immunoglobulin light chain.

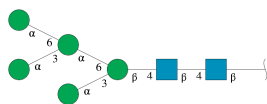
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	P	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	R	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	T	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	V	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	X	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	Z	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	2	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	4	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	6	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	8	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	0	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

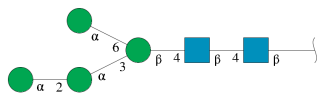
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	d	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	g	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	j	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	m	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	p	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	s	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	v	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	y	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	BA	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	EA	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	HA	7	Total	C	N	O	0	0	0
			83	46	2	35			

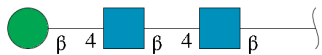
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(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
			Total	C	N	O			
5	b	6	72	40	2	30	0	0	0
5	e	6	72	40	2	30	0	0	0
5	h	6	72	40	2	30	0	0	0
5	k	6	72	40	2	30	0	0	0
5	n	6	72	40	2	30	0	0	0
5	q	6	72	40	2	30	0	0	0
5	t	6	72	40	2	30	0	0	0
5	w	6	72	40	2	30	0	0	0
5	z	6	72	40	2	30	0	0	0
5	CA	6	72	40	2	30	0	0	0
5	FA	6	72	40	2	30	0	0	0
5	IA	6	72	40	2	30	0	0	0

- Molecule 6 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.



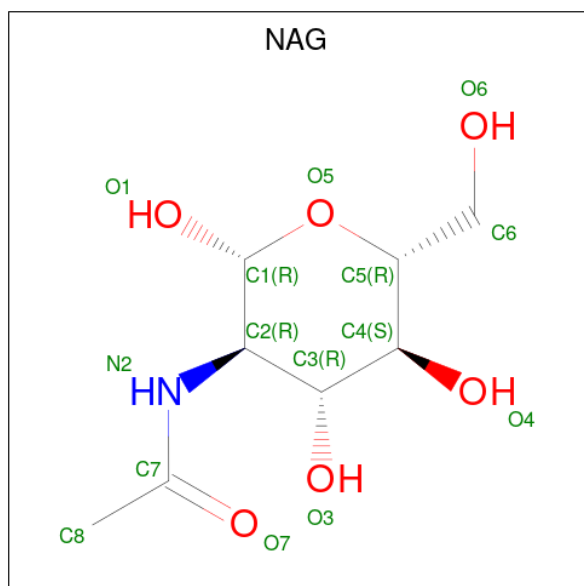
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	c	3	39	22	2	15	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	f	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	i	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	o	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	u	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	x	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	AA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	DA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	GA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	JA	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		

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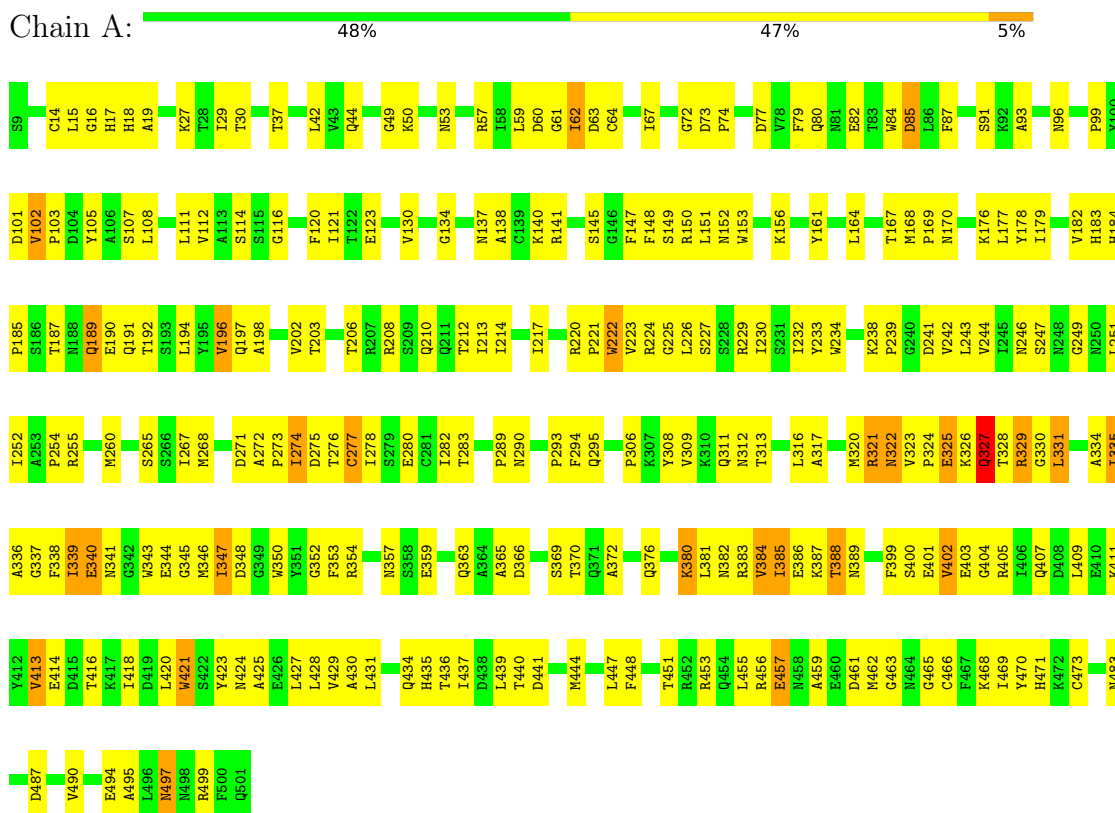
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

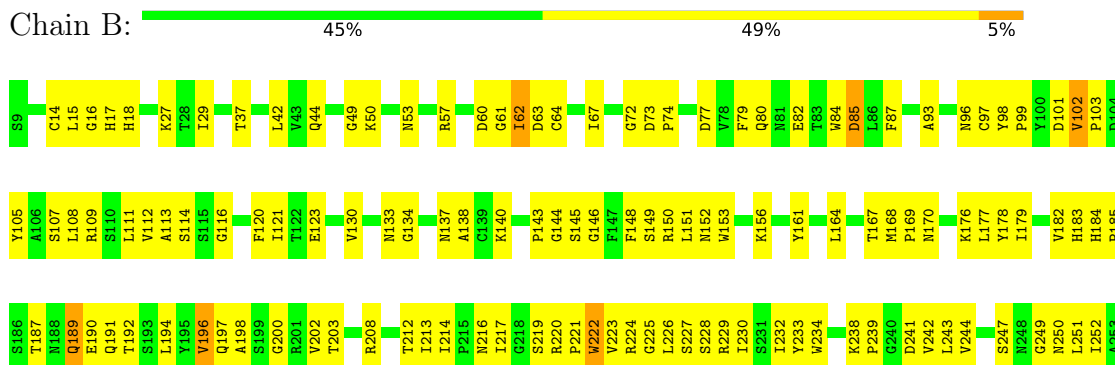
3 Residue-property plots [i](#)

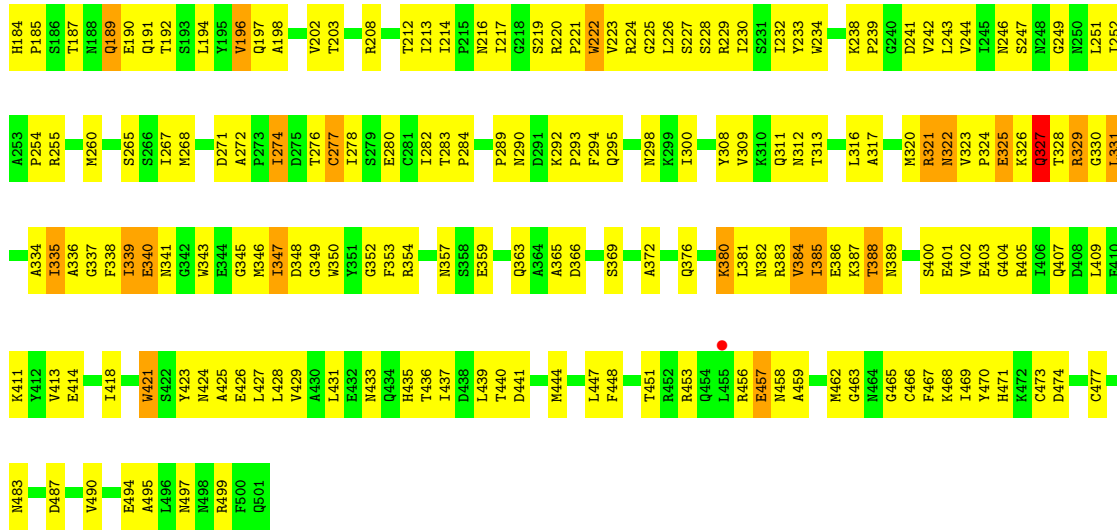
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Hemagglutinin

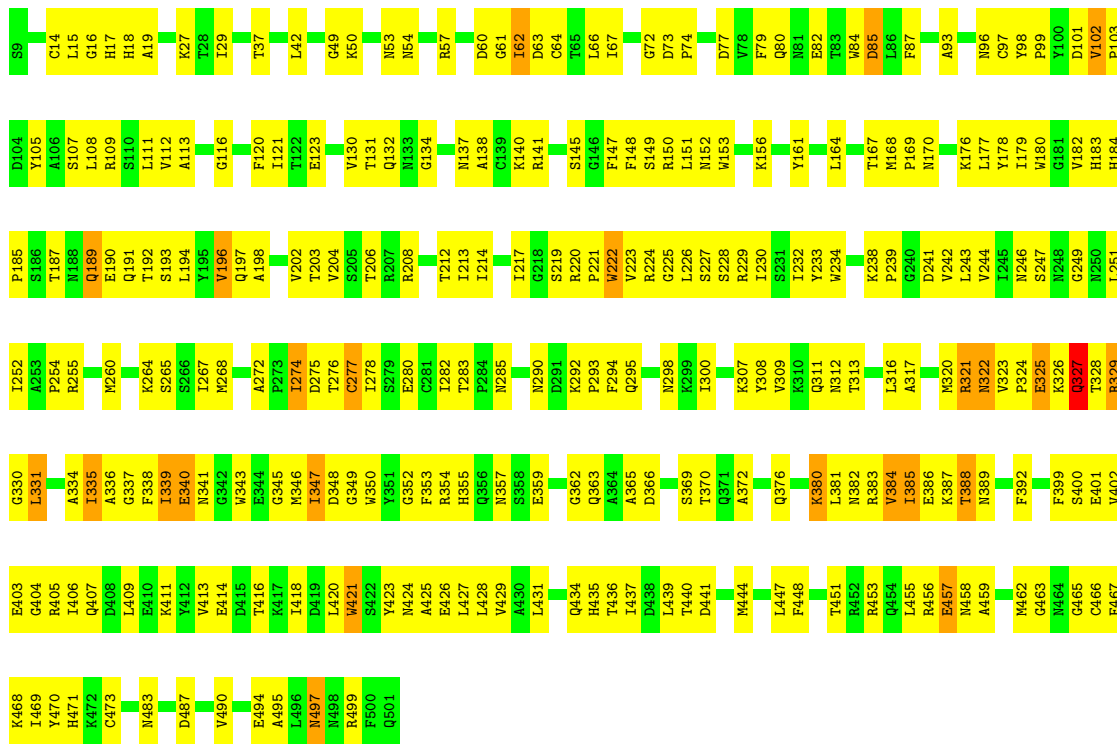


- Molecule 1: Hemagglutinin

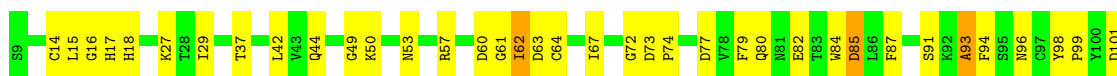


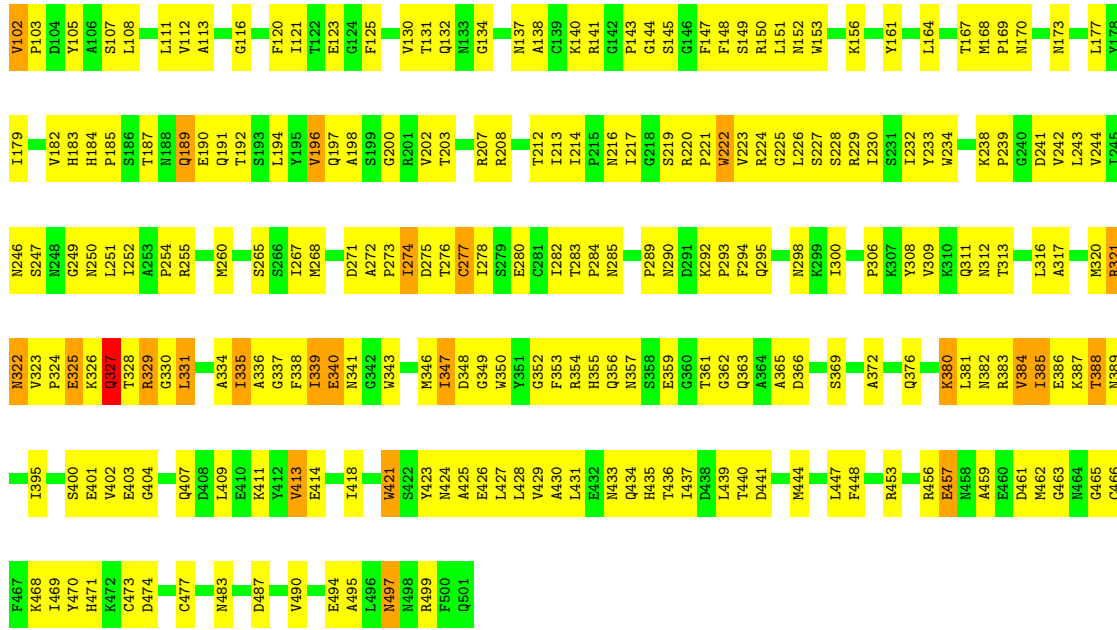


● Molecule 1: Hemagglutinin

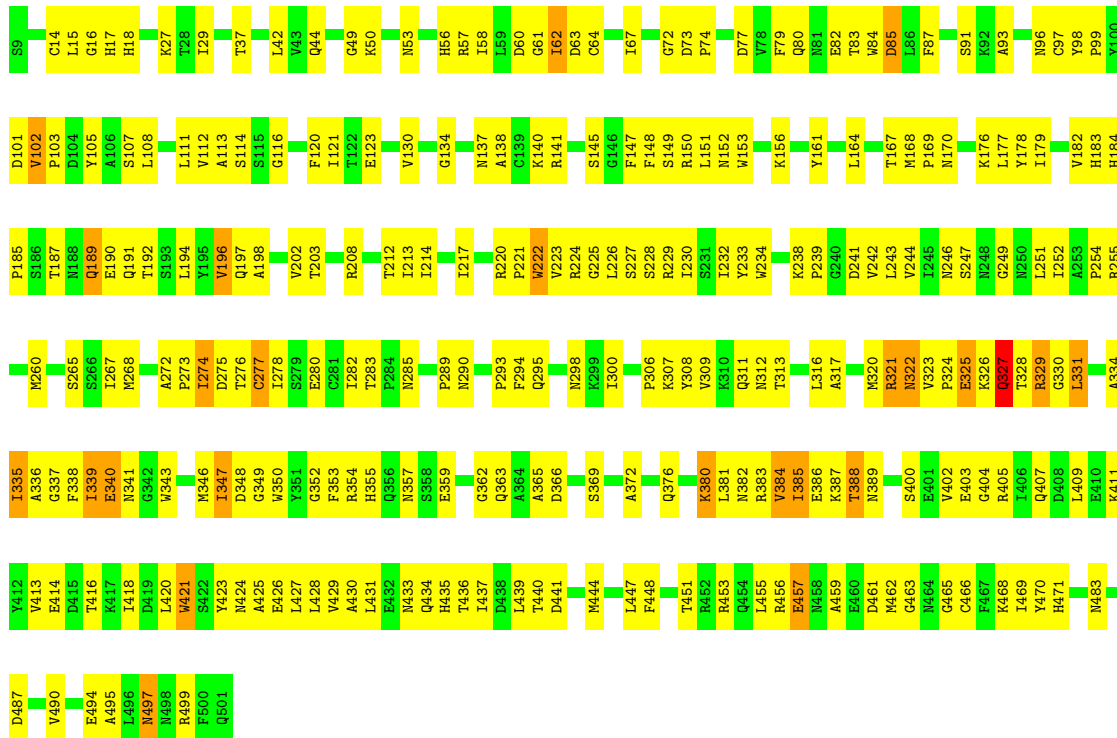


● Molecule 1: Hemagglutinin





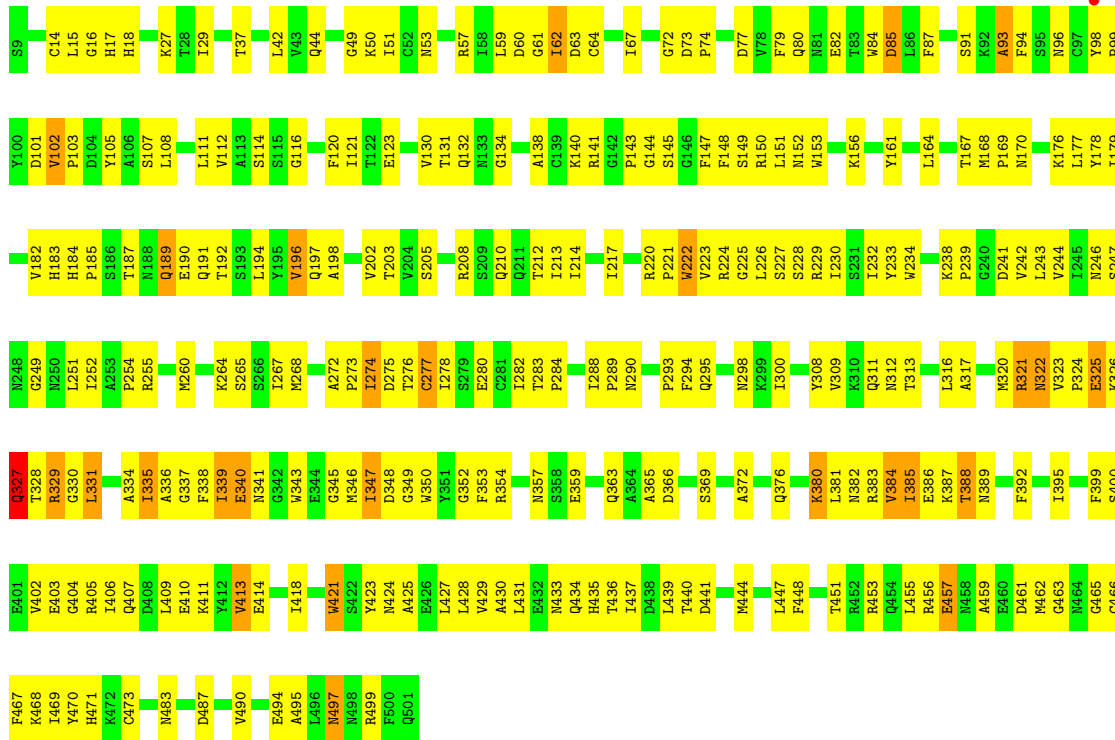
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

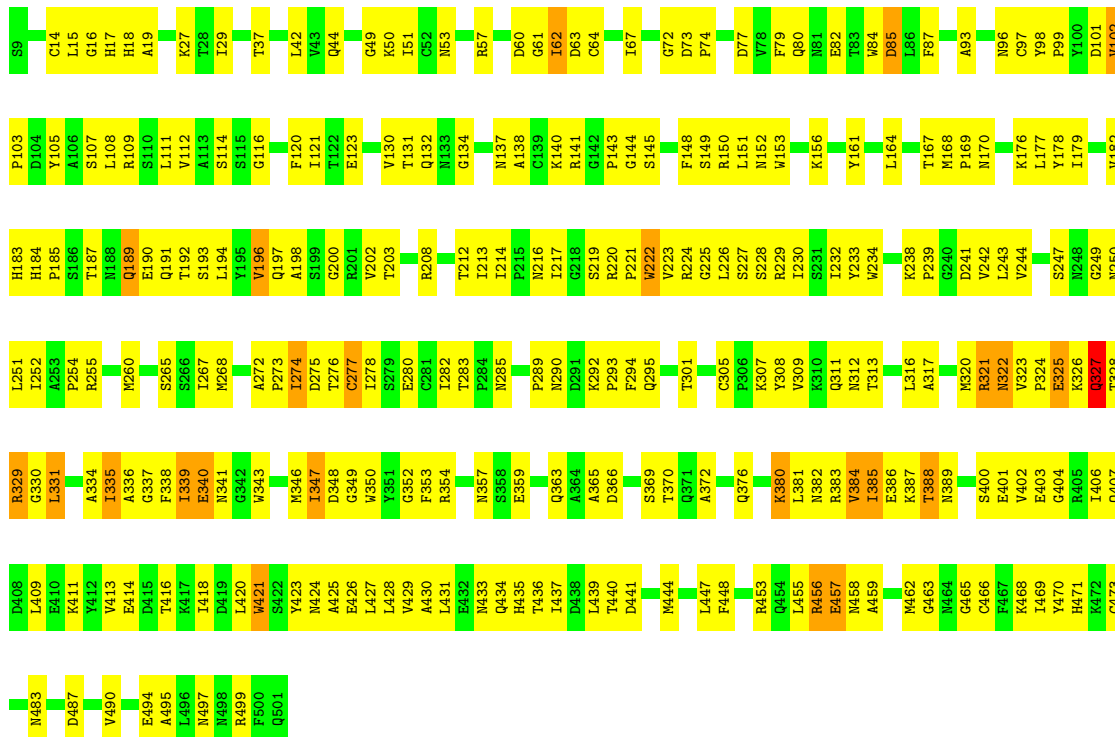


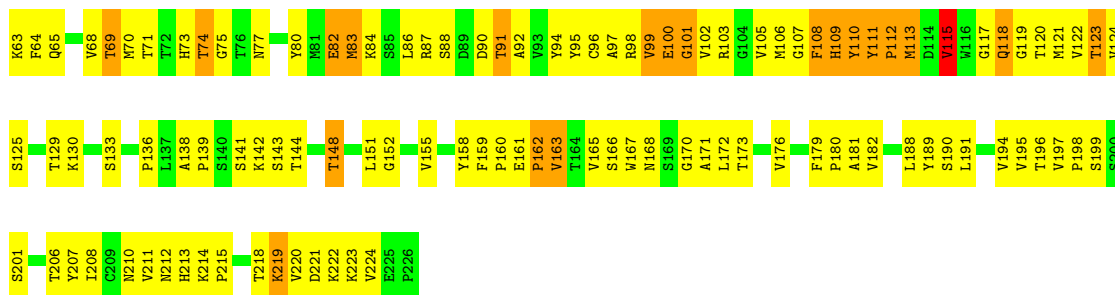
Chain J:  46% 49% 5%



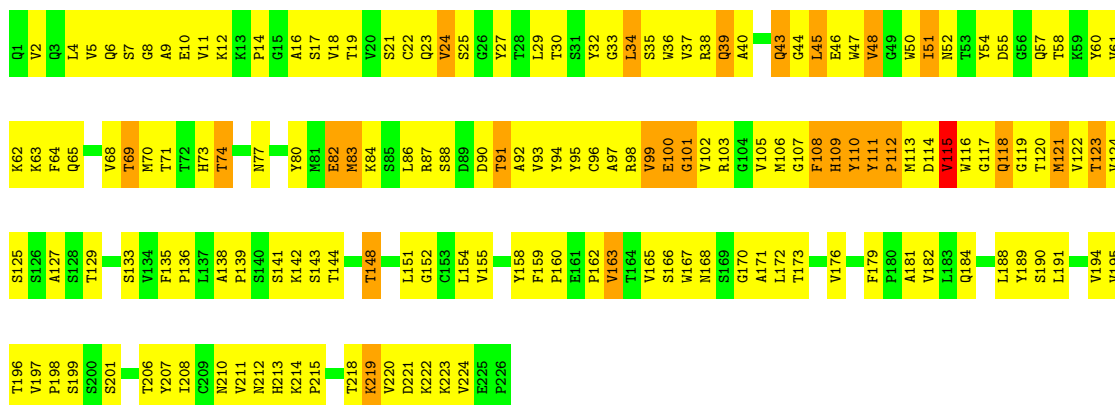
• Molecule 1: Hemagglutinin

Chain K:  46% 49% 5%

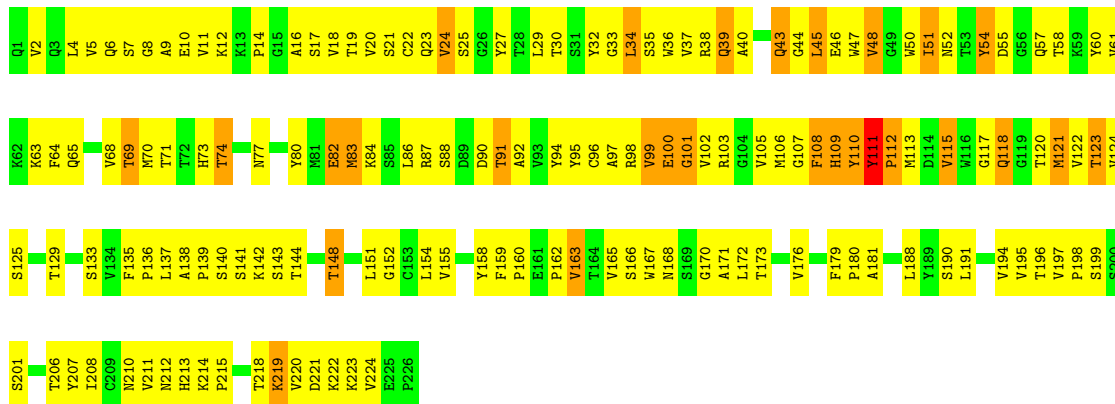




• Molecule 2: immunoglobulin heavy chain

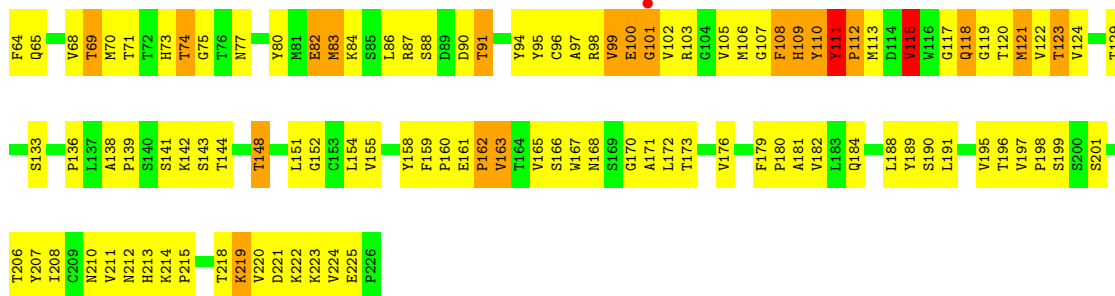


• Molecule 2: immunoglobulin heavy chain

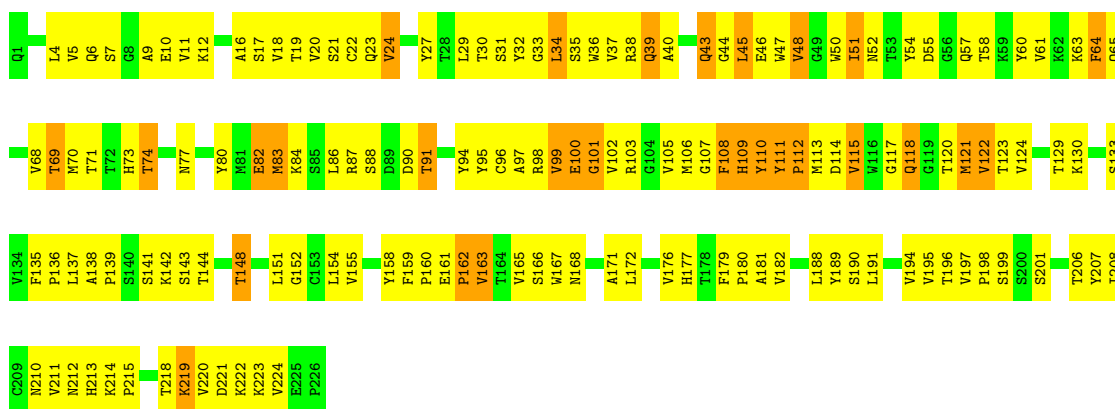


• Molecule 2: immunoglobulin heavy chain

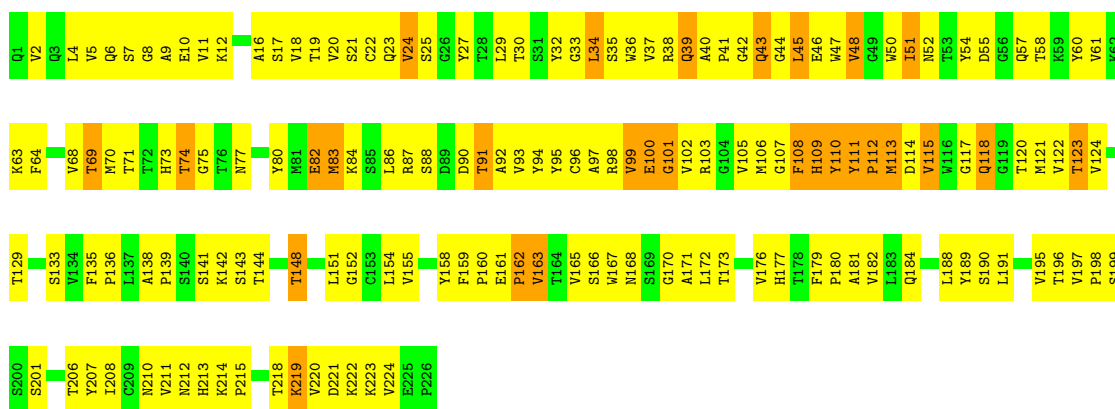




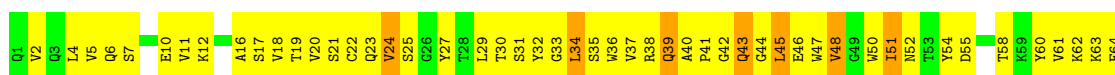
• Molecule 2: immunoglobulin heavy chain

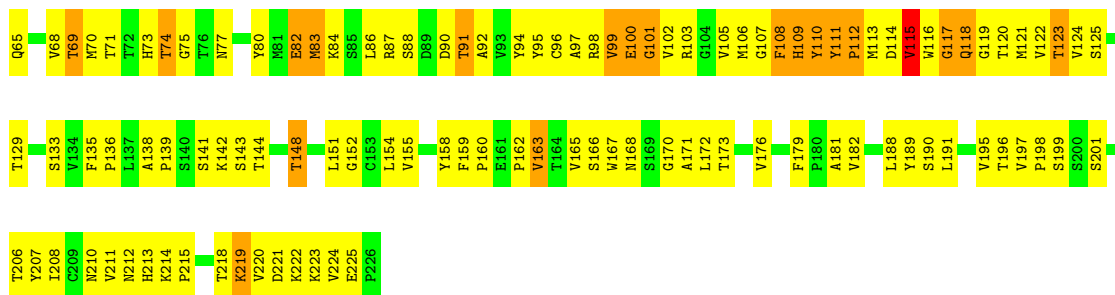


• Molecule 2: immunoglobulin heavy chain

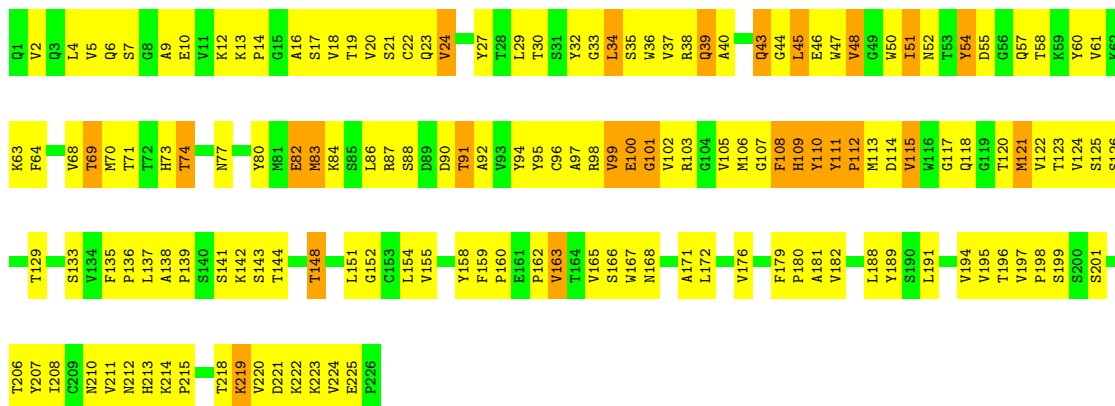


• Molecule 2: immunoglobulin heavy chain

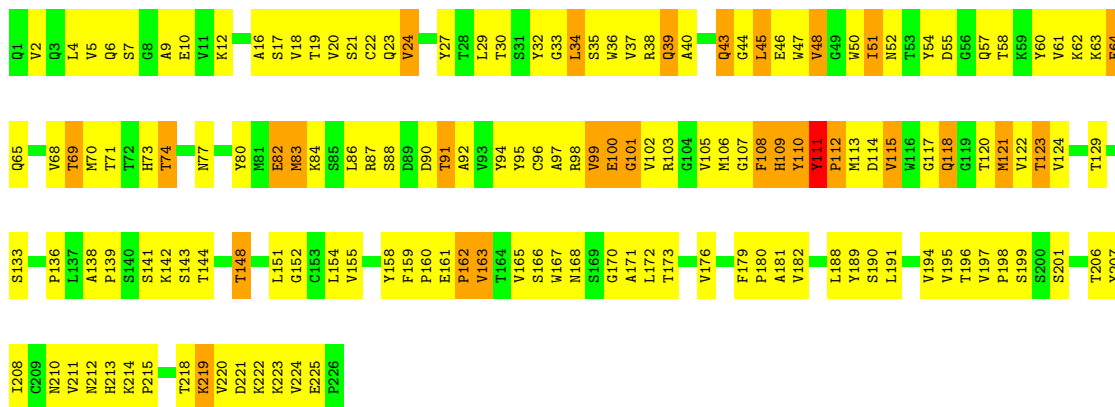




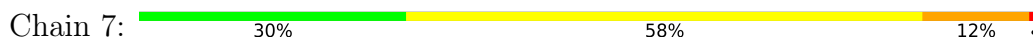
• Molecule 2: immunoglobulin heavy chain

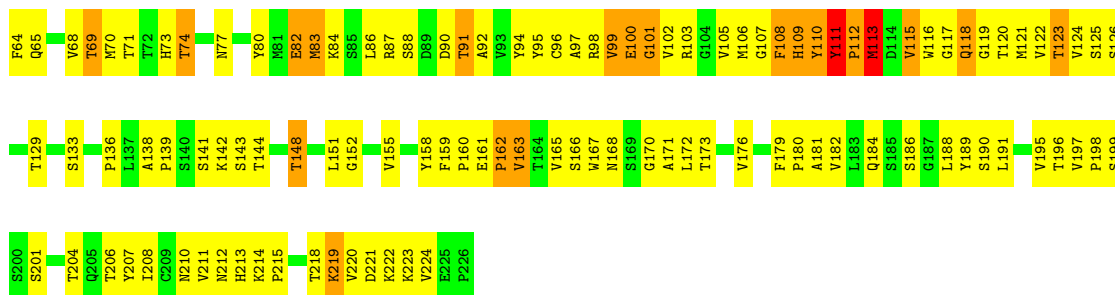


• Molecule 2: immunoglobulin heavy chain

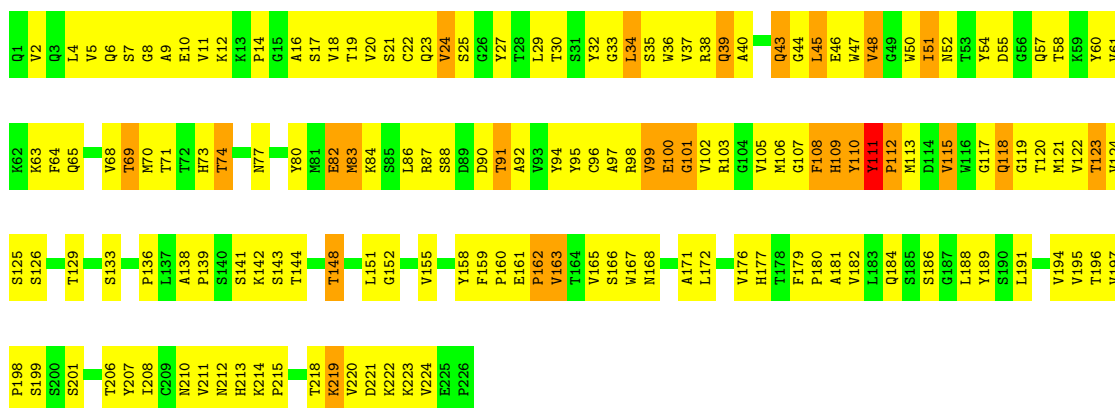


• Molecule 2: immunoglobulin heavy chain

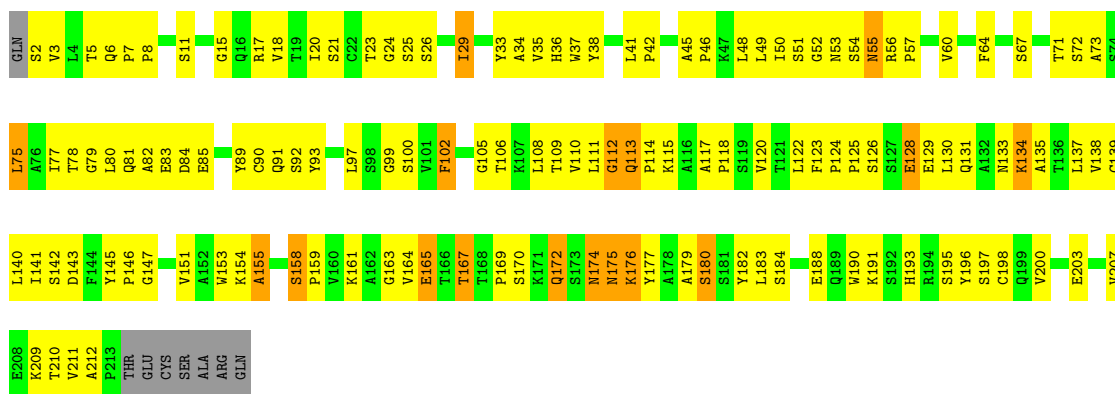




• Molecule 2: immunoglobulin heavy chain

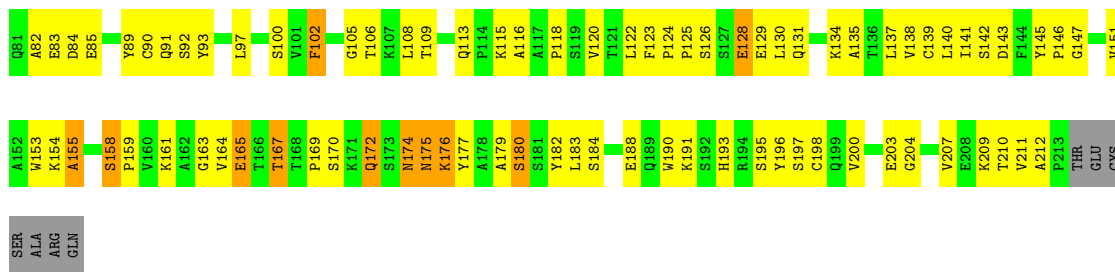


• Molecule 3: immunoglobulin light chain

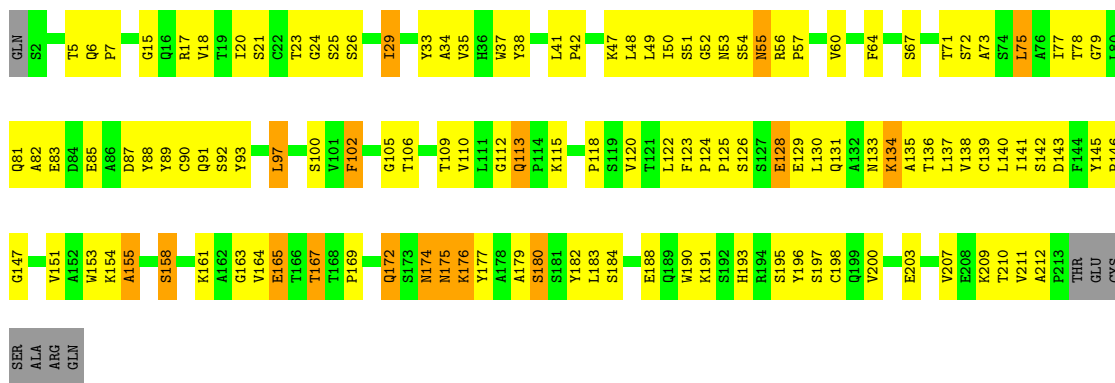


• Molecule 3: immunoglobulin light chain

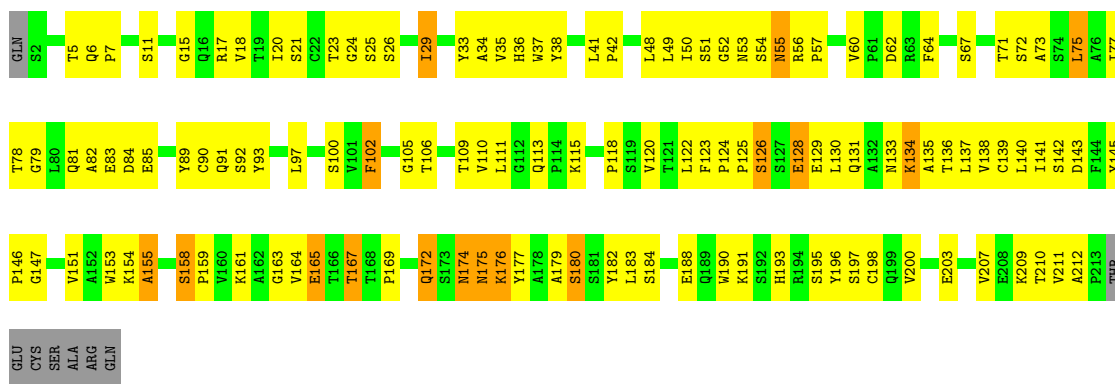




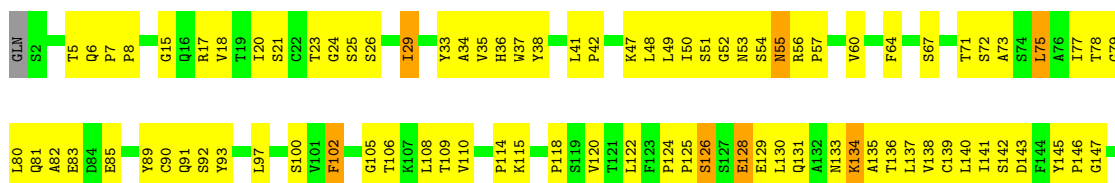
• Molecule 3: immunoglobulin light chain

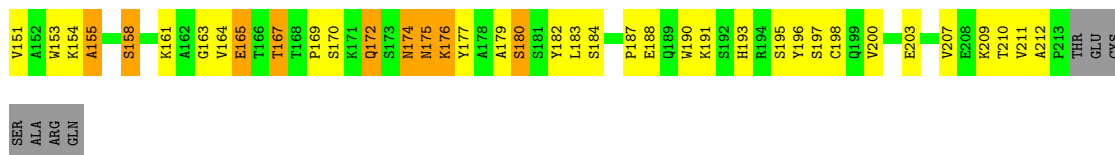


• Molecule 3: immunoglobulin light chain

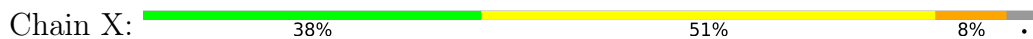


• Molecule 3: immunoglobulin light chain

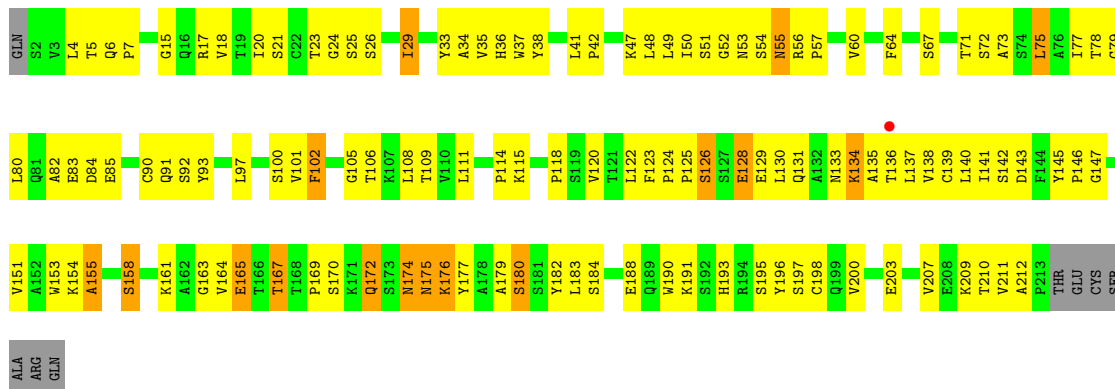
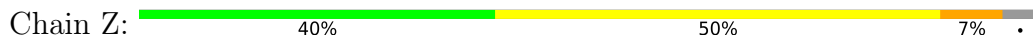




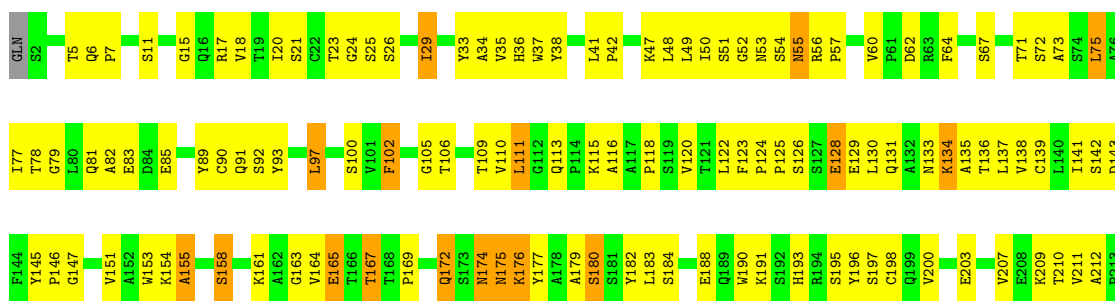
• Molecule 3: immunoglobulin light chain



• Molecule 3: immunoglobulin light chain



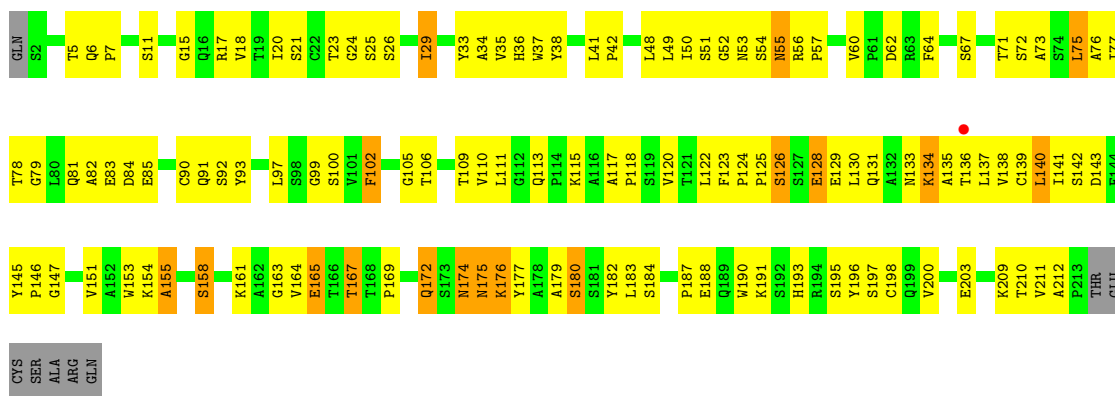
• Molecule 3: immunoglobulin light chain



THR
GLU
CYS
SER
ALA
ARG
GLN

• Molecule 3: immunoglobulin light chain

Chain 4: 39% 50% 8%



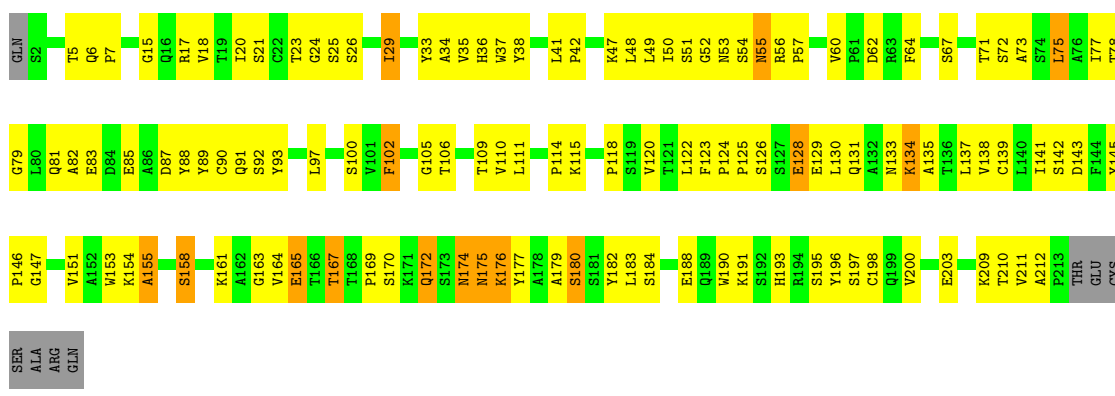
• Molecule 3: immunoglobulin light chain

Chain 6: 39% 50% 8%

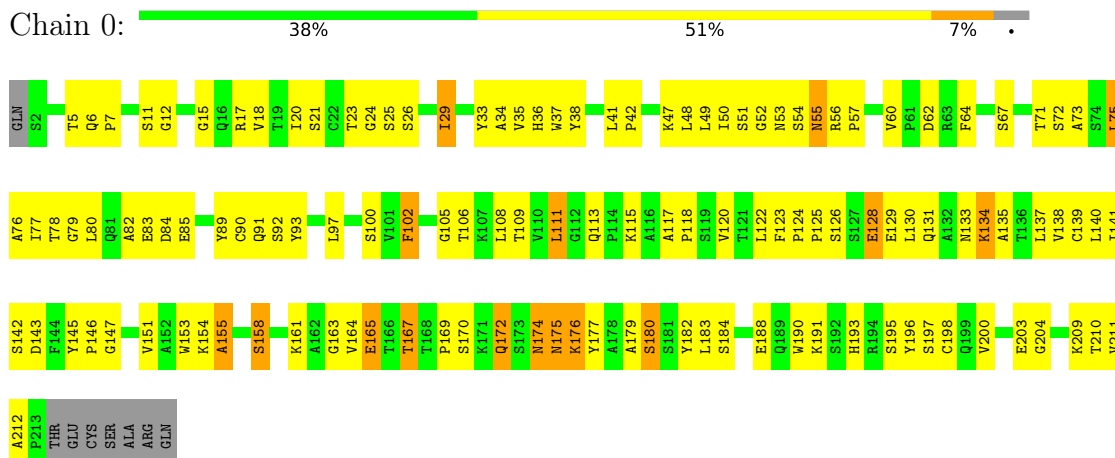


• Molecule 3: immunoglobulin light chain

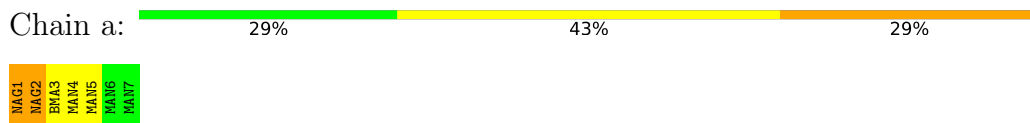
Chain 8: 40% 49% 7%



- Molecule 3: immunoglobulin light chain



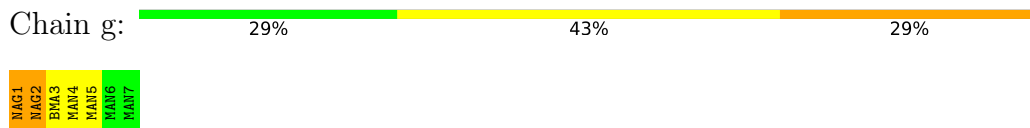
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



- Molecule 4: 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

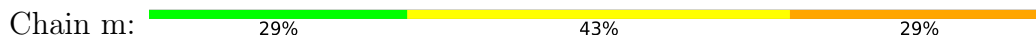


- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 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



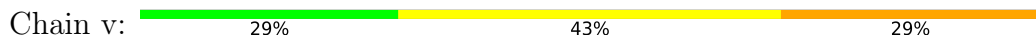
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



- Molecule 4: 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

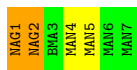


- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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 BA:  43% 29% 29%



- Molecule 4: 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 EA:  29% 43% 29%

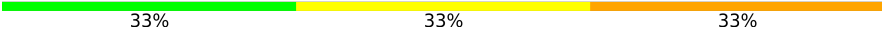


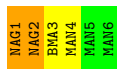
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:  29% 43% 29%



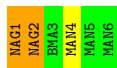
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 33% 33%



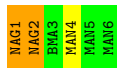
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 17% 33%

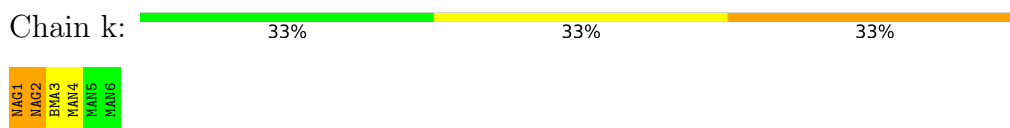


- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  50% 17% 33%



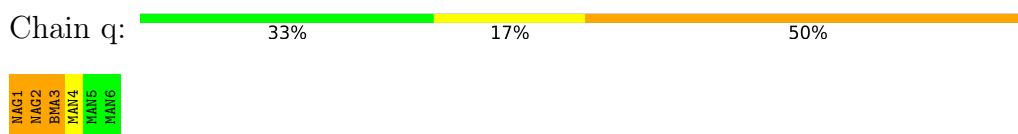
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



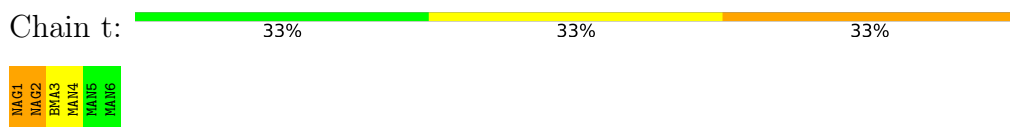
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



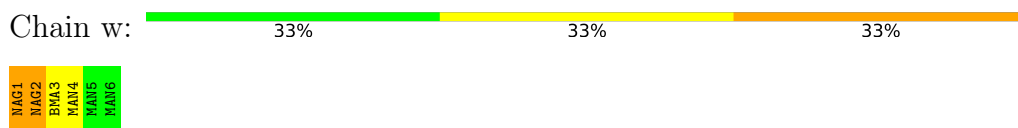
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

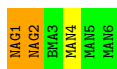


- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

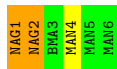


- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

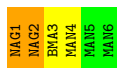




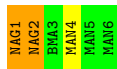
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



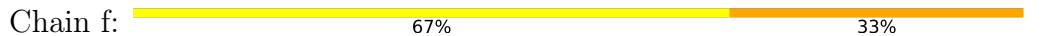
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

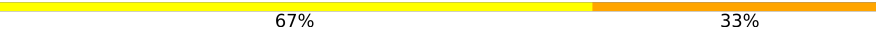


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  67% 33%

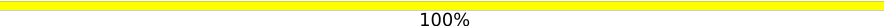
MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%


MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  33% 67%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  67% 33%


MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:  100%

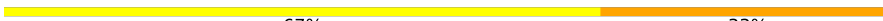
MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:  100%


MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	391.04Å 241.17Å 223.21Å 90.00° 123.62° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-4.00) 98.0 (30.00-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.98Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.235 , 0.308 0.282 , 0.290	Depositor DCC
R_{free} test set	7106 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	180.3	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 164.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.063 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	88152	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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

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	0.28	0/3959	0.79	5/5369 (0.1%)
1	B	0.27	0/3959	0.78	5/5369 (0.1%)
1	C	0.28	0/3959	0.79	5/5369 (0.1%)
1	D	0.28	0/3959	0.78	5/5369 (0.1%)
1	E	0.28	0/3959	0.79	5/5369 (0.1%)
1	F	0.28	0/3959	0.79	5/5369 (0.1%)
1	G	0.28	0/3959	0.79	5/5369 (0.1%)
1	H	0.28	0/3959	0.79	4/5369 (0.1%)
1	I	0.28	0/3959	0.79	6/5369 (0.1%)
1	J	0.28	0/3959	0.79	5/5369 (0.1%)
1	K	0.28	0/3959	0.79	5/5369 (0.1%)
1	L	0.28	0/3959	0.79	5/5369 (0.1%)
2	1	0.29	0/1739	0.82	1/2371 (0.0%)
2	3	0.29	0/1739	0.82	1/2371 (0.0%)
2	5	0.29	0/1739	0.81	2/2371 (0.1%)
2	7	0.30	0/1739	0.83	3/2371 (0.1%)
2	9	0.30	0/1739	0.83	2/2371 (0.1%)
2	M	0.29	0/1739	0.83	2/2371 (0.1%)
2	O	0.29	0/1739	0.82	2/2371 (0.1%)
2	Q	0.30	0/1739	0.84	2/2371 (0.1%)
2	S	0.29	0/1739	0.82	2/2371 (0.1%)
2	U	0.29	0/1739	0.83	2/2371 (0.1%)
2	W	0.29	0/1739	0.82	1/2371 (0.0%)
2	Y	0.29	0/1739	0.83	2/2371 (0.1%)
3	0	0.31	0/1586	0.87	4/2166 (0.2%)
3	2	0.31	0/1586	0.87	4/2166 (0.2%)
3	4	0.31	0/1586	0.87	4/2166 (0.2%)
3	6	0.31	0/1586	0.87	4/2166 (0.2%)
3	8	0.31	0/1586	0.87	4/2166 (0.2%)
3	N	0.31	0/1586	0.92	7/2166 (0.3%)
3	P	0.31	0/1586	0.88	4/2166 (0.2%)
3	R	0.31	0/1586	0.92	7/2166 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	T	0.31	0/1586	0.87	4/2166 (0.2%)
3	V	0.33	0/1586	0.88	4/2166 (0.2%)
3	X	0.32	0/1586	0.87	4/2166 (0.2%)
3	Z	0.31	0/1586	0.87	4/2166 (0.2%)
All	All	0.29	0/87408	0.82	136/118872 (0.1%)

There are no bond length outliers.

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	113	GLN	CA-C-N	8.55	128.62	119.90
3	N	113	GLN	C-N-CA	8.55	128.62	119.90
3	R	113	GLN	CA-C-N	8.54	128.61	119.90
3	R	113	GLN	C-N-CA	8.54	128.61	119.90
3	R	155	ALA	N-CA-C	-8.51	99.63	110.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3743	268	0
1	B	3878	0	3743	286	0
1	C	3878	0	3743	287	0
1	D	3878	0	3743	285	0
1	E	3878	0	3743	293	0
1	F	3878	0	3743	292	0
1	G	3878	0	3743	262	0
1	H	3878	0	3743	272	0
1	I	3878	0	3743	266	0
1	J	3878	0	3743	271	0
1	K	3878	0	3743	267	0
1	L	3878	0	3743	284	0
2	1	1697	0	1668	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	1697	0	1668	199	2
2	5	1697	0	1668	195	0
2	7	1697	0	1668	202	0
2	9	1697	0	1668	198	0
2	M	1697	0	1668	221	0
2	O	1697	0	1668	205	0
2	Q	1697	0	1668	196	0
2	S	1697	0	1668	206	0
2	U	1697	0	1668	213	0
2	W	1697	0	1668	216	0
2	Y	1697	0	1668	198	0
3	0	1549	0	1503	137	0
3	2	1549	0	1503	134	0
3	4	1549	0	1503	138	0
3	6	1549	0	1503	138	0
3	8	1549	0	1503	129	0
3	N	1549	0	1503	157	0
3	P	1549	0	1503	133	0
3	R	1549	0	1503	139	0
3	T	1549	0	1503	137	0
3	V	1549	0	1503	144	0
3	X	1549	0	1503	145	0
3	Z	1549	0	1503	135	0
4	BA	83	0	70	4	0
4	EA	83	0	70	7	0
4	HA	83	0	70	5	0
4	a	83	0	70	4	0
4	d	83	0	70	5	0
4	g	83	0	70	1	0
4	j	83	0	70	4	0
4	m	83	0	70	2	0
4	p	83	0	70	2	0
4	s	83	0	70	2	0
4	v	83	0	70	2	0
4	y	83	0	70	1	0
5	CA	72	0	61	3	0
5	FA	72	0	61	3	0
5	IA	72	0	61	5	0
5	b	72	0	61	3	0
5	e	72	0	61	3	0
5	h	72	0	61	10	0
5	k	72	0	61	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	n	72	0	61	3	0
5	q	72	0	61	12	0
5	t	72	0	61	3	0
5	w	72	0	61	3	0
5	z	72	0	61	5	0
6	AA	39	0	34	1	0
6	DA	39	0	34	1	0
6	GA	39	0	34	1	0
6	JA	39	0	34	1	0
6	c	39	0	34	1	0
6	f	39	0	34	1	0
6	i	39	0	34	1	0
6	l	39	0	34	1	0
6	o	39	0	34	1	0
6	r	39	0	34	1	0
6	u	39	0	34	2	0
6	x	39	0	34	1	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
7	E	28	0	26	0	0
7	F	28	0	26	0	0
7	G	28	0	26	0	0
7	H	28	0	26	0	0
7	I	28	0	26	0	0
7	J	28	0	26	0	0
7	K	28	0	26	0	0
7	L	28	0	26	0	0
All	All	88152	0	85260	6964	2

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 40.

The worst 5 of 6964 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)
2:5:136:PRO:O	3:6:126:SER:HB3	1.52	1.09
3:2:143:ASP:HA	3:2:176:LYS:HG3	1.35	1.08
3:T:143:ASP:HA	3:T:176:LYS:HG3	1.35	1.08
3:0:143:ASP:HA	3:0:176:LYS:HG3	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:LEU:HD22	1:G:331:LEU:H	1.19	1.08

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:171:ALA:CB	2:3:171:ALA:CB[2_556]	1.73	0.47
2:3:206:THR:OG1	2:3:206:THR:OG1[2_556]	1.74	0.46

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	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	10	42
1	B	491/493 (100%)	425 (87%)	60 (12%)	6 (1%)	10	42
1	C	491/493 (100%)	427 (87%)	57 (12%)	7 (1%)	9	39
1	D	491/493 (100%)	429 (87%)	55 (11%)	7 (1%)	9	39
1	E	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	9	39
1	F	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	9	39
1	G	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	10	42
1	H	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	9	39
1	I	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	10	42
1	J	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	9	39
1	K	491/493 (100%)	424 (86%)	60 (12%)	7 (1%)	9	39
1	L	491/493 (100%)	429 (87%)	56 (11%)	6 (1%)	10	42
2	1	224/226 (99%)	200 (89%)	18 (8%)	6 (3%)	4	28
2	3	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5	224/226 (99%)	202 (90%)	17 (8%)	5 (2%)	5	31
2	7	224/226 (99%)	198 (88%)	20 (9%)	6 (3%)	4	28
2	9	224/226 (99%)	201 (90%)	18 (8%)	5 (2%)	5	31
2	M	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	5	31
2	O	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	5	31
2	Q	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	5	31
2	S	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	5	31
2	U	224/226 (99%)	199 (89%)	20 (9%)	5 (2%)	5	31
2	W	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	5	31
2	Y	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	5	31
3	0	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	4	30
3	2	210/220 (96%)	191 (91%)	16 (8%)	3 (1%)	9	39
3	4	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	6	34
3	6	210/220 (96%)	192 (91%)	15 (7%)	3 (1%)	9	39
3	8	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	6	34
3	N	210/220 (96%)	189 (90%)	16 (8%)	5 (2%)	4	30
3	P	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	6	34
3	R	210/220 (96%)	190 (90%)	17 (8%)	3 (1%)	9	39
3	T	210/220 (96%)	192 (91%)	14 (7%)	4 (2%)	6	34
3	V	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	6	34
3	X	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	6	34
3	Z	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	4	30
All	All	11100/11268 (98%)	9822 (88%)	1089 (10%)	189 (2%)	7	36

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	330	GLY
2	5	115	VAL
3	N	175	ASN
3	P	175	ASN
3	R	175	ASN

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	430/430 (100%)	404 (94%)	26 (6%)	17	42
1	B	430/430 (100%)	406 (94%)	24 (6%)	19	43
1	C	430/430 (100%)	404 (94%)	26 (6%)	17	42
1	D	430/430 (100%)	406 (94%)	24 (6%)	19	43
1	E	430/430 (100%)	406 (94%)	24 (6%)	19	43
1	F	430/430 (100%)	405 (94%)	25 (6%)	18	42
1	G	430/430 (100%)	406 (94%)	24 (6%)	19	43
1	H	430/430 (100%)	405 (94%)	25 (6%)	18	42
1	I	430/430 (100%)	404 (94%)	26 (6%)	17	42
1	J	430/430 (100%)	405 (94%)	25 (6%)	18	42
1	K	430/430 (100%)	406 (94%)	24 (6%)	19	43
1	L	430/430 (100%)	406 (94%)	24 (6%)	19	43
2	1	191/191 (100%)	163 (85%)	28 (15%)	3	16
2	3	191/191 (100%)	165 (86%)	26 (14%)	3	18
2	5	191/191 (100%)	165 (86%)	26 (14%)	3	18
2	7	191/191 (100%)	162 (85%)	29 (15%)	3	15
2	9	191/191 (100%)	164 (86%)	27 (14%)	3	17
2	M	191/191 (100%)	164 (86%)	27 (14%)	3	17
2	O	191/191 (100%)	162 (85%)	29 (15%)	3	15
2	Q	191/191 (100%)	164 (86%)	27 (14%)	3	17
2	S	191/191 (100%)	165 (86%)	26 (14%)	3	18
2	U	191/191 (100%)	164 (86%)	27 (14%)	3	17
2	W	191/191 (100%)	165 (86%)	26 (14%)	3	18
2	Y	191/191 (100%)	165 (86%)	26 (14%)	3	18
3	0	174/181 (96%)	160 (92%)	14 (8%)	11	35
3	2	174/181 (96%)	159 (91%)	15 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	174/181 (96%)	158 (91%)	16 (9%)	8	30
3	6	174/181 (96%)	159 (91%)	15 (9%)	10	33
3	8	174/181 (96%)	159 (91%)	15 (9%)	10	33
3	N	174/181 (96%)	160 (92%)	14 (8%)	11	35
3	P	174/181 (96%)	160 (92%)	14 (8%)	11	35
3	R	174/181 (96%)	160 (92%)	14 (8%)	11	35
3	T	174/181 (96%)	159 (91%)	15 (9%)	10	33
3	V	174/181 (96%)	159 (91%)	15 (9%)	10	33
3	X	174/181 (96%)	158 (91%)	16 (9%)	8	30
3	Z	174/181 (96%)	158 (91%)	16 (9%)	8	30
All	All	9540/9624 (99%)	8740 (92%)	800 (8%)	10	33

5 of 800 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	45	LEU
2	7	64	PHE
3	0	180	SER
2	Y	108	PHE
2	Y	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 439 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	54	ASN
2	Q	39	GLN
3	0	199	GLN
3	2	133	ASN
1	K	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

192 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
6	NAG	AA	1	1,6	14,14,15	0.89	1 (7%)	17,19,21	1.18	2 (11%)
6	NAG	AA	2	6	14,14,15	0.75	0	17,19,21	0.70	0
6	BMA	AA	3	6	11,11,12	0.74	0	15,15,17	0.29	0
4	NAG	BA	1	1,4	14,14,15	0.63	0	17,19,21	0.72	1 (5%)
4	NAG	BA	2	4	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
4	BMA	BA	3	4	11,11,12	0.82	0	15,15,17	0.51	0
4	MAN	BA	4	4	11,11,12	1.01	1 (9%)	15,15,17	1.14	1 (6%)
4	MAN	BA	5	4	11,11,12	0.76	0	15,15,17	0.90	1 (6%)
4	MAN	BA	6	4	11,11,12	0.59	0	15,15,17	0.66	0
4	MAN	BA	7	4	11,11,12	0.70	0	15,15,17	0.60	0
5	NAG	CA	1	1,5	14,14,15	0.91	0	17,19,21	1.10	2 (11%)
5	NAG	CA	2	5	14,14,15	0.91	1 (7%)	17,19,21	1.28	2 (11%)
5	BMA	CA	3	5	11,11,12	0.80	0	15,15,17	0.70	0
5	MAN	CA	4	5	11,11,12	0.81	0	15,15,17	1.14	1 (6%)
5	MAN	CA	5	5	11,11,12	0.65	0	15,15,17	0.76	0
5	MAN	CA	6	5	11,11,12	0.75	0	15,15,17	0.75	0
6	NAG	DA	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	DA	2	6	14,14,15	0.73	0	17,19,21	0.74	0
6	BMA	DA	3	6	11,11,12	0.77	0	15,15,17	0.31	0
4	NAG	EA	1	1,4	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
4	NAG	EA	2	4	14,14,15	0.59	0	17,19,21	0.74	1 (5%)
4	BMA	EA	3	4	11,11,12	0.90	1 (9%)	15,15,17	0.48	0
4	MAN	EA	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	EA	5	4	11,11,12	0.68	0	15,15,17	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	EA	6	4	11,11,12	0.63	0	15,15,17	0.69	0
4	MAN	EA	7	4	11,11,12	0.63	0	15,15,17	0.63	0
5	NAG	FA	1	1,5	14,14,15	0.91	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	FA	2	5	14,14,15	0.91	1 (7%)	17,19,21	1.22	2 (11%)
5	BMA	FA	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.69	0
5	MAN	FA	4	5	11,11,12	0.83	0	15,15,17	1.12	1 (6%)
5	MAN	FA	5	5	11,11,12	0.67	0	15,15,17	0.75	0
5	MAN	FA	6	5	11,11,12	0.71	0	15,15,17	0.69	0
6	NAG	GA	1	1,6	14,14,15	0.96	1 (7%)	17,19,21	1.18	2 (11%)
6	NAG	GA	2	6	14,14,15	0.77	1 (7%)	17,19,21	0.70	0
6	BMA	GA	3	6	11,11,12	0.72	0	15,15,17	0.29	0
4	NAG	HA	1	1,4	14,14,15	0.74	0	17,19,21	0.72	1 (5%)
4	NAG	HA	2	4	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
4	BMA	HA	3	4	11,11,12	0.85	1 (9%)	15,15,17	0.47	0
4	MAN	HA	4	4	11,11,12	1.13	1 (9%)	15,15,17	1.18	1 (6%)
4	MAN	HA	5	4	11,11,12	0.76	0	15,15,17	0.91	1 (6%)
4	MAN	HA	6	4	11,11,12	0.66	0	15,15,17	0.65	0
4	MAN	HA	7	4	11,11,12	0.75	0	15,15,17	0.63	0
5	NAG	IA	1	1,5	14,14,15	0.89	0	17,19,21	1.06	2 (11%)
5	NAG	IA	2	5	14,14,15	0.93	1 (7%)	17,19,21	1.25	2 (11%)
5	BMA	IA	3	5	11,11,12	0.82	0	15,15,17	0.70	0
5	MAN	IA	4	5	11,11,12	0.83	0	15,15,17	1.13	1 (6%)
5	MAN	IA	5	5	11,11,12	0.67	0	15,15,17	0.78	0
5	MAN	IA	6	5	11,11,12	0.68	0	15,15,17	0.71	0
6	NAG	JA	1	1,6	14,14,15	0.92	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	JA	2	6	14,14,15	0.73	0	17,19,21	0.73	0
6	BMA	JA	3	6	11,11,12	0.76	0	15,15,17	0.31	0
4	NAG	a	1	1,4	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
4	NAG	a	2	4	14,14,15	0.55	0	17,19,21	0.73	1 (5%)
4	BMA	a	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.47	0
4	MAN	a	4	4	11,11,12	1.05	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	a	5	4	11,11,12	0.73	0	15,15,17	0.86	1 (6%)
4	MAN	a	6	4	11,11,12	0.63	0	15,15,17	0.65	0
4	MAN	a	7	4	11,11,12	0.75	0	15,15,17	0.63	0
5	NAG	b	1	1,5	14,14,15	0.80	0	17,19,21	1.05	2 (11%)
5	NAG	b	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.26	2 (11%)
5	BMA	b	3	5	11,11,12	0.94	1 (9%)	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	b	4	5	11,11,12	0.89	0	15,15,17	1.07	1 (6%)
5	MAN	b	5	5	11,11,12	0.65	0	15,15,17	0.80	0
5	MAN	b	6	5	11,11,12	0.63	0	15,15,17	0.72	0
6	NAG	c	1	1,6	14,14,15	0.78	0	17,19,21	1.21	2 (11%)
6	NAG	c	2	6	14,14,15	0.77	1 (7%)	17,19,21	0.72	0
6	BMA	c	3	6	11,11,12	0.74	0	15,15,17	0.32	0
4	NAG	d	1	1,4	14,14,15	0.61	0	17,19,21	0.70	1 (5%)
4	NAG	d	2	4	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
4	BMA	d	3	4	11,11,12	0.92	1 (9%)	15,15,17	0.51	0
4	MAN	d	4	4	11,11,12	1.03	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	d	5	4	11,11,12	0.81	0	15,15,17	0.91	1 (6%)
4	MAN	d	6	4	11,11,12	0.63	0	15,15,17	0.66	0
4	MAN	d	7	4	11,11,12	0.74	0	15,15,17	0.57	0
5	NAG	e	1	1,5	14,14,15	0.92	1 (7%)	17,19,21	1.07	2 (11%)
5	NAG	e	2	5	14,14,15	0.97	1 (7%)	17,19,21	1.20	2 (11%)
5	BMA	e	3	5	11,11,12	0.78	0	15,15,17	0.69	0
5	MAN	e	4	5	11,11,12	0.89	0	15,15,17	1.13	1 (6%)
5	MAN	e	5	5	11,11,12	0.68	0	15,15,17	0.77	0
5	MAN	e	6	5	11,11,12	0.70	0	15,15,17	0.71	0
6	NAG	f	1	1,6	14,14,15	0.81	0	17,19,21	1.25	2 (11%)
6	NAG	f	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.73	0
6	BMA	f	3	6	11,11,12	0.74	0	15,15,17	0.28	0
4	NAG	g	1	1,4	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
4	NAG	g	2	4	14,14,15	0.51	0	17,19,21	0.75	1 (5%)
4	BMA	g	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.49	0
4	MAN	g	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.11	1 (6%)
4	MAN	g	5	4	11,11,12	0.73	0	15,15,17	0.86	1 (6%)
4	MAN	g	6	4	11,11,12	0.63	0	15,15,17	0.67	0
4	MAN	g	7	4	11,11,12	0.75	0	15,15,17	0.61	0
5	NAG	h	1	1,5	14,14,15	0.80	0	17,19,21	1.12	2 (11%)
5	NAG	h	2	5	14,14,15	0.88	1 (7%)	17,19,21	1.32	2 (11%)
5	BMA	h	3	5	11,11,12	0.74	0	15,15,17	0.78	0
5	MAN	h	4	5	11,11,12	0.81	0	15,15,17	1.13	1 (6%)
5	MAN	h	5	5	11,11,12	0.62	0	15,15,17	0.76	0
5	MAN	h	6	5	11,11,12	0.68	0	15,15,17	0.76	0
6	NAG	i	1	1,6	14,14,15	0.88	1 (7%)	17,19,21	1.18	2 (11%)
6	NAG	i	2	6	14,14,15	0.85	1 (7%)	17,19,21	0.73	0
6	BMA	i	3	6	11,11,12	0.76	0	15,15,17	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	j	1	1,4	14,14,15	0.62	0	17,19,21	0.70	1 (5%)
4	NAG	j	2	4	14,14,15	0.61	0	17,19,21	0.76	1 (5%)
4	BMA	j	3	4	11,11,12	0.85	1 (9%)	15,15,17	0.45	0
4	MAN	j	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.14	1 (6%)
4	MAN	j	5	4	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
4	MAN	j	6	4	11,11,12	0.62	0	15,15,17	0.64	0
4	MAN	j	7	4	11,11,12	0.67	0	15,15,17	0.57	0
5	NAG	k	1	1,5	14,14,15	0.85	0	17,19,21	1.12	2 (11%)
5	NAG	k	2	5	14,14,15	0.91	1 (7%)	17,19,21	1.26	2 (11%)
5	BMA	k	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.71	0
5	MAN	k	4	5	11,11,12	0.90	1 (9%)	15,15,17	1.12	1 (6%)
5	MAN	k	5	5	11,11,12	0.67	0	15,15,17	0.78	0
5	MAN	k	6	5	11,11,12	0.71	0	15,15,17	0.72	0
6	NAG	l	1	1,6	14,14,15	0.86	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	l	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.70	0
6	BMA	l	3	6	11,11,12	0.72	0	15,15,17	0.30	0
4	NAG	m	1	1,4	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
4	NAG	m	2	4	14,14,15	0.41	0	17,19,21	0.78	1 (5%)
4	BMA	m	3	4	11,11,12	1.01	1 (9%)	15,15,17	0.50	0
4	MAN	m	4	4	11,11,12	1.10	1 (9%)	15,15,17	1.12	1 (6%)
4	MAN	m	5	4	11,11,12	0.73	0	15,15,17	0.84	1 (6%)
4	MAN	m	6	4	11,11,12	0.58	0	15,15,17	0.65	0
4	MAN	m	7	4	11,11,12	0.79	0	15,15,17	0.66	0
5	NAG	n	1	1,5	14,14,15	0.83	0	17,19,21	1.07	2 (11%)
5	NAG	n	2	5	14,14,15	0.88	1 (7%)	17,19,21	1.28	2 (11%)
5	BMA	n	3	5	11,11,12	0.85	0	15,15,17	0.71	0
5	MAN	n	4	5	11,11,12	0.86	0	15,15,17	1.11	1 (6%)
5	MAN	n	5	5	11,11,12	0.71	0	15,15,17	0.80	0
5	MAN	n	6	5	11,11,12	0.64	0	15,15,17	0.73	0
6	NAG	o	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.23	2 (11%)
6	NAG	o	2	6	14,14,15	0.72	0	17,19,21	0.73	0
6	BMA	o	3	6	11,11,12	0.71	0	15,15,17	0.30	0
4	NAG	p	1	1,4	14,14,15	0.68	0	17,19,21	0.78	1 (5%)
4	NAG	p	2	4	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
4	BMA	p	3	4	11,11,12	1.00	1 (9%)	15,15,17	0.50	0
4	MAN	p	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.16	1 (6%)
4	MAN	p	5	4	11,11,12	0.74	0	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	p	6	4	11,11,12	0.57	0	15,15,17	0.64	0
4	MAN	p	7	4	11,11,12	0.72	0	15,15,17	0.62	0
5	NAG	q	1	1,5	14,14,15	0.86	0	17,19,21	1.02	2 (11%)
5	NAG	q	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.20	2 (11%)
5	BMA	q	3	5	11,11,12	0.89	1 (9%)	15,15,17	0.78	1 (6%)
5	MAN	q	4	5	11,11,12	0.84	0	15,15,17	1.12	1 (6%)
5	MAN	q	5	5	11,11,12	0.67	0	15,15,17	0.80	0
5	MAN	q	6	5	11,11,12	0.65	0	15,15,17	0.71	0
6	NAG	r	1	1,6	14,14,15	0.80	0	17,19,21	1.23	2 (11%)
6	NAG	r	2	6	14,14,15	0.68	0	17,19,21	0.74	0
6	BMA	r	3	6	11,11,12	0.71	0	15,15,17	0.30	0
4	NAG	s	1	1,4	14,14,15	0.63	0	17,19,21	0.72	1 (5%)
4	NAG	s	2	4	14,14,15	0.54	0	17,19,21	0.79	1 (5%)
4	BMA	s	3	4	11,11,12	0.92	1 (9%)	15,15,17	0.54	0
4	MAN	s	4	4	11,11,12	1.00	1 (9%)	15,15,17	1.10	1 (6%)
4	MAN	s	5	4	11,11,12	0.69	0	15,15,17	0.85	1 (6%)
4	MAN	s	6	4	11,11,12	0.60	0	15,15,17	0.66	0
4	MAN	s	7	4	11,11,12	0.69	0	15,15,17	0.63	0
5	NAG	t	1	1,5	14,14,15	0.94	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	t	2	5	14,14,15	0.94	1 (7%)	17,19,21	1.24	2 (11%)
5	BMA	t	3	5	11,11,12	0.86	1 (9%)	15,15,17	0.68	0
5	MAN	t	4	5	11,11,12	0.75	0	15,15,17	1.15	1 (6%)
5	MAN	t	5	5	11,11,12	0.66	0	15,15,17	0.76	0
5	MAN	t	6	5	11,11,12	0.69	0	15,15,17	0.71	0
6	NAG	u	1	1,6	14,14,15	0.89	1 (7%)	17,19,21	1.24	2 (11%)
6	NAG	u	2	6	14,14,15	0.82	1 (7%)	17,19,21	0.71	0
6	BMA	u	3	6	11,11,12	0.77	0	15,15,17	0.36	0
4	NAG	v	1	1,4	14,14,15	0.65	0	17,19,21	0.69	1 (5%)
4	NAG	v	2	4	14,14,15	0.69	0	17,19,21	0.72	1 (5%)
4	BMA	v	3	4	11,11,12	0.90	1 (9%)	15,15,17	0.42	0
4	MAN	v	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.13	1 (6%)
4	MAN	v	5	4	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
4	MAN	v	6	4	11,11,12	0.65	0	15,15,17	0.68	0
4	MAN	v	7	4	11,11,12	0.73	0	15,15,17	0.58	0
5	NAG	w	1	1,5	14,14,15	0.90	0	17,19,21	1.06	2 (11%)
5	NAG	w	2	5	14,14,15	0.90	1 (7%)	17,19,21	1.23	2 (11%)
5	BMA	w	3	5	11,11,12	0.87	1 (9%)	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	w	4	5	11,11,12	0.87	0	15,15,17	1.12	1 (6%)
5	MAN	w	5	5	11,11,12	0.67	0	15,15,17	0.76	0
5	MAN	w	6	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	x	1	1,6	14,14,15	1.04	1 (7%)	17,19,21	1.13	2 (11%)
6	NAG	x	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.67	0
6	BMA	x	3	6	11,11,12	0.73	0	15,15,17	0.33	0
4	NAG	y	1	1,4	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
4	NAG	y	2	4	14,14,15	0.44	0	17,19,21	0.77	1 (5%)
4	BMA	y	3	4	11,11,12	1.09	1 (9%)	15,15,17	0.50	0
4	MAN	y	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.17	1 (6%)
4	MAN	y	5	4	11,11,12	0.73	0	15,15,17	0.91	1 (6%)
4	MAN	y	6	4	11,11,12	0.65	0	15,15,17	0.66	0
4	MAN	y	7	4	11,11,12	0.83	0	15,15,17	0.66	0
5	NAG	z	1	1,5	14,14,15	0.91	0	17,19,21	1.07	2 (11%)
5	NAG	z	2	5	14,14,15	0.95	1 (7%)	17,19,21	1.22	2 (11%)
5	BMA	z	3	5	11,11,12	0.75	0	15,15,17	0.71	0
5	MAN	z	4	5	11,11,12	0.82	0	15,15,17	1.14	1 (6%)
5	MAN	z	5	5	11,11,12	0.67	0	15,15,17	0.75	0
5	MAN	z	6	5	11,11,12	0.69	0	15,15,17	0.74	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
6	NAG	AA	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	AA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	AA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	BA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	6/6/23/26	0/1/1/1
4	BMA	BA	3	4	-	1/2/19/22	0/1/1/1
4	MAN	BA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	BA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	BA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	BA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	CA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	CA	2	5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	CA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	CA	6	5	-	0/2/19/22	0/1/1/1
6	NAG	DA	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	EA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	EA	2	4	-	6/6/23/26	0/1/1/1
4	BMA	EA	3	4	-	1/2/19/22	0/1/1/1
4	MAN	EA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	EA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	EA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	EA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	FA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	FA	6	5	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	HA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	HA	2	4	-	6/6/23/26	0/1/1/1
4	BMA	HA	3	4	-	2/2/19/22	0/1/1/1
4	MAN	HA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	HA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	HA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	HA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	IA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	IA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	IA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	IA	6	5	-	0/2/19/22	0/1/1/1
6	NAG	JA	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	4/6/23/26	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	n	4	5	-	0/2/19/22	0/1/1/1
5	MAN	n	5	5	-	2/2/19/22	0/1/1/1
5	MAN	n	6	5	-	0/2/19/22	0/1/1/1
6	NAG	o	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	o	2	6	-	4/6/23/26	0/1/1/1
6	BMA	o	3	6	-	1/2/19/22	0/1/1/1
4	NAG	p	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	6/6/23/26	0/1/1/1
4	BMA	p	3	4	-	2/2/19/22	0/1/1/1
4	MAN	p	4	4	-	2/2/19/22	0/1/1/1
4	MAN	p	5	4	-	1/2/19/22	0/1/1/1
4	MAN	p	6	4	-	0/2/19/22	0/1/1/1
4	MAN	p	7	4	-	0/2/19/22	0/1/1/1
5	NAG	q	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	q	2	5	-	4/6/23/26	0/1/1/1
5	BMA	q	3	5	-	0/2/19/22	0/1/1/1
5	MAN	q	4	5	-	0/2/19/22	0/1/1/1
5	MAN	q	5	5	-	2/2/19/22	0/1/1/1
5	MAN	q	6	5	-	0/2/19/22	0/1/1/1
6	NAG	r	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	r	2	6	-	4/6/23/26	0/1/1/1
6	BMA	r	3	6	-	1/2/19/22	0/1/1/1
4	NAG	s	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	s	2	4	-	6/6/23/26	0/1/1/1
4	BMA	s	3	4	-	1/2/19/22	0/1/1/1
4	MAN	s	4	4	-	2/2/19/22	0/1/1/1
4	MAN	s	5	4	-	1/2/19/22	0/1/1/1
4	MAN	s	6	4	-	0/2/19/22	0/1/1/1
4	MAN	s	7	4	-	0/2/19/22	0/1/1/1
5	NAG	t	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	t	2	5	-	4/6/23/26	0/1/1/1
5	BMA	t	3	5	-	0/2/19/22	0/1/1/1
5	MAN	t	4	5	-	0/2/19/22	0/1/1/1
5	MAN	t	5	5	-	2/2/19/22	0/1/1/1
5	MAN	t	6	5	-	0/2/19/22	0/1/1/1
6	NAG	u	1	1,6	-	6/6/23/26	0/1/1/1
6	NAG	u	2	6	-	4/6/23/26	0/1/1/1
6	BMA	u	3	6	-	1/2/19/22	0/1/1/1

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

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	y	3	BMA	C4-C3	2.99	1.60	1.52
6	x	1	NAG	C4-C3	2.91	1.59	1.52
4	m	3	BMA	C4-C3	2.69	1.59	1.52
4	p	3	BMA	C4-C3	2.64	1.59	1.52
4	HA	4	MAN	C4-C3	2.54	1.58	1.52

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	1	NAG	C4-C3-C2	3.63	116.34	111.02
4	d	4	MAN	C1-C2-C3	3.52	114.77	109.64
6	u	1	NAG	C4-C3-C2	3.50	116.15	111.02
6	r	1	NAG	C4-C3-C2	3.50	116.15	111.02
4	BA	4	MAN	C1-C2-C3	3.50	114.73	109.64

There are no chirality outliers.

5 of 410 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2

There are no ring outliers.

74 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	u	1	NAG	1	0
5	b	1	NAG	3	0
6	l	3	BMA	1	0
6	JA	2	NAG	1	0
4	j	1	NAG	1	0
4	p	2	NAG	2	0
6	x	3	BMA	1	0
4	EA	1	NAG	1	0
6	GA	3	BMA	1	0
5	e	2	NAG	2	0
4	m	2	NAG	2	0
5	IA	2	NAG	4	0
5	IA	1	NAG	3	0
4	EA	2	NAG	7	0
5	FA	2	NAG	2	0
4	y	1	NAG	1	0
6	GA	2	NAG	1	0
4	HA	2	NAG	5	0
5	CA	2	NAG	2	0
4	BA	1	NAG	1	0
6	i	3	BMA	1	0

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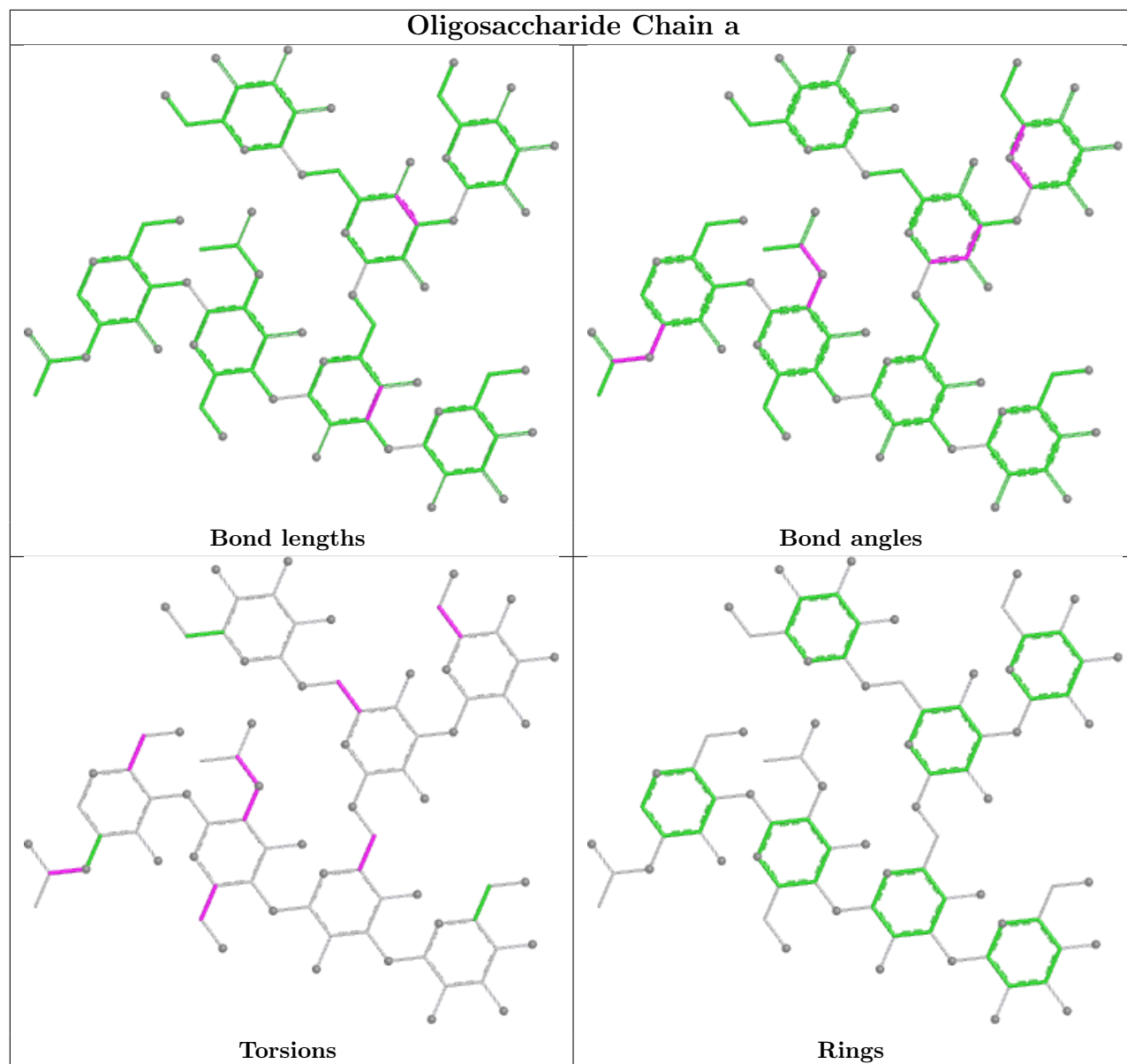
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	l	2	NAG	1	0
4	a	1	NAG	1	0
5	z	2	NAG	4	0
6	AA	2	NAG	1	0
4	d	2	NAG	5	0
4	d	1	NAG	1	0
6	AA	3	BMA	1	0
6	c	2	NAG	1	0
6	u	3	BMA	1	0
4	v	1	NAG	1	0
5	h	2	NAG	9	0
6	c	3	BMA	1	0
5	h	1	NAG	4	0
6	u	2	NAG	1	0
4	g	1	NAG	1	0
5	w	1	NAG	3	0
6	f	3	BMA	1	0
6	DA	3	BMA	1	0
4	s	1	NAG	1	0
5	n	2	NAG	2	0
4	p	1	NAG	1	0
4	y	2	NAG	1	0
6	r	3	BMA	1	0
5	t	2	NAG	2	0
5	CA	1	NAG	3	0
6	o	3	BMA	1	0
6	DA	2	NAG	1	0
5	q	3	BMA	2	0
5	q	1	NAG	3	0
6	r	2	NAG	1	0
6	i	2	NAG	1	0
4	a	2	NAG	4	0
5	e	1	NAG	3	0
6	x	2	NAG	1	0
5	b	2	NAG	2	0
5	k	2	NAG	7	0
4	m	1	NAG	1	0
6	JA	3	BMA	1	0
4	j	2	NAG	4	0
4	BA	2	NAG	4	0
4	v	2	NAG	2	0
5	k	1	NAG	3	0

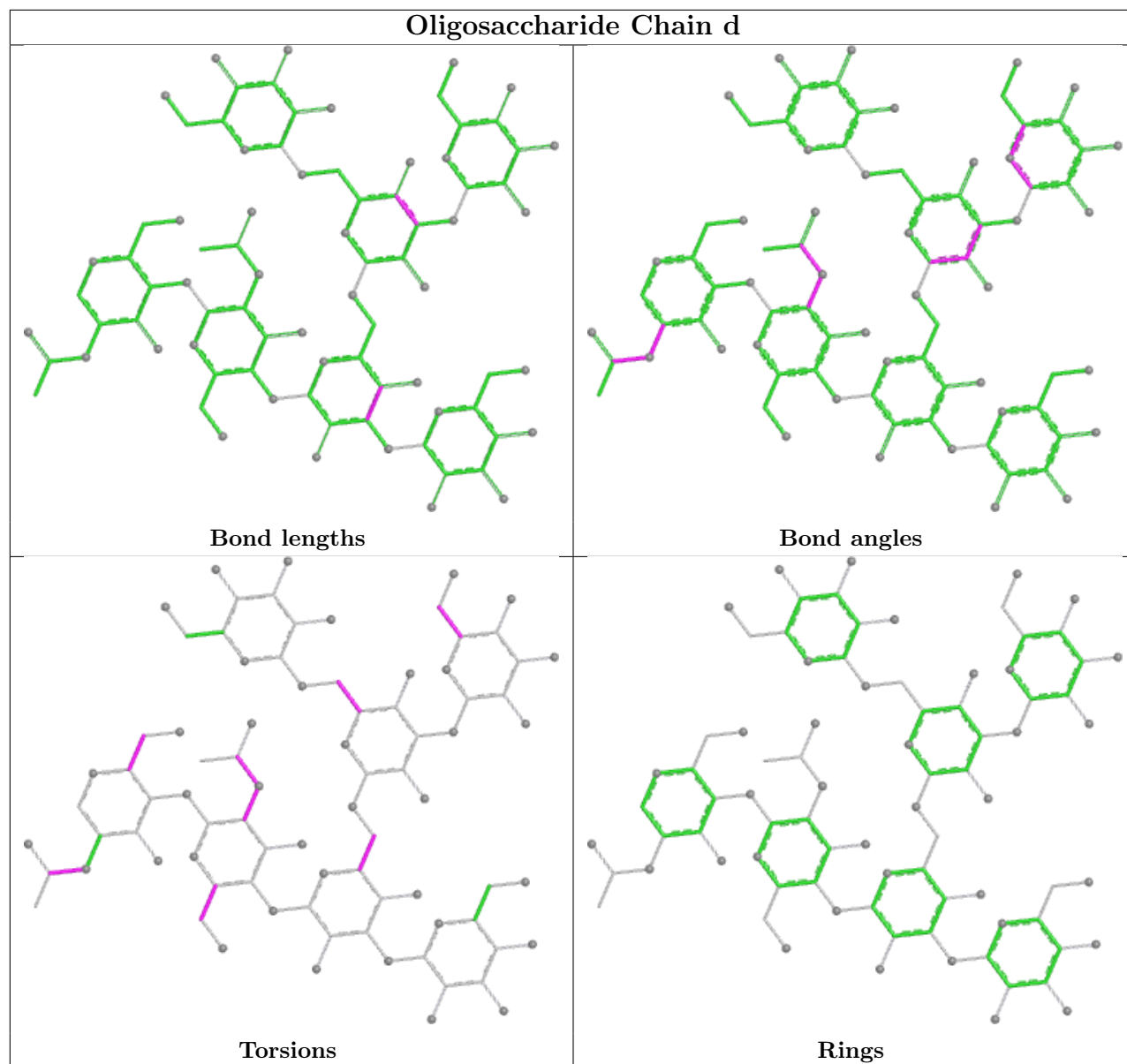
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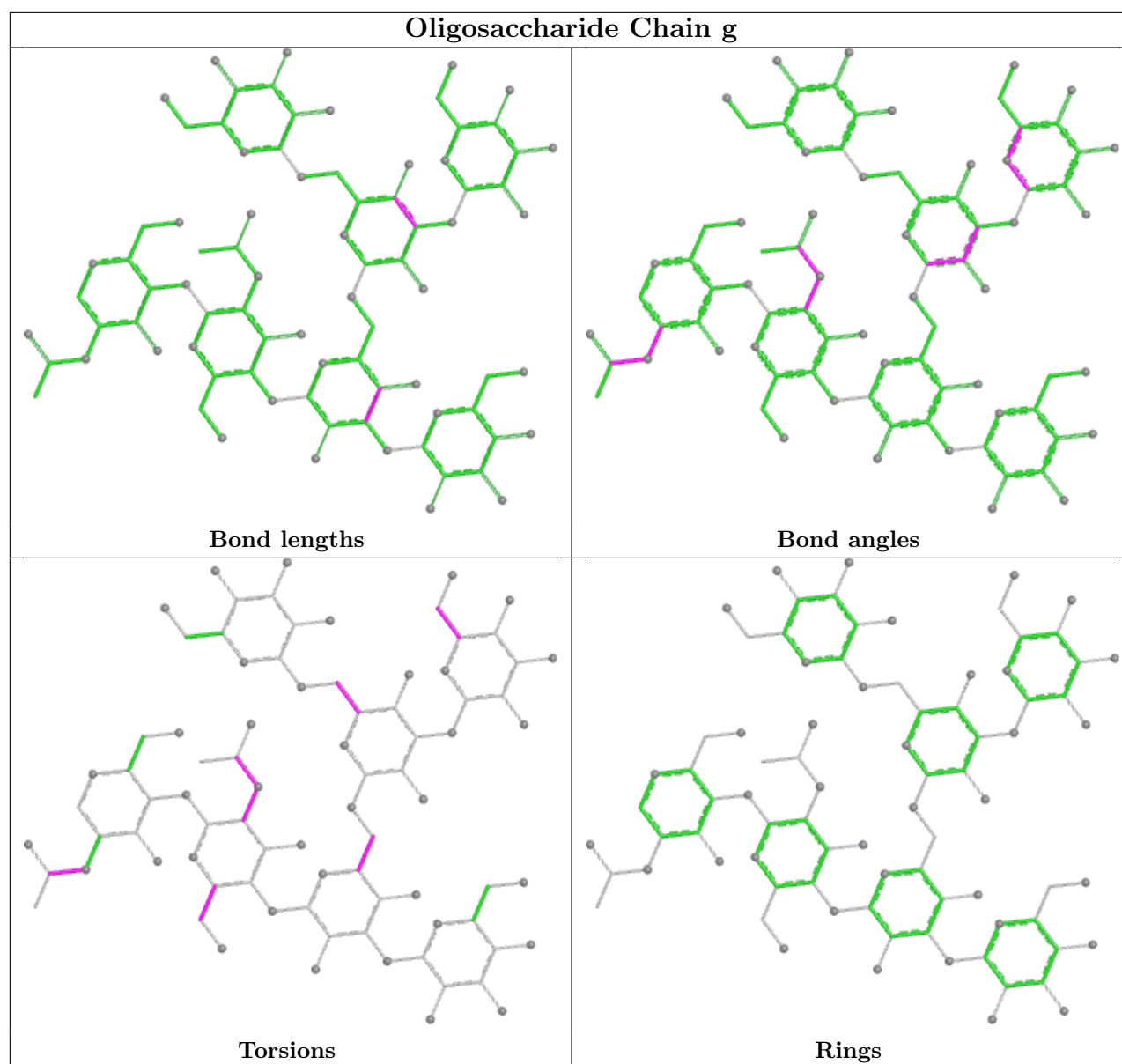
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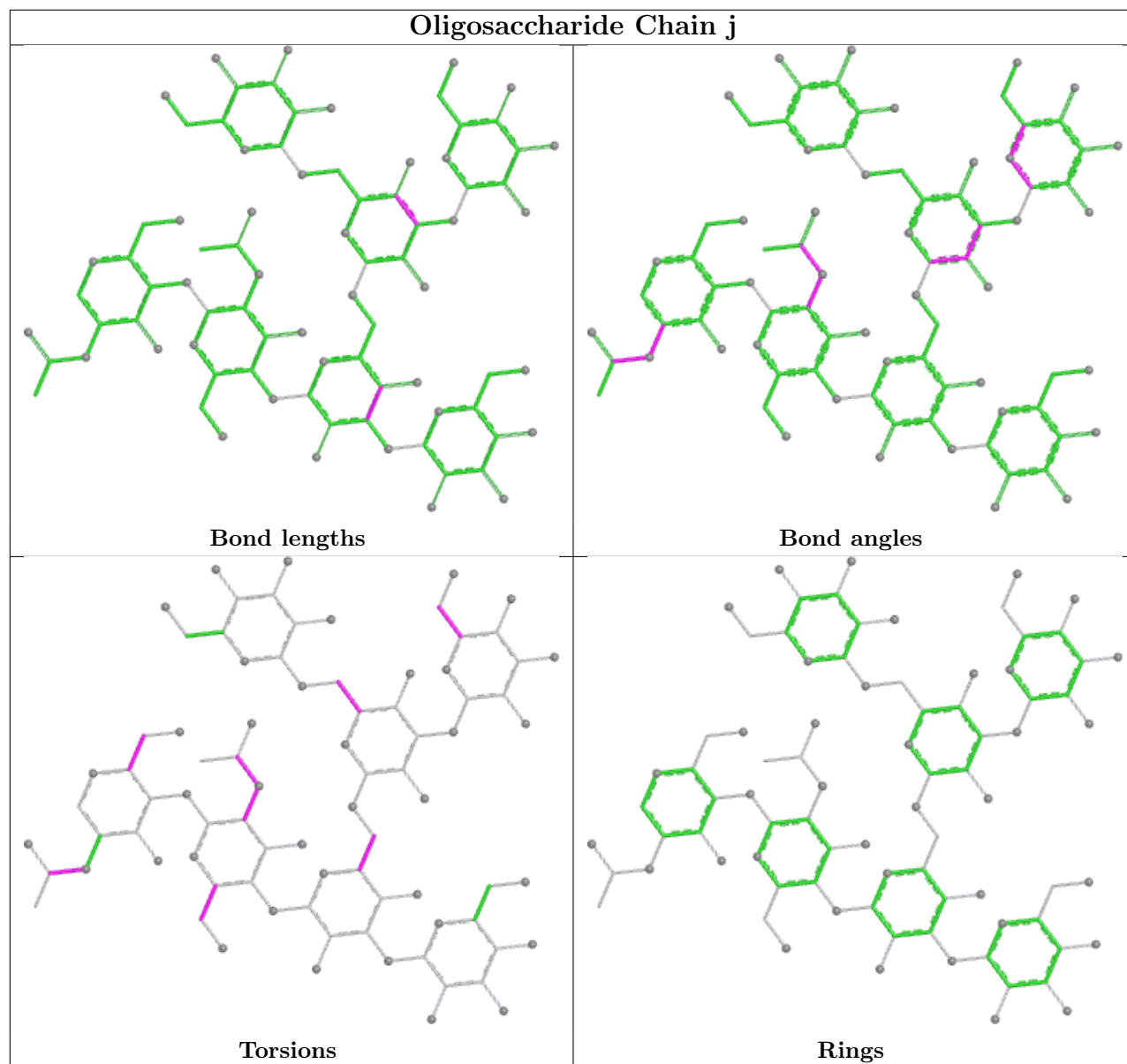
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	n	1	NAG	3	0
5	w	2	NAG	2	0
5	t	1	NAG	3	0
5	FA	1	NAG	3	0
6	f	2	NAG	1	0
6	o	2	NAG	1	0
4	g	2	NAG	1	0
5	q	2	NAG	9	0
5	z	1	NAG	3	0
4	HA	1	NAG	1	0
4	s	2	NAG	2	0

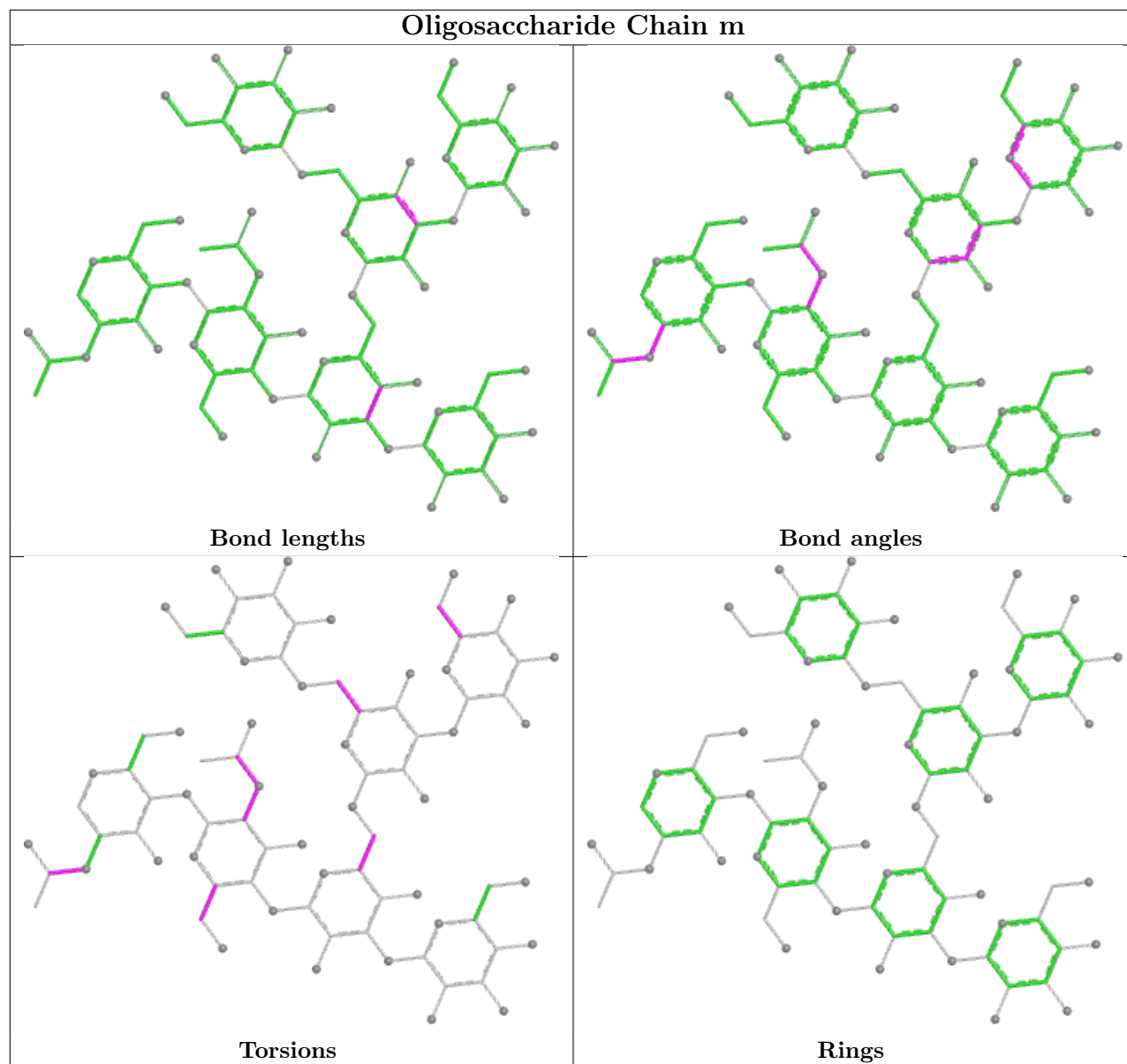
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

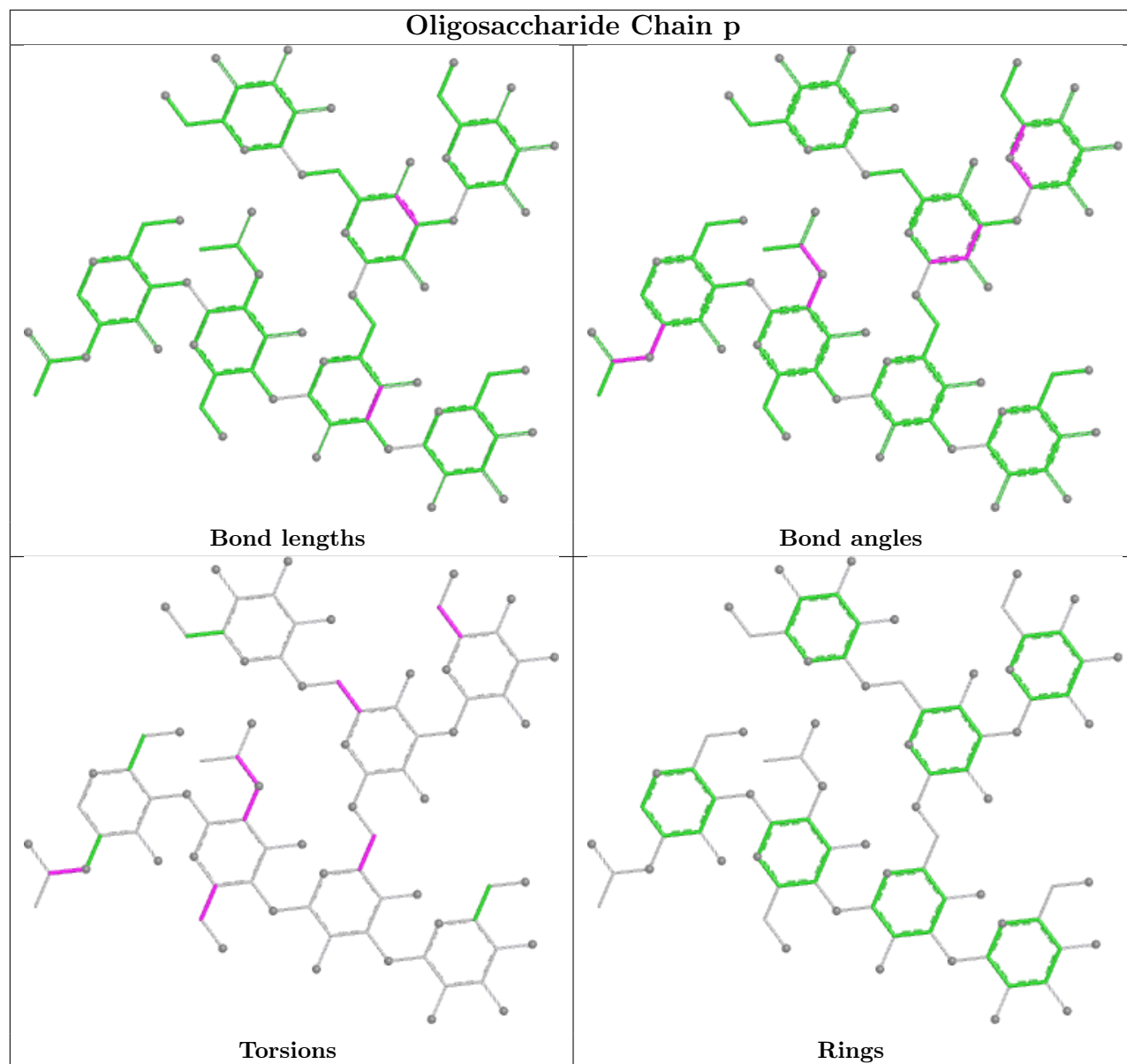


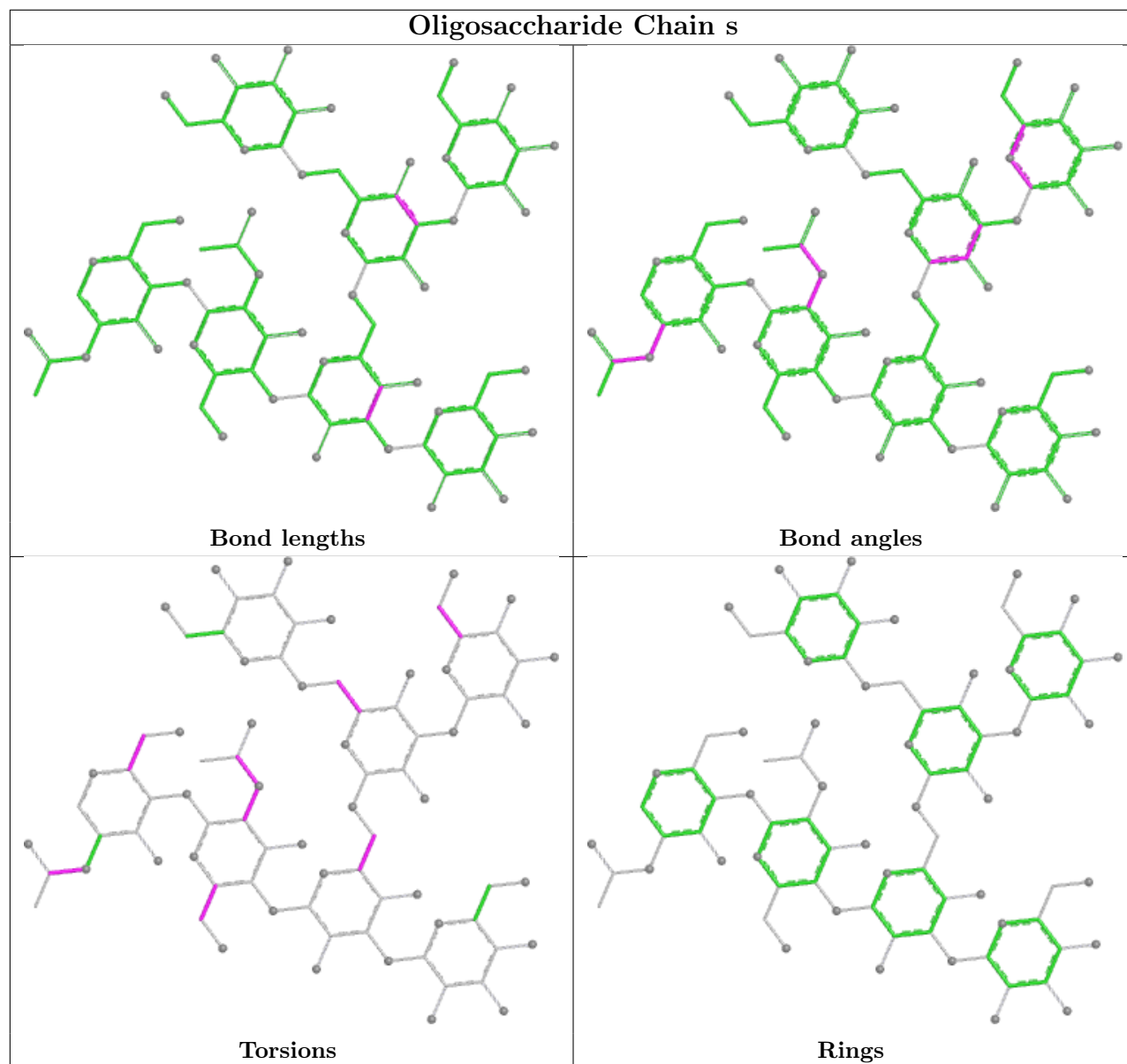


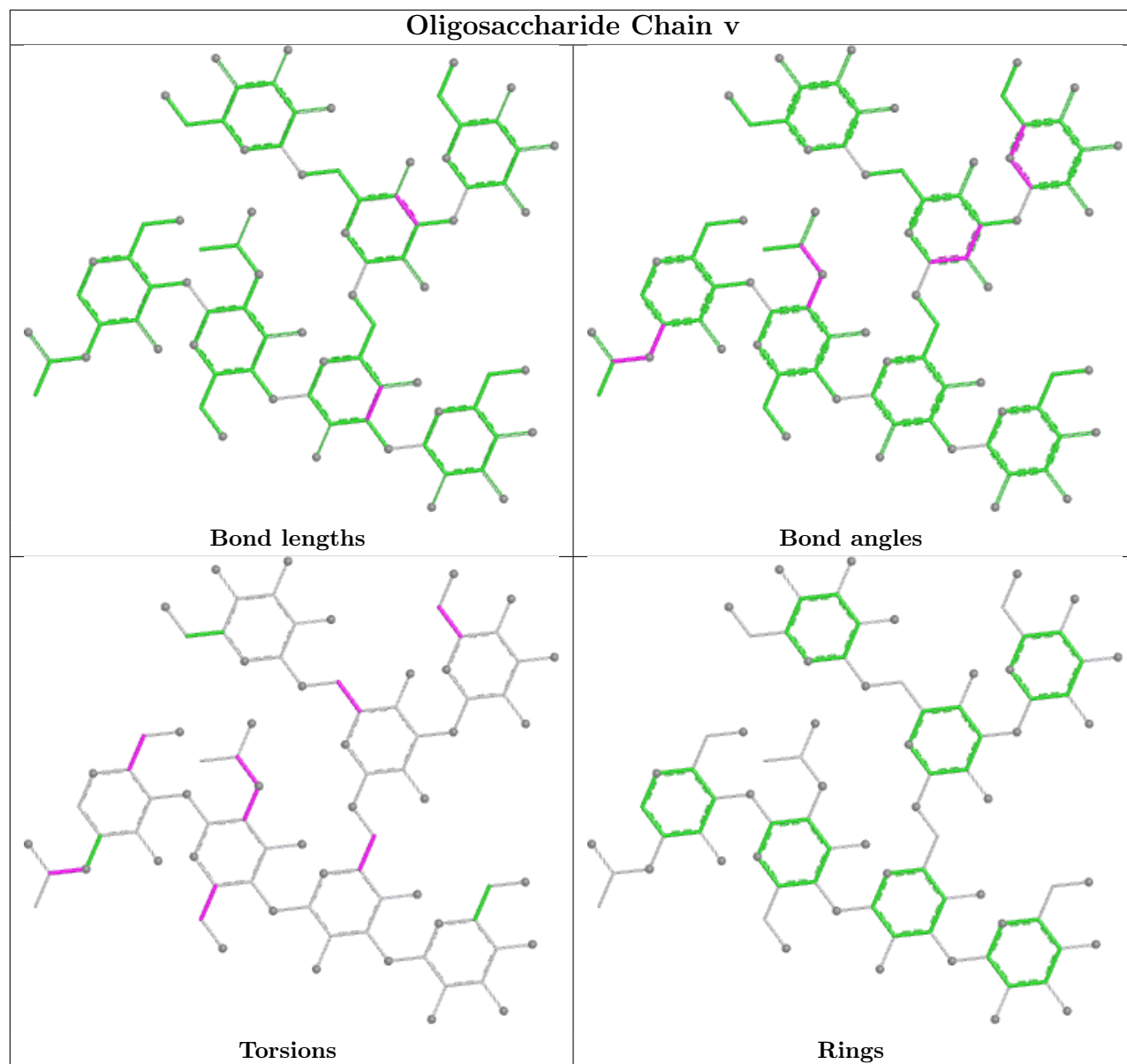


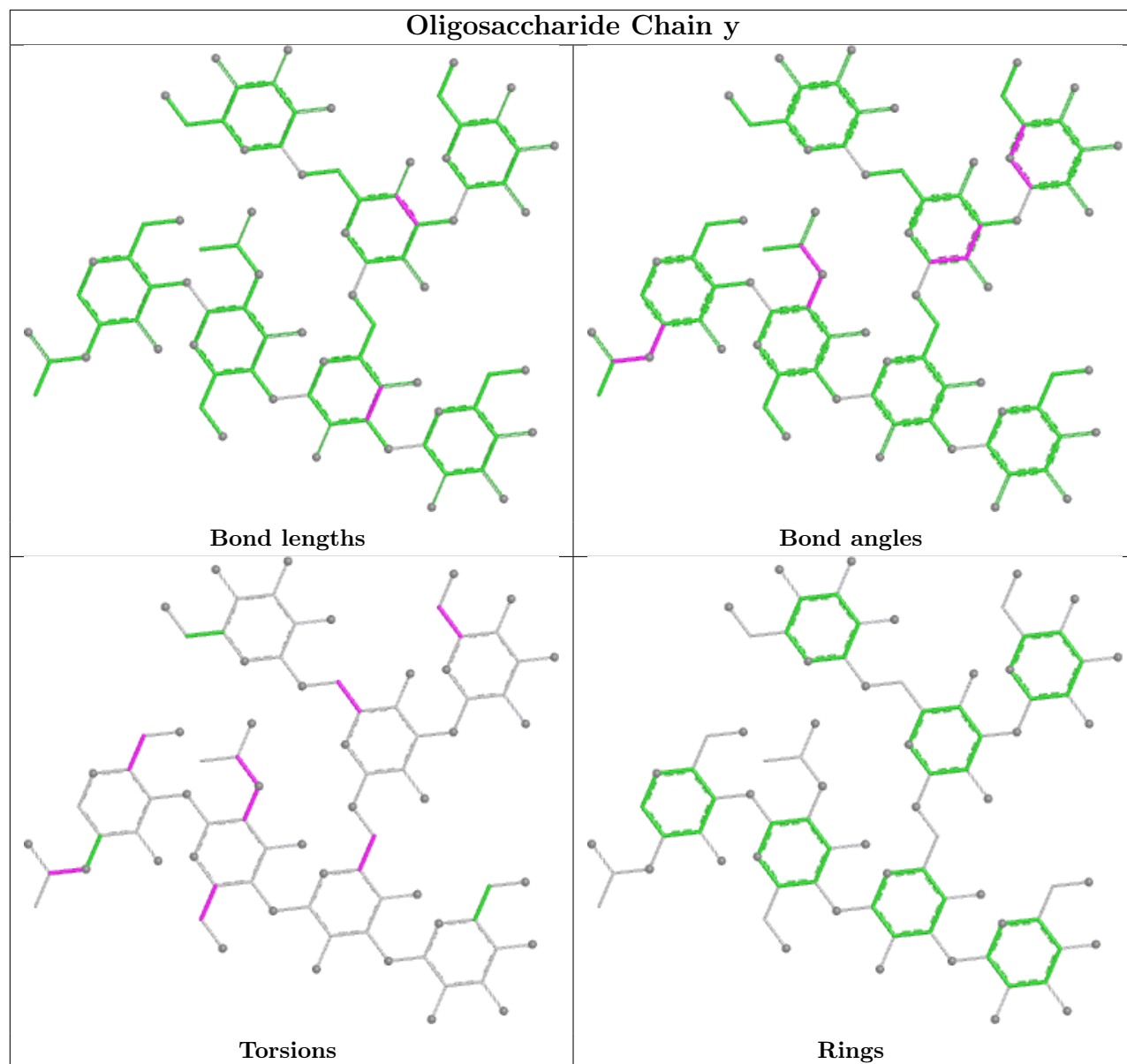


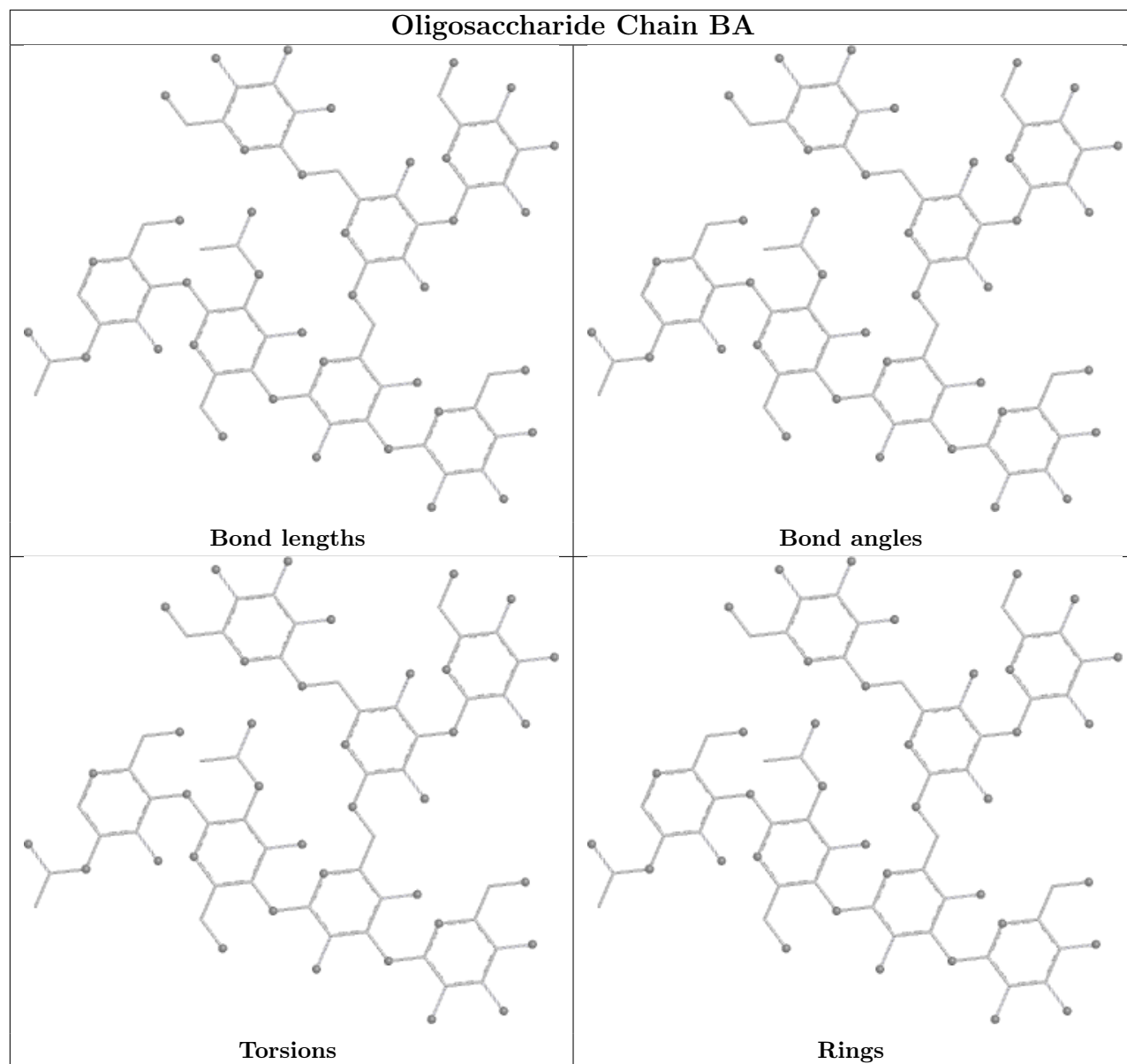


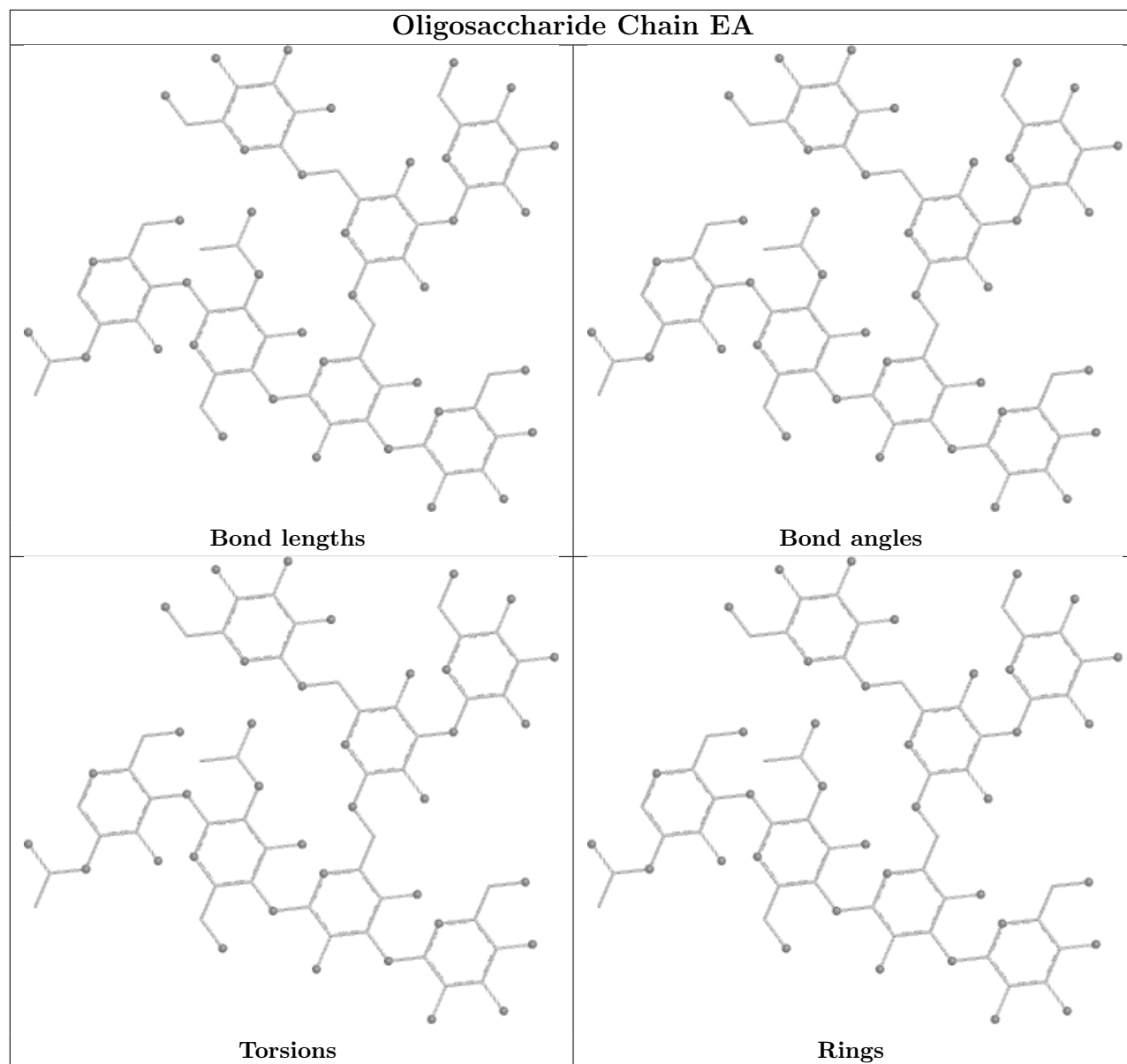


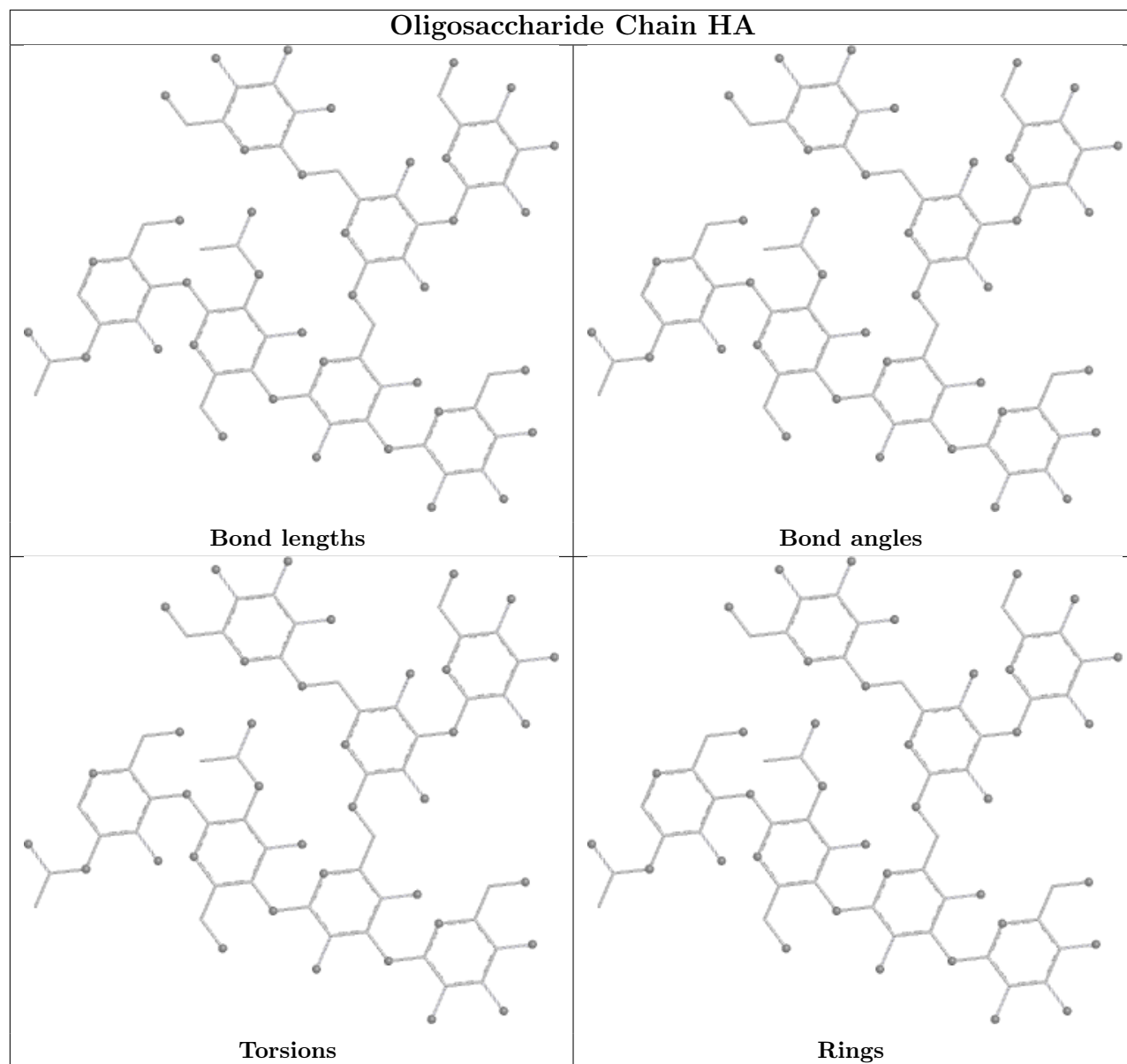


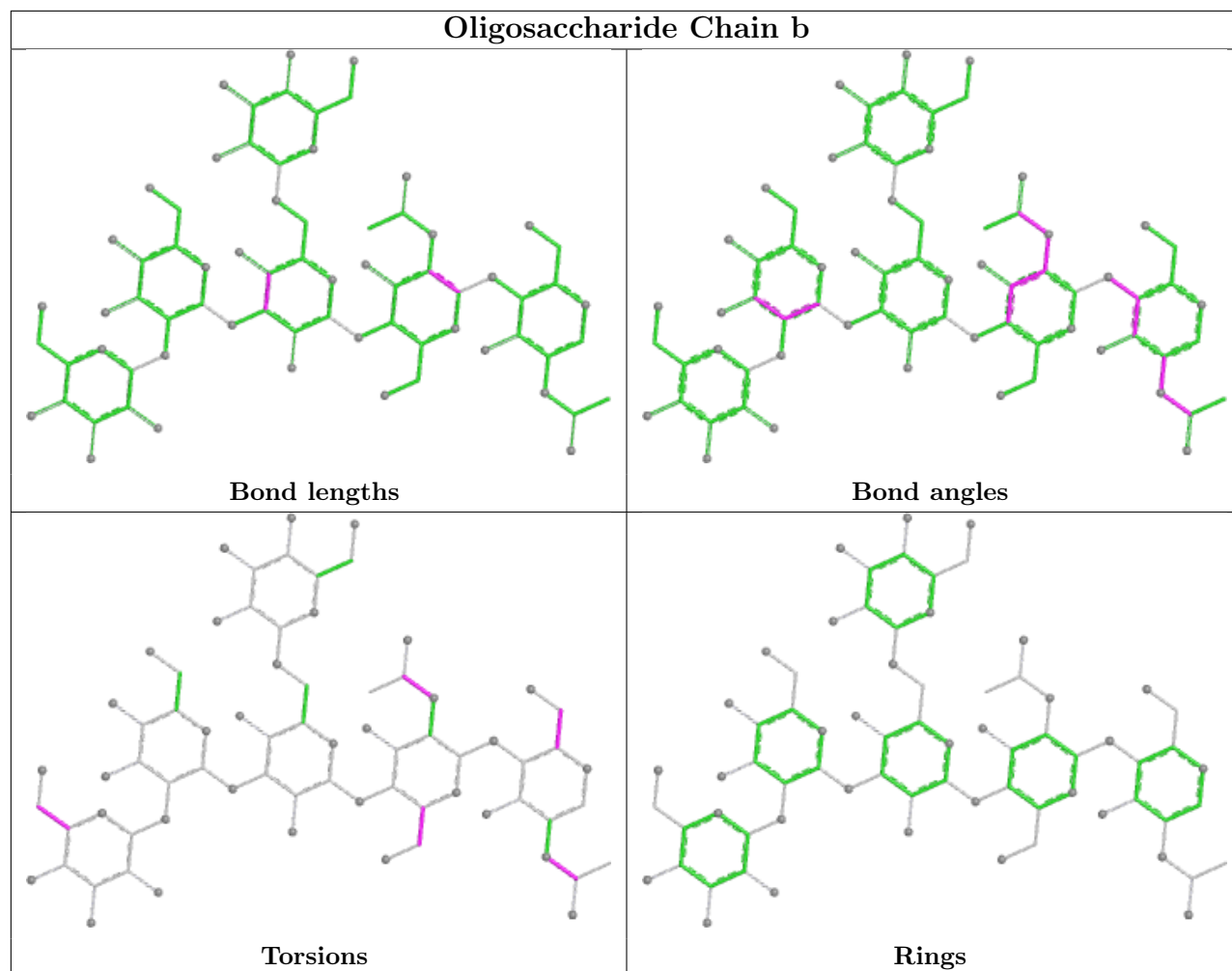


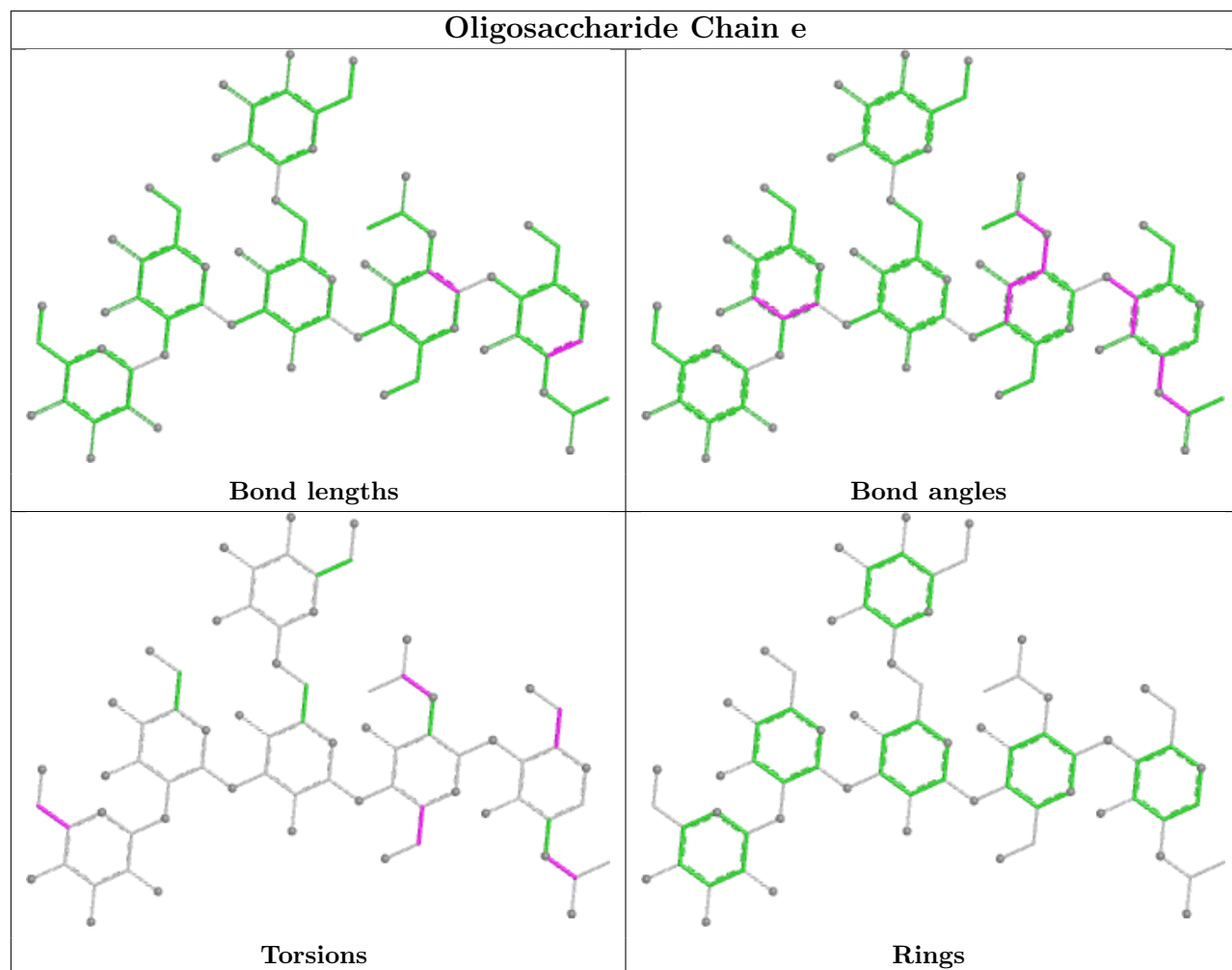


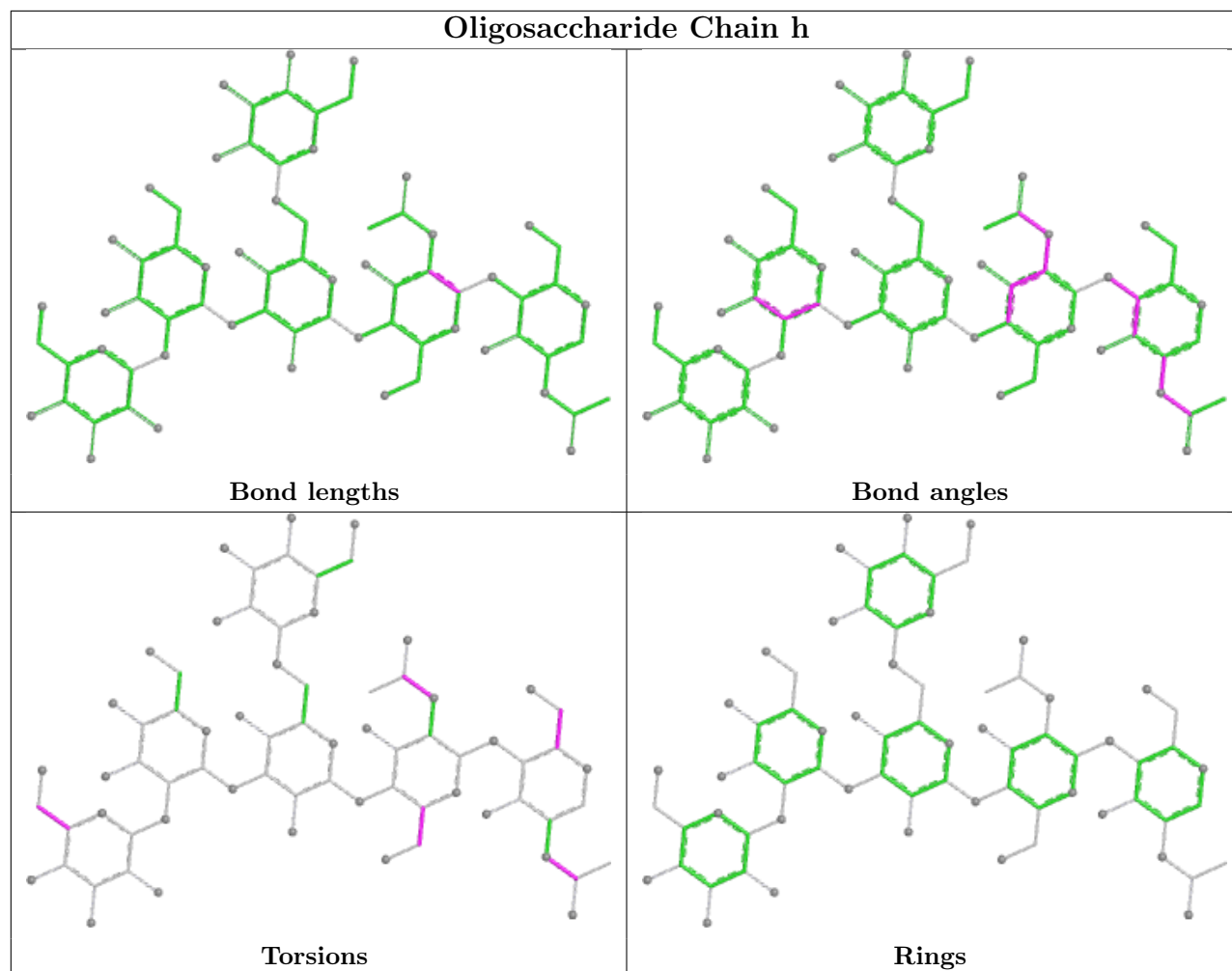


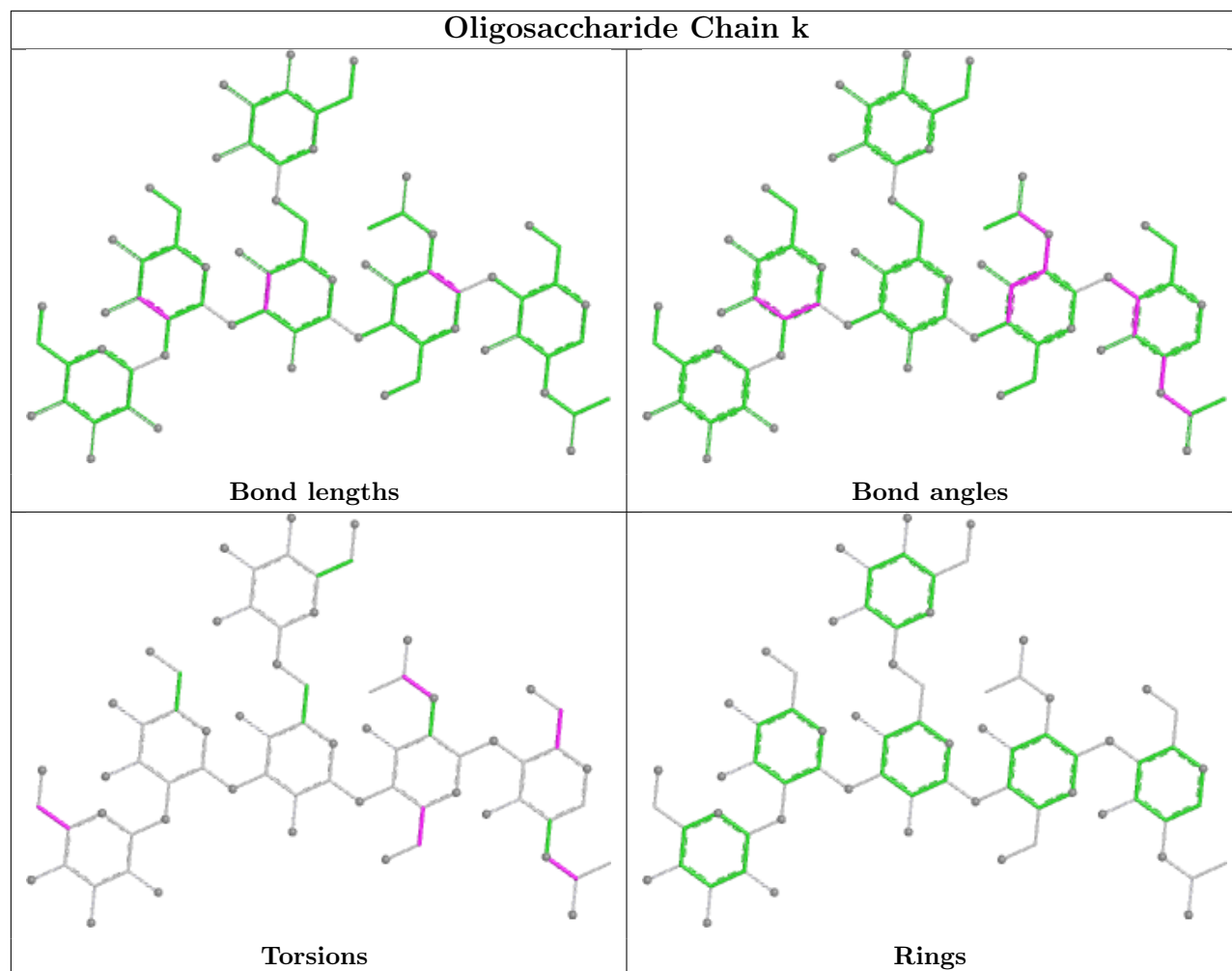


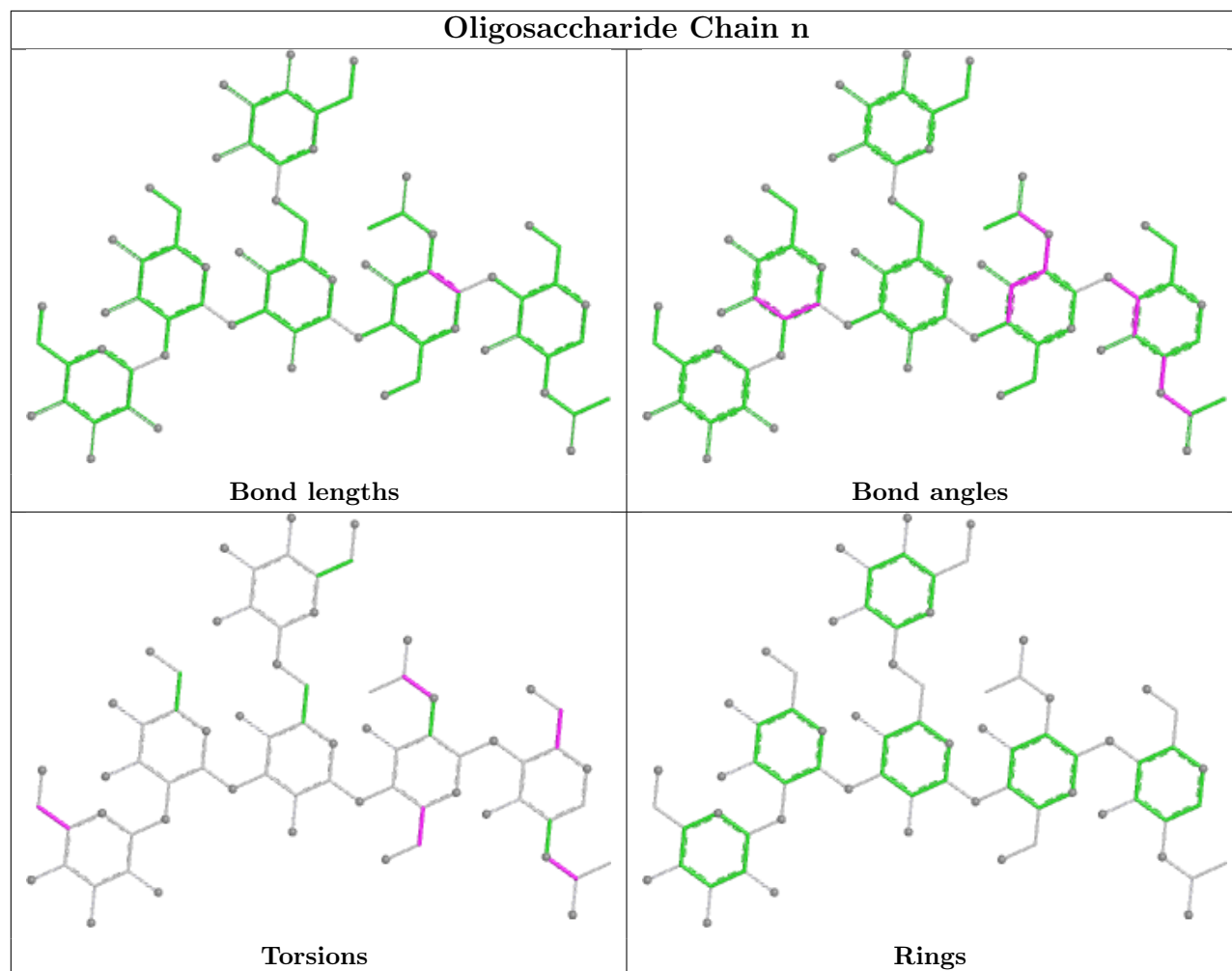


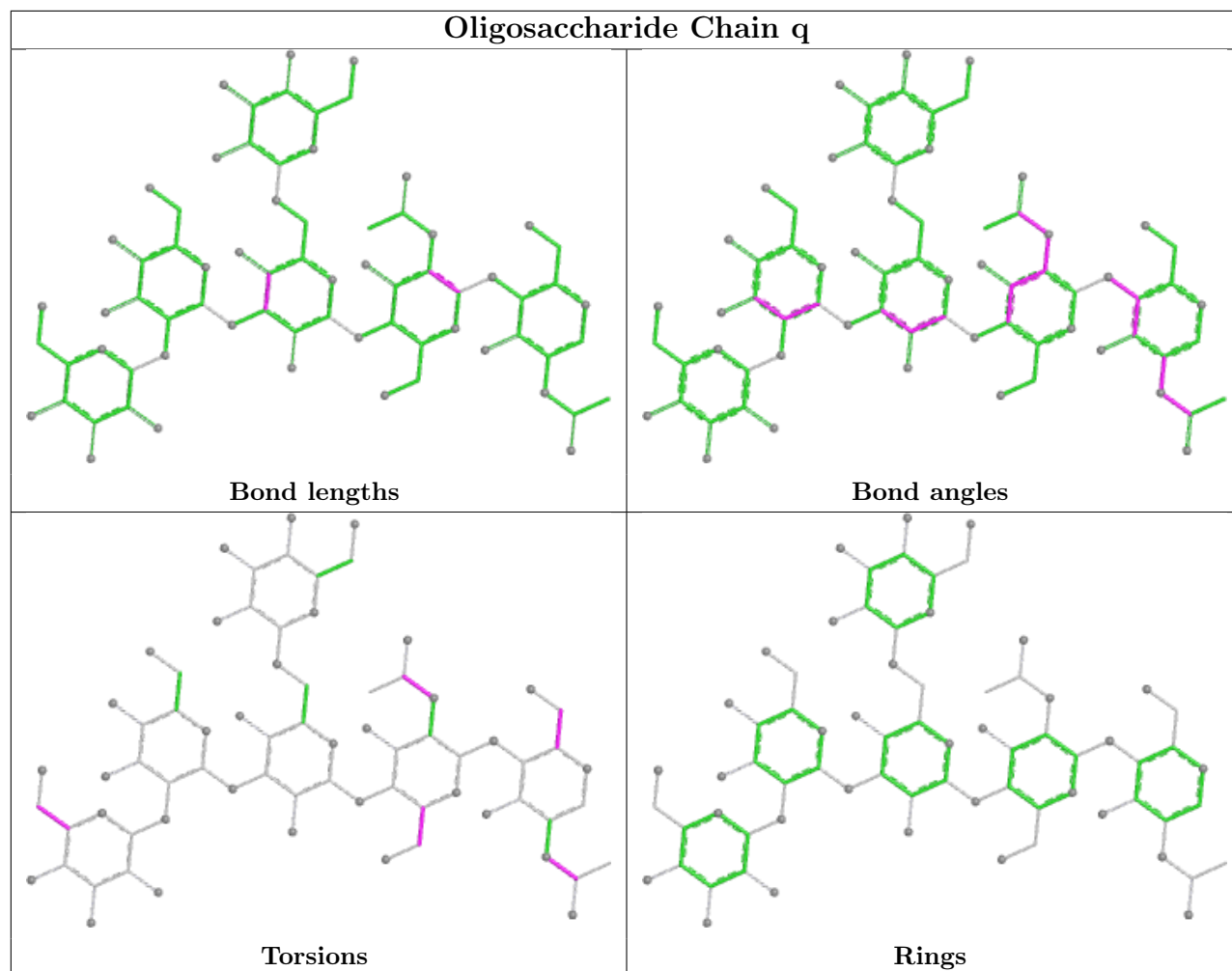


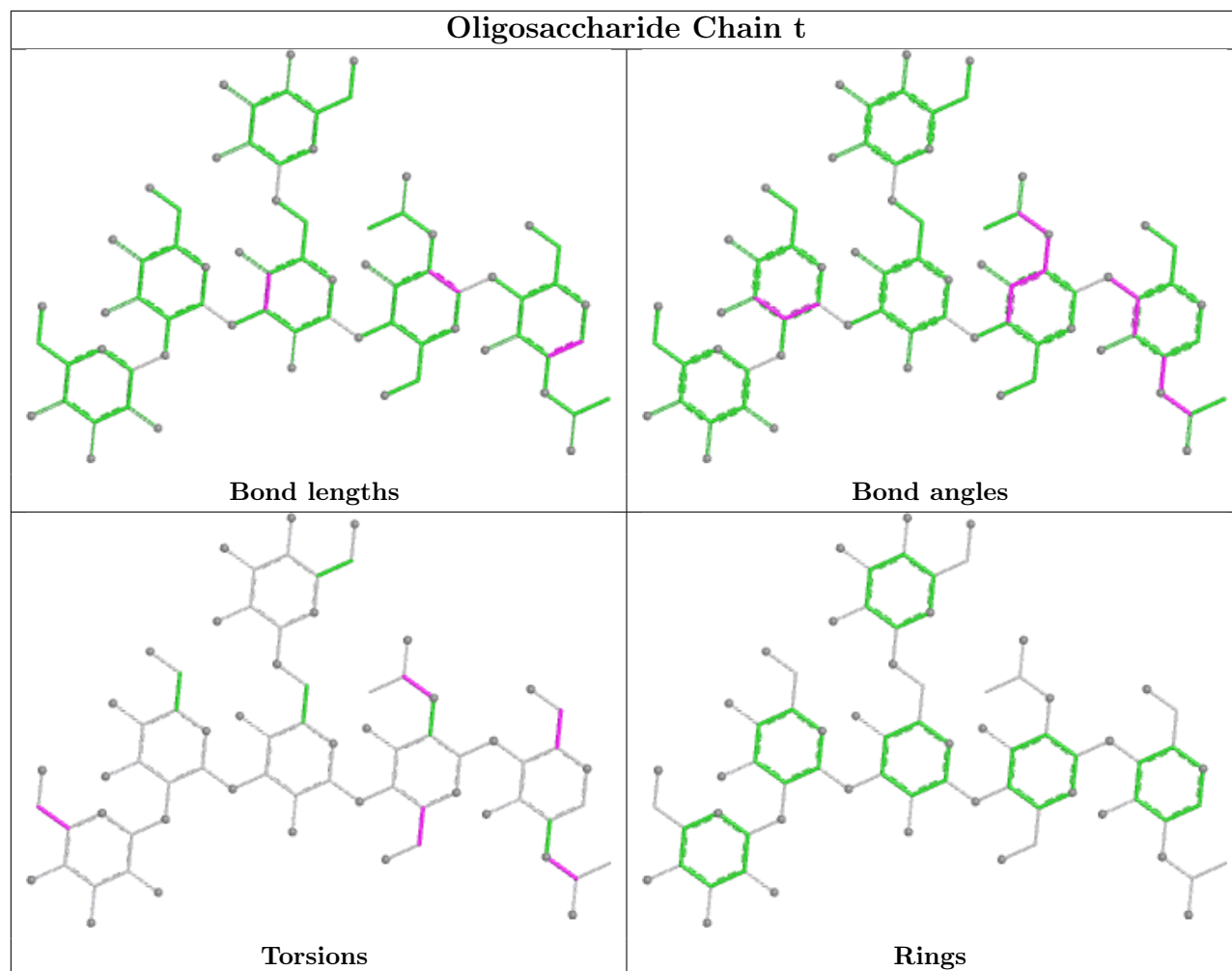


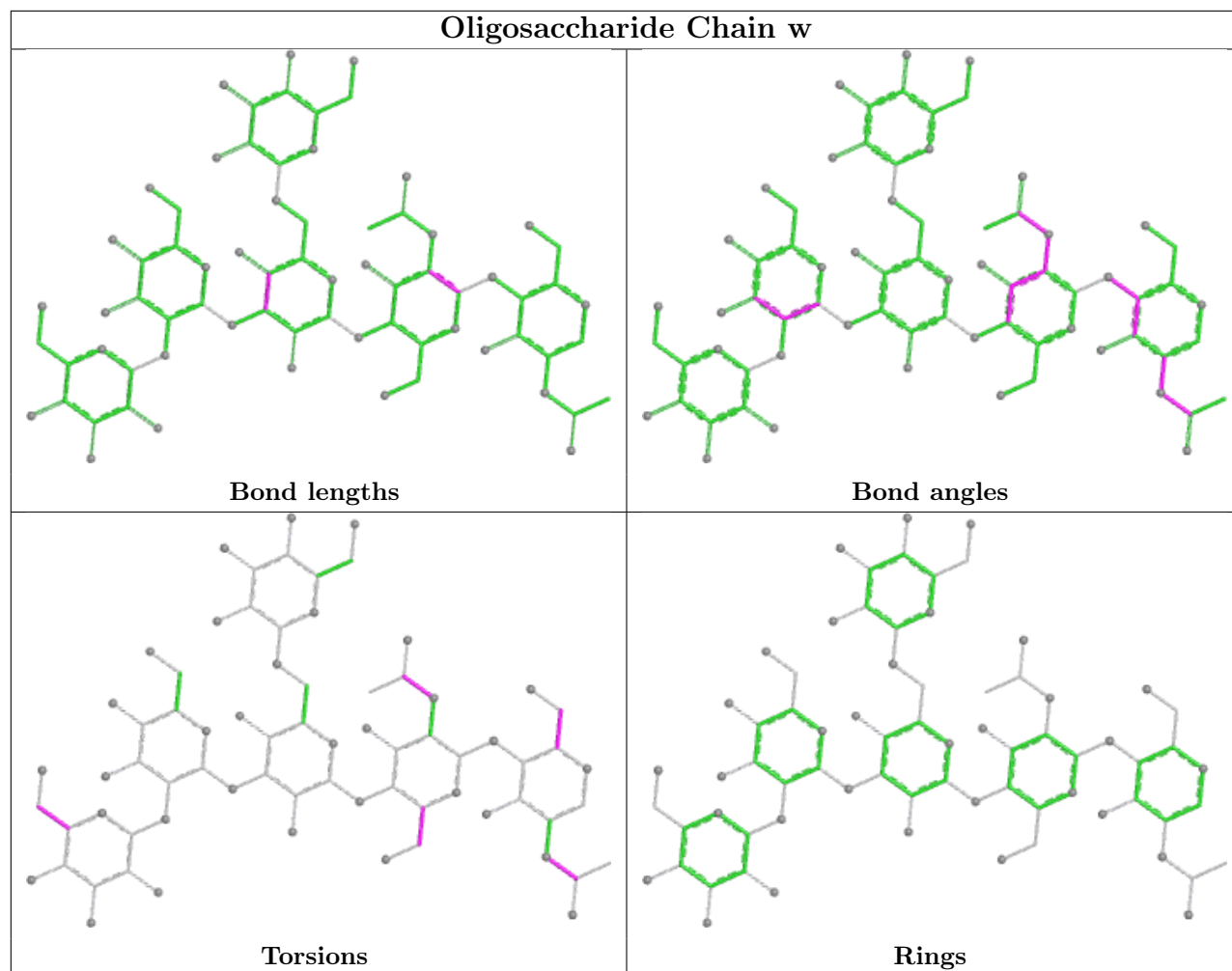


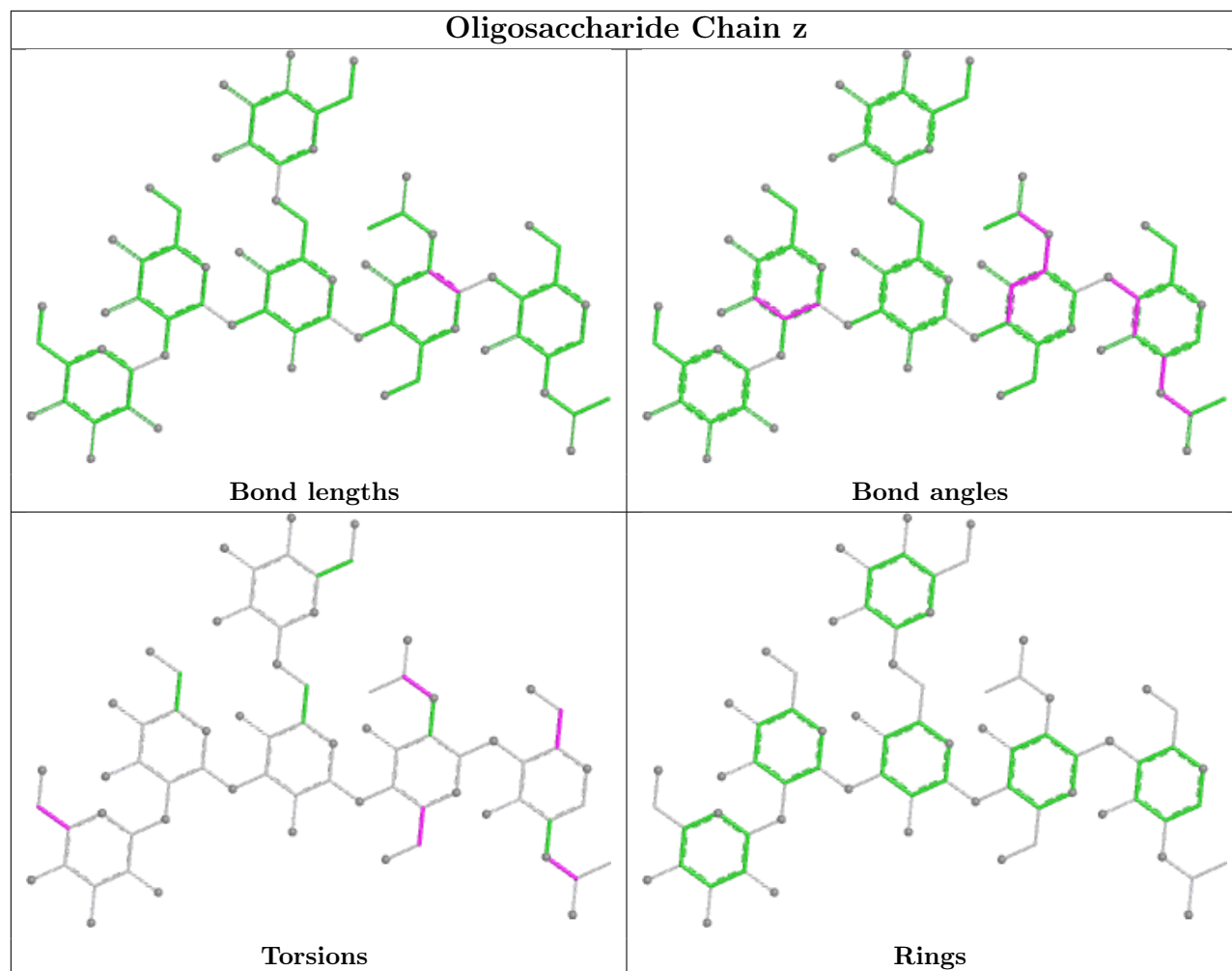


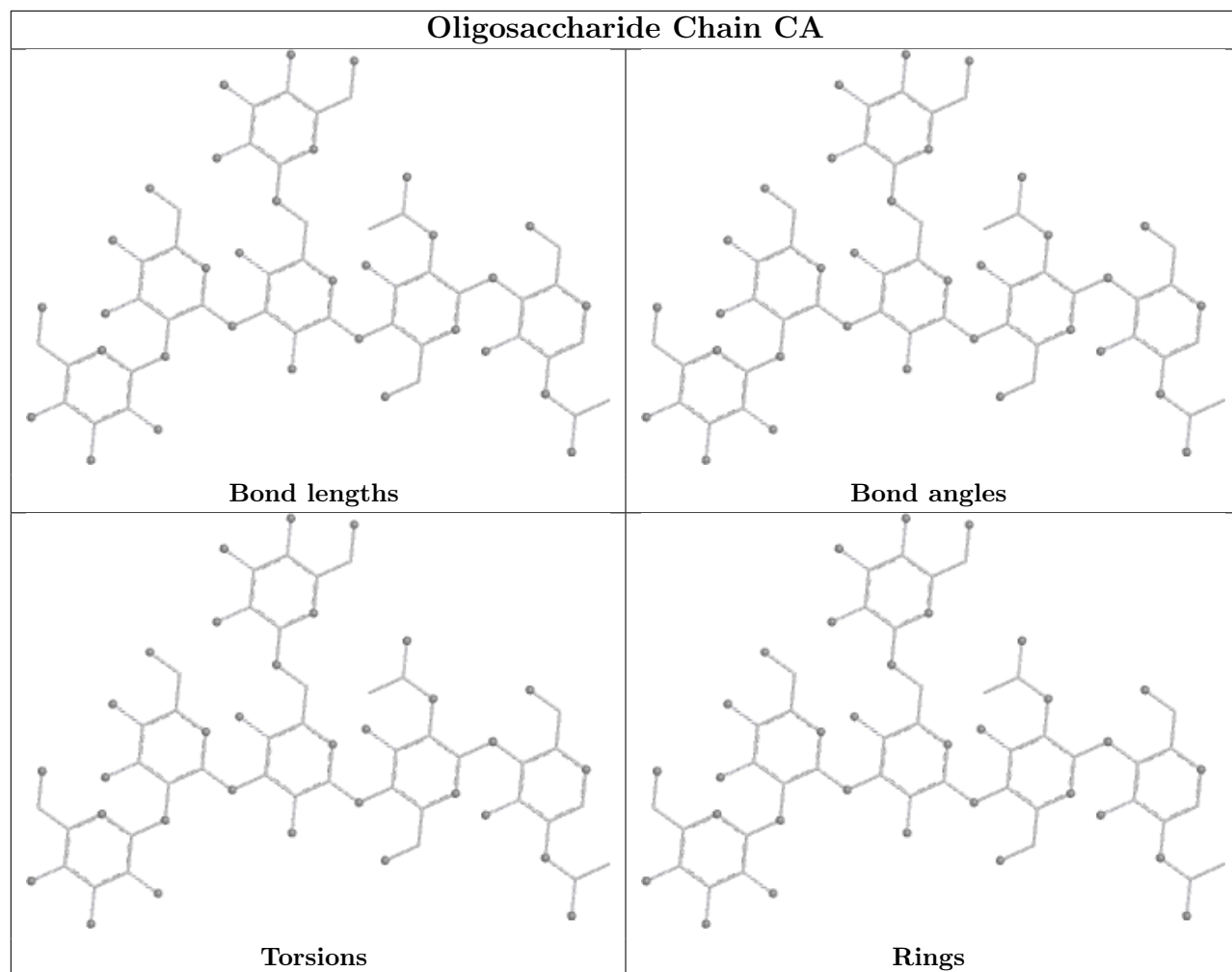


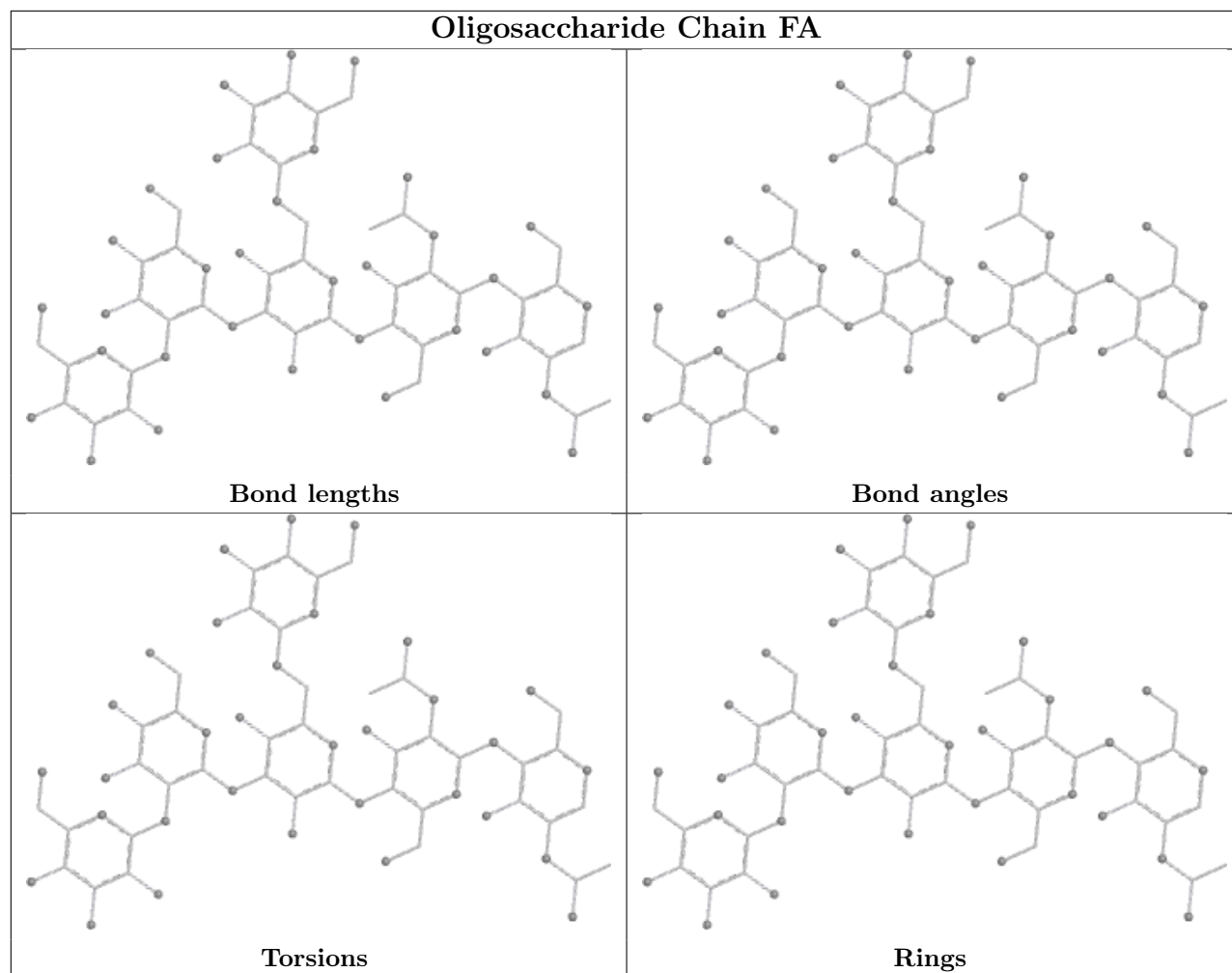


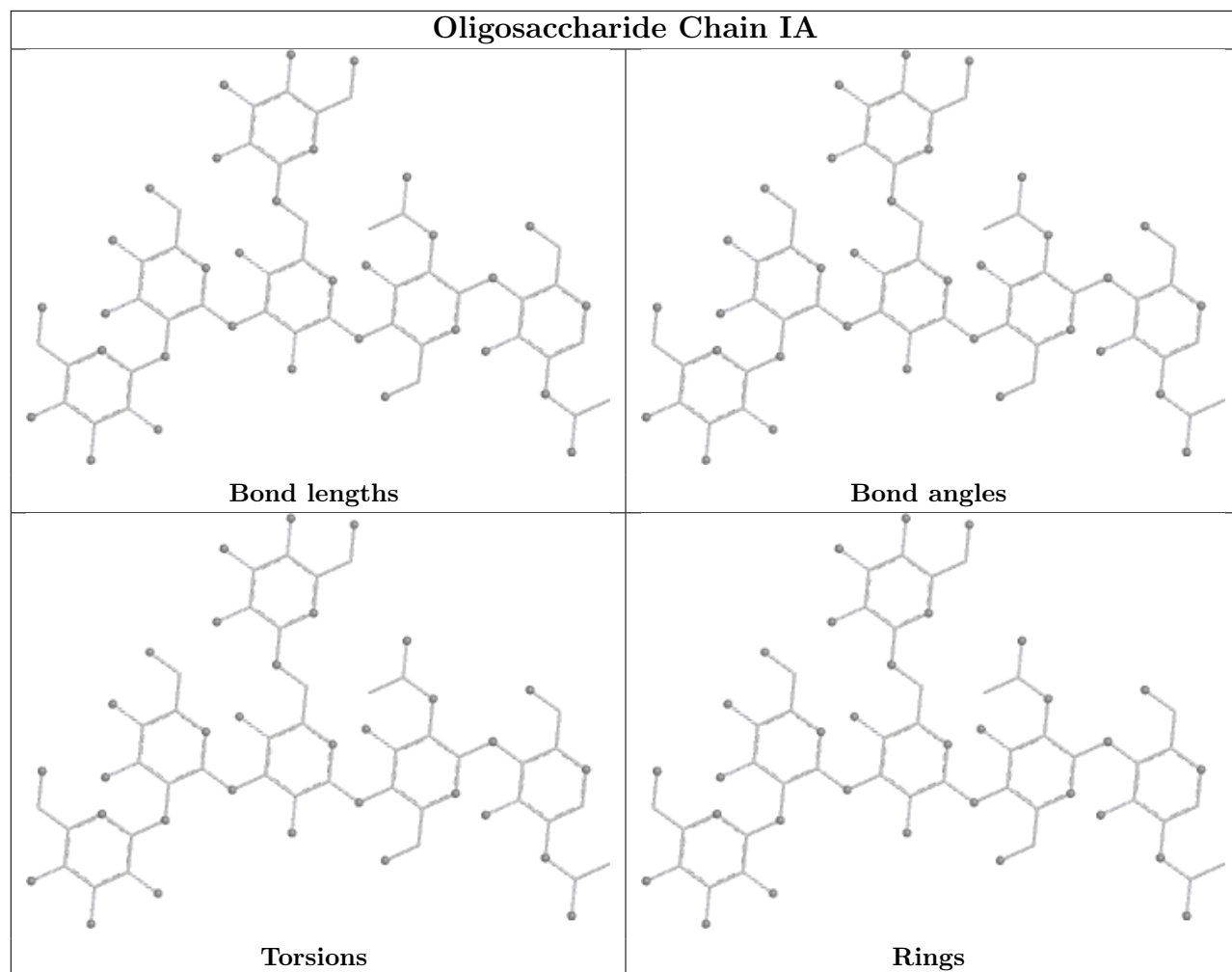


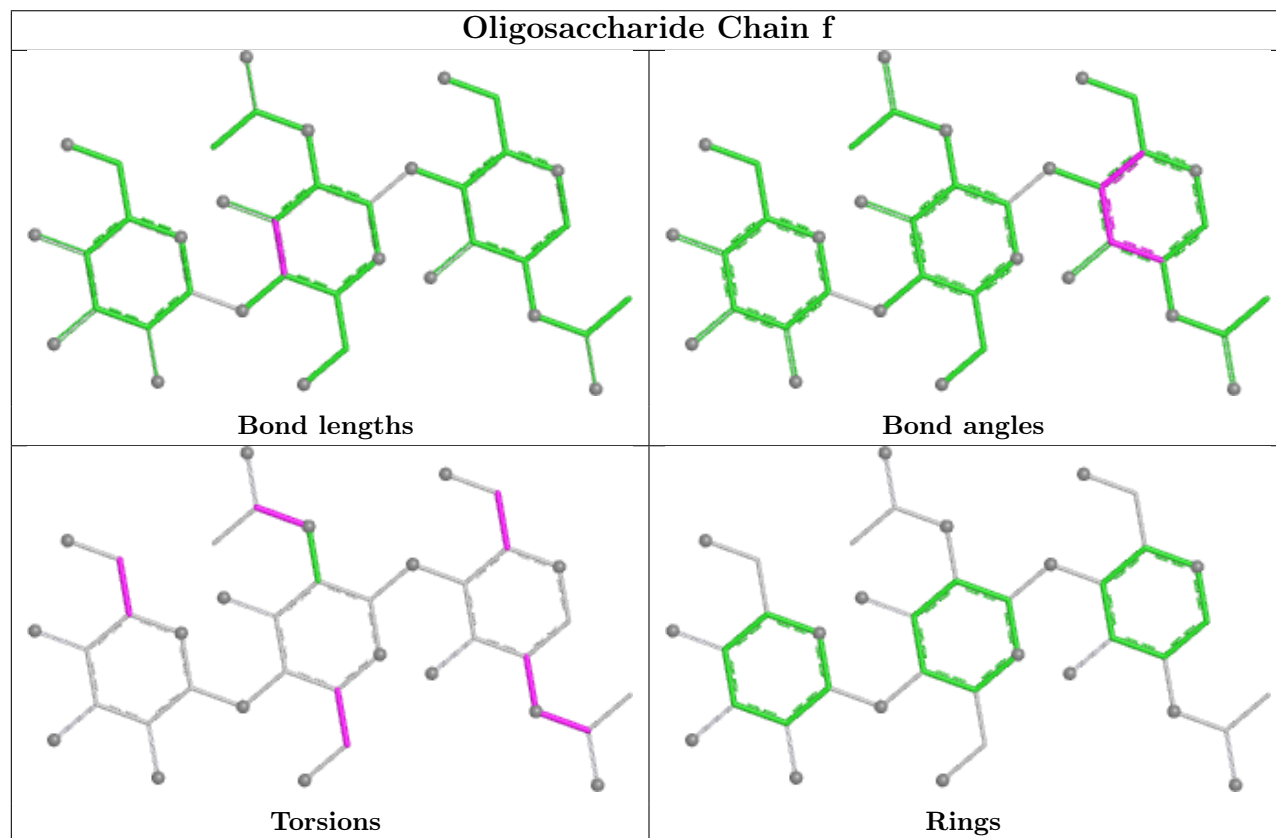
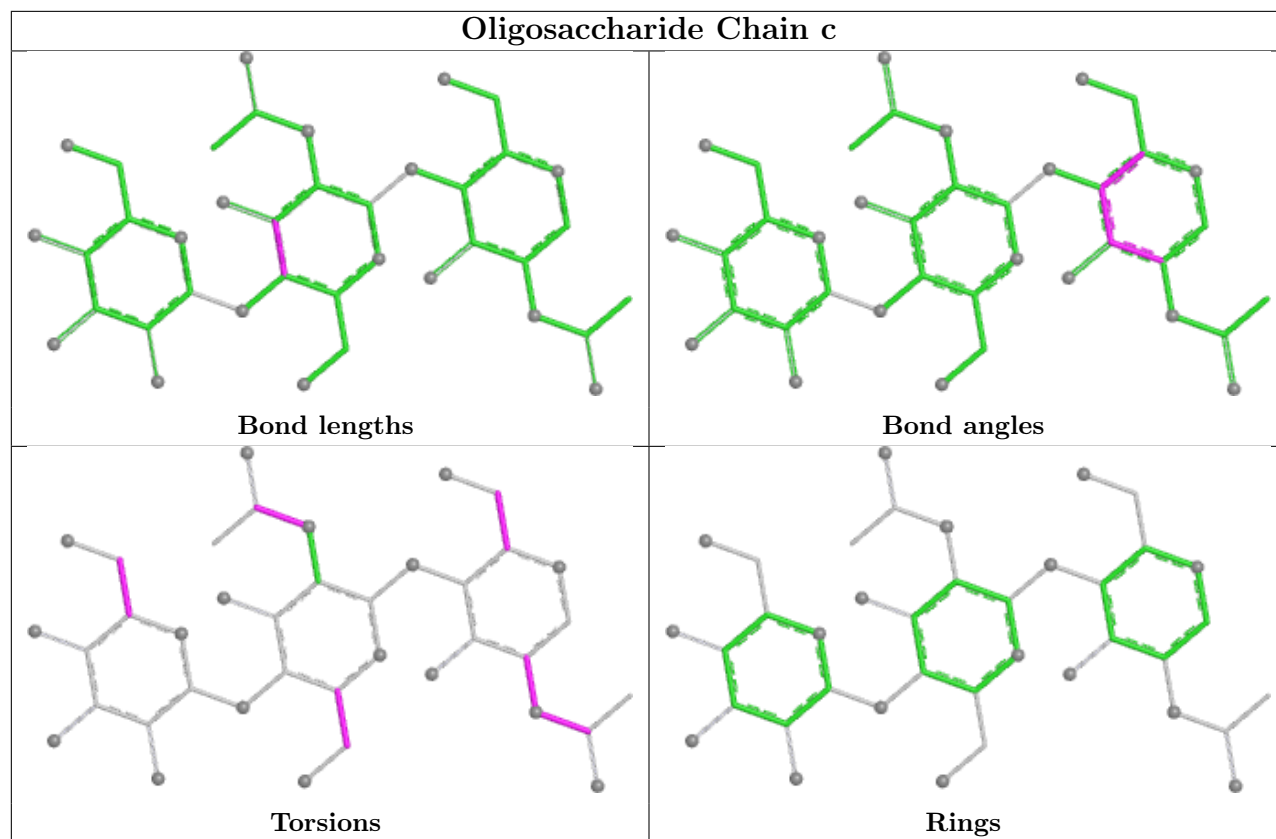


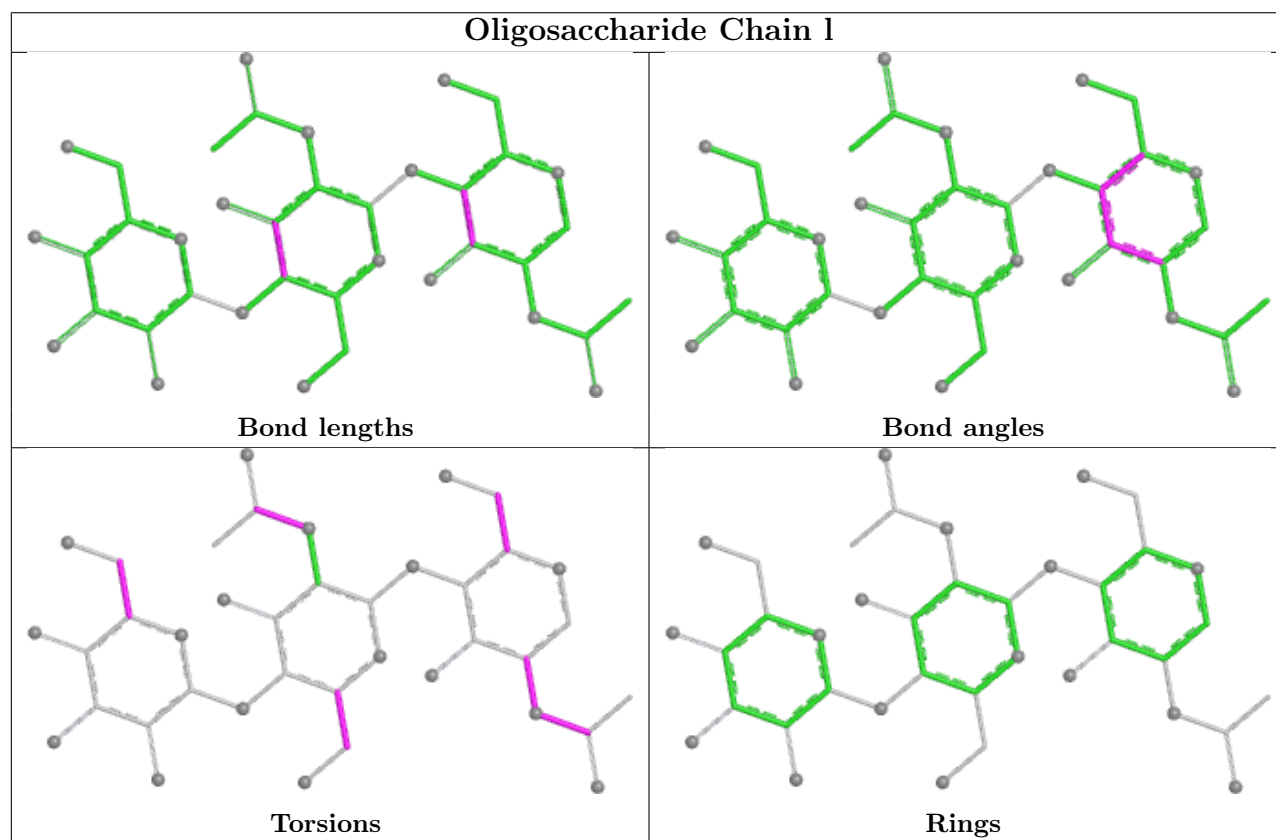
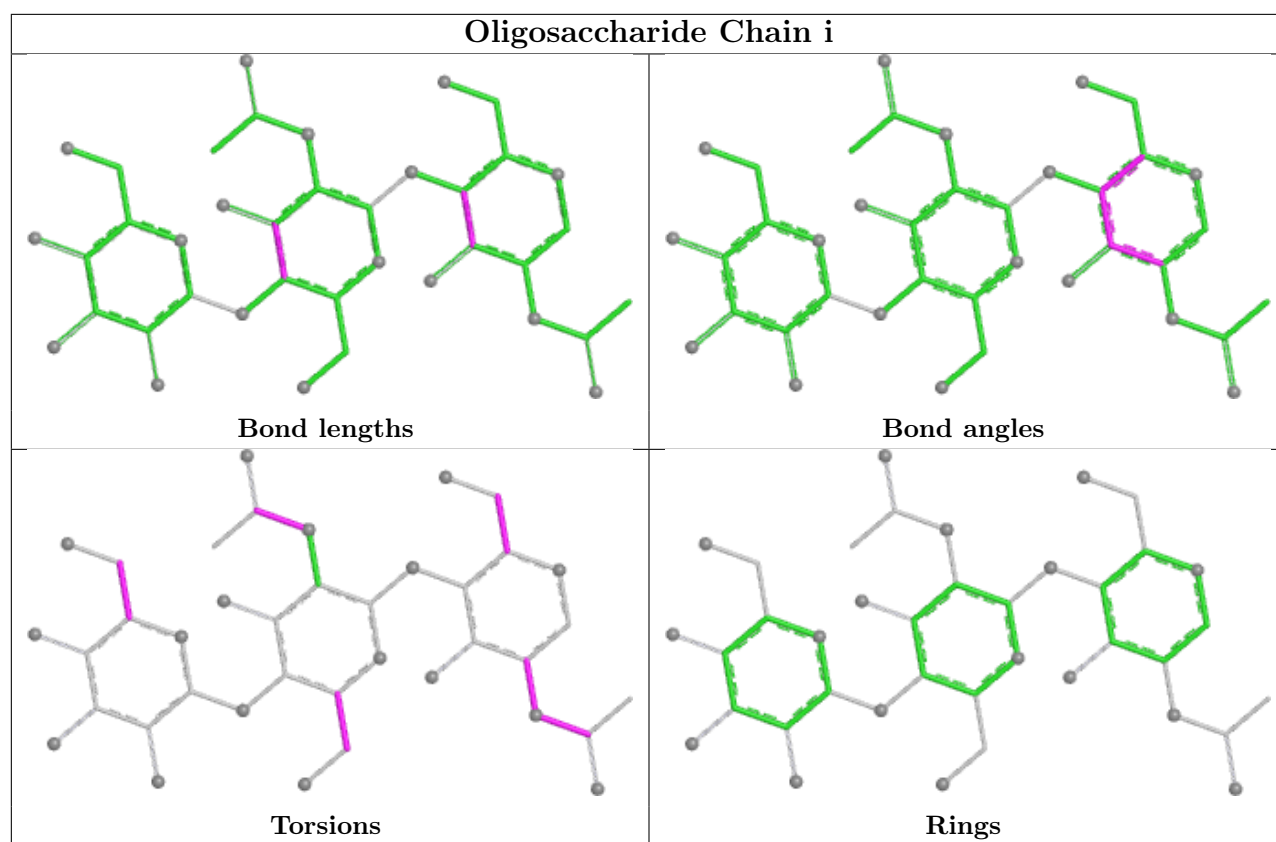


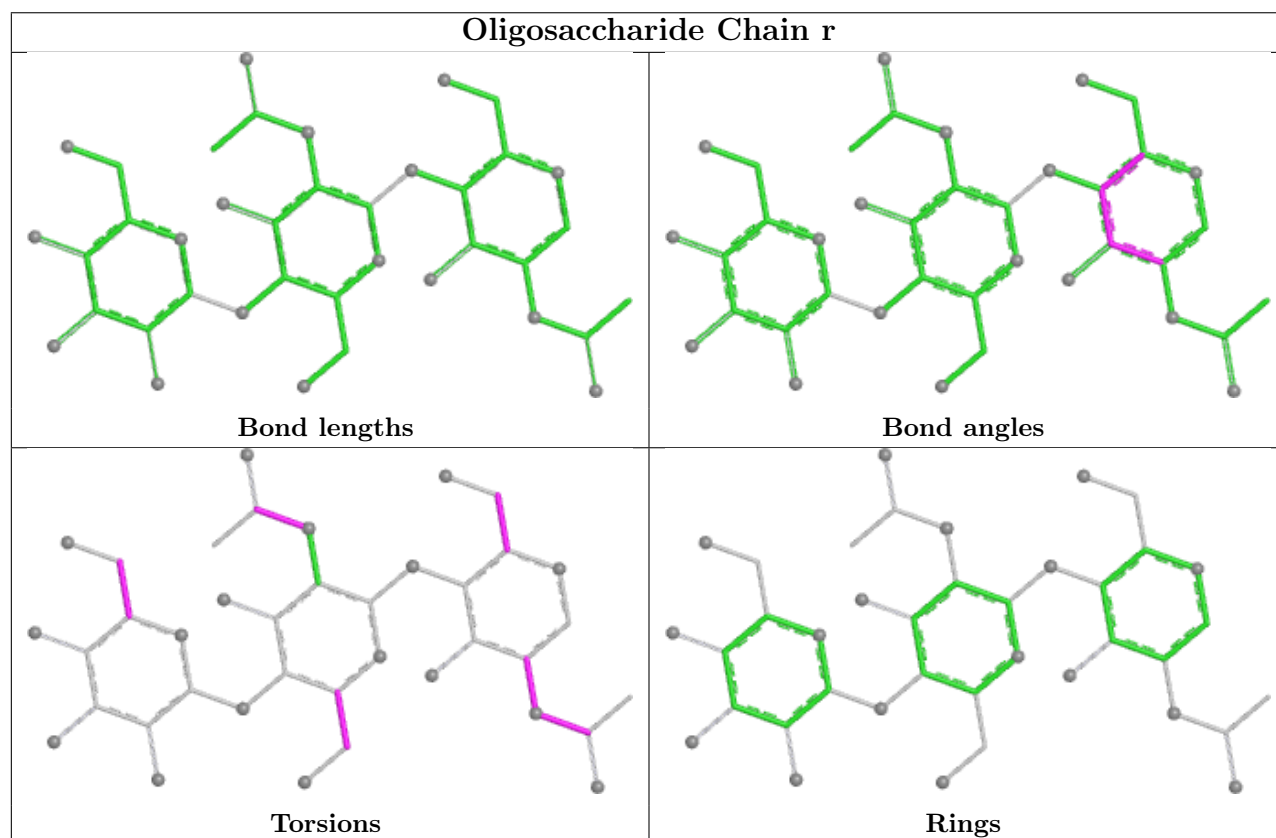
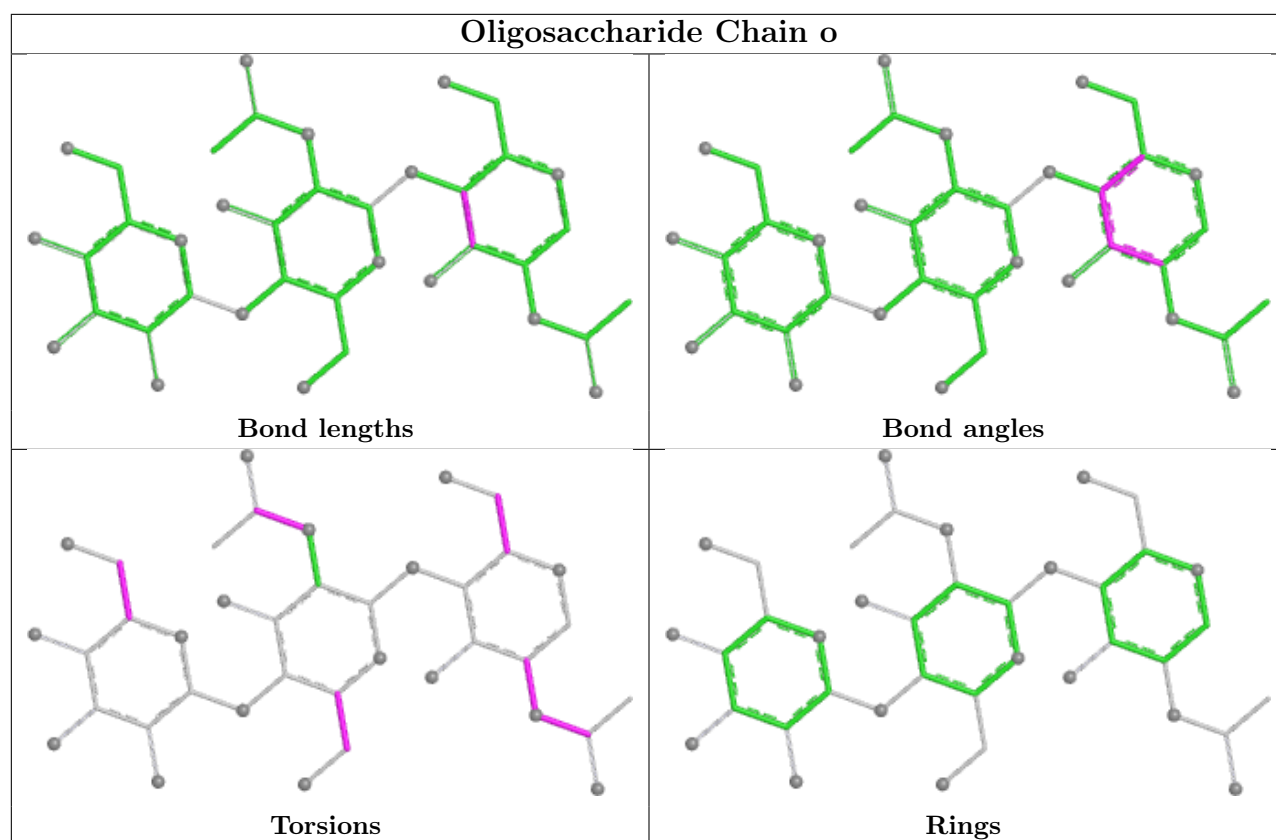


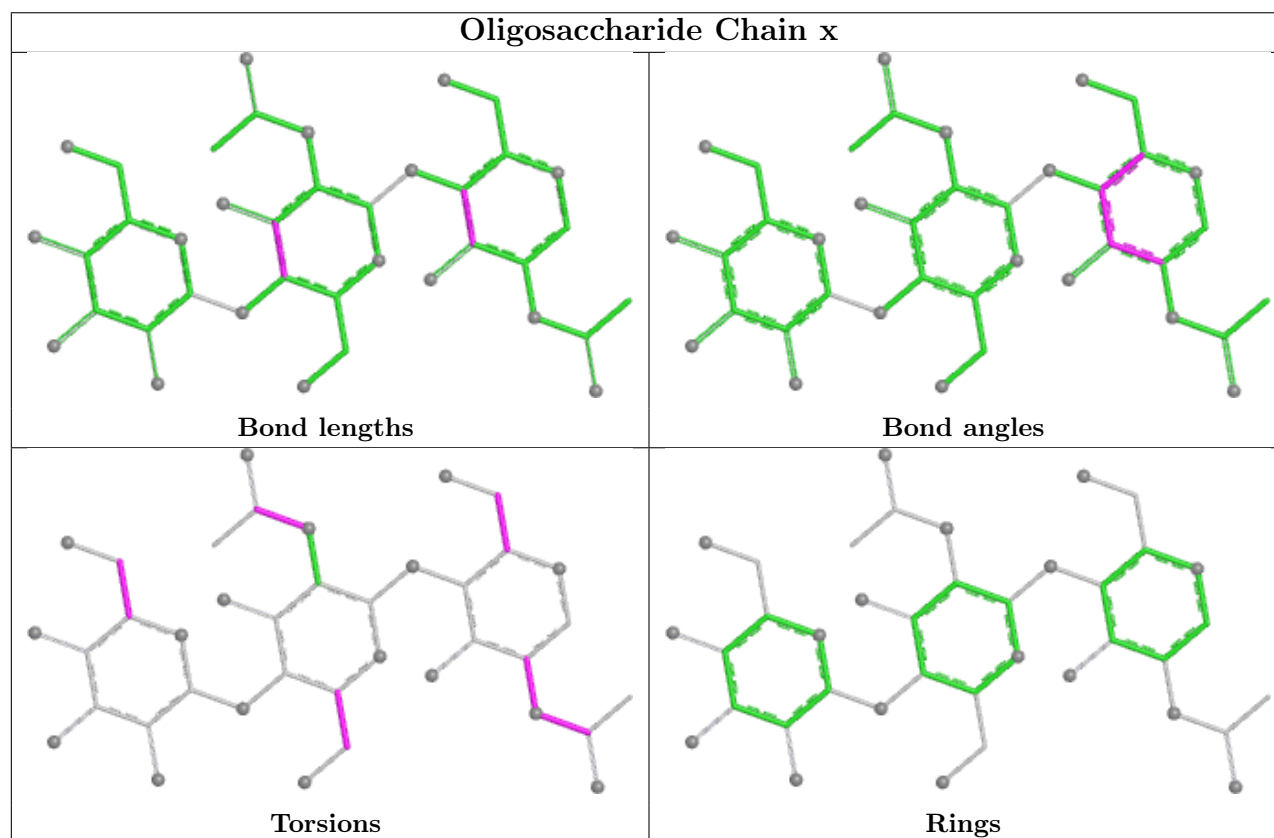
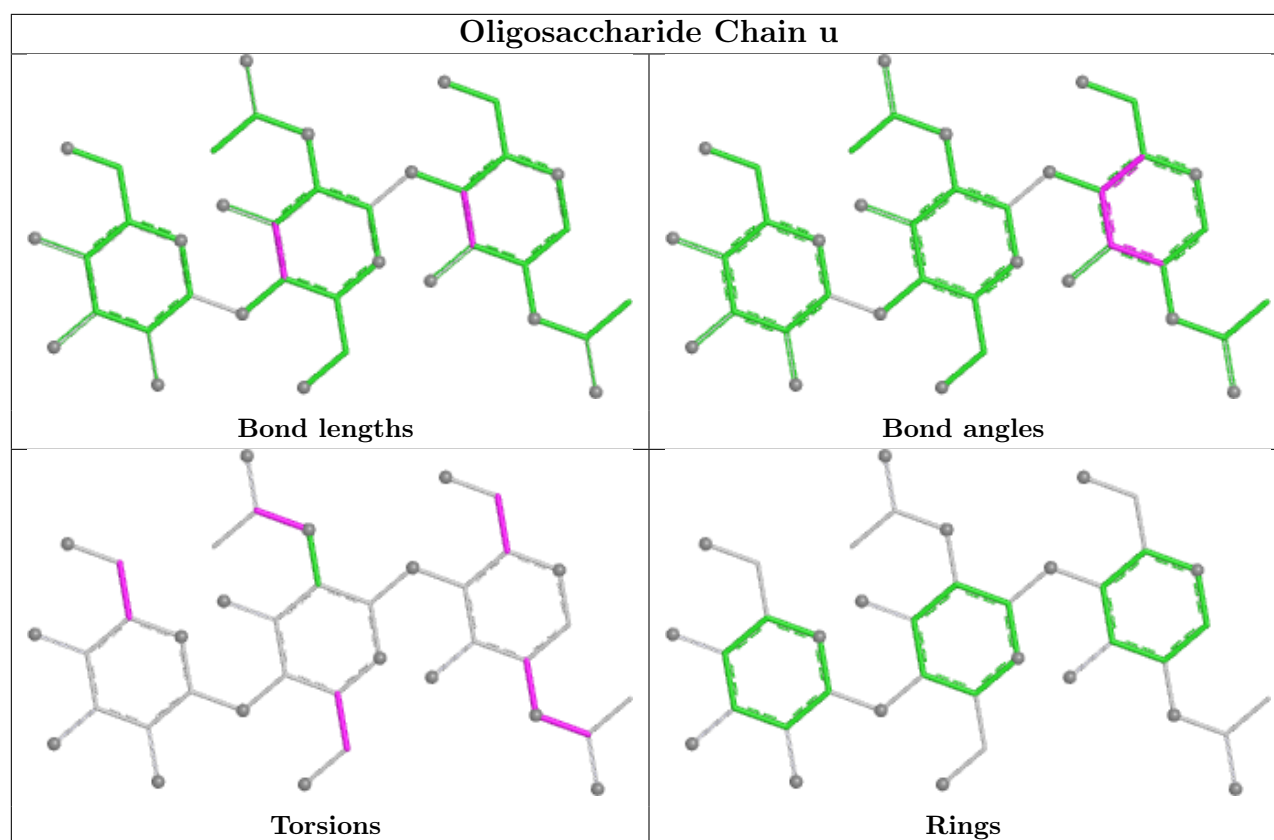


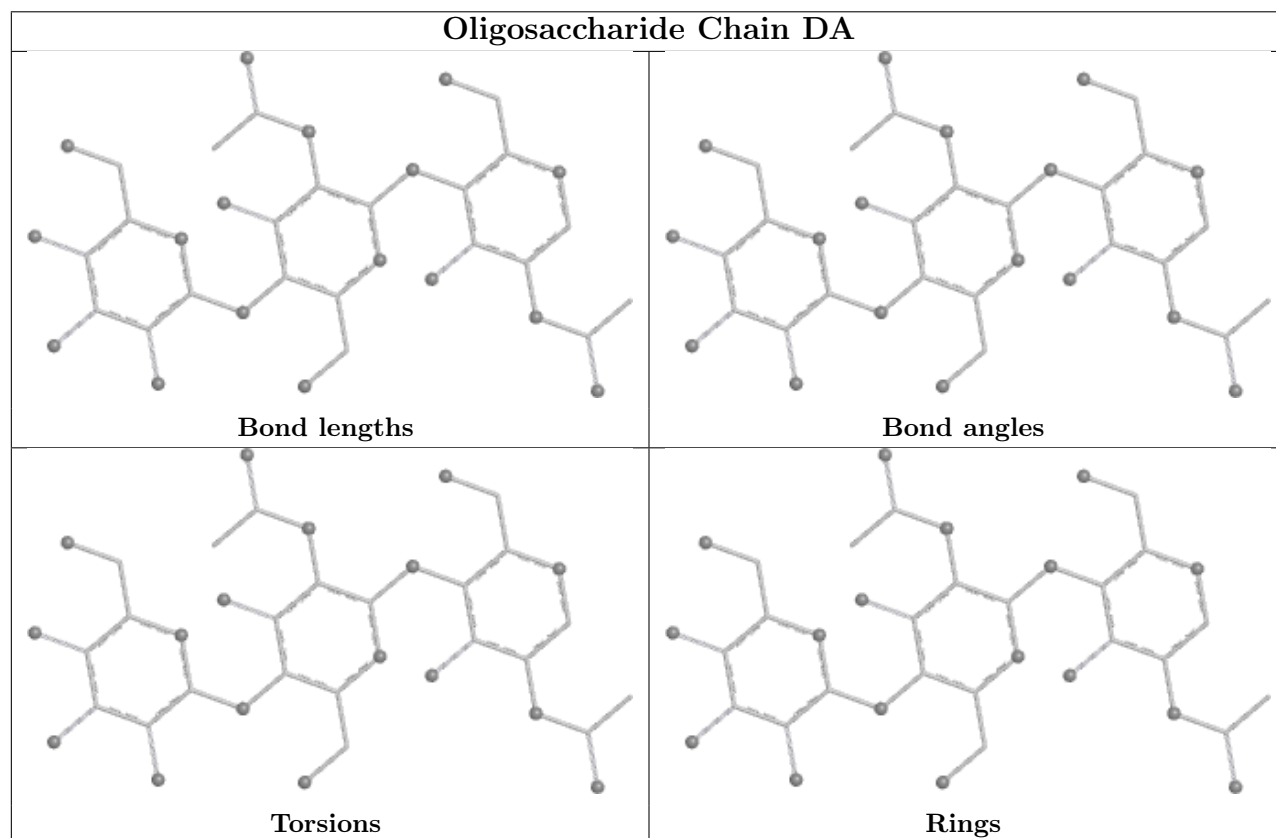
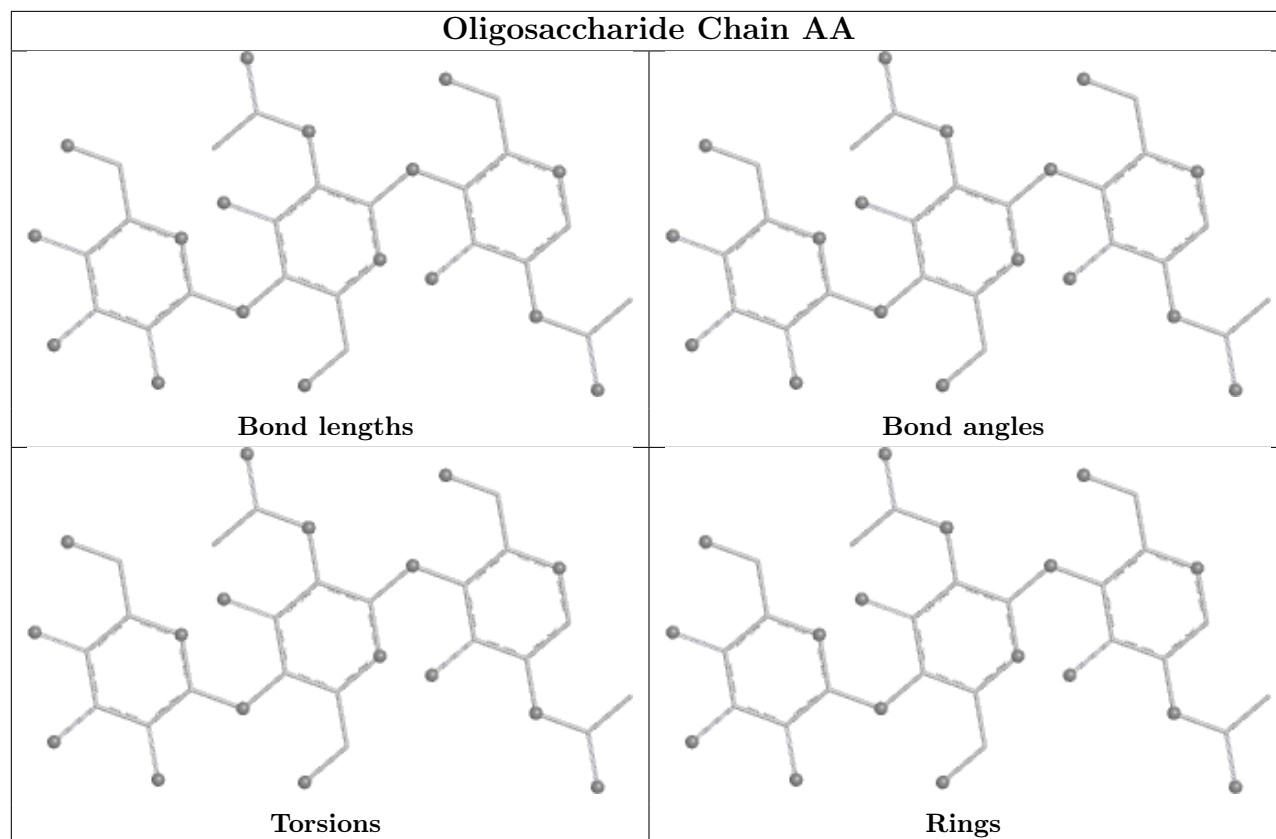


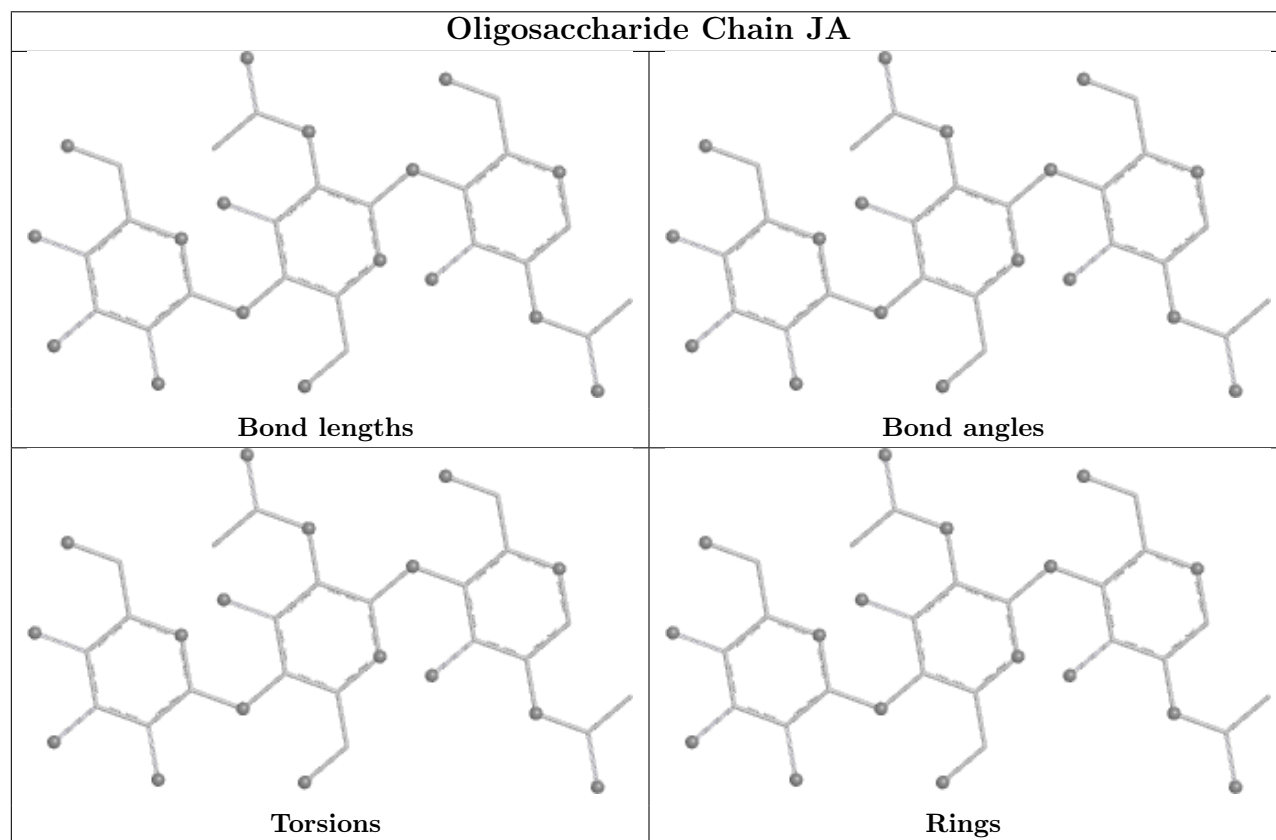
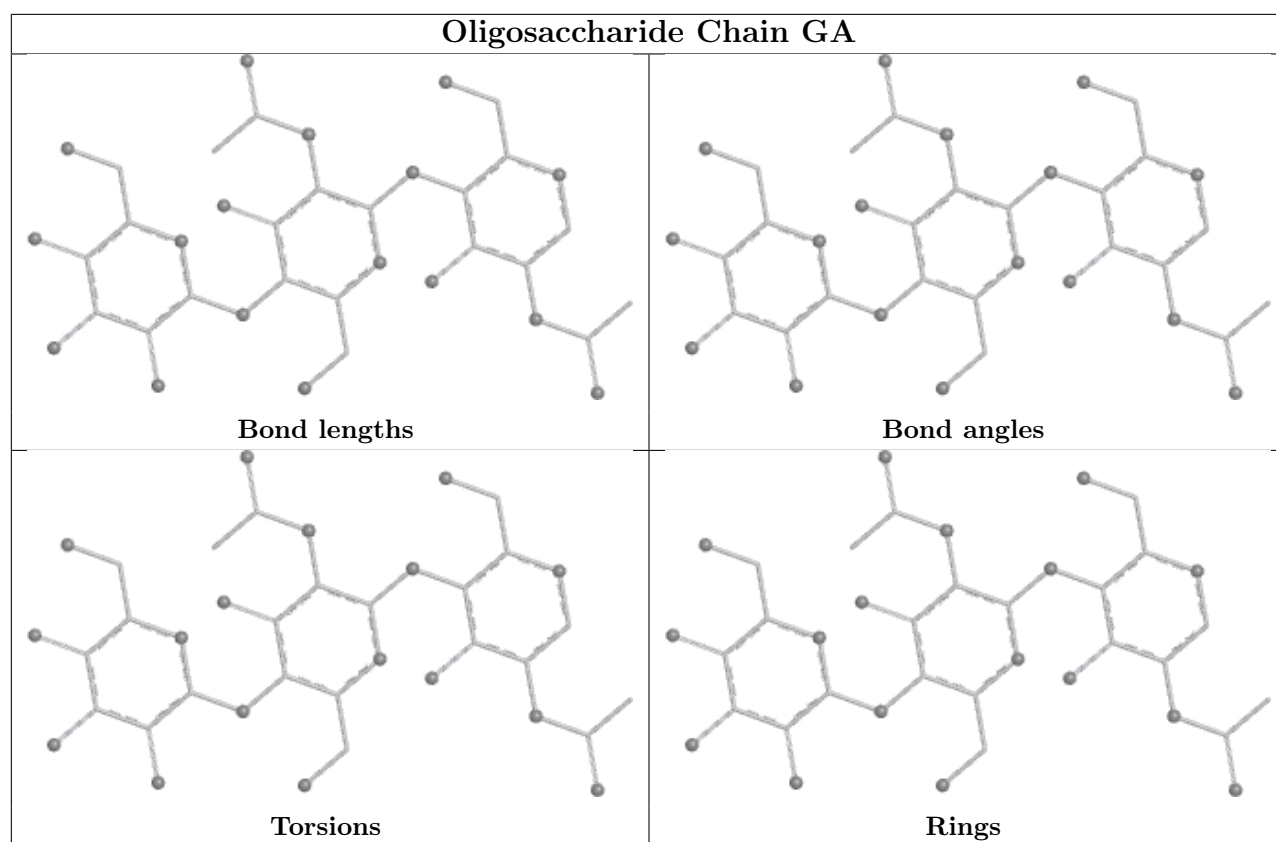












5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	618	1	14,14,15	0.72	0	17,19,21	0.68	0
7	NAG	A	618	1	14,14,15	0.73	0	17,19,21	0.69	0
7	NAG	E	618	1	14,14,15	0.73	0	17,19,21	0.67	0
7	NAG	A	608	1	14,14,15	0.63	0	17,19,21	0.72	1 (5%)
7	NAG	J	608	1	14,14,15	0.66	0	17,19,21	0.70	1 (5%)
7	NAG	H	608	1	14,14,15	0.78	1 (7%)	17,19,21	0.71	1 (5%)
7	NAG	C	618	1	14,14,15	0.74	0	17,19,21	0.68	0
7	NAG	D	618	1	14,14,15	0.77	0	17,19,21	0.68	0
7	NAG	K	608	1	14,14,15	0.71	0	17,19,21	0.71	1 (5%)
7	NAG	C	608	1	14,14,15	0.71	0	17,19,21	0.71	1 (5%)
7	NAG	F	608	1	14,14,15	0.68	0	17,19,21	0.70	1 (5%)
7	NAG	I	618	1	14,14,15	0.75	0	17,19,21	0.68	0
7	NAG	D	608	1	14,14,15	0.80	1 (7%)	17,19,21	0.70	1 (5%)
7	NAG	E	608	1	14,14,15	0.69	0	17,19,21	0.71	1 (5%)
7	NAG	K	618	1	14,14,15	0.76	0	17,19,21	0.67	0
7	NAG	H	618	1	14,14,15	1.18	2 (14%)	17,19,21	1.25	3 (17%)
7	NAG	G	608	1	14,14,15	0.69	0	17,19,21	0.73	1 (5%)
7	NAG	I	608	1	14,14,15	0.71	0	17,19,21	0.71	1 (5%)
7	NAG	L	618	1	14,14,15	0.73	0	17,19,21	0.67	0
7	NAG	F	618	1	14,14,15	0.76	0	17,19,21	0.66	0
7	NAG	J	618	1	14,14,15	0.75	0	17,19,21	0.65	0
7	NAG	B	618	1	14,14,15	0.79	1 (7%)	17,19,21	0.67	0
7	NAG	L	608	1	14,14,15	0.67	0	17,19,21	0.71	1 (5%)
7	NAG	B	608	1	14,14,15	0.78	1 (7%)	17,19,21	0.70	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
7	NAG	G	618	1	-	2/6/23/26	0/1/1/1
7	NAG	A	618	1	-	2/6/23/26	0/1/1/1
7	NAG	E	618	1	-	2/6/23/26	0/1/1/1
7	NAG	A	608	1	-	2/6/23/26	0/1/1/1
7	NAG	J	608	1	-	2/6/23/26	0/1/1/1
7	NAG	H	608	1	-	2/6/23/26	0/1/1/1
7	NAG	C	618	1	-	2/6/23/26	0/1/1/1
7	NAG	D	618	1	-	2/6/23/26	0/1/1/1
7	NAG	K	608	1	-	2/6/23/26	0/1/1/1
7	NAG	C	608	1	-	2/6/23/26	0/1/1/1
7	NAG	F	608	1	-	2/6/23/26	0/1/1/1
7	NAG	I	618	1	-	2/6/23/26	0/1/1/1
7	NAG	D	608	1	-	2/6/23/26	0/1/1/1
7	NAG	E	608	1	-	2/6/23/26	0/1/1/1
7	NAG	K	618	1	-	2/6/23/26	0/1/1/1
7	NAG	H	618	1	-	2/6/23/26	0/1/1/1
7	NAG	G	608	1	-	2/6/23/26	0/1/1/1
7	NAG	I	608	1	-	2/6/23/26	0/1/1/1
7	NAG	L	618	1	-	2/6/23/26	0/1/1/1
7	NAG	F	618	1	-	2/6/23/26	0/1/1/1
7	NAG	J	618	1	-	2/6/23/26	0/1/1/1
7	NAG	B	618	1	-	2/6/23/26	0/1/1/1
7	NAG	L	608	1	-	2/6/23/26	0/1/1/1
7	NAG	B	608	1	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	618	NAG	O5-C5	2.56	1.48	1.43
7	D	608	NAG	C4-C3	2.24	1.58	1.52
7	H	608	NAG	C4-C3	2.22	1.58	1.52
7	B	608	NAG	C4-C3	2.14	1.57	1.52
7	H	618	NAG	C3-C2	2.10	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	618	NAG	O4-C4-C3	2.56	116.42	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	618	NAG	C3-C4-C5	2.55	114.85	110.23
7	L	608	NAG	C2-N2-C7	-2.13	120.04	122.90
7	H	608	NAG	C2-N2-C7	-2.13	120.04	122.90
7	G	608	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	608	NAG	C8-C7-N2-C2
7	A	608	NAG	O7-C7-N2-C2
7	B	608	NAG	C8-C7-N2-C2
7	B	608	NAG	O7-C7-N2-C2
7	C	608	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	493/493 (100%)	-0.51	0 100 100	113, 184, 248, 333	0
1	B	493/493 (100%)	-0.50	0 100 100	113, 184, 249, 332	0
1	C	493/493 (100%)	-0.45	0 100 100	112, 184, 249, 333	0
1	D	493/493 (100%)	-0.40	1 (0%) 91 81	114, 184, 249, 333	0
1	E	493/493 (100%)	-0.40	0 100 100	113, 184, 249, 333	0
1	F	493/493 (100%)	-0.37	0 100 100	114, 184, 248, 333	0
1	G	493/493 (100%)	-0.56	0 100 100	114, 184, 249, 333	0
1	H	493/493 (100%)	-0.55	0 100 100	113, 184, 248, 333	0
1	I	493/493 (100%)	-0.52	1 (0%) 91 81	114, 184, 249, 333	0
1	J	493/493 (100%)	-0.51	1 (0%) 91 81	113, 184, 248, 333	0
1	K	493/493 (100%)	-0.55	0 100 100	113, 184, 249, 333	0
1	L	493/493 (100%)	-0.40	1 (0%) 91 81	114, 184, 249, 333	0
2	1	226/226 (100%)	-0.37	0 100 100	125, 213, 300, 359	0
2	3	226/226 (100%)	-0.36	0 100 100	114, 213, 300, 359	0
2	5	226/226 (100%)	-0.44	0 100 100	134, 215, 300, 359	0
2	7	226/226 (100%)	-0.39	0 100 100	137, 212, 300, 359	0
2	9	226/226 (100%)	-0.32	0 100 100	131, 213, 300, 359	0
2	M	226/226 (100%)	-0.41	0 100 100	133, 213, 304, 359	0
2	O	226/226 (100%)	-0.29	0 100 100	136, 212, 306, 359	0
2	Q	226/226 (100%)	-0.39	0 100 100	140, 214, 306, 359	0
2	S	226/226 (100%)	-0.38	0 100 100	146, 214, 306, 359	0
2	U	226/226 (100%)	-0.25	1 (0%) 88 75	145, 214, 306, 359	0
2	W	226/226 (100%)	-0.32	0 100 100	121, 213, 306, 359	0
2	Y	226/226 (100%)	-0.44	0 100 100	145, 214, 306, 359	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	0	212/220 (96%)	-0.22	0 100 100	146, 221, 284, 324	0
3	2	212/220 (96%)	-0.43	0 100 100	146, 222, 284, 325	0
3	4	212/220 (96%)	-0.31	1 (0%) 87 73	146, 221, 284, 325	0
3	6	212/220 (96%)	-0.48	0 100 100	146, 223, 284, 325	0
3	8	212/220 (96%)	-0.35	0 100 100	146, 223, 284, 324	0
3	N	212/220 (96%)	-0.41	0 100 100	146, 222, 284, 324	0
3	P	212/220 (96%)	-0.25	0 100 100	146, 222, 284, 324	0
3	R	212/220 (96%)	-0.45	0 100 100	146, 224, 284, 324	0
3	T	212/220 (96%)	-0.43	0 100 100	146, 224, 284, 324	0
3	V	212/220 (96%)	-0.28	0 100 100	146, 223, 284, 325	0
3	X	212/220 (96%)	-0.27	0 100 100	146, 222, 284, 325	0
3	Z	212/220 (96%)	-0.48	1 (0%) 87 73	146, 223, 284, 325	0
All	All	11172/11268 (99%)	-0.42	7 (0%) 92 87	112, 200, 279, 359	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	98	TYR	2.8
3	Z	136	THR	2.4
1	L	335	ILE	2.4
3	4	136	THR	2.4
2	U	101	GLY	2.4

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(Å ²)	Q<0.9
4	NAG	a	1	14/15	-	-	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	a	2	14/15	-	-	198,198,198,198	0
4	BMA	a	3	11/12	-	-	212,212,212,212	0
4	MAN	a	4	11/12	-	-	235,235,235,235	0
4	MAN	a	5	11/12	-	-	222,222,222,222	0
4	MAN	a	6	11/12	-	-	244,244,244,244	0
4	MAN	a	7	11/12	-	-	236,236,236,236	0
4	NAG	d	1	14/15	-	-	168,168,168,168	0
4	NAG	d	2	14/15	-	-	198,198,198,198	0
4	BMA	d	3	11/12	-	-	212,212,212,212	0
4	MAN	d	4	11/12	-	-	235,235,235,235	0
4	MAN	d	5	11/12	-	-	222,222,222,222	0
4	MAN	d	6	11/12	-	-	245,245,245,245	0
4	MAN	d	7	11/12	-	-	235,235,235,235	0
4	NAG	g	1	14/15	-	-	168,168,168,168	0
4	NAG	g	2	14/15	-	-	199,199,199,199	0
4	BMA	g	3	11/12	-	-	212,212,212,212	0
4	MAN	g	4	11/12	-	-	235,235,235,235	0
4	MAN	g	5	11/12	-	-	223,223,223,223	0
4	MAN	g	6	11/12	-	-	244,244,244,244	0
4	MAN	g	7	11/12	-	-	236,236,236,236	0
4	NAG	j	1	14/15	-	-	168,168,168,168	0
4	NAG	j	2	14/15	-	-	199,199,199,199	0
4	BMA	j	3	11/12	-	-	212,212,212,212	0
4	MAN	j	4	11/12	-	-	235,235,235,235	0
4	MAN	j	5	11/12	-	-	223,223,223,223	0
4	MAN	j	6	11/12	-	-	244,244,244,244	0
4	MAN	j	7	11/12	-	-	236,236,236,236	0
4	NAG	m	1	14/15	-	-	169,169,169,169	0
4	NAG	m	2	14/15	-	-	198,198,198,198	0
4	BMA	m	3	11/12	-	-	212,212,212,212	0
4	MAN	m	4	11/12	-	-	235,235,235,235	0
4	MAN	m	5	11/12	-	-	222,222,222,222	0
4	MAN	m	6	11/12	-	-	244,244,244,244	0
4	MAN	m	7	11/12	-	-	236,236,236,236	0
4	NAG	p	1	14/15	-	-	169,169,169,169	0
4	NAG	p	2	14/15	-	-	198,198,198,198	0
4	BMA	p	3	11/12	-	-	212,212,212,212	0
4	MAN	p	4	11/12	-	-	235,235,235,235	0
4	MAN	p	5	11/12	-	-	222,222,222,222	0
4	MAN	p	6	11/12	-	-	244,244,244,244	0
4	MAN	p	7	11/12	-	-	236,236,236,236	0
4	NAG	s	1	14/15	-	-	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	s	2	14/15	-	-	198,198,198,198	0
4	BMA	s	3	11/12	-	-	212,212,212,212	0
4	MAN	s	4	11/12	-	-	235,235,235,235	0
4	MAN	s	5	11/12	-	-	222,222,222,222	0
4	MAN	s	6	11/12	-	-	244,244,244,244	0
4	MAN	s	7	11/12	-	-	236,236,236,236	0
4	NAG	v	1	14/15	-	-	168,168,168,168	0
4	NAG	v	2	14/15	-	-	199,199,199,199	0
4	BMA	v	3	11/12	-	-	212,212,212,212	0
4	MAN	v	4	11/12	-	-	235,235,235,235	0
4	MAN	v	5	11/12	-	-	222,222,222,222	0
4	MAN	v	6	11/12	-	-	245,245,245,245	0
4	MAN	v	7	11/12	-	-	235,235,235,235	0
4	NAG	y	1	14/15	-	-	168,168,168,168	0
4	NAG	y	2	14/15	-	-	199,199,199,199	0
4	BMA	y	3	11/12	-	-	212,212,212,212	0
4	MAN	y	4	11/12	-	-	235,235,235,235	0
4	MAN	y	5	11/12	-	-	222,222,222,222	0
4	MAN	y	6	11/12	-	-	245,245,245,245	0
4	MAN	y	7	11/12	-	-	235,235,235,235	0
4	NAG	BA	1	14/15	-	-	169,169,169,169	0
4	NAG	BA	2	14/15	-	-	198,198,198,198	0
4	BMA	BA	3	11/12	-	-	212,212,212,212	0
4	MAN	BA	4	11/12	-	-	235,235,235,235	0
4	MAN	BA	5	11/12	-	-	222,222,222,222	0
4	MAN	BA	6	11/12	-	-	244,244,244,244	0
4	MAN	BA	7	11/12	-	-	236,236,236,236	0
4	NAG	EA	1	14/15	-	-	168,168,168,168	0
4	NAG	EA	2	14/15	-	-	199,199,199,199	0
4	BMA	EA	3	11/12	-	-	212,212,212,212	0
4	MAN	EA	4	11/12	-	-	235,235,235,235	0
4	MAN	EA	5	11/12	-	-	222,222,222,222	0
4	MAN	EA	6	11/12	-	-	244,244,244,244	0
4	MAN	EA	7	11/12	-	-	236,236,236,236	0
4	NAG	HA	1	14/15	-	-	169,169,169,169	0
4	NAG	HA	2	14/15	-	-	199,199,199,199	0
4	BMA	HA	3	11/12	-	-	212,212,212,212	0
4	MAN	HA	4	11/12	-	-	235,235,235,235	0
4	MAN	HA	5	11/12	-	-	222,222,222,222	0
4	MAN	HA	6	11/12	-	-	245,245,245,245	0
4	MAN	HA	7	11/12	-	-	236,236,236,236	0
5	NAG	b	1	14/15	-	-	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	b	2	14/15	-	-	201,201,201,201	0
5	BMA	b	3	11/12	-	-	223,223,223,223	0
5	MAN	b	4	11/12	-	-	271,271,271,271	0
5	MAN	b	5	11/12	-	-	293,293,293,293	0
5	MAN	b	6	11/12	-	-	253,253,253,253	0
5	NAG	e	1	14/15	-	-	181,181,181,181	0
5	NAG	e	2	14/15	-	-	202,202,202,202	0
5	BMA	e	3	11/12	-	-	223,223,223,223	0
5	MAN	e	4	11/12	-	-	271,271,271,271	0
5	MAN	e	5	11/12	-	-	294,294,294,294	0
5	MAN	e	6	11/12	-	-	254,254,254,254	0
5	NAG	h	1	14/15	-	-	180,180,180,180	0
5	NAG	h	2	14/15	-	-	201,201,201,201	0
5	BMA	h	3	11/12	-	-	223,223,223,223	0
5	MAN	h	4	11/12	-	-	271,271,271,271	0
5	MAN	h	5	11/12	-	-	294,294,294,294	0
5	MAN	h	6	11/12	-	-	253,253,253,253	0
5	NAG	k	1	14/15	-	-	181,181,181,181	0
5	NAG	k	2	14/15	-	-	202,202,202,202	0
5	BMA	k	3	11/12	-	-	224,224,224,224	0
5	MAN	k	4	11/12	-	-	271,271,271,271	0
5	MAN	k	5	11/12	-	-	294,294,294,294	0
5	MAN	k	6	11/12	-	-	254,254,254,254	0
5	NAG	n	1	14/15	-	-	180,180,180,180	0
5	NAG	n	2	14/15	-	-	201,201,201,201	0
5	BMA	n	3	11/12	-	-	223,223,223,223	0
5	MAN	n	4	11/12	-	-	271,271,271,271	0
5	MAN	n	5	11/12	-	-	293,293,293,293	0
5	MAN	n	6	11/12	-	-	253,253,253,253	0
5	NAG	q	1	14/15	-	-	181,181,181,181	0
5	NAG	q	2	14/15	-	-	202,202,202,202	0
5	BMA	q	3	11/12	-	-	224,224,224,224	0
5	MAN	q	4	11/12	-	-	271,271,271,271	0
5	MAN	q	5	11/12	-	-	293,293,293,293	0
5	MAN	q	6	11/12	-	-	253,253,253,253	0
5	NAG	t	1	14/15	-	-	181,181,181,181	0
5	NAG	t	2	14/15	-	-	202,202,202,202	0
5	BMA	t	3	11/12	-	-	224,224,224,224	0
5	MAN	t	4	11/12	-	-	271,271,271,271	0
5	MAN	t	5	11/12	-	-	294,294,294,294	0
5	MAN	t	6	11/12	-	-	254,254,254,254	0
5	NAG	w	1	14/15	-	-	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	w	2	14/15	-	-	202,202,202,202	0
5	BMA	w	3	11/12	-	-	223,223,223,223	0
5	MAN	w	4	11/12	-	-	271,271,271,271	0
5	MAN	w	5	11/12	-	-	294,294,294,294	0
5	MAN	w	6	11/12	-	-	253,253,253,253	0
5	NAG	z	1	14/15	-	-	181,181,181,181	0
5	NAG	z	2	14/15	-	-	202,202,202,202	0
5	BMA	z	3	11/12	-	-	224,224,224,224	0
5	MAN	z	4	11/12	-	-	271,271,271,271	0
5	MAN	z	5	11/12	-	-	294,294,294,294	0
5	MAN	z	6	11/12	-	-	254,254,254,254	0
5	NAG	CA	1	14/15	-	-	181,181,181,181	0
5	NAG	CA	2	14/15	-	-	202,202,202,202	0
5	BMA	CA	3	11/12	-	-	223,223,223,223	0
5	MAN	CA	4	11/12	-	-	271,271,271,271	0
5	MAN	CA	5	11/12	-	-	294,294,294,294	0
5	MAN	CA	6	11/12	-	-	254,254,254,254	0
5	NAG	FA	1	14/15	-	-	181,181,181,181	0
5	NAG	FA	2	14/15	-	-	202,202,202,202	0
5	BMA	FA	3	11/12	-	-	224,224,224,224	0
5	MAN	FA	4	11/12	-	-	271,271,271,271	0
5	MAN	FA	5	11/12	-	-	294,294,294,294	0
5	MAN	FA	6	11/12	-	-	254,254,254,254	0
5	NAG	IA	1	14/15	-	-	181,181,181,181	0
5	NAG	IA	2	14/15	-	-	202,202,202,202	0
5	BMA	IA	3	11/12	-	-	223,223,223,223	0
5	MAN	IA	4	11/12	-	-	271,271,271,271	0
5	MAN	IA	5	11/12	-	-	294,294,294,294	0
5	MAN	IA	6	11/12	-	-	254,254,254,254	0
6	NAG	c	1	14/15	-	-	250,250,250,250	0
6	NAG	c	2	14/15	-	-	271,271,271,271	0
6	BMA	c	3	11/12	-	-	301,301,301,301	0
6	NAG	f	1	14/15	-	-	251,251,251,251	0
6	NAG	f	2	14/15	-	-	270,270,270,270	0
6	BMA	f	3	11/12	-	-	301,301,301,301	0
6	NAG	i	1	14/15	-	-	251,251,251,251	0
6	NAG	i	2	14/15	-	-	270,270,270,270	0
6	BMA	i	3	11/12	-	-	301,301,301,301	0
6	NAG	l	1	14/15	-	-	250,250,250,250	0
6	NAG	l	2	14/15	-	-	270,270,270,270	0
6	BMA	l	3	11/12	-	-	301,301,301,301	0
6	NAG	o	1	14/15	-	-	251,251,251,251	0

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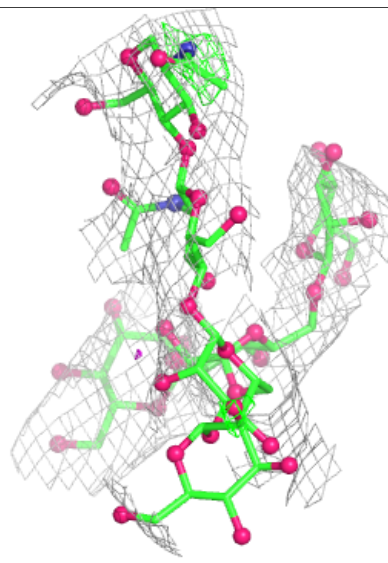
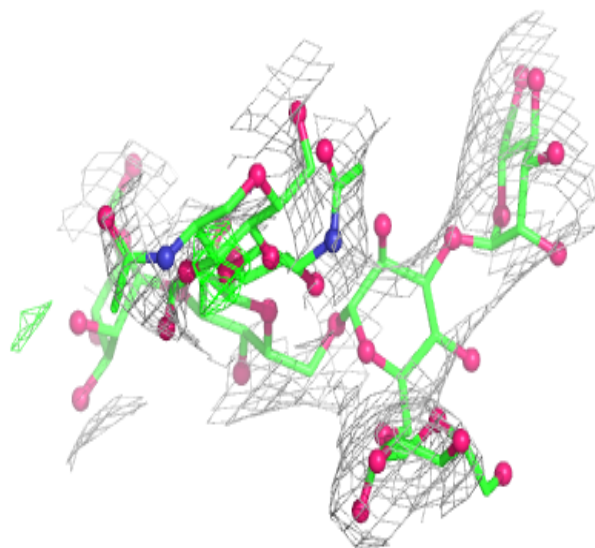
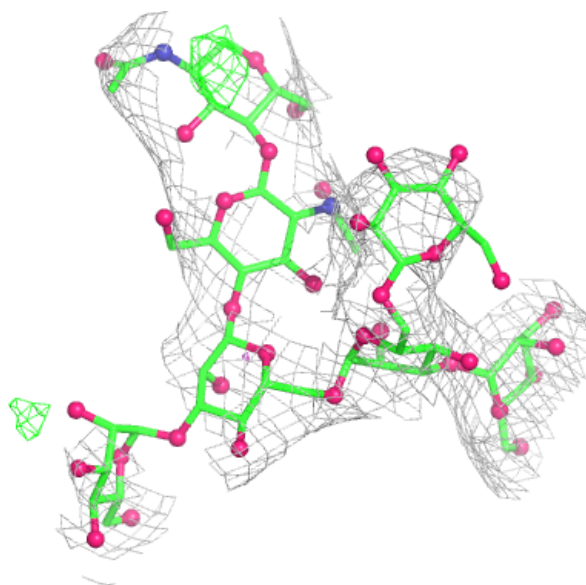
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	o	2	14/15	-	-	270,270,270,270	0
6	BMA	o	3	11/12	-	-	301,301,301,301	0
6	NAG	r	1	14/15	-	-	250,250,250,250	0
6	NAG	r	2	14/15	-	-	270,270,270,270	0
6	BMA	r	3	11/12	-	-	301,301,301,301	0
6	NAG	u	1	14/15	-	-	251,251,251,251	0
6	NAG	u	2	14/15	-	-	270,270,270,270	0
6	BMA	u	3	11/12	-	-	301,301,301,301	0
6	NAG	x	1	14/15	-	-	251,251,251,251	0
6	NAG	x	2	14/15	-	-	270,270,270,270	0
6	BMA	x	3	11/12	-	-	301,301,301,301	0
6	NAG	AA	1	14/15	-	-	250,250,250,250	0
6	NAG	AA	2	14/15	-	-	270,270,270,270	0
6	BMA	AA	3	11/12	-	-	301,301,301,301	0
6	NAG	DA	1	14/15	-	-	251,251,251,251	0
6	NAG	DA	2	14/15	-	-	270,270,270,270	0
6	BMA	DA	3	11/12	-	-	301,301,301,301	0
6	NAG	GA	1	14/15	-	-	251,251,251,251	0
6	NAG	GA	2	14/15	-	-	270,270,270,270	0
6	BMA	GA	3	11/12	-	-	301,301,301,301	0
6	NAG	JA	1	14/15	-	-	251,251,251,251	0
6	NAG	JA	2	14/15	-	-	270,270,270,270	0
6	BMA	JA	3	11/12	-	-	301,301,301,301	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.

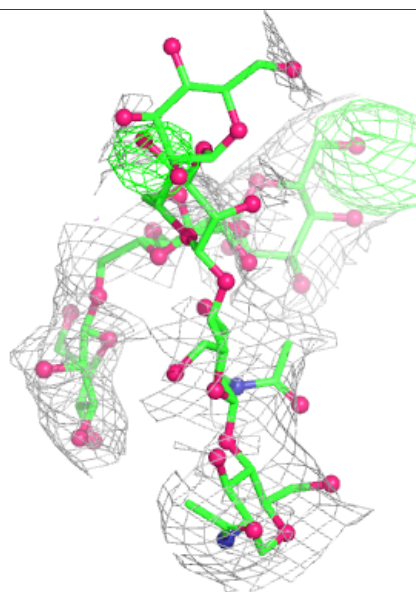
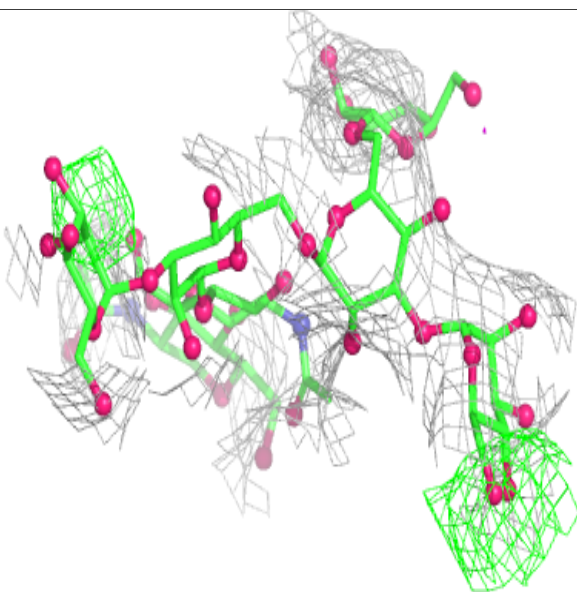
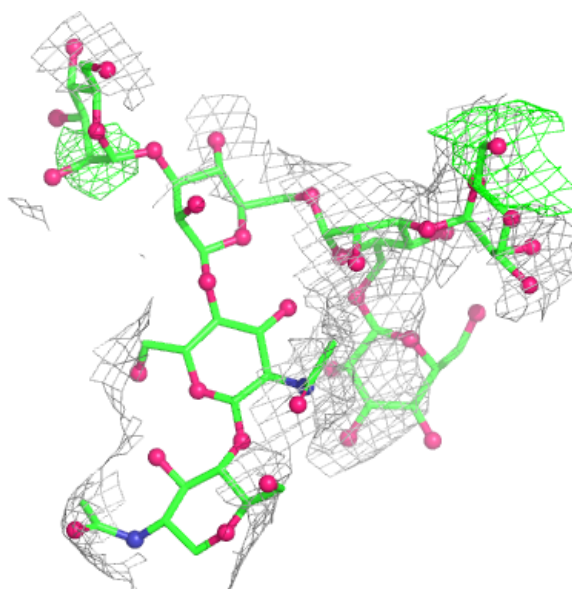
Electron density around Chain a:

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



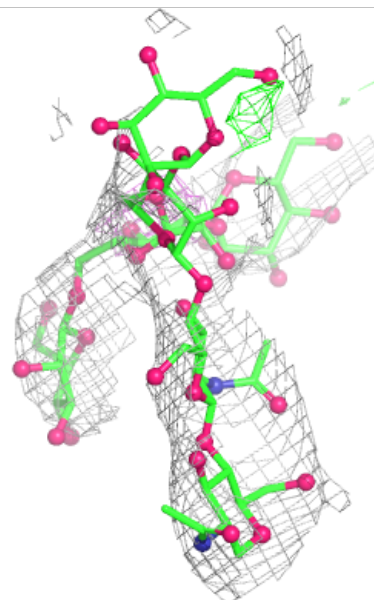
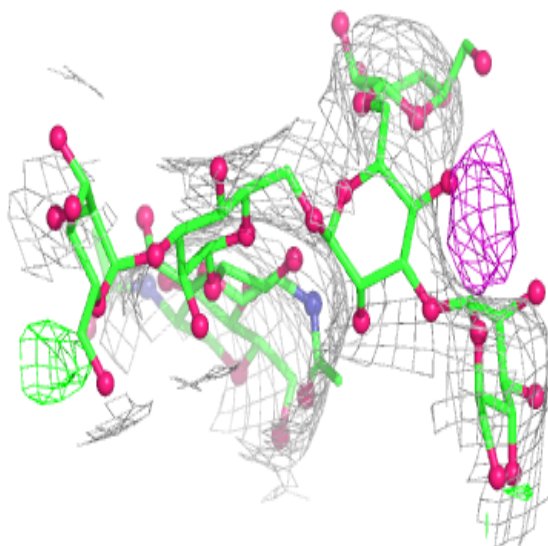
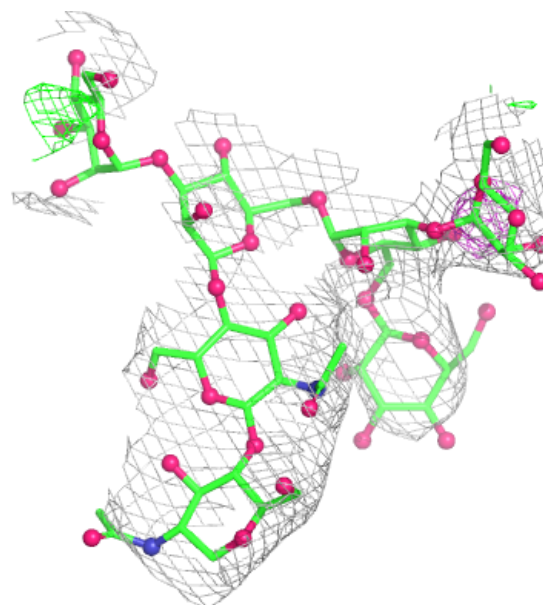
Electron density around Chain d:

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



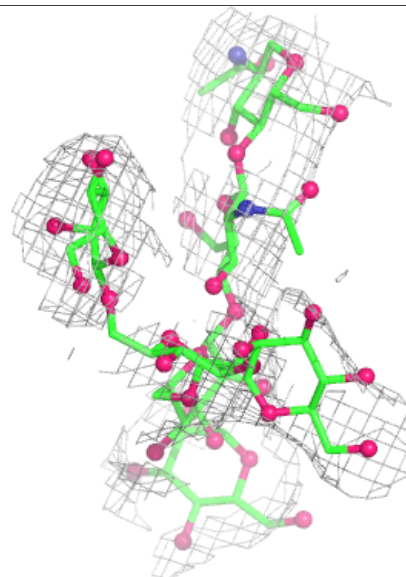
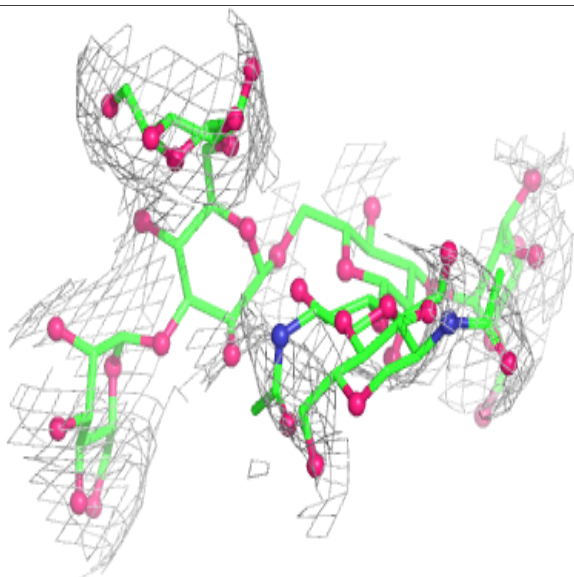
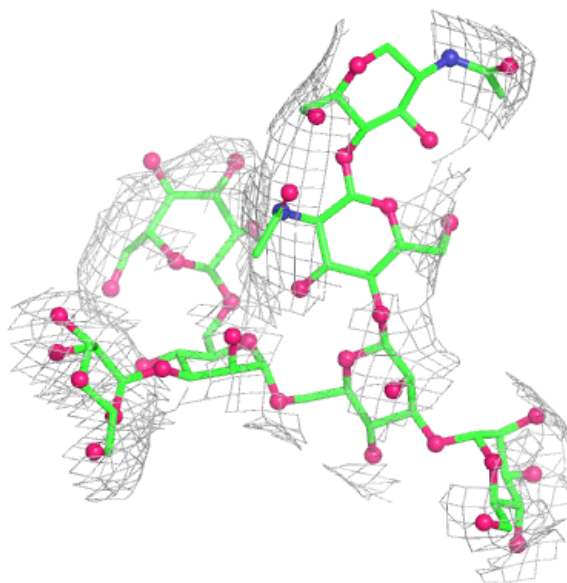
Electron density around Chain g:

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



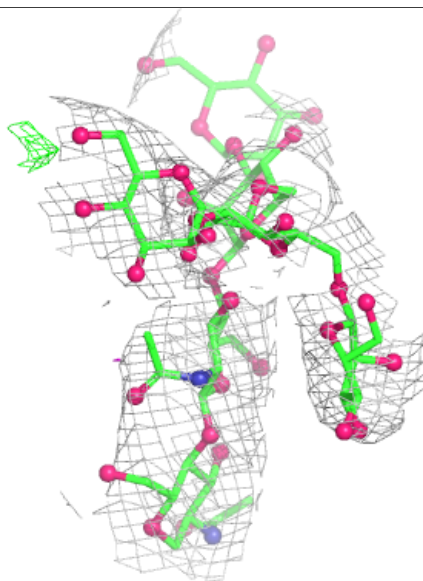
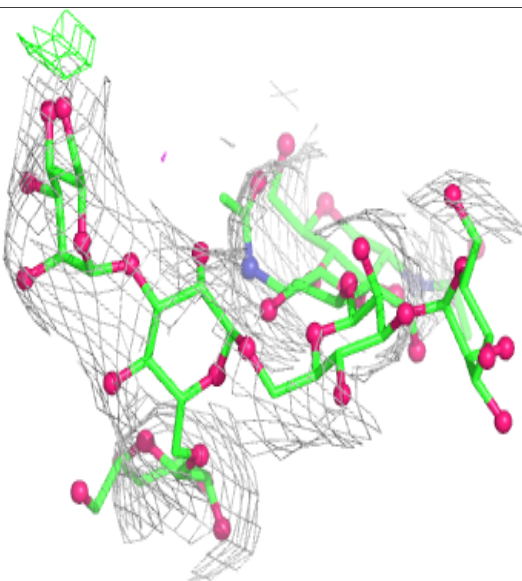
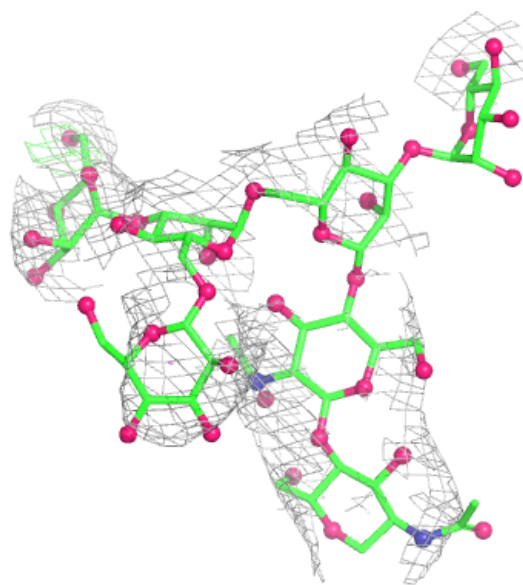
Electron density around Chain j:

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



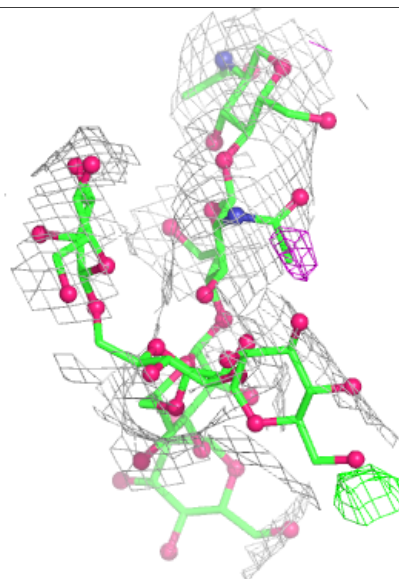
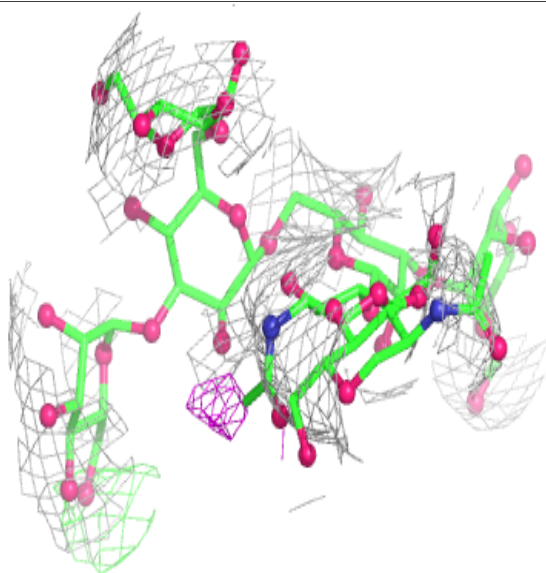
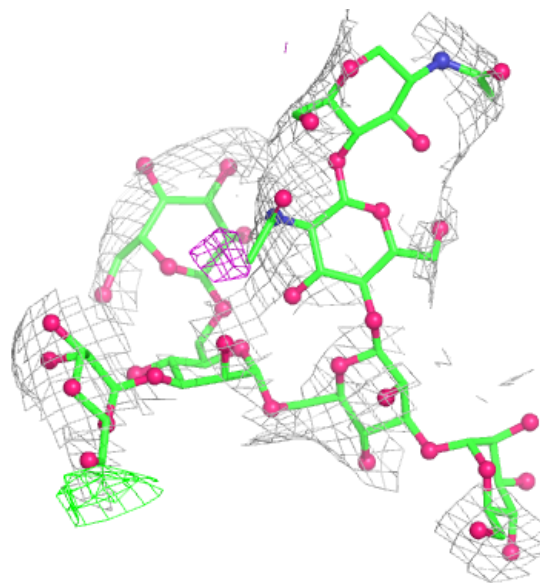
Electron density around Chain m:

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



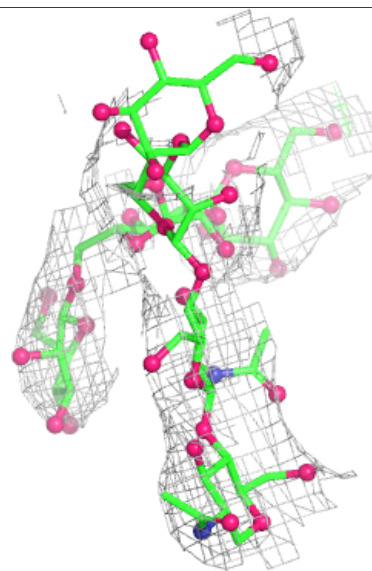
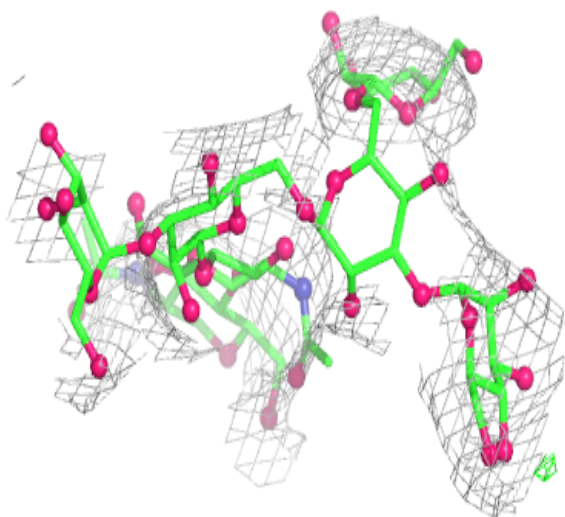
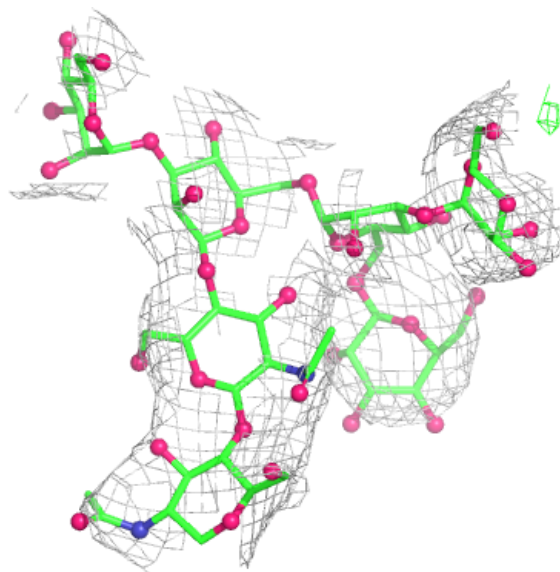
Electron density around Chain p:

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



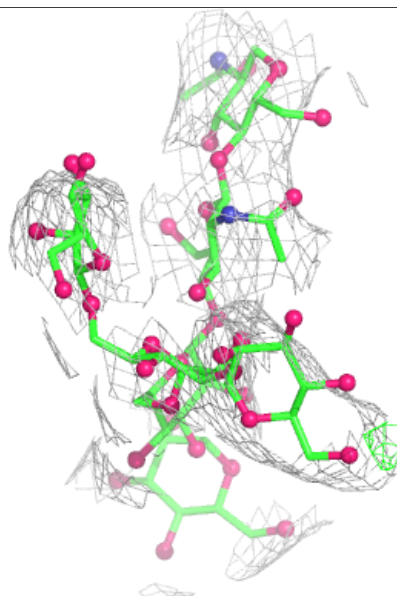
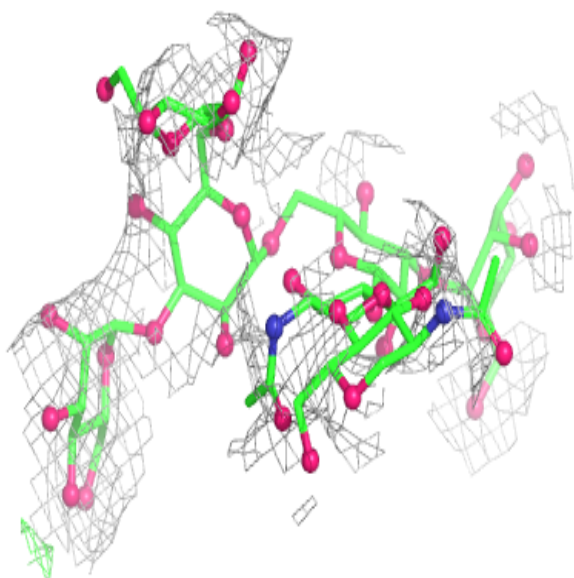
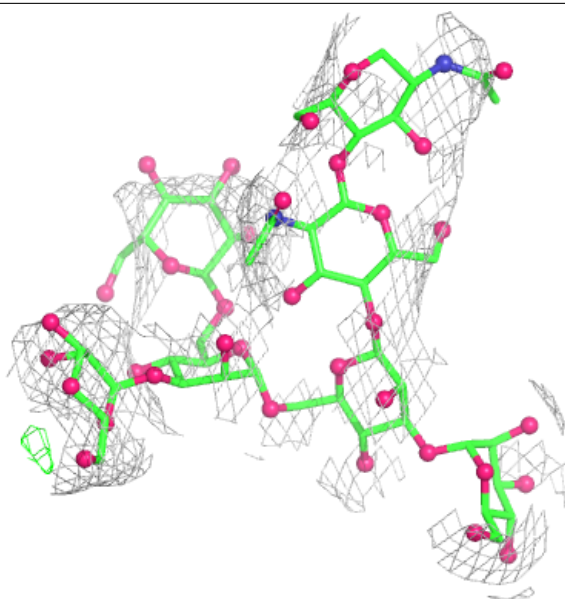
Electron density around Chain s:

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



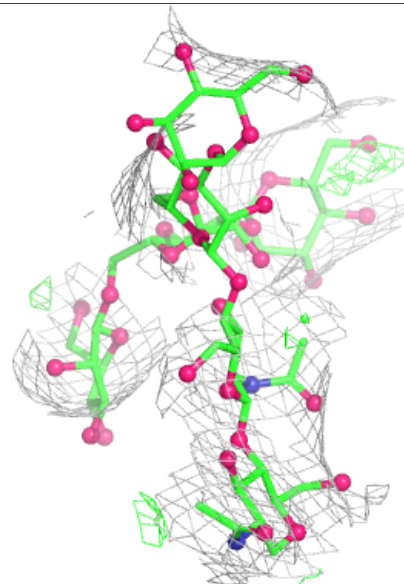
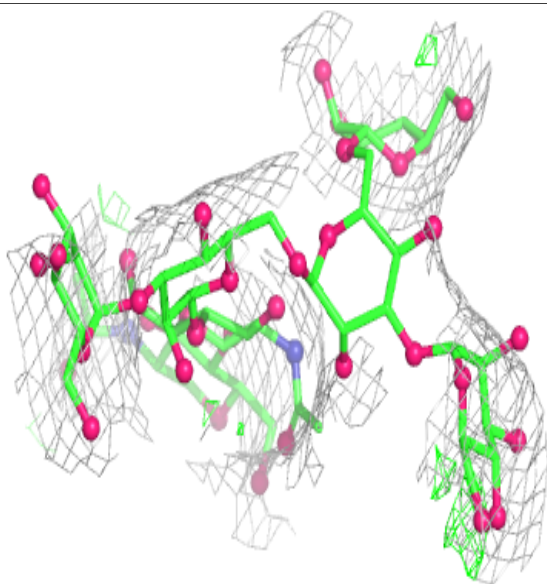
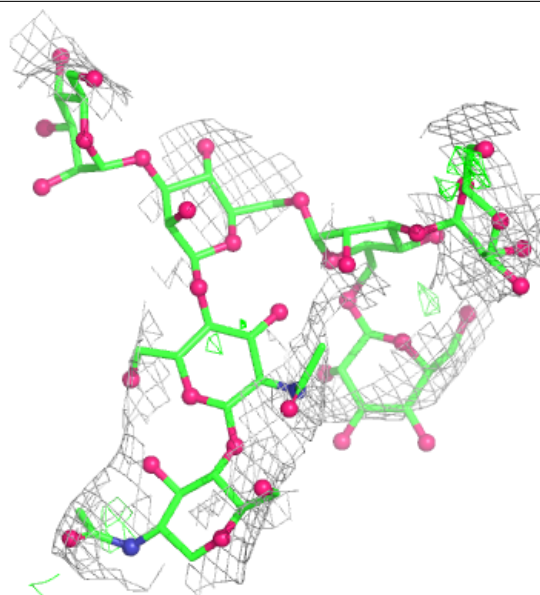
Electron density around Chain v:

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



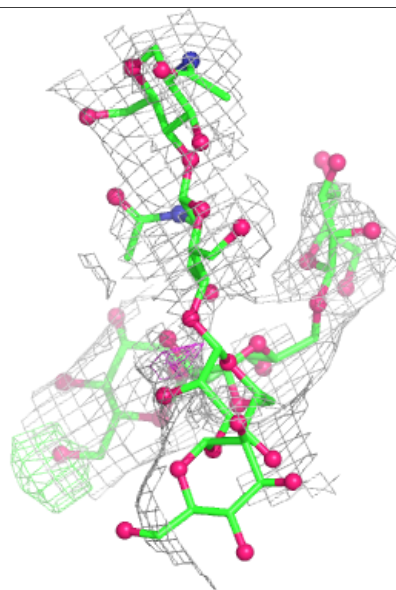
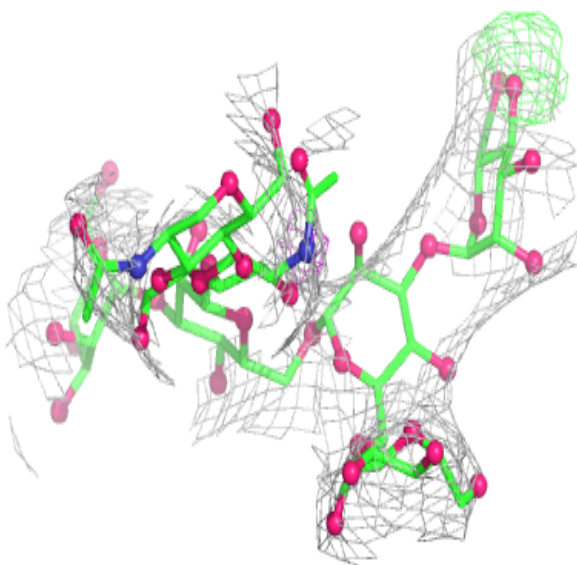
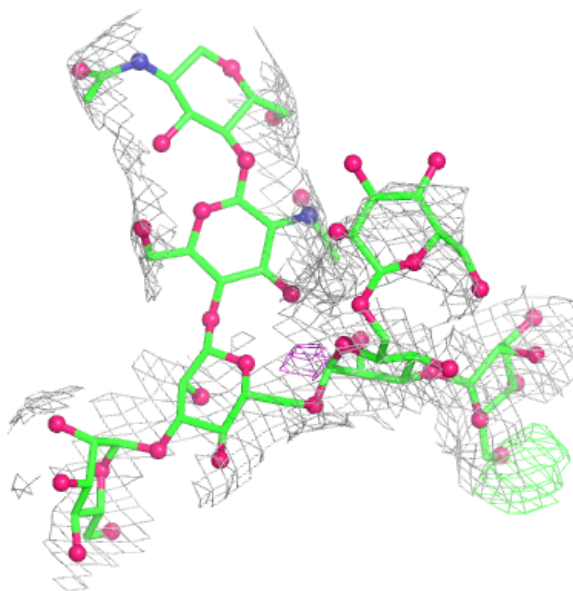
Electron density around Chain y:

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



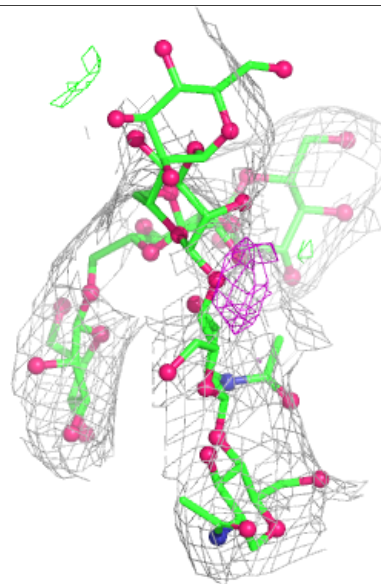
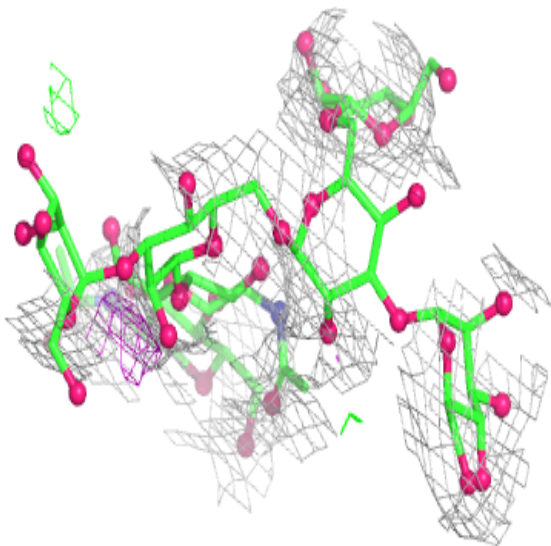
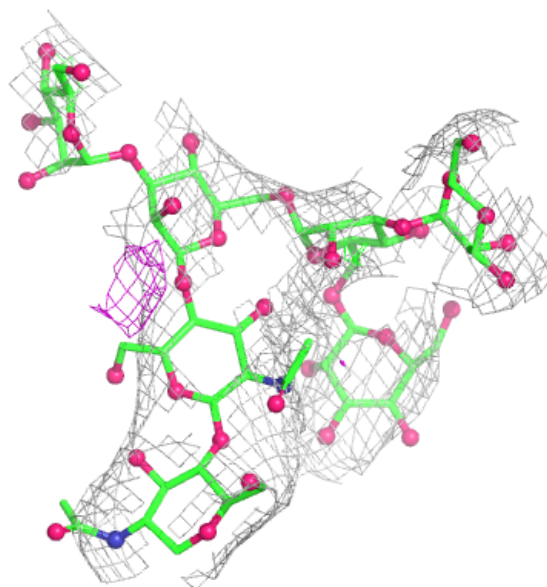
Electron density around Chain BA:

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



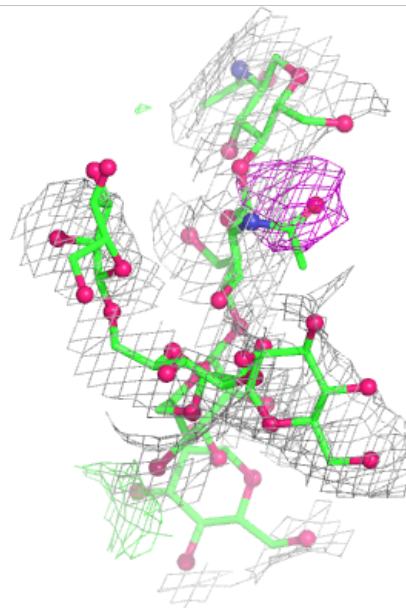
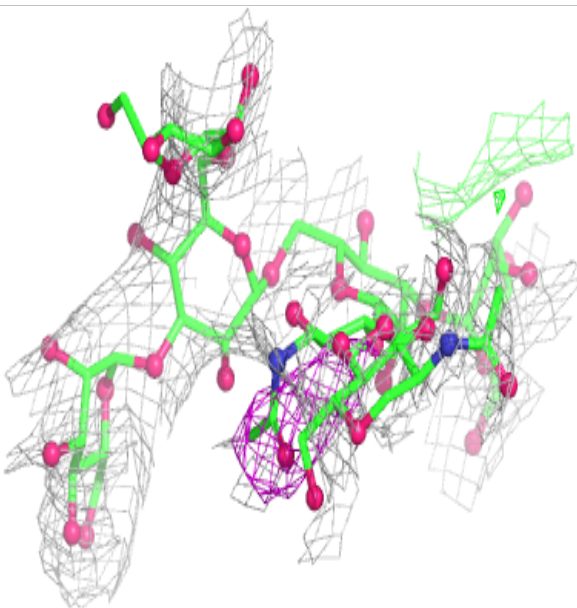
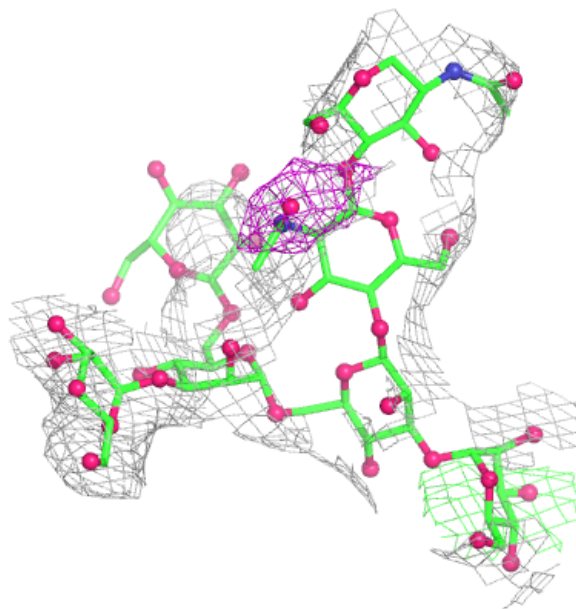
Electron density around Chain EA:

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and green (positive)



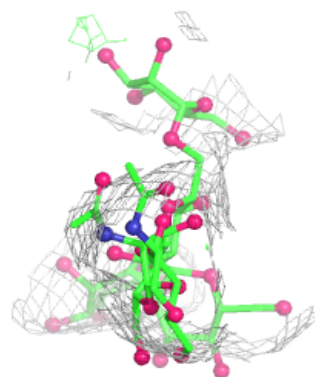
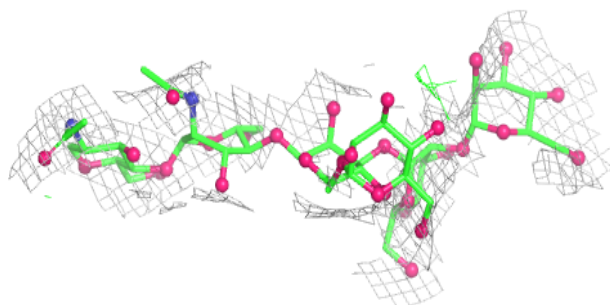
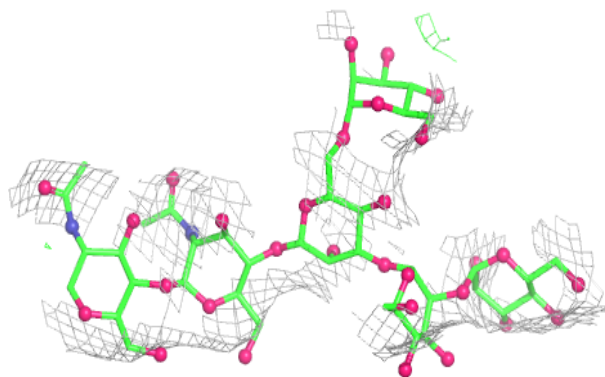
Electron density around Chain HA:

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

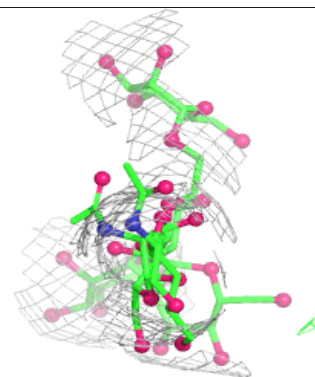
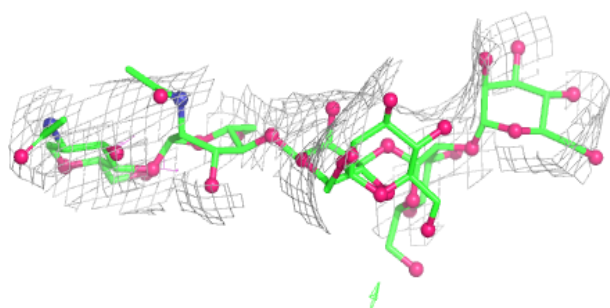
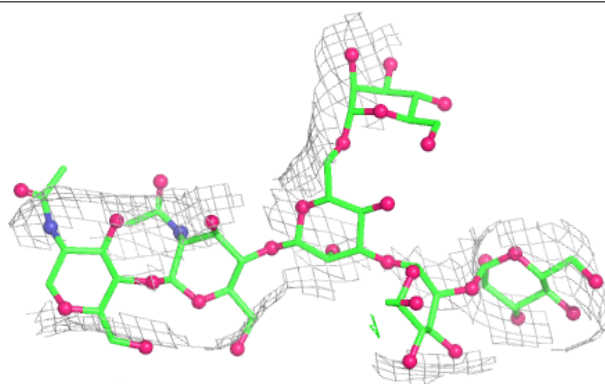


Electron density around Chain b:

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

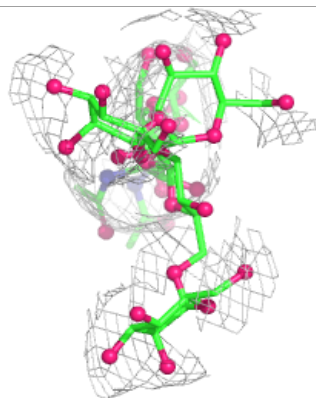
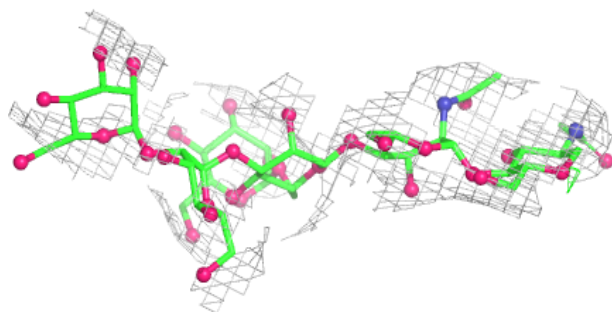
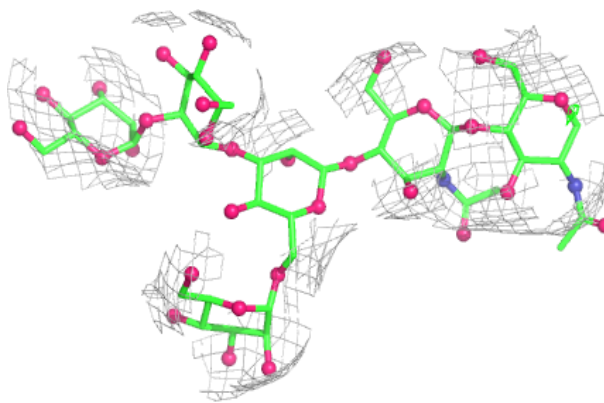
**Electron density around Chain e:**

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

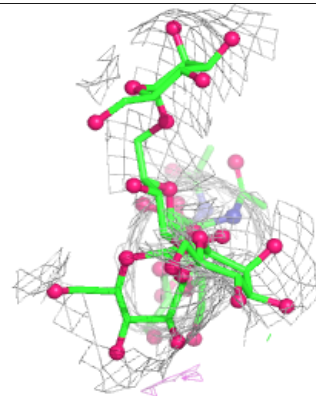
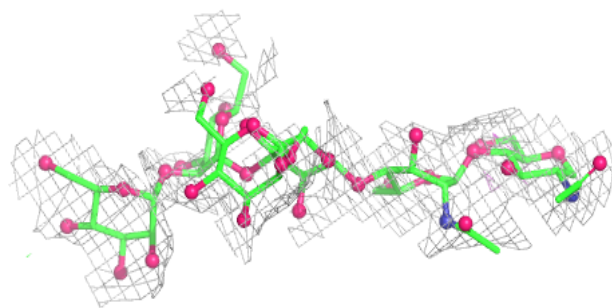
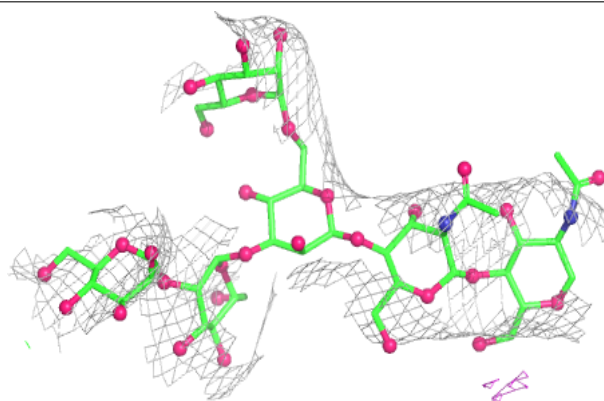


Electron density around Chain h:

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

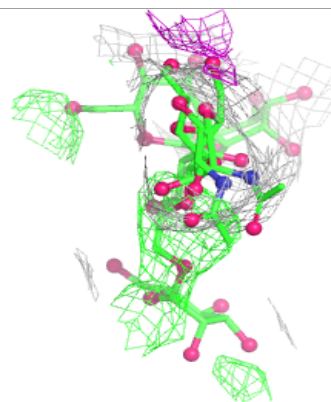
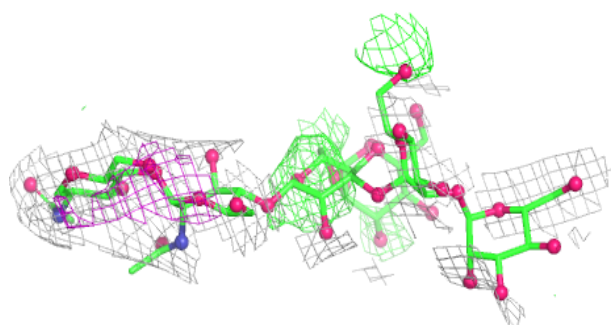
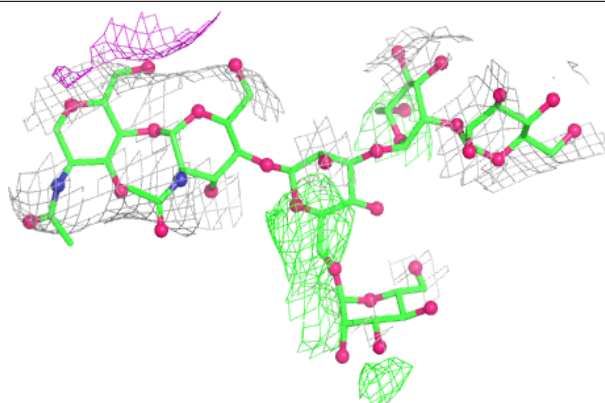
**Electron density around Chain k:**

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

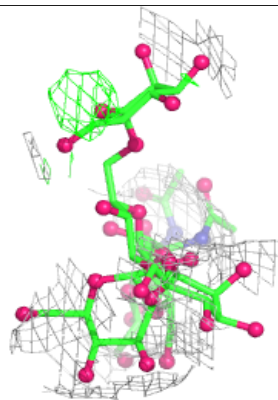
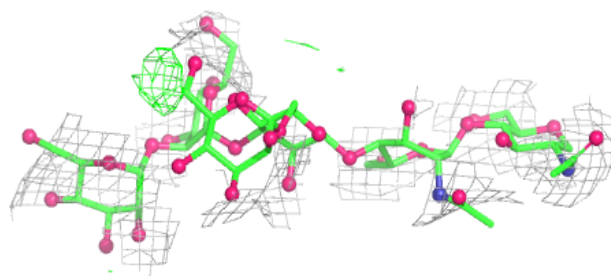
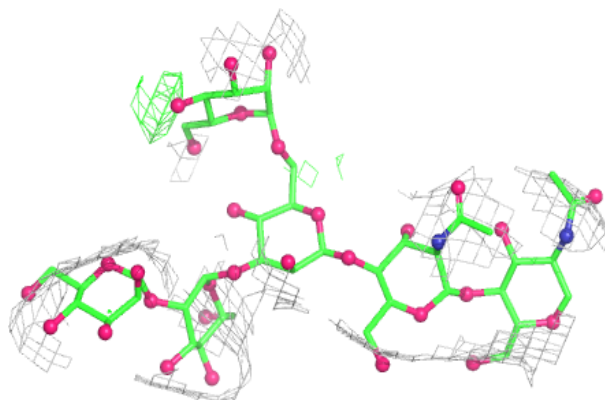


Electron density around Chain n:

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

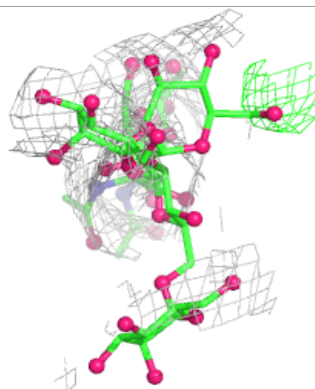
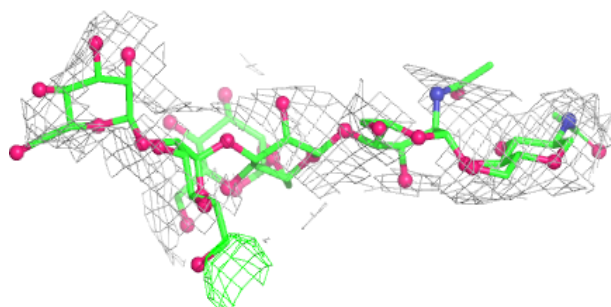
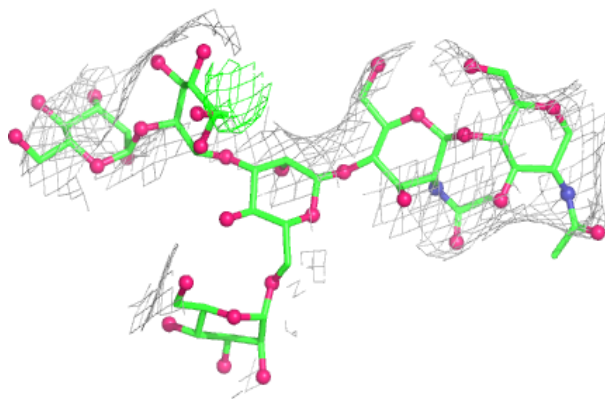
**Electron density around Chain q:**

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

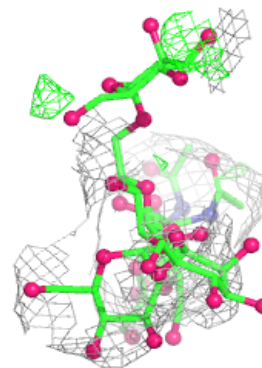
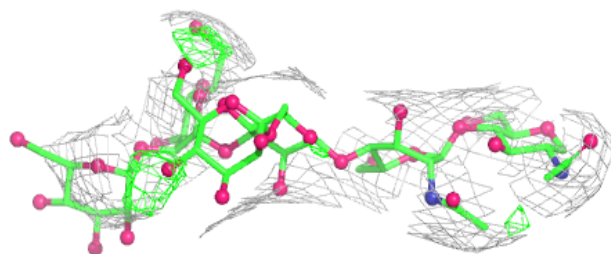
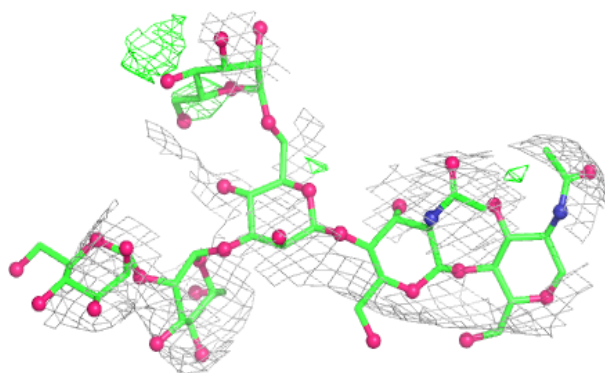


Electron density around Chain t:

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

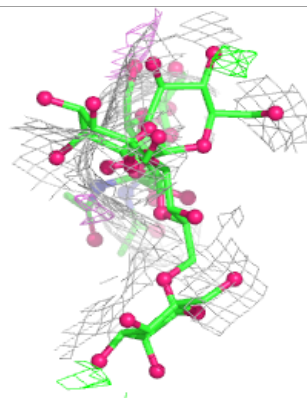
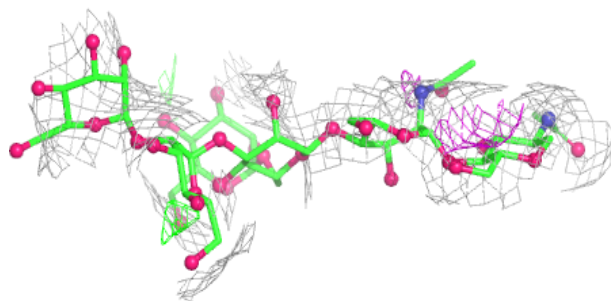
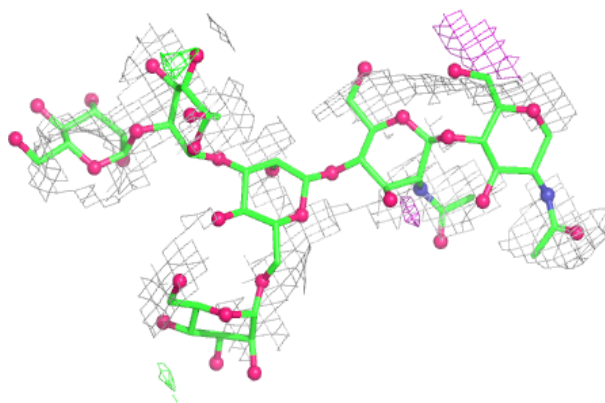
**Electron density around Chain w:**

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

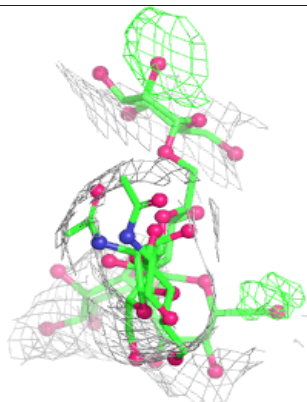
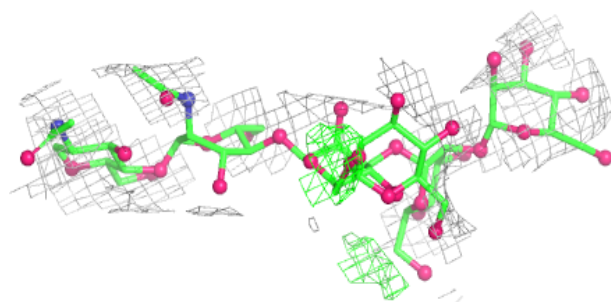
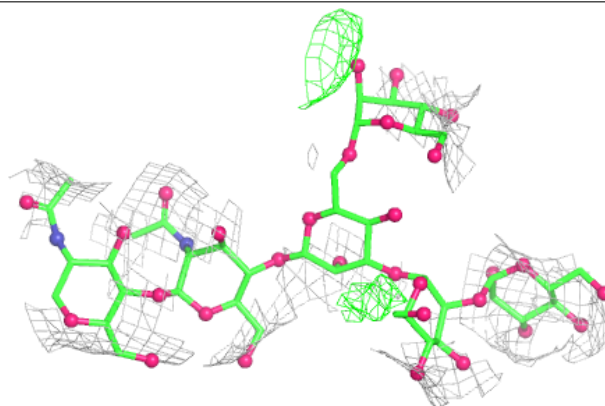


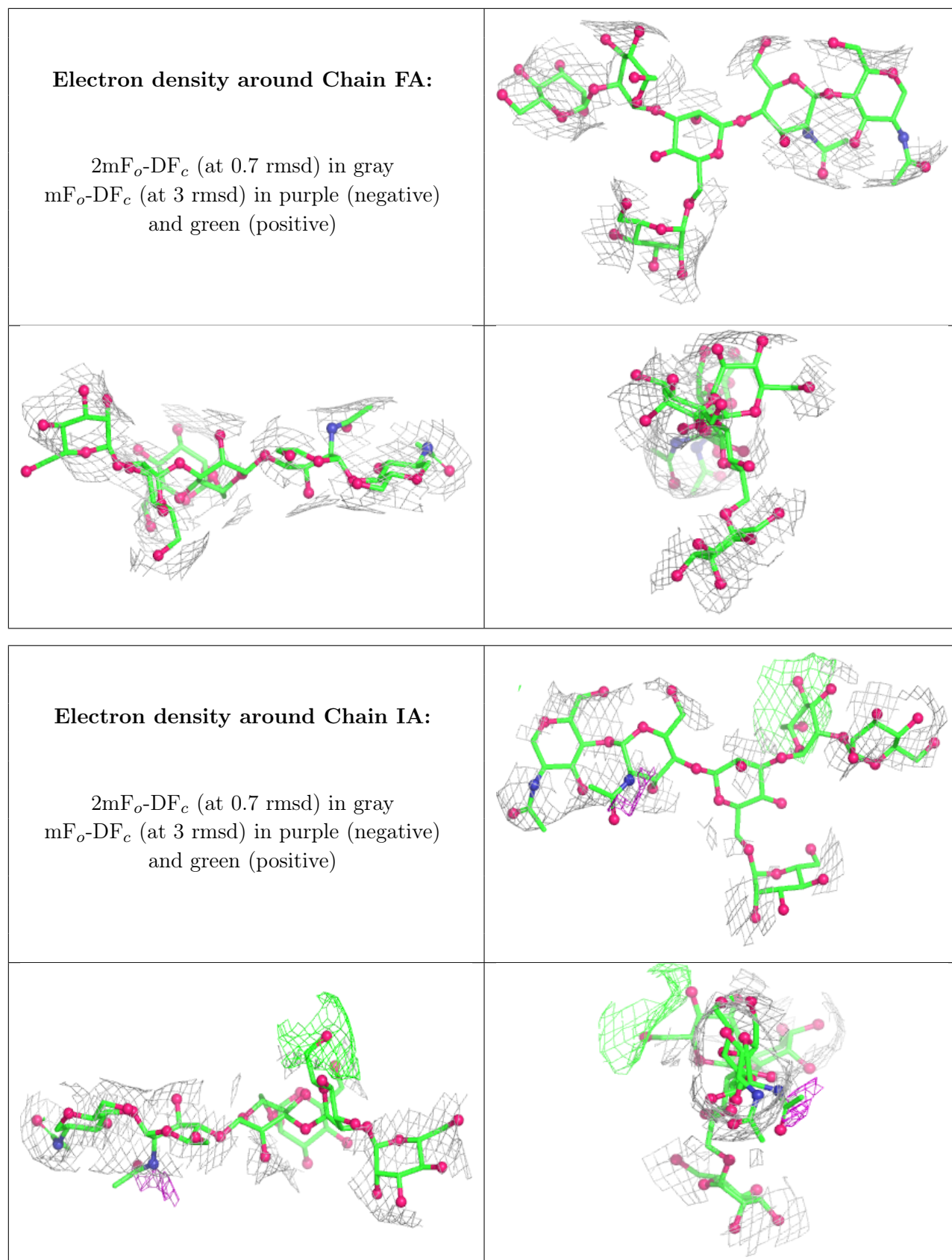
Electron density around Chain z:

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

**Electron density around Chain CA:**

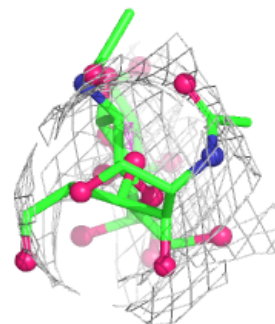
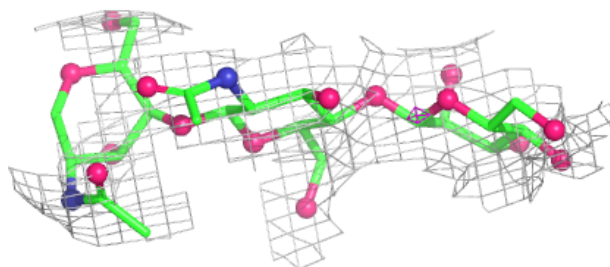
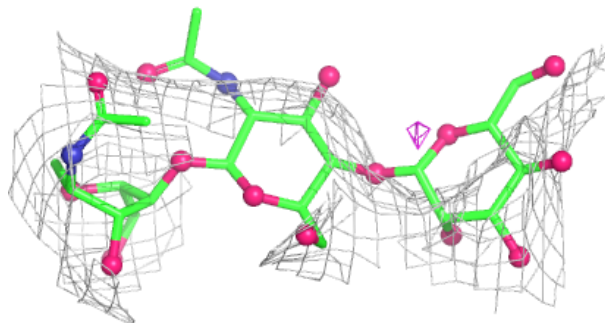
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



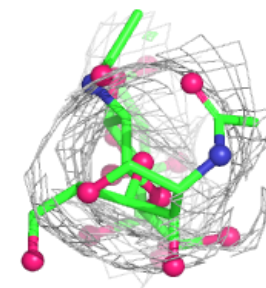
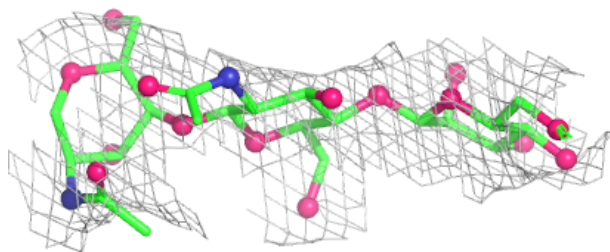
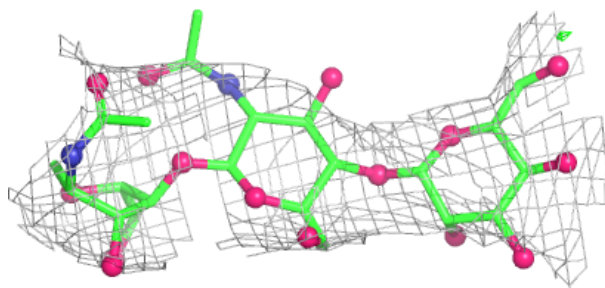


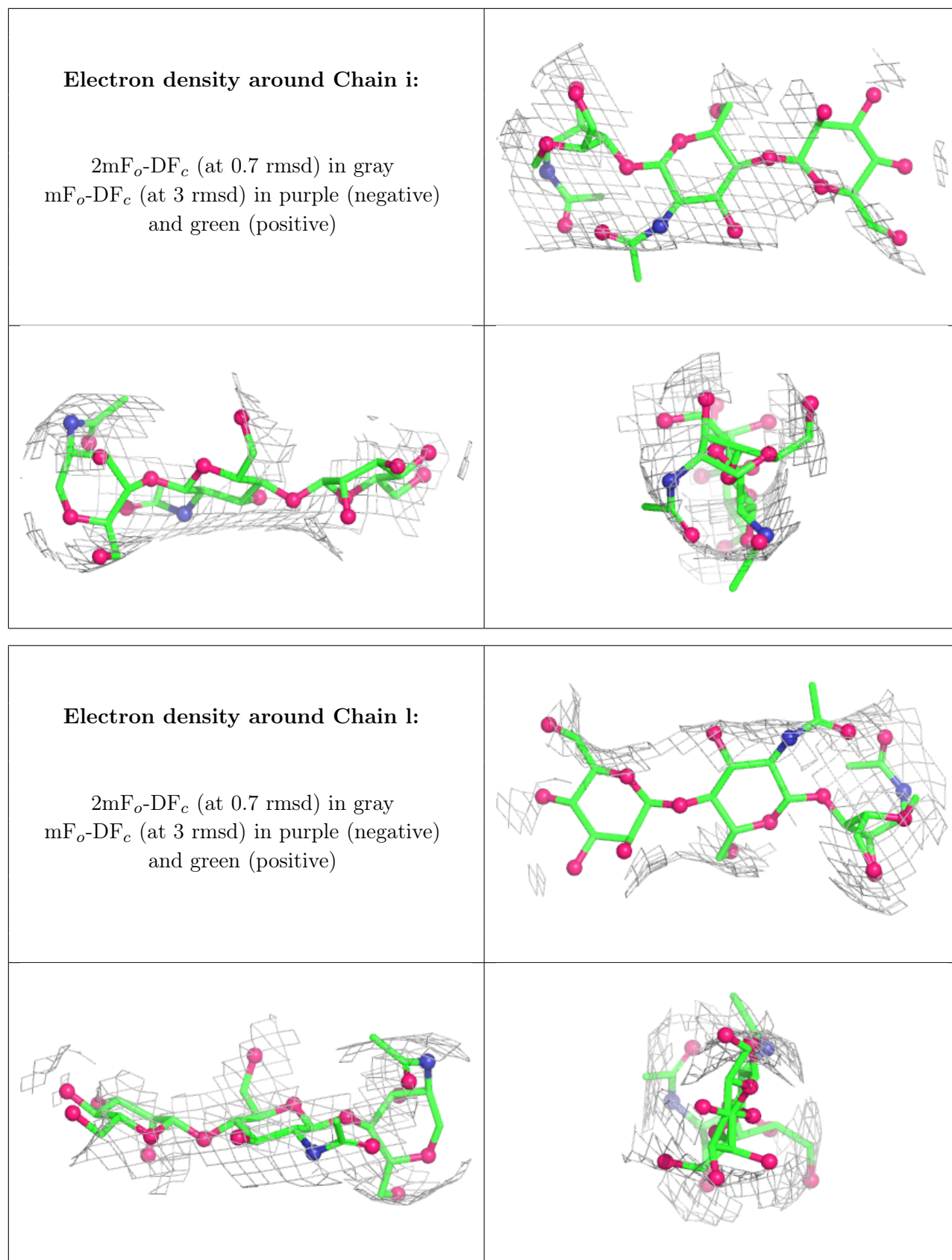
Electron density around Chain c:

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

**Electron density around Chain f:**

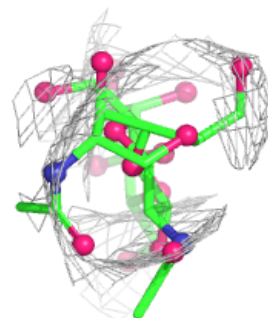
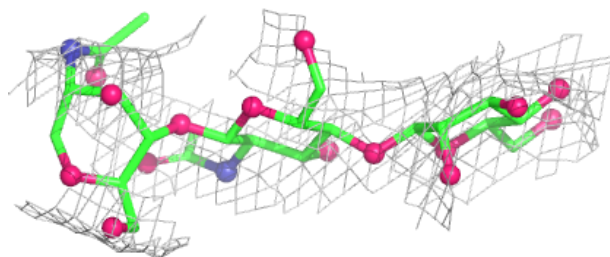
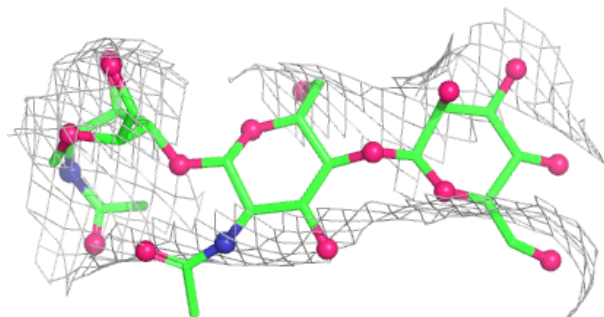
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



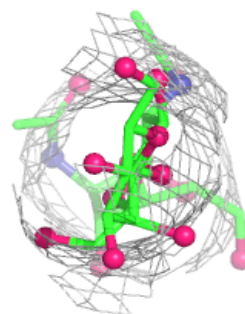
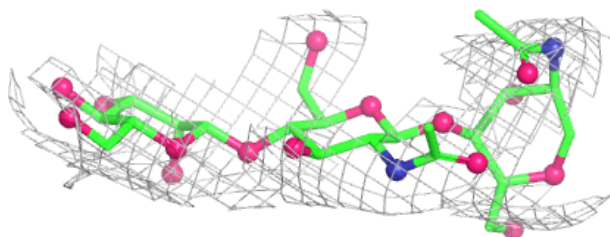
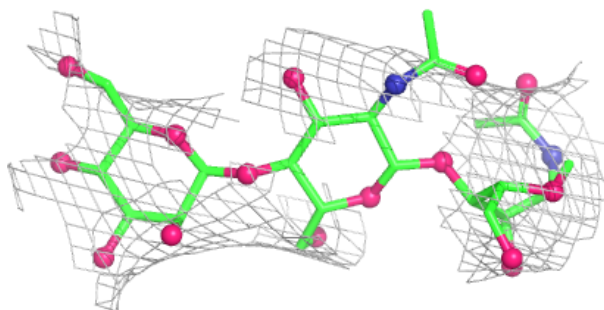


Electron density around Chain o:

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

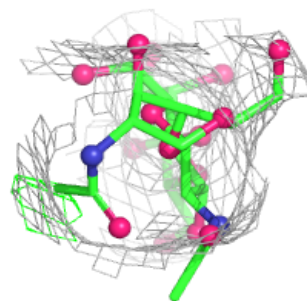
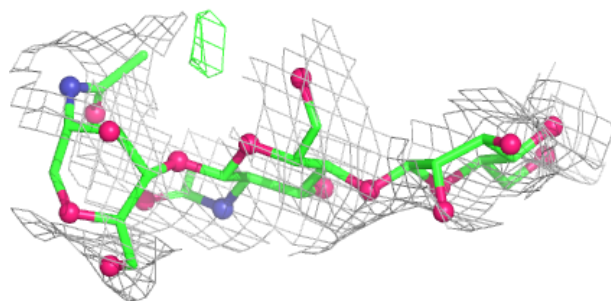
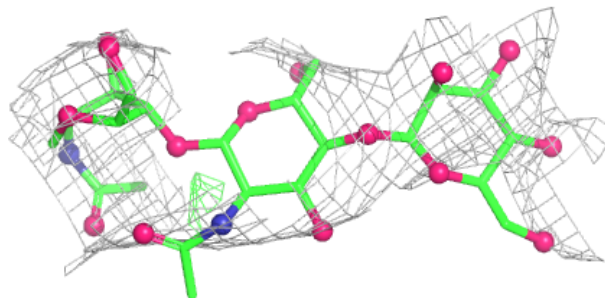
**Electron density around Chain r:**

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

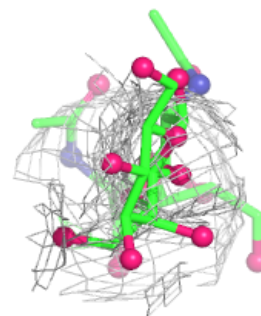
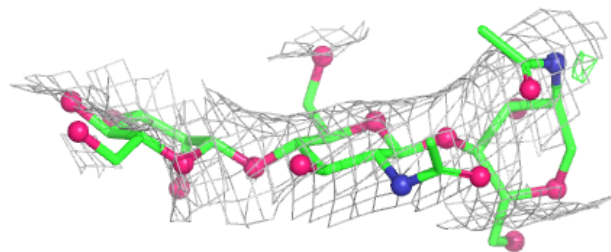
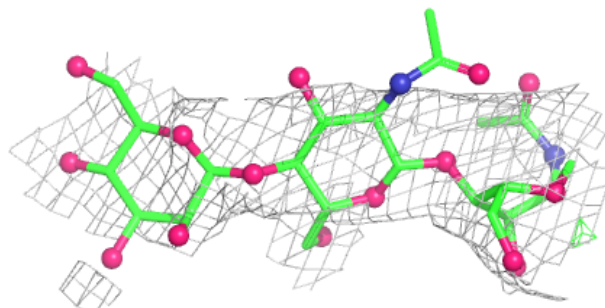


Electron density around Chain u:

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

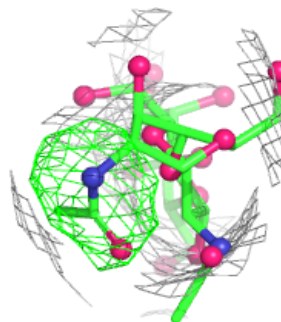
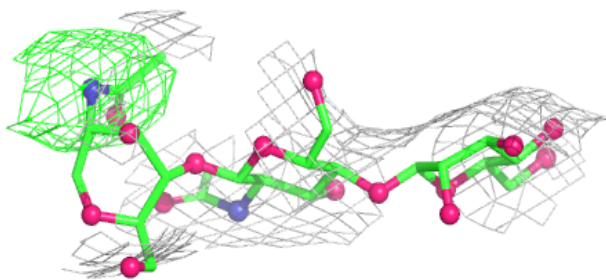
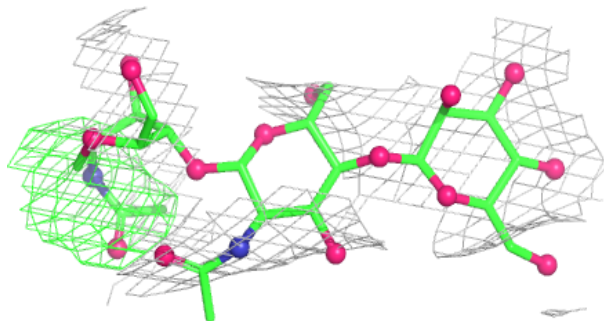
**Electron density around Chain x:**

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

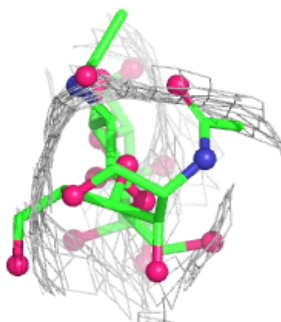
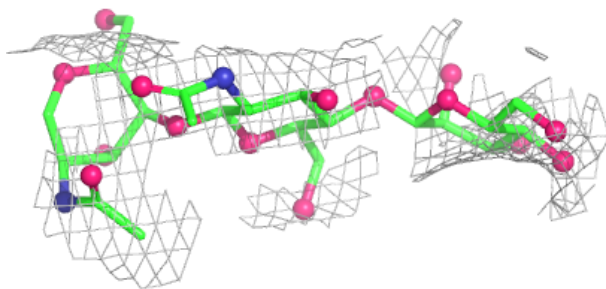
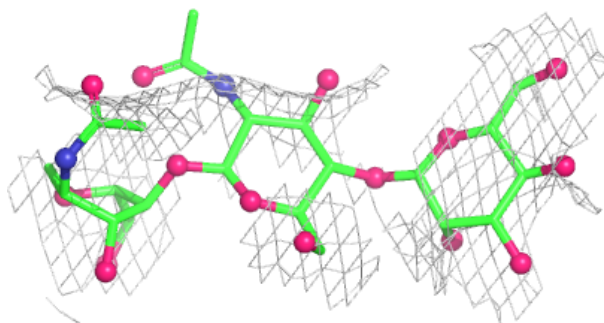


Electron density around Chain AA:

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

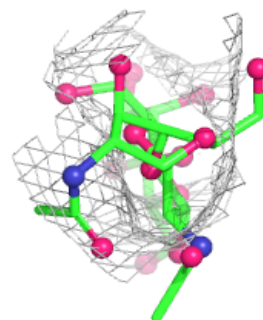
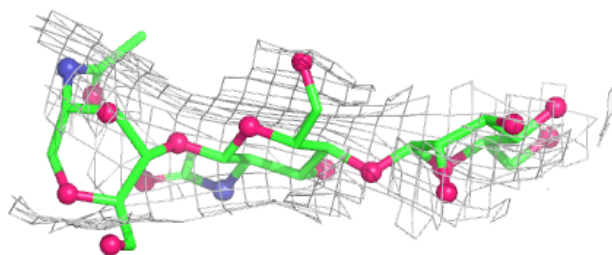
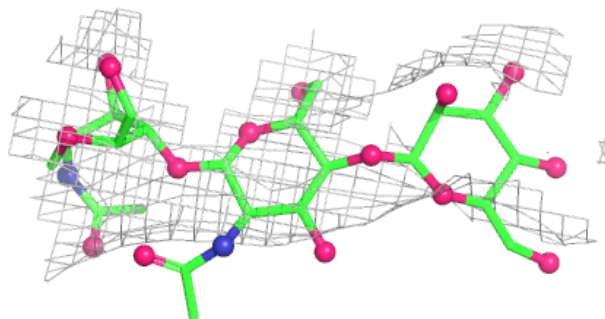
**Electron density around Chain DA:**

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

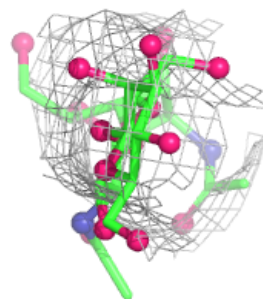
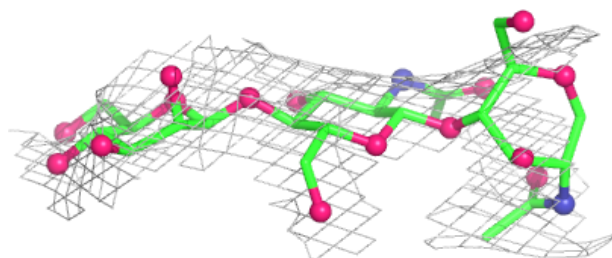
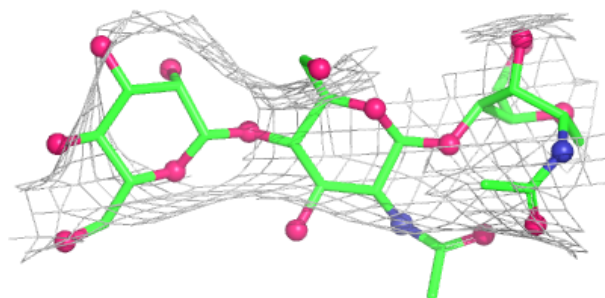


Electron density around Chain GA:

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

**Electron density around Chain JA:**

$2mF_o-DF_c$ (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
7	NAG	H	608	14/15	0.13	0.15	238,238,238,238	0
7	NAG	K	618	14/15	0.15	0.10	291,291,291,291	0
7	NAG	L	618	14/15	0.25	0.08	291,291,291,291	0
7	NAG	A	618	14/15	0.37	0.08	291,291,291,291	0
7	NAG	D	618	14/15	0.39	0.10	291,291,291,291	0
7	NAG	G	618	14/15	0.40	0.08	291,291,291,291	0
7	NAG	B	608	14/15	0.40	0.15	238,238,238,238	0
7	NAG	H	618	14/15	0.51	0.09	291,291,291,291	0
7	NAG	I	618	14/15	0.51	0.10	290,290,290,290	0
7	NAG	E	608	14/15	0.55	0.09	238,238,238,238	0
7	NAG	L	608	14/15	0.56	0.11	238,238,238,238	0
7	NAG	J	618	14/15	0.58	0.07	291,291,291,291	0
7	NAG	B	618	14/15	0.58	0.08	291,291,291,291	0
7	NAG	C	618	14/15	0.59	0.09	290,290,290,290	0
7	NAG	F	608	14/15	0.62	0.07	238,238,238,238	0
7	NAG	K	608	14/15	0.63	0.09	238,238,238,238	0
7	NAG	G	608	14/15	0.65	0.07	238,238,238,238	0
7	NAG	E	618	14/15	0.66	0.06	291,291,291,291	0
7	NAG	F	618	14/15	0.66	0.09	291,291,291,291	0
7	NAG	D	608	14/15	0.72	0.08	238,238,238,238	0
7	NAG	C	608	14/15	0.73	0.08	238,238,238,238	0
7	NAG	A	608	14/15	0.73	0.08	238,238,238,238	0
7	NAG	I	608	14/15	0.75	0.07	238,238,238,238	0
7	NAG	J	608	14/15	0.79	0.06	238,238,238,238	0

6.5 Other polymers [i](#)

There are no such residues in this entry.