



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 08:10 PM UTC

PDB ID : 4O5I / pdb_00004o5i
Title : Crystal structure of broadly neutralizing antibody F045-092 in complex with A/Victoria/361/2011 (H3N2) influenza hemagglutinin
Authors : Lee, P.S.; Wilson, I.A.
Deposited on : 2013-12-19
Resolution : 6.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

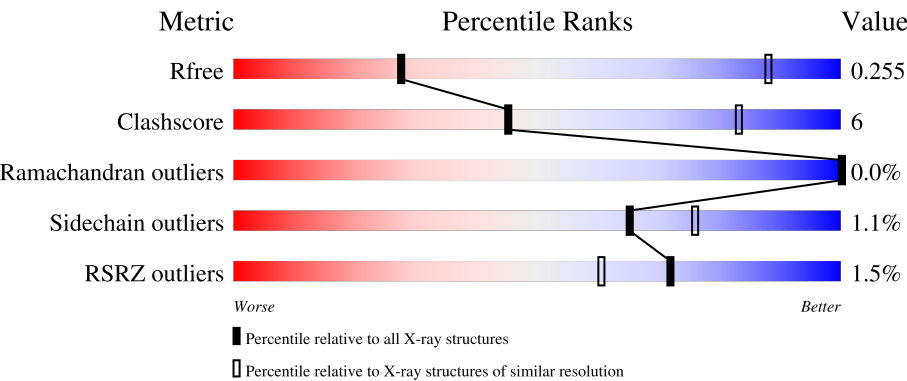
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	323	2% 84% 14% ..
1	C	323	% 84% 14% .
1	E	323	3% 84% 13% ..
1	G	323	85% 13% ..
1	I	323	2% 85% 12% ..

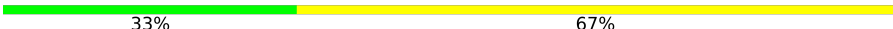
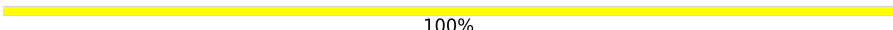
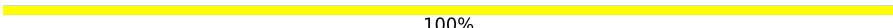
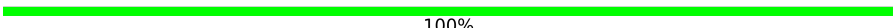
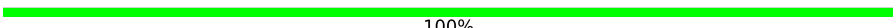
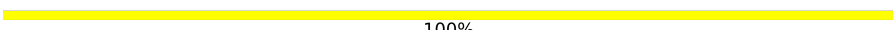
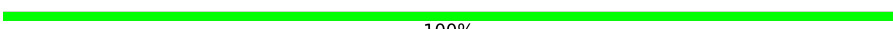
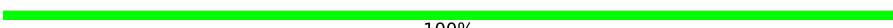
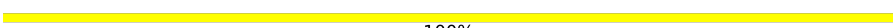
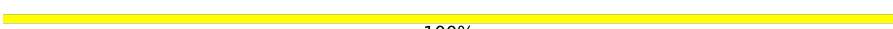
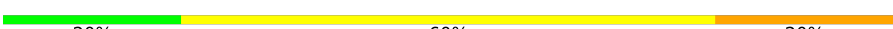
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Mol	Chain	Length	Quality of chain
1	K	323	 85% 12% ..
2	B	176	 90% 9% .
2	D	176	 91% 7% .
2	F	176	 93% 5% .
2	H	176	 91% 7% .
2	J	176	 91% 7% .
2	L	176	 90% 9% .
3	M	240	 73% 19% . 6%
3	O	240	 70% 22% . 6%
3	Q	240	 75% 15% . 6%
3	S	240	 78% 15% . 6%
3	U	240	 75% 18% . 6%
3	W	240	 75% 18% . 6%
4	N	216	 88% 10% .
4	P	216	 84% 15% .
4	R	216	 82% 17% .
4	T	216	 81% 17% .
4	V	216	 86% 12% .
4	X	216	 82% 15% ..
5	0	3	 67% 33%
5	3	3	 67% 33%
5	5	3	 67% 33%
5	6	3	 67% 33%
5	Y	3	 33% 67%
5	i	3	 100%

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Mol	Chain	Length	Quality of chain
5	j	3	 67% 33%
5	l	3	 67% 33%
5	p	3	 33% 67%
5	t	3	 67% 33%
5	u	3	 100%
5	y	3	 100%
5	z	3	 67% 33%
6	1	2	 100%
6	2	2	 100%
6	4	2	 50% 50%
6	Z	2	 50% 50%
6	a	2	 50% 50%
6	c	2	 100%
6	d	2	 50% 50%
6	f	2	 100%
6	o	2	 100%
6	q	2	 50% 50%
6	r	2	 50% 50%
6	s	2	 50% 50%
6	v	2	 100%
6	w	2	 100%
6	x	2	 50% 50%
7	b	5	 20% 60% 20%
7	h	5	 20% 80%
7	k	5	 80% 20%

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Mol	Chain	Length	Quality of chain
7	n	5	 20% 40% 40%
8	e	4	 75% 25%
8	g	4	 50% 50%
8	m	4	 50% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44305 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	C	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	E	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	G	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	I	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	K	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP R9U684
A	8	ASP	-	expression tag	UNP R9U684
A	9	PRO	-	expression tag	UNP R9U684
A	10	GLY	-	expression tag	UNP R9U684
C	7	ALA	-	expression tag	UNP R9U684
C	8	ASP	-	expression tag	UNP R9U684
C	9	PRO	-	expression tag	UNP R9U684
C	10	GLY	-	expression tag	UNP R9U684
E	7	ALA	-	expression tag	UNP R9U684
E	8	ASP	-	expression tag	UNP R9U684
E	9	PRO	-	expression tag	UNP R9U684
E	10	GLY	-	expression tag	UNP R9U684
G	7	ALA	-	expression tag	UNP R9U684
G	8	ASP	-	expression tag	UNP R9U684
G	9	PRO	-	expression tag	UNP R9U684
G	10	GLY	-	expression tag	UNP R9U684
I	7	ALA	-	expression tag	UNP R9U684

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	expression tag	UNP R9U684
I	9	PRO	-	expression tag	UNP R9U684
I	10	GLY	-	expression tag	UNP R9U684
K	7	ALA	-	expression tag	UNP R9U684
K	8	ASP	-	expression tag	UNP R9U684
K	9	PRO	-	expression tag	UNP R9U684
K	10	GLY	-	expression tag	UNP R9U684

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	D	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	F	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	H	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	J	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	L	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			

- Molecule 3 is a protein called Fab F045-092 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	O	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	Q	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	S	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	U	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	W	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	217	HIS	-	expression tag	UNP S6C4S0
M	218	HIS	-	expression tag	UNP S6C4S0
M	219	HIS	-	expression tag	UNP S6C4S0
M	220	HIS	-	expression tag	UNP S6C4S0
M	221	HIS	-	expression tag	UNP S6C4S0
M	222	HIS	-	expression tag	UNP S6C4S0
O	217	HIS	-	expression tag	UNP S6C4S0
O	218	HIS	-	expression tag	UNP S6C4S0
O	219	HIS	-	expression tag	UNP S6C4S0
O	220	HIS	-	expression tag	UNP S6C4S0
O	221	HIS	-	expression tag	UNP S6C4S0
O	222	HIS	-	expression tag	UNP S6C4S0
Q	217	HIS	-	expression tag	UNP S6C4S0
Q	218	HIS	-	expression tag	UNP S6C4S0
Q	219	HIS	-	expression tag	UNP S6C4S0
Q	220	HIS	-	expression tag	UNP S6C4S0
Q	221	HIS	-	expression tag	UNP S6C4S0
Q	222	HIS	-	expression tag	UNP S6C4S0
S	217	HIS	-	expression tag	UNP S6C4S0
S	218	HIS	-	expression tag	UNP S6C4S0
S	219	HIS	-	expression tag	UNP S6C4S0
S	220	HIS	-	expression tag	UNP S6C4S0
S	221	HIS	-	expression tag	UNP S6C4S0
S	222	HIS	-	expression tag	UNP S6C4S0
U	217	HIS	-	expression tag	UNP S6C4S0
U	218	HIS	-	expression tag	UNP S6C4S0
U	219	HIS	-	expression tag	UNP S6C4S0
U	220	HIS	-	expression tag	UNP S6C4S0
U	221	HIS	-	expression tag	UNP S6C4S0
U	222	HIS	-	expression tag	UNP S6C4S0
W	217	HIS	-	expression tag	UNP S6C4S0
W	218	HIS	-	expression tag	UNP S6C4S0
W	219	HIS	-	expression tag	UNP S6C4S0
W	220	HIS	-	expression tag	UNP S6C4S0
W	221	HIS	-	expression tag	UNP S6C4S0
W	222	HIS	-	expression tag	UNP S6C4S0

- Molecule 4 is a protein called Fab F045-092 light chain.

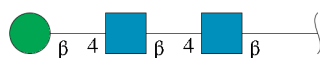
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	P	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	T	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	V	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	X	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

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



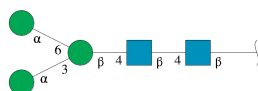
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	i	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	p	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	t	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	u	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	z	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	0	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	3	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	5	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	6	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	o	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	r	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	s	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	v	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	w	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	x	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	1	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	2	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	4	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



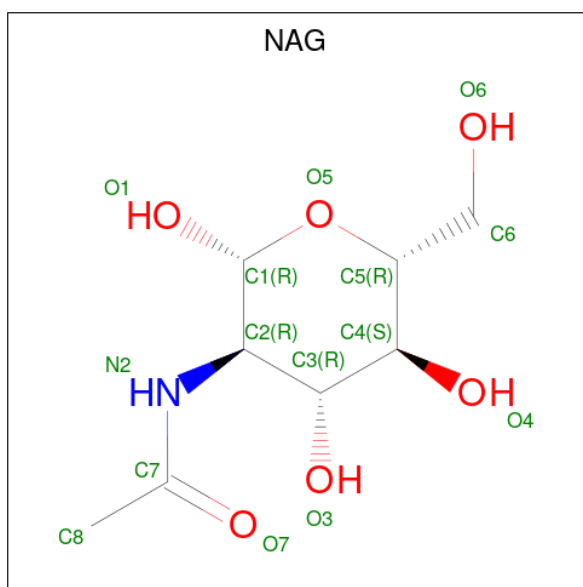
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	b	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	h	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	k	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	n	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	e	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	g	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	m	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

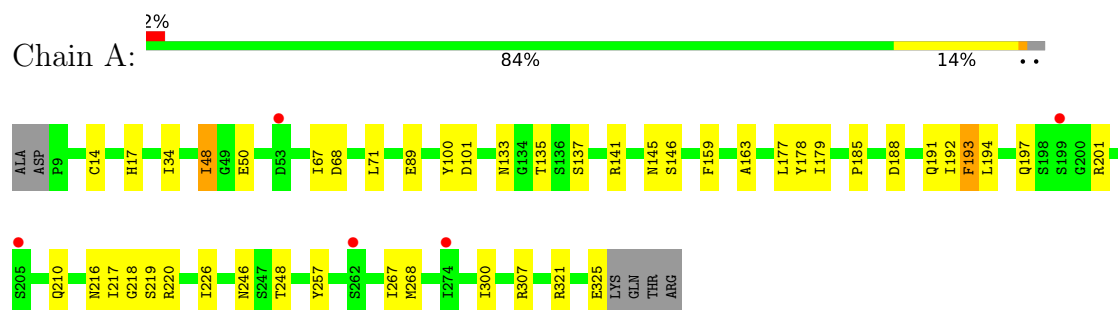


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	H	1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

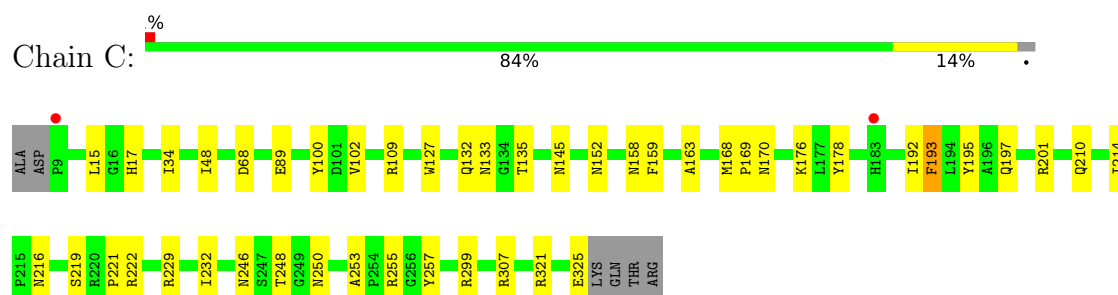
3 Residue-property plots [i](#)

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.

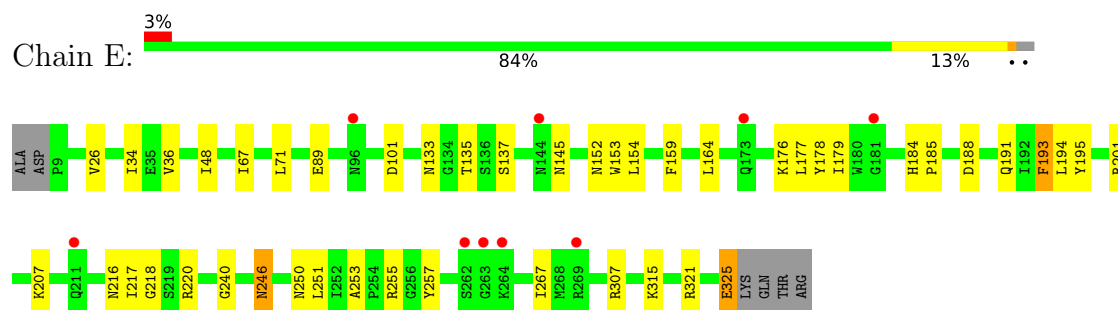
- Molecule 1: Hemagglutinin HA1 chain



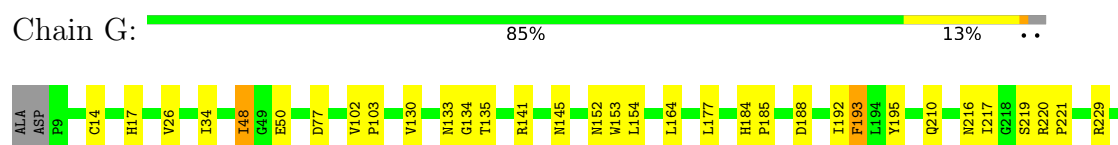
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

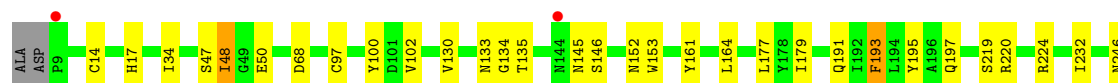
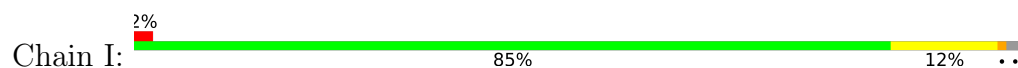


- Molecule 1: Hemagglutinin HA1 chain

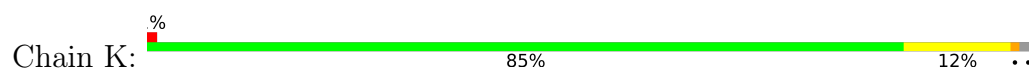




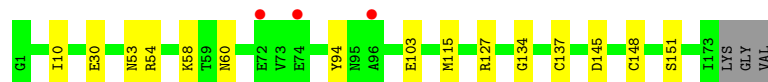
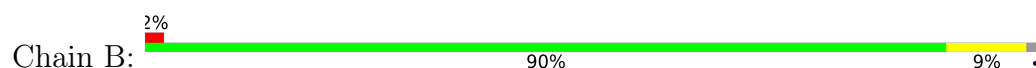
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain



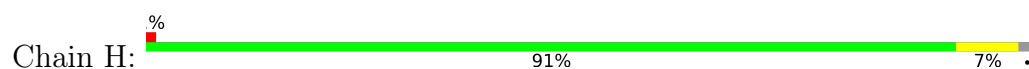
• Molecule 2: Hemagglutinin HA2 chain

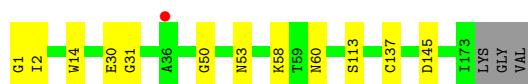


• Molecule 2: Hemagglutinin HA2 chain

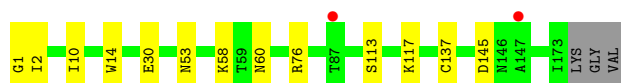
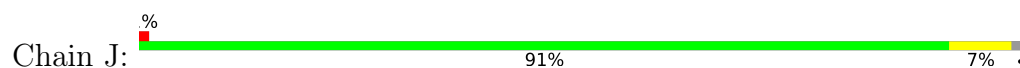


• Molecule 2: Hemagglutinin HA2 chain

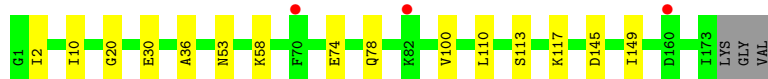
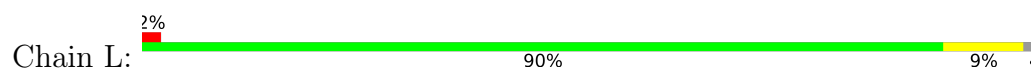




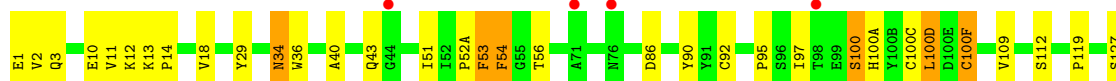
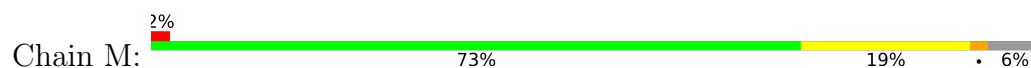
- Molecule 2: Hemagglutinin HA2 chain



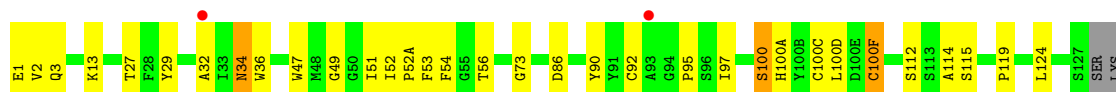
- Molecule 2: Hemagglutinin HA2 chain



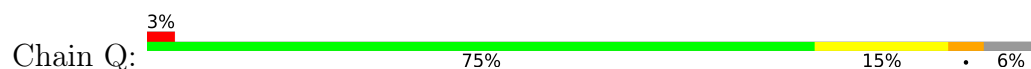
- Molecule 3: Fab F045-092 heavy chain



- Molecule 3: Fab F045-092 heavy chain

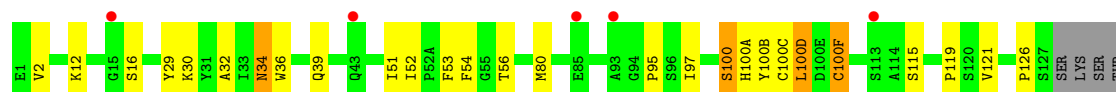
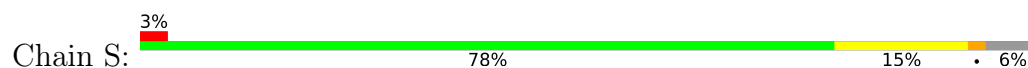


- Molecule 3: Fab F045-092 heavy chain

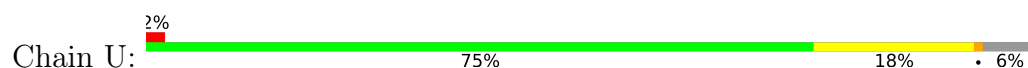




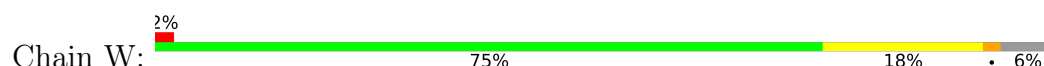
• Molecule 3: Fab F045-092 heavy chain



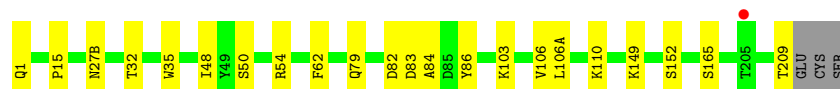
• Molecule 3: Fab F045-092 heavy chain



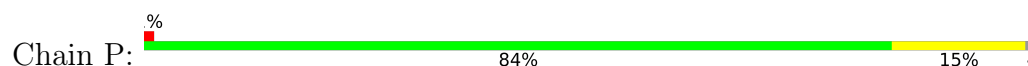
• Molecule 3: Fab F045-092 heavy chain

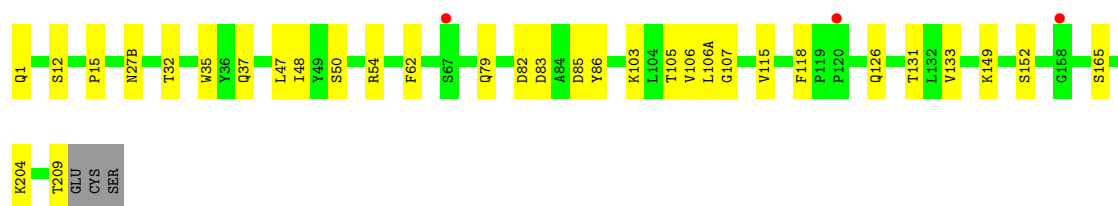


• Molecule 4: Fab F045-092 light chain



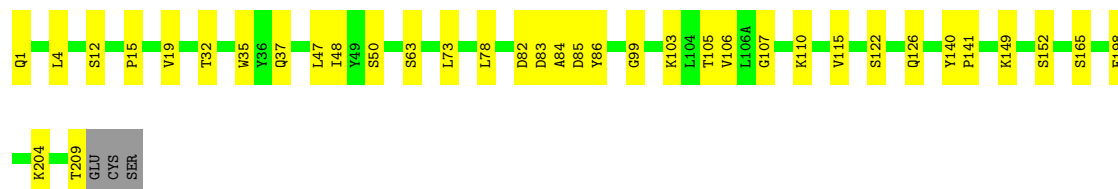
• Molecule 4: Fab F045-092 light chain





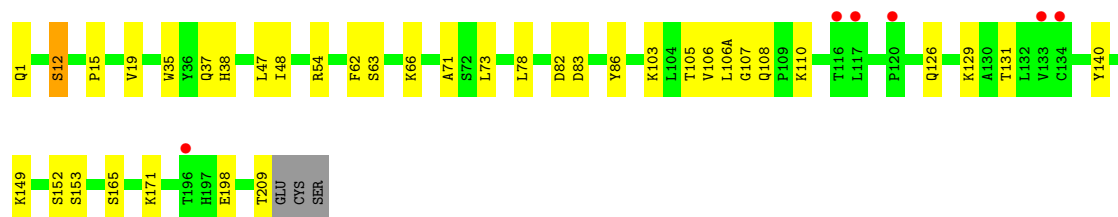
- Molecule 4: Fab F045-092 light chain

Chain R: 82% 17%



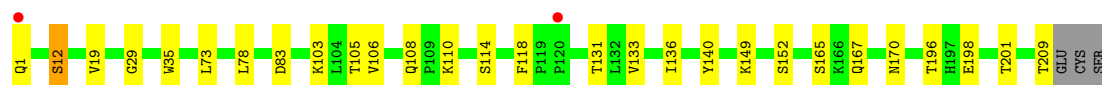
- Molecule 4: Fab F045-092 light chain

Chain T: 3% 81% 17%



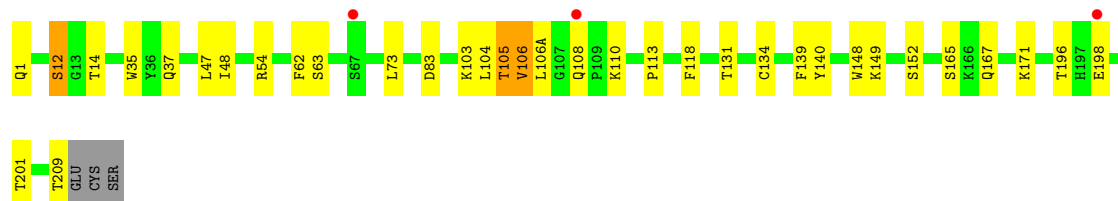
- Molecule 4: Fab F045-092 light chain

Chain V: 86% 12%



- Molecule 4: Fab F045-092 light chain

Chain X: 82% 15%



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

Chain Y:  33% 67%

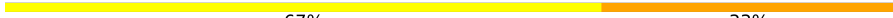


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



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

Chain j:  67% 33%



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

Chain l:  67% 33%



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

Chain p:  33% 67%

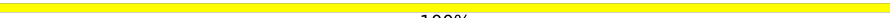


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  67% 33%



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

Chain u:  100%



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

Chain y:  100%

MAG1
MAG2
BMA3

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

Chain z:  67% 33%

MAG1
MAG2
BMA3

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

Chain 0:  67% 33%

MAG1
MAG2
BMA3

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

Chain 3:  67% 33%

MAG1
MAG2
BMA3

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

Chain 5:  67% 33%

MAG1
MAG2
BMA3

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

Chain 6:  67% 33%

MAG1
MAG2
BMA3

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

Chain Z:  50% 50%



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

Chain a:  50% 50%



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

Chain c:  100%



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

Chain d:  50% 50%



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

Chain f:  100%



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

Chain o:  100%



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

Chain q:  50% 50%



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

Chain r:  50% 50%

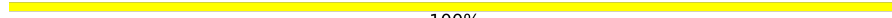
MAG1
MAG2

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

Chain s:  50% 50%

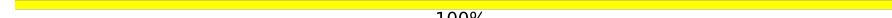
MAG1
MAG2

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

Chain v:  100%

MAG1
MAG2

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

Chain w:  100%

MAG1
MAG2

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

Chain x:  50% 50%

MAG1
MAG2

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

Chain 1:  100%

MAG1
MAG2

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

Chain 2:  100%



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



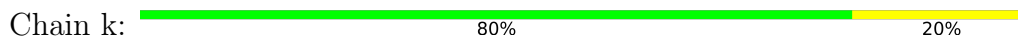
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



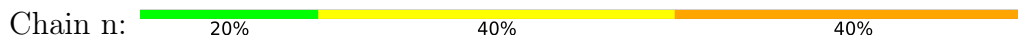
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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 8: 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 g:  50% 50%



- Molecule 8: 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 m:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	318.12Å 187.17Å 353.64Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	49.00 – 6.50 49.00 – 6.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.00-6.50) 89.4 (49.00-6.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.201 , 0.248 0.213 , 0.255	Depositor DCC
R_{free} test set	1926 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	209.5	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 676.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.038 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.039 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.297 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.289 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.047 for -h,-k,l	Xtriage
F_o , F_c correlation	0.86	EDS
Total number of atoms	44305	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% 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

5.1 Standard geometry

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

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	0.43	0/2532	0.90	3/3443 (0.1%)
1	C	0.41	0/2532	0.88	2/3443 (0.1%)
1	E	0.41	0/2532	0.88	1/3443 (0.0%)
1	G	0.38	0/2532	0.87	2/3443 (0.1%)
1	I	0.40	0/2532	0.89	4/3443 (0.1%)
1	K	0.39	0/2532	0.89	4/3443 (0.1%)
2	B	0.40	0/1420	0.88	1/1906 (0.1%)
2	D	0.39	0/1420	0.86	0/1906
2	F	0.38	0/1420	0.87	1/1906 (0.1%)
2	H	0.37	0/1420	0.86	1/1906 (0.1%)
2	J	0.39	0/1420	0.87	0/1906
2	L	0.38	0/1420	0.86	1/1906 (0.1%)
3	M	0.44	0/1740	0.91	5/2373 (0.2%)
3	O	0.46	0/1740	0.93	5/2373 (0.2%)
3	Q	0.46	0/1740	0.93	7/2373 (0.3%)
3	S	0.46	0/1740	0.93	3/2373 (0.1%)
3	U	0.45	0/1740	0.94	2/2373 (0.1%)
3	W	0.44	0/1740	0.92	5/2373 (0.2%)
4	N	0.46	0/1604	0.89	1/2190 (0.0%)
4	P	0.42	0/1604	0.86	1/2190 (0.0%)
4	R	0.41	0/1604	0.88	1/2190 (0.0%)
4	T	0.42	0/1604	0.90	3/2190 (0.1%)
4	V	0.45	0/1604	0.89	3/2190 (0.1%)
4	X	0.45	0/1604	0.96	5/2190 (0.2%)
All	All	0.42	0/43776	0.89	61/59472 (0.1%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	105	THR	CA-C-N	8.62	137.22	121.70
4	X	105	THR	C-N-CA	8.62	137.22	121.70
1	C	193	PHE	N-CA-C	8.13	120.14	111.28
1	I	193	PHE	N-CA-C	8.03	120.04	111.28
1	K	161	TYR	CA-C-N	-7.59	112.18	119.85
1	K	161	TYR	C-N-CA	-7.59	112.18	119.85
1	G	193	PHE	N-CA-C	7.46	119.41	111.28
3	S	100(D)	LEU	N-CA-C	6.84	121.79	113.38
3	U	100(D)	LEU	N-CA-C	6.75	121.68	113.38
3	W	100	SER	N-CA-C	-6.73	104.03	111.36
3	Q	53	PHE	N-CA-C	-6.71	103.99	111.71
3	U	100	SER	N-CA-C	-6.64	104.12	111.36
4	X	105	THR	CA-C-O	-6.49	113.35	120.36
3	Q	100(D)	LEU	N-CA-C	6.43	121.27	113.17
3	O	100(D)	LEU	N-CA-C	6.40	121.25	113.38
1	K	193	PHE	N-CA-C	6.39	118.25	111.28
3	O	100(F)	CYS	N-CA-C	6.37	119.95	110.52
3	W	100(B)	TYR	N-CA-C	6.35	119.86	109.76
4	X	104	LEU	N-CA-C	6.34	119.98	109.46
2	B	94	TYR	N-CA-C	6.29	117.80	111.07
1	E	193	PHE	N-CA-C	6.27	118.11	111.28
4	T	12	SER	N-CA-C	6.15	118.20	108.79
3	Q	100	SER	N-CA-C	-6.12	104.69	111.36
3	M	100(F)	CYS	N-CA-C	6.07	119.50	110.52
3	O	114	ALA	N-CA-C	6.06	119.05	109.96
3	M	100	SER	N-CA-C	-6.04	104.78	111.36
4	X	12	SER	N-CA-C	6.04	118.02	108.79
3	Q	54	PHE	CA-CB-CG	6.02	119.82	113.80
1	A	192	ILE	N-CA-C	-5.83	104.83	110.72
3	S	100	SER	N-CA-C	-5.79	105.05	111.36
1	I	191	GLN	N-CA-C	5.68	117.93	111.11
3	O	100	SER	N-CA-C	-5.67	105.18	111.36
3	Q	100(F)	CYS	N-CA-C	5.67	118.91	110.52
1	A	193	PHE	N-CA-C	5.62	117.41	111.28
3	W	100(D)	LEU	N-CA-C	5.61	120.23	113.17
4	R	12	SER	N-CA-C	5.60	117.35	108.79
3	Q	11	VAL	N-CA-C	5.58	116.32	108.17
4	T	153	SER	CA-C-N	5.56	125.48	119.76
4	T	153	SER	C-N-CA	5.56	125.48	119.76
4	V	29	GLY	N-CA-C	5.53	120.62	113.27
4	V	12	SER	N-CA-C	5.49	117.19	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	161	TYR	CA-C-N	-5.48	114.31	119.85
1	I	161	TYR	C-N-CA	-5.48	114.31	119.85
3	Q	113	SER	N-CA-C	-5.46	106.57	113.18
1	C	192	ILE	N-CA-C	-5.40	105.11	110.62
3	M	100(D)	LEU	N-CA-C	5.37	119.94	113.17
1	K	133	ASN	N-CA-C	5.33	118.94	111.74
3	W	100(C)	CYS	N-CA-C	5.20	117.77	109.96
4	P	27(B)	ASN	N-CA-C	5.14	116.95	108.48
3	O	137	ALA	N-CA-C	5.13	117.33	109.07
2	L	100	VAL	N-CA-C	5.13	115.90	110.72
2	F	163	ARG	N-CA-C	5.10	116.53	111.07
3	S	100(F)	CYS	N-CA-C	5.10	118.07	110.52
3	W	190	GLY	N-CA-C	5.10	120.20	113.37
2	H	31	GLY	N-CA-C	5.09	117.30	110.43
3	M	54	PHE	CA-CB-CG	5.08	118.88	113.80
1	G	192	ILE	N-CA-C	-5.06	105.46	110.62
4	N	27(B)	ASN	N-CA-C	5.06	116.83	108.48
3	M	53	PHE	N-CA-C	-5.05	105.91	111.71
1	A	226	ILE	N-CA-C	5.01	113.45	107.73
4	V	170	ASN	N-CA-C	5.01	119.24	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2475	0	2423	40	0
1	C	2475	0	2422	45	0
1	E	2475	0	2422	42	0
1	G	2475	0	2422	40	0
1	I	2475	0	2422	40	0
1	K	2475	0	2422	36	0
2	B	1396	0	1327	10	0
2	D	1396	0	1327	10	0
2	F	1396	0	1327	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1396	0	1327	11	0
2	J	1396	0	1327	13	0
2	L	1396	0	1327	11	0
3	M	1698	0	1649	44	0
3	O	1698	0	1649	48	0
3	Q	1698	0	1649	42	0
3	S	1698	0	1649	35	0
3	U	1698	0	1649	38	0
3	W	1698	0	1649	41	0
4	N	1567	0	1515	11	0
4	P	1567	0	1515	19	0
4	R	1567	0	1515	22	0
4	T	1567	0	1515	25	0
4	V	1567	0	1515	14	0
4	X	1567	0	1515	21	0
5	0	39	0	34	1	0
5	3	39	0	34	0	0
5	5	39	0	34	1	0
5	6	39	0	34	1	0
5	Y	39	0	34	0	0
5	i	39	0	34	0	0
5	j	39	0	34	2	0
5	l	39	0	34	0	0
5	p	39	0	34	0	0
5	t	39	0	34	1	0
5	u	39	0	34	0	0
5	y	39	0	34	2	0
5	z	39	0	34	0	0
6	1	28	0	25	0	0
6	2	28	0	25	0	0
6	4	28	0	25	2	0
6	Z	28	0	25	0	0
6	a	28	0	25	0	0
6	c	28	0	25	1	0
6	d	28	0	25	1	0
6	f	28	0	25	0	0
6	o	28	0	25	0	0
6	q	28	0	25	0	0
6	r	28	0	25	0	0
6	s	28	0	25	3	0
6	v	28	0	25	0	0
6	w	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	x	28	0	25	1	0
7	b	61	0	52	1	0
7	h	61	0	52	1	0
7	k	61	0	52	0	0
7	n	61	0	52	3	0
8	e	50	0	43	0	0
8	g	50	0	43	0	0
8	m	50	0	43	0	0
9	B	14	0	13	0	0
9	C	14	0	13	0	0
9	D	14	0	13	0	0
9	E	14	0	13	0	0
9	F	14	0	13	0	0
9	G	28	0	26	0	0
9	H	14	0	13	0	0
9	I	14	0	13	0	0
9	J	14	0	13	0	0
9	K	14	0	13	0	0
9	L	14	0	13	0	0
All	All	44305	0	42789	515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (515) 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)
1:G:145:ASN:ND2	3:S:100(F):CYS:SG	2.44	0.90
1:C:145:ASN:ND2	3:O:100(F):CYS:SG	2.46	0.89
1:K:145:ASN:ND2	3:W:100(F):CYS:SG	2.48	0.86
3:O:195:ILE:HG12	3:O:210:ARG:HG2	1.54	0.86
3:Q:195:ILE:HG12	3:Q:210:ARG:HG2	1.62	0.82
1:A:145:ASN:ND2	3:M:100(F):CYS:SG	2.52	0.82
1:I:145:ASN:ND2	3:U:100(F):CYS:SG	2.54	0.79
4:X:83:ASP:OD2	4:X:103:LYS:NZ	2.15	0.79
4:X:106:VAL:O	4:X:140:TYR:OH	2.01	0.78
4:R:105:THR:HG21	4:R:141:PRO:HB3	1.63	0.77
1:E:145:ASN:ND2	3:Q:100(F):CYS:SG	2.57	0.77
1:G:307:ARG:HH21	2:H:60:ASN:HD22	1.33	0.76
1:G:216:ASN:HB3	1:G:220:ARG:HH22	1.51	0.76
3:O:115:SER:HB2	4:T:126:GLN:HE22	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:15:PRO:HG3	4:T:107:GLY:HA2	1.70	0.73
3:O:188:SER:HB3	3:O:192:GLN:HG3	1.72	0.72
3:U:13:LYS:HG2	3:U:113:SER:HA	1.72	0.71
1:C:34:ILE:HD11	1:C:321:ARG:HD2	1.73	0.71
3:M:29:TYR:CE1	3:M:53:PHE:HA	2.27	0.69
1:C:307:ARG:HH21	2:D:60:ASN:HD22	1.39	0.69
4:T:106:VAL:O	4:T:140:TYR:OH	2.11	0.68
4:V:83:ASP:OD2	4:V:103:LYS:NZ	2.27	0.67
2:L:53:ASN:O	2:L:58:LYS:NZ	2.25	0.67
4:T:108:GLN:OE1	4:T:171:LYS:NZ	2.27	0.67
4:X:108:GLN:OE1	4:X:171:LYS:NZ	2.28	0.66
3:Q:188:SER:HB3	3:Q:192:GLN:HG3	1.76	0.66
4:P:126:GLN:NE2	3:S:115:SER:HB2	2.11	0.65
1:G:135:THR:HG21	3:S:100(A):HIS:HD2	1.62	0.65
3:W:23:ARG:NH1	3:W:75:THR:O	2.30	0.65
1:E:34:ILE:HD11	1:E:321:ARG:HD2	1.78	0.64
4:N:82:ASP:O	4:N:86:TYR:OH	2.10	0.64
4:T:15:PRO:HD3	4:T:106(A):LEU:O	1.98	0.64
3:Q:29:TYR:CE1	3:Q:53:PHE:HA	2.33	0.64
1:K:102:VAL:HG22	1:K:232:ILE:HB	1.80	0.64
2:J:53:ASN:O	2:J:58:LYS:NZ	2.31	0.64
1:K:135:THR:CG2	3:W:100(A):HIS:HB2	2.29	0.63
3:O:163:VAL:HG22	3:O:182:VAL:HG22	1.81	0.63
4:T:149:LYS:HE3	4:T:152:SER:HA	1.81	0.63
3:U:143:LYS:NZ	4:V:131:THR:OG1	2.29	0.62
1:K:197:GLN:NE2	1:K:248:THR:O	2.31	0.62
1:G:219:SER:HB2	5:y:1:NAG:HN2	1.64	0.62
3:U:11:VAL:HG21	3:U:146:PHE:HE2	1.64	0.62
4:N:83:ASP:OD2	4:N:103:LYS:NZ	2.32	0.62
1:A:34:ILE:HD11	1:A:321:ARG:HD2	1.82	0.62
1:E:193:PHE:CE1	3:Q:53:PHE:HD2	2.17	0.62
4:R:106:VAL:O	4:R:140:TYR:OH	2.18	0.61
1:A:135:THR:HG23	3:M:100(A):HIS:HB2	1.83	0.61
1:K:146:SER:HA	3:W:100(A):HIS:HD2	1.65	0.61
1:I:135:THR:HG21	3:U:100(A):HIS:CD2	2.35	0.60
4:R:37:GLN:HB2	4:R:47:LEU:HD11	1.83	0.60
4:X:14:THR:HG22	4:X:106(A):LEU:HB3	1.83	0.60
3:W:143:LYS:NZ	4:X:131:THR:OG1	2.28	0.60
1:E:193:PHE:CZ	3:Q:53:PHE:HD2	2.18	0.60
3:O:115:SER:CB	4:T:126:GLN:HE22	2.14	0.60
1:E:218:GLY:O	1:E:220:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:THR:HG21	3:S:100(A):HIS:CD2	2.37	0.60
1:C:152:ASN:N	1:C:253:ALA:O	2.30	0.60
4:R:83:ASP:OD2	4:R:103:LYS:NZ	2.34	0.59
1:A:101:ASP:OD2	1:C:210:GLN:NE2	2.35	0.59
1:K:193:PHE:HE1	3:W:54:PHE:HA	1.67	0.59
2:J:2:ILE:O	2:L:113:SER:OG	2.20	0.59
3:M:86:ASP:O	3:M:90:TYR:OH	2.17	0.59
3:O:29:TYR:CE1	3:O:53:PHE:HA	2.38	0.59
4:X:37:GLN:HB2	4:X:47:LEU:HD11	1.83	0.59
3:O:86:ASP:O	3:O:90:TYR:OH	2.16	0.59
2:F:53:ASN:O	2:F:58:LYS:NZ	2.34	0.59
1:K:159:PHE:HE2	3:W:73:GLY:HA3	1.66	0.59
4:P:115:VAL:O	4:P:204:LYS:NZ	2.33	0.59
1:I:197:GLN:NE2	1:I:248:THR:O	2.36	0.58
2:H:2:ILE:O	2:J:113:SER:OG	2.20	0.58
1:I:133:ASN:HB3	3:U:100(A):HIS:HB3	1.86	0.58
3:Q:163:VAL:HG22	3:Q:182:VAL:HG22	1.85	0.58
1:I:135:THR:HG21	3:U:100(A):HIS:HD2	1.69	0.58
4:N:149:LYS:HE3	4:N:152:SER:HA	1.85	0.58
1:A:218:GLY:O	1:A:220:ARG:NH1	2.36	0.57
1:K:216:ASN:HB3	1:K:220:ARG:HH22	1.69	0.57
1:A:307:ARG:HH21	2:B:60:ASN:HD22	1.52	0.57
1:C:221:PRO:O	1:C:229:ARG:NH2	2.34	0.57
4:V:110:LYS:HE3	4:V:198:GLU:HG3	1.85	0.57
3:W:95:PRO:HB2	3:W:97:ILE:HG12	1.85	0.57
1:K:34:ILE:HD11	1:K:321:ARG:HD2	1.86	0.57
4:R:110:LYS:NZ	4:R:198:GLU:HB2	2.19	0.57
3:S:36:TRP:CE2	3:S:80:MET:HB2	2.39	0.57
1:C:197:GLN:NE2	1:C:248:THR:O	2.37	0.57
1:E:135:THR:HG21	3:Q:100(A):HIS:HD2	1.70	0.57
1:K:194:LEU:HD22	3:W:100(D):LEU:HD13	1.86	0.57
3:W:29:TYR:CZ	3:W:53:PHE:HA	2.40	0.57
1:K:135:THR:HG23	3:W:100(A):HIS:HB2	1.86	0.56
1:A:135:THR:CG2	3:M:100(A):HIS:HB2	2.36	0.56
1:G:216:ASN:HB3	1:G:220:ARG:NH2	2.20	0.56
1:K:152:ASN:HB3	1:K:253:ALA:HB3	1.87	0.56
1:A:135:THR:HG21	3:M:100(A):HIS:HD2	1.71	0.56
4:R:32:THR:HB	4:R:50:SER:HA	1.88	0.56
3:W:185:PRO:HG2	3:W:188:SER:HB2	1.88	0.56
1:I:307:ARG:HH21	2:J:60:ASN:HD22	1.53	0.56
2:B:127:ARG:NH2	2:F:131:GLU:OE1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:186:SER:HA	3:O:189:LEU:HD13	1.88	0.56
4:X:14:THR:HG22	4:X:106(A):LEU:HG	1.87	0.56
1:E:135:THR:HG23	3:Q:100(A):HIS:HB2	1.87	0.56
4:P:32:THR:HB	4:P:50:SER:HA	1.87	0.56
1:K:146:SER:HA	3:W:100(A):HIS:CD2	2.39	0.55
1:C:222:ARG:NH2	7:n:2:NAG:O6	2.39	0.55
4:X:149:LYS:HE3	4:X:152:SER:HA	1.88	0.55
3:S:32:ALA:HB2	3:S:52:ILE:HG12	1.89	0.55
1:A:163:ALA:CB	6:d:1:NAG:H4	2.36	0.55
4:T:37:GLN:HB2	4:T:47:LEU:HD11	1.89	0.55
1:G:133:ASN:HB3	3:S:100(A):HIS:HB3	1.88	0.55
1:C:219:SER:HB2	7:n:1:NAG:HN2	1.71	0.55
3:M:188:SER:HB3	3:M:192:GLN:HG3	1.89	0.55
1:K:219:SER:HB2	6:s:1:NAG:HN2	1.71	0.55
4:R:115:VAL:O	4:R:204:LYS:NZ	2.32	0.55
2:J:30:GLU:OE2	2:J:145:ASP:HB2	2.07	0.54
3:O:124:LEU:HB3	4:P:118:PHE:CD1	2.42	0.54
3:Q:115:SER:OG	3:Q:116:THR:N	2.40	0.54
4:V:149:LYS:HE3	4:V:152:SER:HA	1.88	0.54
1:E:135:THR:HG21	3:Q:100(A):HIS:CD2	2.42	0.54
2:H:53:ASN:O	2:H:58:LYS:NZ	2.40	0.54
1:I:48:ILE:HD13	1:I:50:GLU:HG2	1.89	0.54
3:O:144:ASP:OD1	3:O:171:GLN:NE2	2.36	0.54
1:A:185:PRO:HG2	1:A:217:ILE:HG12	1.89	0.54
1:G:34:ILE:HD11	1:G:321:ARG:HD2	1.88	0.54
1:I:34:ILE:HD11	1:I:321:ARG:HD2	1.89	0.54
3:W:100:SER:OG	3:W:100(A):HIS:ND1	2.37	0.54
1:E:135:THR:CG2	3:Q:100(A):HIS:HB2	2.37	0.54
1:I:220:ARG:NE	1:K:210:GLN:OE1	2.40	0.54
3:S:167:PRO:HG2	4:T:165:SER:OG	2.07	0.54
1:C:135:THR:HG21	3:O:100(A):HIS:HD2	1.73	0.54
3:M:40:ALA:HB3	3:M:43:GLN:HG3	1.90	0.54
1:G:307:ARG:HH21	2:H:60:ASN:ND2	2.02	0.54
3:Q:29:TYR:CZ	3:Q:53:PHE:HA	2.43	0.54
3:U:100:SER:OG	3:U:100(A):HIS:ND1	2.35	0.54
4:T:82:ASP:HB2	4:T:106:VAL:HG21	1.90	0.53
3:U:167:PRO:HG2	4:V:165:SER:OG	2.08	0.53
3:U:188:SER:HB3	3:U:192:GLN:HG3	1.91	0.53
4:R:149:LYS:HE3	4:R:152:SER:HA	1.90	0.53
6:w:1:NAG:H61	6:w:2:NAG:C7	2.38	0.53
1:K:13:LEU:HD13	2:L:149:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:GLU:OE2	2:L:145:ASP:HB2	2.08	0.53
1:I:193:PHE:CZ	3:U:54:PHE:CE1	2.97	0.53
4:N:32:THR:HB	4:N:50:SER:HA	1.91	0.53
1:I:135:THR:HG23	3:U:100(A):HIS:HB2	1.89	0.53
1:A:193:PHE:CE1	3:M:53:PHE:HD2	2.27	0.53
1:K:135:THR:HG21	3:W:100(A):HIS:CD2	2.43	0.53
3:M:186:SER:HA	3:M:189:LEU:HD13	1.90	0.53
3:Q:36:TRP:CH2	3:Q:92:CYS:HB3	2.44	0.53
1:A:135:THR:HG21	3:M:100(A):HIS:CD2	2.44	0.52
3:M:119:PRO:HB3	3:M:145:TYR:HB3	1.90	0.52
3:O:29:TYR:CZ	3:O:53:PHE:HA	2.44	0.52
3:O:32:ALA:HB2	3:O:52:ILE:HG12	1.91	0.52
3:S:39:GLN:OE1	4:T:38:HIS:NE2	2.30	0.52
1:A:14:CYS:HA	2:B:137:CYS:HA	1.92	0.52
3:O:47:TRP:CH2	3:O:49:GLY:HA2	2.45	0.52
3:Q:14:PRO:HD3	3:Q:112:SER:C	2.34	0.52
1:E:159:PHE:CZ	3:Q:73:GLY:HA3	2.44	0.52
3:U:11:VAL:HG21	3:U:146:PHE:CE2	2.42	0.52
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.09	0.52
3:S:95:PRO:HB2	3:S:97:ILE:HG12	1.91	0.52
3:U:95:PRO:HB2	3:U:97:ILE:HG12	1.91	0.52
4:R:82:ASP:O	4:R:86:TYR:OH	2.17	0.52
3:S:119:PRO:HD2	3:S:205:THR:HG21	1.92	0.52
3:S:138:LEU:HB2	3:S:211:VAL:HG11	1.92	0.52
4:T:110:LYS:HE3	4:T:198:GLU:HG3	1.91	0.52
1:G:297:VAL:HA	5:t:1:NAG:H82	1.92	0.52
4:T:15:PRO:CG	4:T:107:GLY:HA2	2.38	0.52
3:W:163:VAL:HG22	3:W:182:VAL:HG22	1.92	0.52
3:O:36:TRP:CH2	3:O:92:CYS:HB3	2.44	0.52
1:C:133:ASN:HB3	3:O:100(A):HIS:HB3	1.92	0.51
1:C:216:ASN:CG	1:E:201:ARG:HH12	2.19	0.51
1:E:133:ASN:HB3	3:Q:100(A):HIS:HB3	1.92	0.51
1:E:195:TYR:CZ	1:E:250:ASN:HA	2.45	0.51
3:U:36:TRP:CE2	3:U:80:MET:HB2	2.45	0.51
1:I:219:SER:HB2	6:4:1:NAG:HN2	1.76	0.51
4:P:37:GLN:HB2	4:P:47:LEU:HD11	1.91	0.51
3:W:186:SER:HA	3:W:189:LEU:HD13	1.91	0.51
1:A:193:PHE:CZ	3:M:53:PHE:HD2	2.28	0.51
4:R:19:VAL:HG13	4:R:78:LEU:HD11	1.91	0.51
3:S:29:TYR:CE1	3:S:53:PHE:HA	2.45	0.51
1:A:210:GLN:NE2	1:E:101:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:MET:HE2	1:A:300:ILE:HG22	1.92	0.51
1:I:133:ASN:N	1:I:152:ASN:OD1	2.36	0.51
3:O:119:PRO:HD2	3:O:205:THR:HG21	1.93	0.51
3:W:147:PRO:O	3:W:200:HIS:NE2	2.31	0.51
1:I:135:THR:CG2	3:U:100(A):HIS:HB2	2.40	0.51
3:M:11:VAL:HG21	3:M:146:PHE:CZ	2.45	0.51
1:C:195:TYR:CZ	1:C:250:ASN:HA	2.46	0.51
1:A:216:ASN:ND2	1:C:201:ARG:HH12	2.09	0.51
1:K:193:PHE:CZ	3:W:54:PHE:CD1	2.98	0.51
3:O:100:SER:OG	3:O:100(A):HIS:ND1	2.40	0.51
1:E:159:PHE:CE1	3:Q:29:TYR:CZ	2.99	0.51
1:E:193:PHE:CE1	3:Q:54:PHE:CD1	2.98	0.51
1:G:221:PRO:O	1:G:229:ARG:NH2	2.39	0.51
1:I:307:ARG:HH21	2:J:60:ASN:ND2	2.09	0.51
1:I:152:ASN:HB3	1:I:253:ALA:HB3	1.92	0.50
4:N:79:GLN:C	4:N:106:VAL:HG11	2.36	0.50
3:U:147:PRO:O	3:U:200:HIS:NE2	2.36	0.50
4:X:63:SER:O	4:X:73:LEU:HD12	2.11	0.50
3:S:29:TYR:CZ	3:S:53:PHE:HA	2.46	0.50
3:W:29:TYR:CE1	3:W:53:PHE:HA	2.46	0.50
3:M:195:ILE:HG12	3:M:210:ARG:HG2	1.93	0.50
4:P:15:PRO:HD3	4:P:106(A):LEU:O	2.12	0.50
1:A:193:PHE:CZ	3:M:54:PHE:CE1	3.00	0.50
1:G:307:ARG:NH2	2:H:60:ASN:HD22	2.05	0.49
3:M:163:VAL:HG22	3:M:182:VAL:HG22	1.94	0.49
4:R:63:SER:O	4:R:73:LEU:HD12	2.11	0.49
1:A:133:ASN:HB3	3:M:100(A):HIS:HB3	1.94	0.49
4:T:12:SER:HA	4:T:105:THR:O	2.12	0.49
1:E:185:PRO:HG2	1:E:217:ILE:HG12	1.94	0.49
1:I:177:LEU:HD21	1:I:179:ILE:HD11	1.95	0.49
1:E:154:LEU:HD12	1:E:251:LEU:HD23	1.94	0.49
1:K:156:HIS:HE1	3:W:29:TYR:CE1	2.31	0.49
1:G:135:THR:HG23	3:S:100(A):HIS:HB2	1.94	0.49
1:A:191:GLN:NE2	1:A:197:GLN:O	2.25	0.49
4:R:15:PRO:CG	4:R:107:GLY:HA2	2.43	0.49
3:W:188:SER:HB3	3:W:192:GLN:HG3	1.93	0.49
1:E:193:PHE:CZ	3:Q:53:PHE:CD2	3.00	0.49
1:I:193:PHE:CE1	3:U:54:PHE:CD1	3.01	0.49
4:P:82:ASP:O	4:P:86:TYR:OH	2.31	0.49
4:R:35:TRP:HB2	4:R:48:ILE:HB	1.94	0.49
1:A:194:LEU:HD22	3:M:100(D):LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:63:SER:O	4:T:73:LEU:HD12	2.13	0.49
1:A:193:PHE:CE1	3:M:53:PHE:CD2	3.01	0.48
1:C:163:ALA:CB	5:j:1:NAG:H4	2.43	0.48
2:B:53:ASN:O	2:B:58:LYS:NZ	2.46	0.48
1:G:154:LEU:HD12	1:G:251:LEU:HD23	1.96	0.48
2:L:74:GLU:HB2	2:L:78:GLN:HB2	1.94	0.48
3:M:12:LYS:HG3	3:M:18:VAL:HB	1.94	0.48
1:E:137:SER:HB3	3:Q:100(F):CYS:SG	2.53	0.48
3:Q:110:THR:HG21	3:Q:146:PHE:HE1	1.78	0.48
4:V:118:PHE:HB2	4:V:133:VAL:HB	1.94	0.48
4:X:54:ARG:HD3	4:X:62:PHE:O	2.13	0.48
1:A:216:ASN:CG	1:C:201:ARG:HH12	2.22	0.48
1:G:219:SER:CB	5:y:1:NAG:HN2	2.26	0.48
4:T:19:VAL:HG13	4:T:78:LEU:HD11	1.95	0.48
1:G:153:TRP:CD2	3:S:100(D):LEU:HD12	2.48	0.48
3:M:11:VAL:HG21	3:M:146:PHE:HZ	1.79	0.48
3:M:13:LYS:HA	3:M:112:SER:O	2.13	0.48
3:U:32:ALA:HB2	3:U:52:ILE:HG12	1.96	0.48
4:P:79:GLN:C	4:P:106:VAL:HG11	2.39	0.48
1:A:89:GLU:HG3	1:A:267:ILE:HD11	1.95	0.48
1:A:193:PHE:CZ	3:M:53:PHE:CD2	3.02	0.48
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.12	0.48
4:T:54:ARG:HD3	4:T:62:PHE:O	2.14	0.48
3:W:47:TRP:CH2	3:W:49:GLY:HA2	2.48	0.48
1:G:102:VAL:HG22	1:G:232:ILE:HB	1.96	0.48
1:G:193:PHE:CZ	3:S:54:PHE:CD1	3.01	0.48
3:S:30:LYS:HB3	3:S:100(B):TYR:CE1	2.48	0.48
1:C:219:SER:CB	7:n:1:NAG:HN2	2.27	0.47
1:E:193:PHE:CZ	3:Q:54:PHE:CE1	3.01	0.47
4:X:110:LYS:HE3	4:X:198:GLU:HG3	1.96	0.47
1:C:193:PHE:CZ	3:O:54:PHE:CD1	3.02	0.47
1:G:135:THR:CG2	3:S:100(A):HIS:HB2	2.45	0.47
1:I:193:PHE:CZ	3:U:54:PHE:CD1	3.02	0.47
1:C:163:ALA:HB1	5:j:1:NAG:H4	1.95	0.47
1:E:152:ASN:HB3	1:E:253:ALA:HB3	1.97	0.47
2:H:113:SER:OG	2:L:2:ILE:O	2.28	0.47
4:R:110:LYS:HZ1	4:R:198:GLU:HB2	1.78	0.47
1:A:137:SER:HB3	3:M:100(F):CYS:SG	2.54	0.47
3:M:34:ASN:HD22	3:M:34:ASN:N	2.13	0.47
3:W:167:PRO:HG2	4:X:165:SER:OG	2.15	0.47
3:M:100:SER:OG	3:M:100(A):HIS:ND1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:13:LYS:HA	3:Q:112:SER:O	2.15	0.47
3:W:70:THR:O	3:W:79:TYR:N	2.43	0.47
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.97	0.47
1:I:47:SER:HB2	1:I:288:ILE:HG22	1.97	0.47
1:A:48:ILE:HD13	1:A:50:GLU:HG2	1.97	0.47
1:K:48:ILE:HD13	1:K:50:GLU:HG2	1.95	0.47
1:K:219:SER:CB	6:s:1:NAG:HN2	2.28	0.47
3:M:1:GLU:O	3:M:3:GLN:NE2	2.47	0.47
2:D:53:ASN:O	2:D:58:LYS:NZ	2.44	0.47
3:O:95:PRO:HB2	3:O:97:ILE:HG12	1.96	0.47
3:S:34:ASN:N	3:S:34:ASN:HD22	2.13	0.47
1:G:133:ASN:N	1:G:152:ASN:OD1	2.35	0.46
1:G:152:ASN:HB3	1:G:253:ALA:HB3	1.96	0.46
1:I:14:CYS:HA	2:J:137:CYS:HA	1.97	0.46
3:U:86:ASP:HB2	3:U:111:VAL:HG21	1.97	0.46
3:Q:1:GLU:O	3:Q:3:GLN:NE2	2.47	0.46
1:G:14:CYS:HA	2:H:137:CYS:HA	1.98	0.46
1:I:153:TRP:CD2	3:U:100(D):LEU:HD12	2.49	0.46
1:K:156:HIS:HE1	3:W:29:TYR:HE1	1.61	0.46
3:U:34:ASN:N	3:U:34:ASN:HD22	2.14	0.46
1:A:178:TYR:CE1	1:A:257:TYR:HB3	2.50	0.46
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.44	0.46
3:O:143:LYS:NZ	4:P:131:THR:OG1	2.45	0.46
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.98	0.46
3:M:51:ILE:HG13	3:M:56:THR:O	2.15	0.46
1:C:135:THR:HG21	3:O:100(A):HIS:CD2	2.49	0.46
1:E:159:PHE:HE1	3:Q:29:TYR:CZ	2.32	0.46
1:G:210:GLN:NE2	1:K:101:ASP:OD2	2.49	0.46
3:W:34:ASN:HD22	3:W:34:ASN:N	2.13	0.46
6:c:1:NAG:H61	6:c:2:NAG:C7	2.46	0.46
4:P:118:PHE:HB2	4:P:133:VAL:HB	1.97	0.46
3:U:47:TRP:CH2	3:U:49:GLY:HA2	2.51	0.46
3:W:138:LEU:O	3:W:181:VAL:HG13	2.16	0.46
4:V:19:VAL:HG13	4:V:78:LEU:HD11	1.97	0.46
4:X:106:VAL:O	4:X:106:VAL:HG12	2.16	0.46
1:I:307:ARG:NH2	2:J:60:ASN:HD22	2.13	0.46
3:Q:51:ILE:O	3:Q:52(A):PRO:HD3	2.16	0.46
3:W:164:HIS:HE1	4:X:167:GLN:OE1	1.99	0.46
4:X:196:THR:HA	4:X:201:THR:HA	1.97	0.46
1:G:188:ASP:OD1	5:0:2:NAG:O6	2.25	0.46
1:I:102:VAL:HG22	1:I:232:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1:GLU:O	3:O:3:GLN:NE2	2.49	0.46
3:Q:38:ARG:NH1	3:Q:86:ASP:HA	2.31	0.46
3:S:119:PRO:HB3	3:S:145:TYR:HB3	1.98	0.46
1:I:146:SER:HA	3:U:100(A):HIS:HD2	1.81	0.45
3:O:138:LEU:O	3:O:181:VAL:HG13	2.16	0.45
3:Q:100:SER:OG	3:Q:100(A):HIS:ND1	2.42	0.45
1:A:67:ILE:O	1:A:71:LEU:HG	2.17	0.45
3:O:208:ASP:O	3:S:204:ASN:O	2.34	0.45
3:S:100:SER:OG	3:S:100(A):HIS:ND1	2.40	0.45
1:A:188:ASP:O	1:A:191:GLN:HB3	2.16	0.45
1:E:207:LYS:NZ	1:E:240:GLY:O	2.32	0.45
1:G:48:ILE:HD13	1:G:50:GLU:HG2	1.98	0.45
3:Q:34:ASN:N	3:Q:34:ASN:HD22	2.15	0.45
1:A:159:PHE:CE1	3:M:29:TYR:CE1	3.04	0.45
3:O:34:ASN:N	3:O:34:ASN:HD22	2.15	0.45
4:R:122:SER:O	4:R:126:GLN:HG3	2.16	0.45
2:L:110:LEU:O	2:L:113:SER:HB3	2.16	0.45
4:V:12:SER:HA	4:V:105:THR:O	2.16	0.45
1:E:193:PHE:CE1	3:Q:53:PHE:CD2	3.01	0.45
2:H:30:GLU:OE2	2:H:145:ASP:HB2	2.17	0.45
3:O:51:ILE:HG13	3:O:56:THR:O	2.17	0.45
1:I:97:CYS:O	1:I:224:ARG:NH2	2.36	0.45
3:M:151:THR:OG1	3:M:199:ASN:HB3	2.17	0.45
3:Q:167:PRO:HG2	4:R:165:SER:OG	2.17	0.45
4:N:79:GLN:O	4:N:106:VAL:HG11	2.17	0.45
4:X:35:TRP:HB2	4:X:48:ILE:HB	1.99	0.45
3:W:32:ALA:HB2	3:W:52:ILE:HG12	1.98	0.45
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.49	0.44
1:I:17:HIS:O	2:J:14:TRP:N	2.41	0.44
3:O:185:PRO:HG2	3:O:188:SER:HB2	1.99	0.44
4:X:113:PRO:HA	4:X:139:PHE:HB3	1.99	0.44
1:C:193:PHE:CZ	3:O:53:PHE:CD2	3.05	0.44
1:G:193:PHE:HE1	3:S:54:PHE:HA	1.82	0.44
1:I:68:ASP:OD1	1:I:100:TYR:OH	2.27	0.44
1:I:193:PHE:CZ	3:U:53:PHE:CD2	3.05	0.44
4:P:12:SER:HA	4:P:105:THR:O	2.18	0.44
3:W:1:GLU:O	3:W:3:GLN:NE2	2.48	0.44
3:Q:95:PRO:HB2	3:Q:97:ILE:HG12	2.00	0.44
3:U:124:LEU:HB3	4:V:118:PHE:CD1	2.53	0.44
1:C:135:THR:HG23	3:O:100(A):HIS:HB2	1.99	0.44
1:E:184:HIS:HB3	1:E:216:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:17:HIS:CD2	2:L:10:ILE:HG21	2.52	0.44
3:M:167:PRO:HG2	4:N:165:SER:OG	2.18	0.44
4:T:83:ASP:OD2	4:T:103:LYS:NZ	2.48	0.44
1:E:176:LYS:HD3	1:E:178:TYR:OH	2.17	0.44
2:H:1:GLY:O	2:J:117:LYS:NZ	2.43	0.44
1:I:134:GLY:CA	1:I:153:TRP:HB3	2.48	0.44
3:Q:47:TRP:CH2	3:Q:49:GLY:HA2	2.53	0.44
1:C:15:LEU:HD21	2:D:122:THR:HG21	2.00	0.44
3:S:143:LYS:NZ	4:T:131:THR:OG1	2.47	0.44
1:K:137:SER:HB3	3:W:100(F):CYS:SG	2.57	0.44
3:O:29:TYR:O	3:O:53:PHE:HB2	2.18	0.44
3:O:167:PRO:HG2	4:P:165:SER:OG	2.18	0.44
4:R:85:ASP:OD1	4:R:103:LYS:HD3	2.18	0.44
1:G:130:VAL:HG11	1:G:164:LEU:HD11	1.99	0.44
3:M:14:PRO:HD3	3:M:112:SER:C	2.43	0.44
3:M:51:ILE:O	3:M:52(A):PRO:HD3	2.16	0.44
4:R:37:GLN:HG3	4:R:86:TYR:CE2	2.53	0.44
3:S:188:SER:HB3	3:S:192:GLN:HG3	2.00	0.44
1:A:17:HIS:CD2	2:B:10:ILE:HG21	2.53	0.43
1:C:178:TYR:CE1	1:C:257:TYR:HB3	2.53	0.43
1:E:67:ILE:O	1:E:71:LEU:HG	2.18	0.43
4:T:129:LYS:HE3	4:T:129:LYS:HB3	1.88	0.43
4:X:12:SER:HA	4:X:105:THR:O	2.18	0.43
1:C:216:ASN:OD1	1:E:201:ARG:NH1	2.49	0.43
3:Q:12:LYS:HG3	3:Q:18:VAL:HB	1.99	0.43
7:b:1:NAG:H61	7:b:2:NAG:C7	2.47	0.43
1:A:219:SER:HB2	7:h:1:NAG:HN2	1.84	0.43
1:C:193:PHE:CZ	3:O:53:PHE:HD2	2.36	0.43
1:E:325:GLU:OE1	2:F:15:GLU:HG3	2.17	0.43
1:I:130:VAL:HG11	1:I:164:LEU:HD11	1.99	0.43
4:R:84:ALA:HB3	4:R:86:TYR:CZ	2.53	0.43
3:S:121:VAL:HB	3:S:207:VAL:HG11	2.00	0.43
1:E:153:TRP:CD2	3:Q:100(D):LEU:HD12	2.52	0.43
3:U:138:LEU:HB2	3:U:211:VAL:HG11	1.99	0.43
2:H:50:GLY:HA3	1:K:30:THR:O	2.18	0.43
1:K:79:PHE:HA	1:K:82:LYS:HD3	2.01	0.43
4:T:35:TRP:CD2	4:T:73:LEU:HB2	2.53	0.43
4:V:35:TRP:CD2	4:V:73:LEU:HB2	2.54	0.43
3:Q:14:PRO:HD3	3:Q:112:SER:O	2.19	0.43
1:G:77:ASP:OD2	1:G:141:ARG:NE	2.34	0.43
1:G:195:TYR:CZ	1:G:250:ASN:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:66:LYS:HA	4:T:71:ALA:HA	1.99	0.43
1:E:307:ARG:HH21	2:F:60:ASN:HD22	1.67	0.43
1:G:17:HIS:O	2:H:14:TRP:N	2.42	0.43
1:I:268:MET:HE2	1:I:300:ILE:HG22	1.99	0.43
1:K:135:THR:N	3:W:100(B):TYR:O	2.39	0.43
2:L:20:GLY:HA3	2:L:36:ALA:HB1	2.01	0.43
3:M:138:LEU:O	3:M:181:VAL:HG13	2.18	0.43
3:U:164:HIS:HE1	4:V:167:GLN:OE1	2.01	0.43
2:B:115:MET:HE3	2:B:115:MET:HA	2.01	0.43
1:E:89:GLU:HG3	1:E:267:ILE:HD11	2.00	0.43
1:I:281:CYS:HB2	1:I:304:ALA:O	2.19	0.43
3:M:10:GLU:O	3:M:109:VAL:HA	2.19	0.43
1:A:193:PHE:CE1	3:M:54:PHE:CD1	3.07	0.43
1:A:197:GLN:NE2	1:A:248:THR:O	2.52	0.43
2:D:90:ASP:OD2	2:F:62:LYS:NZ	2.32	0.43
1:E:177:LEU:HD21	1:E:179:ILE:HD11	2.00	0.43
1:I:219:SER:CB	6:4:1:NAG:HN2	2.32	0.43
1:K:159:PHE:CE2	3:W:73:GLY:HA3	2.51	0.43
3:U:51:ILE:HG13	3:U:56:THR:O	2.19	0.43
1:C:193:PHE:CE1	3:O:54:PHE:HA	2.54	0.42
2:J:76:ARG:HH22	2:L:74:GLU:CD	2.25	0.42
6:s:1:NAG:H61	6:s:2:NAG:C7	2.49	0.42
1:C:17:HIS:CD2	2:D:10:ILE:HG21	2.54	0.42
1:C:152:ASN:HB3	1:C:253:ALA:HB3	2.01	0.42
1:G:193:PHE:CZ	3:S:53:PHE:HD2	2.38	0.42
3:M:95:PRO:HB2	3:M:97:ILE:HG12	2.00	0.42
4:P:15:PRO:HG3	4:P:107:GLY:HA2	2.00	0.42
5:5:1:NAG:H61	5:5:2:NAG:C7	2.49	0.42
1:C:89:GLU:OE1	1:C:109:ARG:NH2	2.40	0.42
3:M:165:THR:HA	3:M:180:SER:HA	2.01	0.42
4:N:15:PRO:HD3	4:N:106(A):LEU:O	2.20	0.42
3:W:36:TRP:CH2	3:W:92:CYS:HB3	2.54	0.42
3:W:47:TRP:CZ2	3:W:49:GLY:HA2	2.55	0.42
2:B:134:GLY:HA2	2:D:124:LYS:HD3	2.02	0.42
1:C:159:PHE:CE1	3:O:29:TYR:CZ	3.07	0.42
1:G:26:VAL:HG12	1:G:315:LYS:CB	2.49	0.42
1:I:193:PHE:CZ	3:U:53:PHE:HD2	2.37	0.42
2:J:1:GLY:O	2:L:117:LYS:NZ	2.37	0.42
4:N:35:TRP:HB2	4:N:48:ILE:HB	2.02	0.42
4:N:54:ARG:HD3	4:N:62:PHE:O	2.18	0.42
3:Q:119:PRO:HD2	3:Q:205:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:84:ALA:HB3	4:R:86:TYR:CE1	2.54	0.42
1:A:68:ASP:OD1	1:A:100:TYR:OH	2.38	0.42
1:I:195:TYR:CZ	1:I:250:ASN:HA	2.54	0.42
3:W:124:LEU:HB3	4:X:118:PHE:CD1	2.55	0.42
1:A:201:ARG:HH12	1:E:216:ASN:ND2	2.17	0.42
3:O:209:LYS:HA	3:S:204:ASN:O	2.19	0.42
1:K:195:TYR:CZ	1:K:250:ASN:HA	2.54	0.42
4:P:149:LYS:HE3	4:P:152:SER:HA	2.01	0.42
1:A:135:THR:OG1	3:M:100(C):CYS:HA	2.20	0.42
1:G:193:PHE:CZ	3:S:53:PHE:CD2	3.07	0.42
1:C:133:ASN:N	1:C:152:ASN:OD1	2.41	0.42
1:C:201:ARG:HD2	1:C:214:ILE:HD11	2.02	0.42
1:E:36:VAL:HG12	1:E:321:ARG:HA	2.01	0.42
3:M:36:TRP:CH2	3:M:92:CYS:HB3	2.54	0.42
3:S:126:PRO:HB2	3:S:189:LEU:HD21	2.00	0.42
3:U:186:SER:HA	3:U:189:LEU:HD13	2.02	0.42
1:C:159:PHE:CZ	3:O:73:GLY:HA3	2.54	0.42
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.55	0.42
1:G:103:PRO:HD2	1:G:232:ILE:O	2.20	0.42
1:I:17:HIS:CD2	2:J:10:ILE:HG21	2.55	0.42
1:K:163:ALA:HB3	5:6:1:NAG:O6	2.20	0.42
1:C:193:PHE:HE1	3:O:54:PHE:HA	1.84	0.41
1:C:299:ARG:O	2:D:68:LYS:NZ	2.48	0.41
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.47	0.41
3:M:100(A):HIS:ND1	3:M:100(A):HIS:N	2.68	0.41
3:O:13:LYS:HA	3:O:112:SER:O	2.19	0.41
4:R:4:LEU:O	4:R:99:GLY:HA2	2.20	0.41
4:T:37:GLN:HG3	4:T:86:TYR:CE2	2.55	0.41
4:X:113:PRO:CA	4:X:139:PHE:HB3	2.50	0.41
3:O:151:THR:OG1	3:O:199:ASN:HB3	2.21	0.41
3:S:12:LYS:HB3	3:S:16:SER:OG	2.19	0.41
2:D:133:MET:SD	2:D:139:LYS:HB2	2.60	0.41
4:T:35:TRP:HB2	4:T:48:ILE:HB	2.02	0.41
1:E:188:ASP:O	1:E:191:GLN:HB3	2.19	0.41
1:E:178:TYR:CE1	1:E:257:TYR:HB3	2.55	0.41
1:I:146:SER:HA	3:U:100(A):HIS:CD2	2.55	0.41
3:O:51:ILE:O	3:O:52(A):PRO:HD3	2.20	0.41
4:P:54:ARG:HD3	4:P:62:PHE:O	2.21	0.41
4:P:85:ASP:OD1	4:P:103:LYS:HD3	2.21	0.41
3:U:90:TYR:CE1	3:U:109:VAL:HB	2.55	0.41
1:C:158:ASN:OD1	3:O:27:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:GLY:CA	1:G:153:TRP:HB3	2.50	0.41
1:K:135:THR:HG21	3:W:100(A):HIS:HD2	1.86	0.41
3:S:185:PRO:HG2	3:S:188:SER:HB2	2.02	0.41
3:U:138:LEU:O	3:U:181:VAL:HG13	2.20	0.41
2:B:148:CYS:O	2:B:151:SER:OG	2.36	0.41
1:I:135:THR:OG1	3:U:100(C):CYS:HA	2.21	0.41
3:Q:155:ASN:ND2	3:Q:159:LEU:HD12	2.36	0.41
4:X:134:CYS:HB2	4:X:148:TRP:CH2	2.55	0.41
1:C:68:ASP:OD1	1:C:100:TYR:OH	2.31	0.41
1:I:134:GLY:N	1:I:153:TRP:HB3	2.35	0.41
1:K:72:GLY:HA3	1:K:149:SER:OG	2.20	0.41
3:O:140:CYS:N	3:O:180:SER:O	2.47	0.41
3:U:116:THR:HG21	3:U:202:PRO:O	2.21	0.41
4:V:114:SER:O	4:V:136:ILE:HA	2.21	0.41
1:C:135:THR:HG1	3:O:100(C):CYS:HA	1.86	0.41
1:E:164:LEU:O	1:E:246:ASN:HA	2.21	0.41
1:G:135:THR:OG1	3:S:100(C):CYS:HA	2.21	0.41
1:K:127:TRP:HD1	1:K:132:GLN:OE1	2.03	0.41
4:N:84:ALA:HB3	4:N:86:TYR:CZ	2.56	0.41
3:O:124:LEU:HD22	4:P:118:PHE:HB3	2.03	0.41
4:P:83:ASP:OD2	4:P:103:LYS:NZ	2.54	0.41
4:V:196:THR:HA	4:V:201:THR:HA	2.02	0.41
3:W:70:THR:HB	3:W:79:TYR:HB2	2.03	0.41
3:W:150:VAL:HG22	3:W:200:HIS:HB2	2.02	0.41
3:W:151:THR:OG1	3:W:199:ASN:HB3	2.20	0.41
1:C:127:TRP:HB2	1:C:132:GLN:NE2	2.36	0.40
1:E:26:VAL:HG12	1:E:315:LYS:CB	2.51	0.40
1:G:177:LEU:HD11	1:G:234:TRP:HB2	2.02	0.40
1:G:185:PRO:HG2	1:G:217:ILE:HG12	2.02	0.40
3:Q:209:LYS:HE2	3:Q:209:LYS:HB2	1.84	0.40
4:T:78:LEU:HD22	4:T:106:VAL:HG22	2.01	0.40
4:V:106:VAL:O	4:V:140:TYR:OH	2.39	0.40
1:A:141:ARG:NH1	1:A:146:SER:OG	2.54	0.40
1:A:177:LEU:HD21	1:A:179:ILE:HD11	2.04	0.40
1:C:135:THR:CG2	3:O:100(A):HIS:HB2	2.52	0.40
1:C:168:MET:HA	1:C:169:PRO:HD3	1.84	0.40
2:D:115:MET:HA	2:D:115:MET:HE3	2.03	0.40
3:M:127:SER:O	3:M:127:SER:OG	2.33	0.40
3:Q:11:VAL:HG21	3:Q:146:PHE:HE2	1.87	0.40
1:C:170:ASN:HA	1:C:176:LYS:NZ	2.37	0.40
1:E:194:LEU:HD22	3:Q:100(D):LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:HIS:HB3	1:G:216:ASN:O	2.22	0.40
1:K:295:GLN:CG	1:K:306:PRO:HB2	2.52	0.40
1:K:295:GLN:HG2	1:K:306:PRO:HB2	2.03	0.40
3:M:29:TYR:O	3:M:53:PHE:HB2	2.22	0.40
3:O:100(A):HIS:ND1	3:O:100(A):HIS:N	2.69	0.40
3:S:51:ILE:HG13	3:S:56:THR:O	2.22	0.40
4:R:4:LEU:HB2	4:R:99:GLY:CA	2.52	0.40
3:U:119:PRO:HD2	3:U:205:THR:HG21	2.04	0.40
6:x:1:NAG:H61	6:x:2:NAG:C7	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	C	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	E	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	G	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	I	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
1	K	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
2	B	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	D	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	F	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	H	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	J	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	L	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
3	M	222/240 (92%)	217 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	222/240 (92%)	216 (97%)	6 (3%)	0	100	100
3	Q	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	S	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	U	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
3	W	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
4	N	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	P	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
4	R	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	T	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	V	211/216 (98%)	208 (99%)	3 (1%)	0	100	100
4	X	211/216 (98%)	205 (97%)	5 (2%)	1 (0%)	24	63
All	All	5514/5730 (96%)	5369 (97%)	144 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	106	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/285 (98%)	277 (99%)	3 (1%)	65	76
1	C	280/285 (98%)	277 (99%)	3 (1%)	65	76
1	E	280/285 (98%)	277 (99%)	3 (1%)	65	76
1	G	280/285 (98%)	277 (99%)	3 (1%)	65	76
1	I	280/285 (98%)	277 (99%)	3 (1%)	65	76
1	K	280/285 (98%)	277 (99%)	3 (1%)	65	76
2	B	146/148 (99%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	146/148 (99%)	146 (100%)	0	100	100
2	F	146/148 (99%)	146 (100%)	0	100	100
2	H	146/148 (99%)	146 (100%)	0	100	100
2	J	146/148 (99%)	146 (100%)	0	100	100
2	L	146/148 (99%)	146 (100%)	0	100	100
3	M	188/201 (94%)	185 (98%)	3 (2%)	55	70
3	O	188/201 (94%)	185 (98%)	3 (2%)	55	70
3	Q	188/201 (94%)	183 (97%)	5 (3%)	39	61
3	S	188/201 (94%)	185 (98%)	3 (2%)	55	70
3	U	188/201 (94%)	184 (98%)	4 (2%)	47	65
3	W	188/201 (94%)	185 (98%)	3 (2%)	55	70
4	N	178/181 (98%)	175 (98%)	3 (2%)	53	69
4	P	178/181 (98%)	176 (99%)	2 (1%)	65	76
4	R	178/181 (98%)	176 (99%)	2 (1%)	65	76
4	T	178/181 (98%)	176 (99%)	2 (1%)	65	76
4	V	178/181 (98%)	175 (98%)	3 (2%)	53	69
4	X	178/181 (98%)	176 (99%)	2 (1%)	65	76
All	All	4752/4890 (97%)	4699 (99%)	53 (1%)	65	76

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	246	ASN
1	A	325	GLU
1	C	48	ILE
1	C	246	ASN
1	C	325	GLU
1	E	48	ILE
1	E	246	ASN
1	E	325	GLU
1	G	48	ILE
1	G	246	ASN
1	G	325	GLU
1	I	48	ILE
1	I	246	ASN

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Mol	Chain	Res	Type
1	I	325	GLU
1	K	48	ILE
1	K	246	ASN
1	K	325	GLU
3	M	2	VAL
3	M	34	ASN
3	M	159	LEU
4	N	1	GLN
4	N	110	LYS
4	N	209	THR
3	O	2	VAL
3	O	34	ASN
3	O	159	LEU
4	P	1	GLN
4	P	209	THR
3	Q	2	VAL
3	Q	34	ASN
3	Q	113	SER
3	Q	115	SER
3	Q	159	LEU
4	R	1	GLN
4	R	209	THR
3	S	2	VAL
3	S	34	ASN
3	S	159	LEU
4	T	1	GLN
4	T	209	THR
3	U	2	VAL
3	U	34	ASN
3	U	115	SER
3	U	159	LEU
4	V	1	GLN
4	V	108	GLN
4	V	209	THR
3	W	2	VAL
3	W	34	ASN
3	W	159	LEU
4	X	1	GLN
4	X	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	HIS
1	A	296	ASN
2	B	47	GLN
2	B	60	ASN
2	B	116	ASN
1	C	17	HIS
1	C	296	ASN
2	D	60	ASN
2	D	78	GLN
1	E	17	HIS
1	E	216	ASN
2	F	60	ASN
2	F	159	HIS
1	G	17	HIS
1	G	144	ASN
1	G	145	ASN
2	H	60	ASN
1	I	17	HIS
1	I	44	GLN
1	I	145	ASN
1	I	296	ASN
2	J	60	ASN
1	K	17	HIS
1	K	144	ASN
1	K	156	HIS
1	K	216	ASN
2	L	129	ASN
3	M	34	ASN
3	M	204	ASN
4	N	37	GLN
4	N	188	HIS
4	N	194	GLN
3	O	34	ASN
3	O	76	ASN
3	O	204	ASN
4	P	53	GLN
4	P	126	GLN
4	P	197	HIS
3	S	43	GLN
3	S	58	ASN
3	S	164	HIS
3	U	43	GLN

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Mol	Chain	Res	Type
3	U	164	HIS
4	V	53	GLN
3	W	34	ASN
3	W	164	HIS
4	X	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

101 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	$\# Z > 2$
5	NAG	0	1	5,1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
5	NAG	0	2	5	14,14,15	0.57	0	17,19,21	0.91	1 (5%)
5	BMA	0	3	5	11,11,12	0.63	0	15,15,17	0.92	1 (6%)
6	NAG	1	1	6,1	14,14,15	0.57	0	17,19,21	0.83	0
6	NAG	1	2	6	14,14,15	0.53	0	17,19,21	0.80	0
6	NAG	2	1	6,1	14,14,15	0.55	0	17,19,21	0.70	0
6	NAG	2	2	6	14,14,15	0.54	0	17,19,21	0.65	0
5	NAG	3	1	5,1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
5	NAG	3	2	5	14,14,15	0.53	0	17,19,21	0.72	0
5	BMA	3	3	5	11,11,12	0.62	0	15,15,17	0.74	0
6	NAG	4	1	6,1	14,14,15	0.54	0	17,19,21	0.72	0
6	NAG	4	2	6	14,14,15	0.60	0	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	5	1	5,1	14,14,15	0.44	0	17,19,21	0.74	1 (5%)
5	NAG	5	2	5	14,14,15	0.49	0	17,19,21	0.80	0
5	BMA	5	3	5	11,11,12	0.61	0	15,15,17	0.83	1 (6%)
5	NAG	6	1	5,1	14,14,15	1.36	3 (21%)	17,19,21	1.99	3 (17%)
5	NAG	6	2	5	14,14,15	0.63	0	17,19,21	1.04	2 (11%)
5	BMA	6	3	5	11,11,12	0.51	0	15,15,17	0.87	1 (6%)
5	NAG	Y	1	5,1	14,14,15	0.64	0	17,19,21	0.95	1 (5%)
5	NAG	Y	2	5	14,14,15	0.62	0	17,19,21	1.46	1 (5%)
5	BMA	Y	3	5	11,11,12	0.61	0	15,15,17	0.67	0
6	NAG	Z	1	6,1	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
6	NAG	Z	2	6	14,14,15	0.57	0	17,19,21	0.80	0
6	NAG	a	1	6,1	14,14,15	0.64	0	17,19,21	0.86	2 (11%)
6	NAG	a	2	6	14,14,15	0.53	0	17,19,21	0.76	0
7	NAG	b	1	1,7	14,14,15	0.50	0	17,19,21	0.82	0
7	NAG	b	2	7	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
7	BMA	b	3	7	11,11,12	0.58	0	15,15,17	1.05	1 (6%)
7	MAN	b	4	7	11,11,12	0.60	0	15,15,17	0.78	0
7	MAN	b	5	7	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
6	NAG	c	1	6,1	14,14,15	0.49	0	17,19,21	0.77	0
6	NAG	c	2	6	14,14,15	0.49	0	17,19,21	0.73	0
6	NAG	d	1	6,1	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
6	NAG	d	2	6	14,14,15	0.60	0	17,19,21	0.76	0
8	NAG	e	1	1,8	14,14,15	0.61	0	17,19,21	0.96	2 (11%)
8	NAG	e	2	8	14,14,15	0.61	0	17,19,21	0.73	0
8	BMA	e	3	8	11,11,12	0.63	0	15,15,17	0.81	0
8	MAN	e	4	8	11,11,12	0.59	0	15,15,17	0.76	0
6	NAG	f	1	6,1	14,14,15	0.52	0	17,19,21	0.75	0
6	NAG	f	2	6	14,14,15	0.57	0	17,19,21	0.58	0
8	NAG	g	1	1,8	14,14,15	0.59	0	17,19,21	0.72	1 (5%)
8	NAG	g	2	8	14,14,15	0.51	0	17,19,21	0.66	0
8	BMA	g	3	8	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
8	MAN	g	4	8	11,11,12	0.61	0	15,15,17	0.59	0
7	NAG	h	1	1,7	14,14,15	0.55	0	17,19,21	0.74	0
7	NAG	h	2	7	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
7	BMA	h	3	7	11,11,12	0.66	0	15,15,17	0.99	1 (6%)
7	MAN	h	4	7	11,11,12	0.55	0	15,15,17	0.96	1 (6%)
7	MAN	h	5	7	11,11,12	0.65	0	15,15,17	0.60	0
5	NAG	i	1	5,1	14,14,15	0.52	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	i	2	5	14,14,15	0.51	0	17,19,21	0.70	0
5	BMA	i	3	5	11,11,12	0.56	0	15,15,17	0.81	0
5	NAG	j	1	5,1	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
5	NAG	j	2	5	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
5	BMA	j	3	5	11,11,12	0.60	0	15,15,17	0.90	1 (6%)
7	NAG	k	1	1,7	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
7	NAG	k	2	7	14,14,15	0.57	0	17,19,21	0.75	0
7	BMA	k	3	7	11,11,12	0.58	0	15,15,17	0.74	0
7	MAN	k	4	7	11,11,12	0.58	0	15,15,17	0.66	0
7	MAN	k	5	7	11,11,12	0.69	0	15,15,17	0.83	0
5	NAG	l	1	5,1	14,14,15	0.55	0	17,19,21	0.81	0
5	NAG	l	2	5	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
5	BMA	l	3	5	11,11,12	0.66	0	15,15,17	0.61	0
8	NAG	m	1	1,8	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
8	NAG	m	2	8	14,14,15	0.51	0	17,19,21	0.81	0
8	BMA	m	3	8	11,11,12	0.55	0	15,15,17	1.09	2 (13%)
8	MAN	m	4	8	11,11,12	0.57	0	15,15,17	0.73	0
7	NAG	n	1	1,7	14,14,15	0.47	0	17,19,21	0.79	1 (5%)
7	NAG	n	2	7	14,14,15	0.56	0	17,19,21	0.86	2 (11%)
7	BMA	n	3	7	11,11,12	0.54	0	15,15,17	0.79	0
7	MAN	n	4	7	11,11,12	0.55	0	15,15,17	0.91	1 (6%)
7	MAN	n	5	7	11,11,12	0.50	0	15,15,17	1.43	2 (13%)
6	NAG	o	1	6,1	14,14,15	0.50	0	17,19,21	0.62	0
6	NAG	o	2	6	14,14,15	0.54	0	17,19,21	0.62	0
5	NAG	p	1	5,1	14,14,15	0.47	0	17,19,21	1.12	1 (5%)
5	NAG	p	2	5	14,14,15	0.58	0	17,19,21	0.93	1 (5%)
5	BMA	p	3	5	11,11,12	0.61	0	15,15,17	0.92	0
6	NAG	q	1	6,1	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
6	NAG	q	2	6	14,14,15	0.54	0	17,19,21	0.68	0
6	NAG	r	1	6,1	14,14,15	0.48	0	17,19,21	0.71	0
6	NAG	r	2	6	14,14,15	0.53	0	17,19,21	0.82	1 (5%)
6	NAG	s	1	6,1	14,14,15	0.49	0	17,19,21	0.73	0
6	NAG	s	2	6	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
5	NAG	t	1	5,1	14,14,15	0.44	0	17,19,21	0.53	0
5	NAG	t	2	5	14,14,15	0.50	0	17,19,21	0.72	0
5	BMA	t	3	5	11,11,12	0.59	0	15,15,17	0.69	0
5	NAG	u	1	5,1	14,14,15	0.48	0	17,19,21	1.36	4 (23%)
5	NAG	u	2	5	14,14,15	0.56	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	u	3	5	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
6	NAG	v	1	6,1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
6	NAG	v	2	6	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
6	NAG	w	1	6,1	14,14,15	0.67	0	17,19,21	0.98	0
6	NAG	w	2	6	14,14,15	0.53	0	17,19,21	0.70	0
6	NAG	x	1	6,1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)
6	NAG	x	2	6	14,14,15	0.49	0	17,19,21	0.70	0
5	NAG	y	1	5,1	14,14,15	0.47	0	17,19,21	0.66	0
5	NAG	y	2	5	14,14,15	0.59	0	17,19,21	0.83	1 (5%)
5	BMA	y	3	5	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
5	NAG	z	1	5,1	14,14,15	0.48	0	17,19,21	0.61	0
5	NAG	z	2	5	14,14,15	0.54	0	17,19,21	0.79	1 (5%)
5	BMA	z	3	5	11,11,12	0.65	0	15,15,17	0.68	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
5	NAG	0	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	2/2/19/22	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	1/6/23/26	0/1/1/1
6	NAG	2	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	2	2	6	-	0/6/23/26	0/1/1/1
5	NAG	3	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	3	2	5	-	2/6/23/26	0/1/1/1
5	BMA	3	3	5	-	2/2/19/22	0/1/1/1
6	NAG	4	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	4	2	6	-	2/6/23/26	0/1/1/1
5	NAG	5	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
5	BMA	5	3	5	-	2/2/19/22	0/1/1/1
5	NAG	6	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	2/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	k	4	7	-	0/2/19/22	0/1/1/1
7	MAN	k	5	7	-	2/2/19/22	0/1/1/1
5	NAG	l	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
5	BMA	l	3	5	-	2/2/19/22	0/1/1/1
8	NAG	m	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	m	2	8	-	0/6/23/26	0/1/1/1
8	BMA	m	3	8	-	2/2/19/22	0/1/1/1
8	MAN	m	4	8	-	0/2/19/22	0/1/1/1
7	NAG	n	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
7	BMA	n	3	7	-	2/2/19/22	0/1/1/1
7	MAN	n	4	7	-	0/2/19/22	0/1/1/1
7	MAN	n	5	7	-	2/2/19/22	1/1/1/1
6	NAG	o	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	o	2	6	-	0/6/23/26	0/1/1/1
5	NAG	p	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	0/6/23/26	0/1/1/1
5	BMA	p	3	5	-	1/2/19/22	0/1/1/1
6	NAG	q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	q	2	6	-	0/6/23/26	0/1/1/1
6	NAG	r	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	r	2	6	-	0/6/23/26	0/1/1/1
6	NAG	s	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
5	NAG	t	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	0/6/23/26	0/1/1/1
5	BMA	t	3	5	-	2/2/19/22	0/1/1/1
5	NAG	u	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	u	2	5	-	0/6/23/26	0/1/1/1
5	BMA	u	3	5	-	0/2/19/22	0/1/1/1
6	NAG	v	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	v	2	6	-	0/6/23/26	0/1/1/1
6	NAG	w	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	w	2	6	-	0/6/23/26	0/1/1/1
6	NAG	x	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	x	2	6	-	0/6/23/26	0/1/1/1
5	NAG	y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	y	2	5	-	2/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	1	NAG	C2-N2	-2.70	1.41	1.46
5	6	1	NAG	O5-C1	-2.61	1.39	1.43
5	6	1	NAG	C1-C2	-2.01	1.49	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	1	NAG	C1-C2-N2	-6.05	100.90	110.43
5	Y	2	NAG	C1-O5-C5	5.11	119.03	112.19
7	n	5	MAN	C1-O5-C5	4.02	117.58	112.19
7	k	1	NAG	C1-O5-C5	3.60	117.02	112.19
7	b	5	MAN	C1-C2-C3	3.10	114.16	109.64
5	p	2	NAG	C4-C3-C2	3.09	115.55	111.02
5	0	1	NAG	C1-C2-N2	-3.06	105.61	110.43
5	Y	1	NAG	C1-O5-C5	2.97	116.17	112.19
7	n	5	MAN	O5-C5-C6	2.94	113.38	107.66
5	j	2	NAG	C4-C3-C2	2.93	115.31	111.02
5	p	1	NAG	O5-C5-C6	2.78	113.08	107.66
8	m	1	NAG	C1-O5-C5	2.77	115.90	112.19
7	h	3	BMA	C1-C2-C3	2.71	113.58	109.64
5	u	1	NAG	O5-C5-C6	2.66	112.84	107.66
6	d	1	NAG	O5-C5-C6	2.66	112.83	107.66
5	3	1	NAG	C1-O5-C5	2.64	115.73	112.19
6	v	1	NAG	C1-O5-C5	2.62	115.70	112.19
6	q	1	NAG	C1-O5-C5	2.62	115.69	112.19
5	j	1	NAG	O5-C5-C6	2.61	112.74	107.66
7	b	5	MAN	C1-O5-C5	2.61	115.68	112.19
5	u	2	NAG	C4-C3-C2	2.61	114.84	111.02
5	6	1	NAG	O7-C7-C8	2.55	126.59	122.05
5	u	1	NAG	C3-C4-C5	-2.52	105.66	110.23
5	6	3	BMA	O5-C5-C6	2.48	112.48	107.66
8	m	3	BMA	O5-C5-C6	2.47	112.47	107.66
7	h	4	MAN	C1-O5-C5	2.46	115.48	112.19
5	y	2	NAG	C4-C3-C2	2.44	114.59	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	2	NAG	C4-C3-C2	2.42	114.57	111.02
5	0	2	NAG	C4-C3-C2	2.42	114.56	111.02
5	u	1	NAG	C1-C2-N2	-2.40	106.65	110.43
5	0	1	NAG	C3-C4-C5	-2.33	106.01	110.23
8	g	3	BMA	O5-C5-C6	2.30	112.14	107.66
5	u	3	BMA	O5-C5-C6	2.28	112.09	107.66
7	b	3	BMA	C6-C5-C4	-2.27	107.45	113.02
7	b	2	NAG	C4-C3-C2	2.26	114.33	111.02
5	y	3	BMA	O5-C5-C6	2.26	112.06	107.66
7	n	1	NAG	C1-O5-C5	2.25	115.21	112.19
8	m	3	BMA	C1-C2-C3	2.23	112.90	109.64
5	0	3	BMA	C1-C2-C3	2.22	112.88	109.64
5	z	2	NAG	C4-C3-C2	2.22	114.27	111.02
7	b	5	MAN	O5-C1-C2	2.19	116.02	110.79
5	6	1	NAG	C4-C3-C2	-2.18	107.83	111.02
5	5	1	NAG	C1-O5-C5	2.17	115.09	112.19
6	v	2	NAG	C1-O5-C5	2.17	115.09	112.19
6	a	1	NAG	C2-N2-C7	-2.15	120.02	122.90
8	e	1	NAG	C2-N2-C7	-2.15	120.02	122.90
6	x	1	NAG	C1-O5-C5	2.12	115.03	112.19
7	h	2	NAG	C4-C3-C2	2.12	114.13	111.02
7	n	2	NAG	C4-C3-C2	2.12	114.12	111.02
8	e	1	NAG	C1-O5-C5	2.12	115.02	112.19
7	n	2	NAG	C2-N2-C7	-2.11	120.07	122.90
5	y	3	BMA	C1-C2-C3	2.11	112.72	109.64
6	a	1	NAG	C1-O5-C5	2.09	114.98	112.19
6	r	2	NAG	C1-O5-C5	2.08	114.97	112.19
7	n	4	MAN	C1-O5-C5	2.07	114.96	112.19
5	j	3	BMA	O5-C5-C6	2.07	111.68	107.66
6	Z	1	NAG	C4-C3-C2	2.05	114.02	111.02
6	s	2	NAG	O5-C5-C6	2.04	111.63	107.66
5	5	3	BMA	O5-C5-C6	2.03	111.62	107.66
5	l	2	NAG	C4-C3-C2	2.03	113.99	111.02
8	g	1	NAG	C2-N2-C7	-2.02	120.19	122.90
5	6	2	NAG	C1-O5-C5	2.02	114.90	112.19
5	u	1	NAG	C2-N2-C7	-2.01	120.20	122.90

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	p	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	p	1	NAG	O7-C7-N2-C2
5	t	1	NAG	O7-C7-N2-C2
5	u	1	NAG	O7-C7-N2-C2
5	z	1	NAG	C8-C7-N2-C2
5	z	1	NAG	O7-C7-N2-C2
5	0	1	NAG	O7-C7-N2-C2
5	3	1	NAG	C8-C7-N2-C2
5	3	1	NAG	O7-C7-N2-C2
5	5	1	NAG	C8-C7-N2-C2
5	5	1	NAG	O7-C7-N2-C2
6	w	1	NAG	C8-C7-N2-C2
6	w	1	NAG	O7-C7-N2-C2
6	x	1	NAG	C8-C7-N2-C2
6	x	1	NAG	O7-C7-N2-C2
8	m	1	NAG	O7-C7-N2-C2
6	4	2	NAG	C4-C5-C6-O6
5	i	2	NAG	C8-C7-N2-C2
5	i	2	NAG	O7-C7-N2-C2
5	j	1	NAG	C8-C7-N2-C2
5	j	1	NAG	O7-C7-N2-C2
5	t	1	NAG	C8-C7-N2-C2
5	u	1	NAG	C8-C7-N2-C2
5	0	1	NAG	C8-C7-N2-C2
8	m	1	NAG	C8-C7-N2-C2
7	k	5	MAN	C4-C5-C6-O6
6	s	2	NAG	C4-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
7	k	3	BMA	O5-C5-C6-O6
6	4	2	NAG	O5-C5-C6-O6
7	n	3	BMA	C4-C5-C6-O6
7	k	5	MAN	O5-C5-C6-O6
5	3	3	BMA	O5-C5-C6-O6
5	0	1	NAG	C4-C5-C6-O6
7	n	3	BMA	O5-C5-C6-O6
8	g	1	NAG	C8-C7-N2-C2
5	Y	3	BMA	C4-C5-C6-O6
8	g	3	BMA	O5-C5-C6-O6
5	3	3	BMA	C4-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
5	l	3	BMA	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
7	k	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	Y	2	NAG	C8-C7-N2-C2
6	a	1	NAG	C8-C7-N2-C2
8	g	1	NAG	O7-C7-N2-C2
8	g	3	BMA	C4-C5-C6-O6
7	h	3	BMA	O5-C5-C6-O6
5	l	3	BMA	C4-C5-C6-O6
8	e	3	BMA	C4-C5-C6-O6
6	a	1	NAG	O7-C7-N2-C2
5	6	3	BMA	C4-C5-C6-O6
5	6	3	BMA	O5-C5-C6-O6
5	Y	2	NAG	O7-C7-N2-C2
6	4	1	NAG	C8-C7-N2-C2
5	0	1	NAG	O5-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
5	3	2	NAG	C4-C5-C6-O6
5	3	2	NAG	O5-C5-C6-O6
7	n	5	MAN	O5-C5-C6-O6
7	n	5	MAN	C4-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
5	t	3	BMA	O5-C5-C6-O6
6	4	1	NAG	O7-C7-N2-C2
5	t	3	BMA	C4-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	j	1	NAG	C4-C5-C6-O6
5	j	1	NAG	O5-C5-C6-O6
5	y	2	NAG	C4-C5-C6-O6
7	h	3	BMA	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
7	k	2	NAG	C4-C5-C6-O6
5	0	3	BMA	C4-C5-C6-O6
8	m	3	BMA	C4-C5-C6-O6
5	j	3	BMA	C4-C5-C6-O6
5	i	3	BMA	C4-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	0	3	BMA	O5-C5-C6-O6
5	Y	2	NAG	C3-C2-N2-C7
7	k	2	NAG	O5-C5-C6-O6
5	y	2	NAG	O5-C5-C6-O6
5	j	3	BMA	O5-C5-C6-O6
8	m	3	BMA	O5-C5-C6-O6
5	i	3	BMA	O5-C5-C6-O6
5	z	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	5	3	BMA	C4-C5-C6-O6
5	z	3	BMA	C4-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
6	1	2	NAG	C4-C5-C6-O6
5	p	3	BMA	C4-C5-C6-O6
5	5	3	BMA	O5-C5-C6-O6

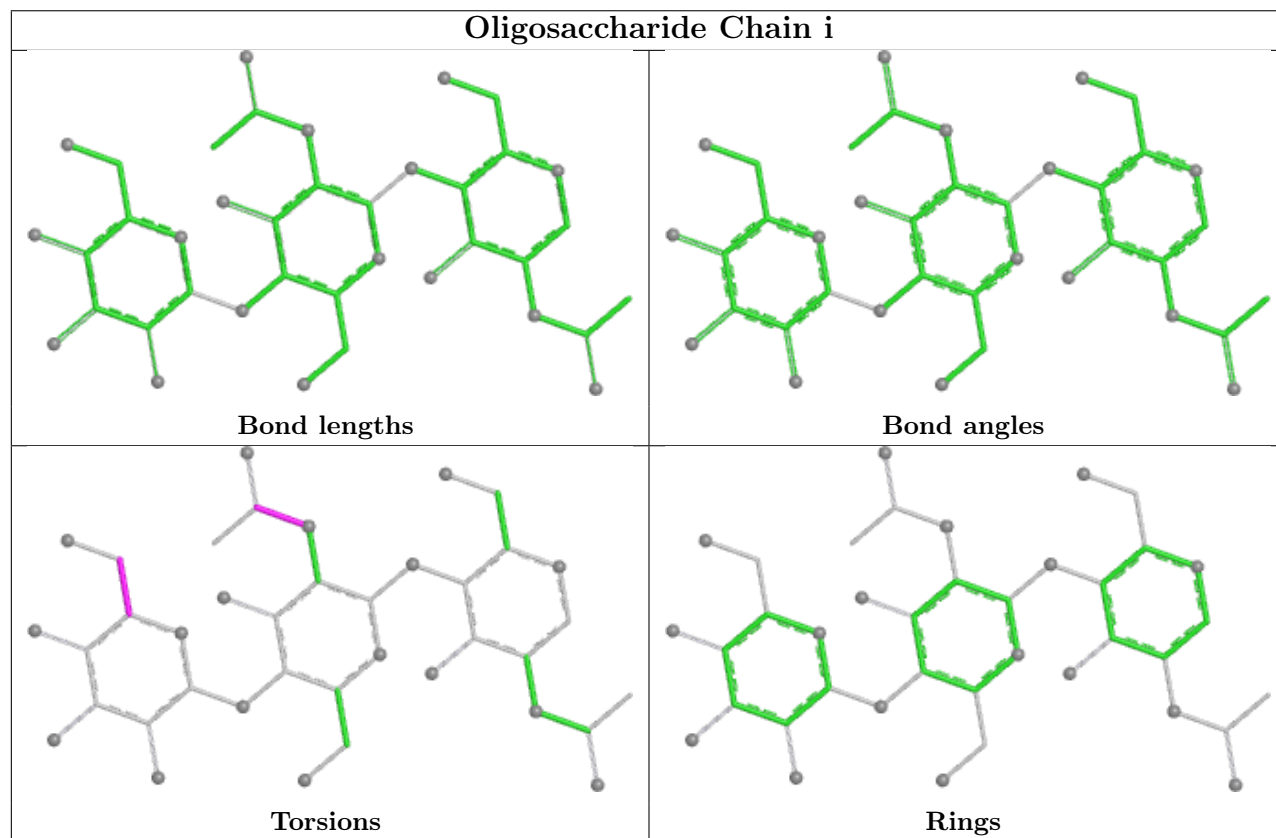
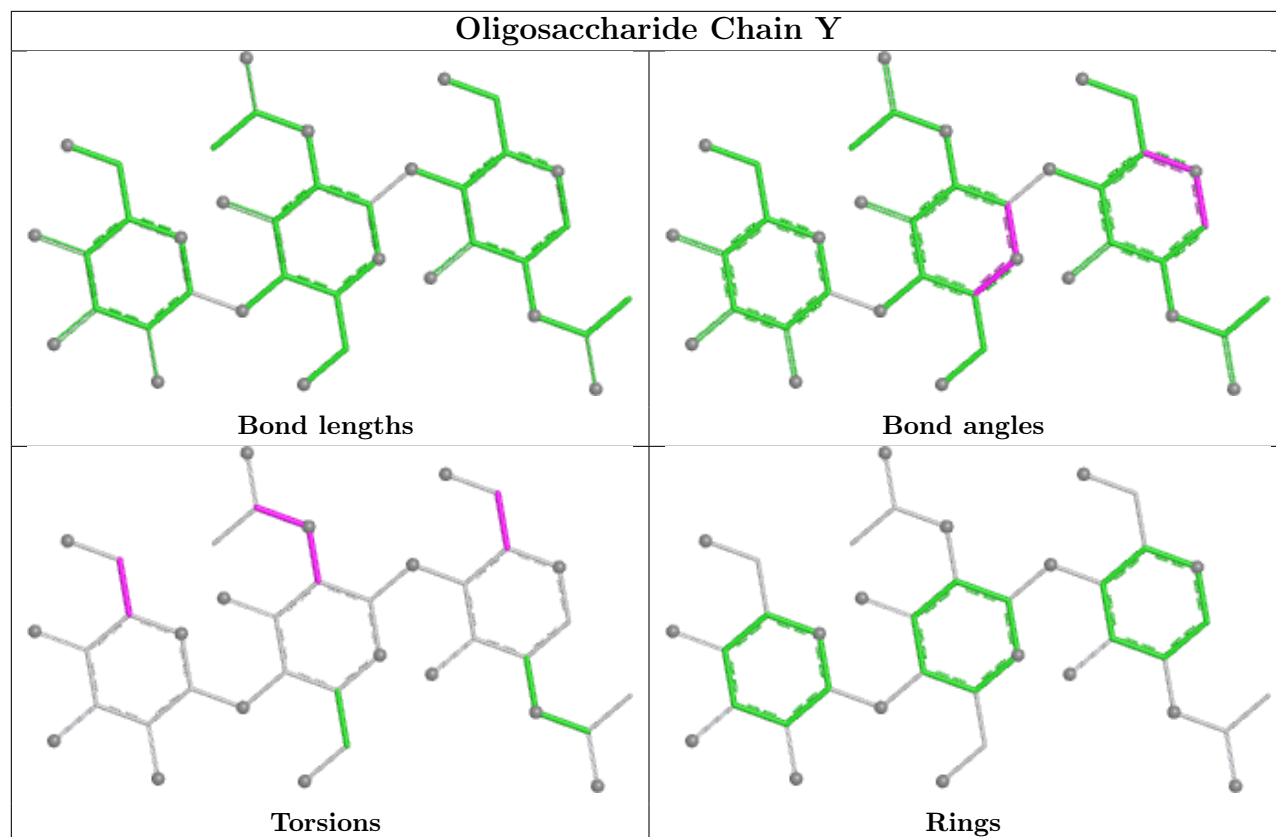
All (1) ring outliers are listed below:

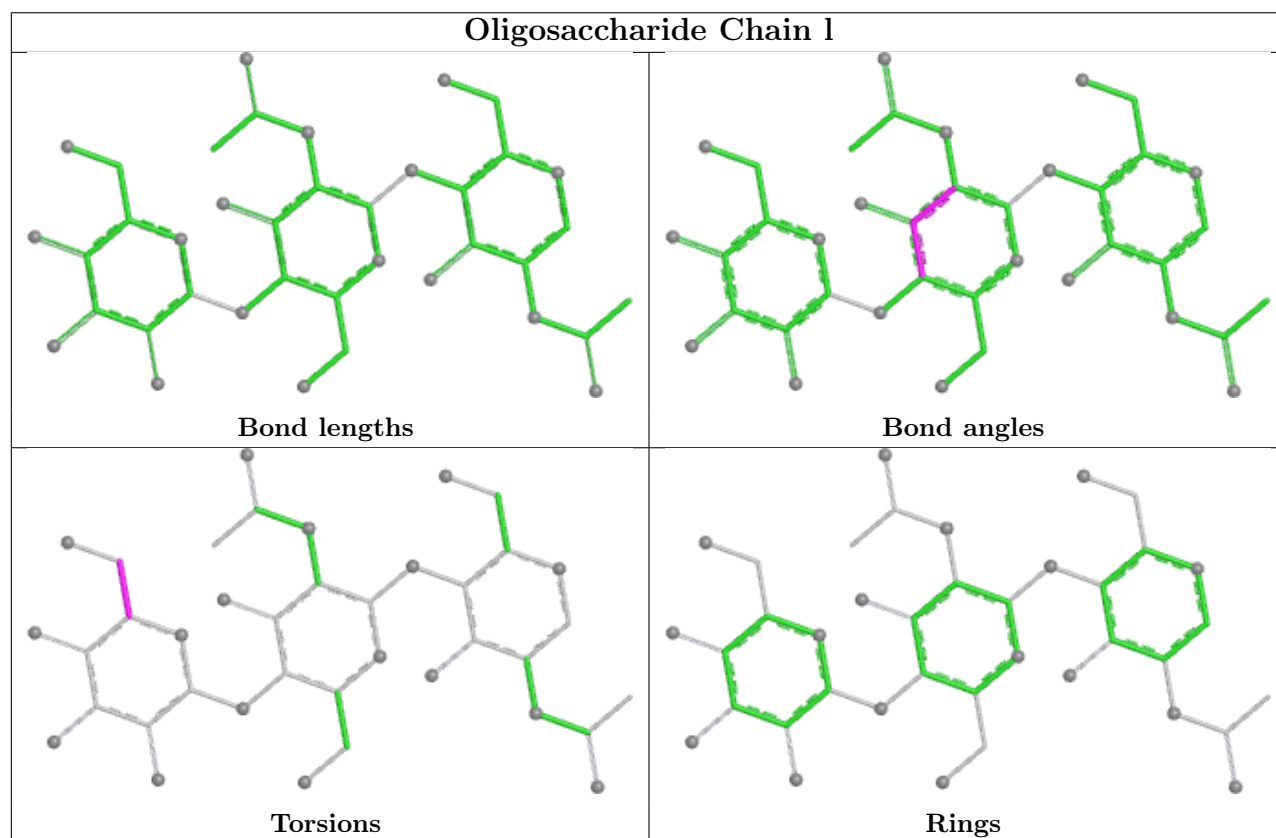
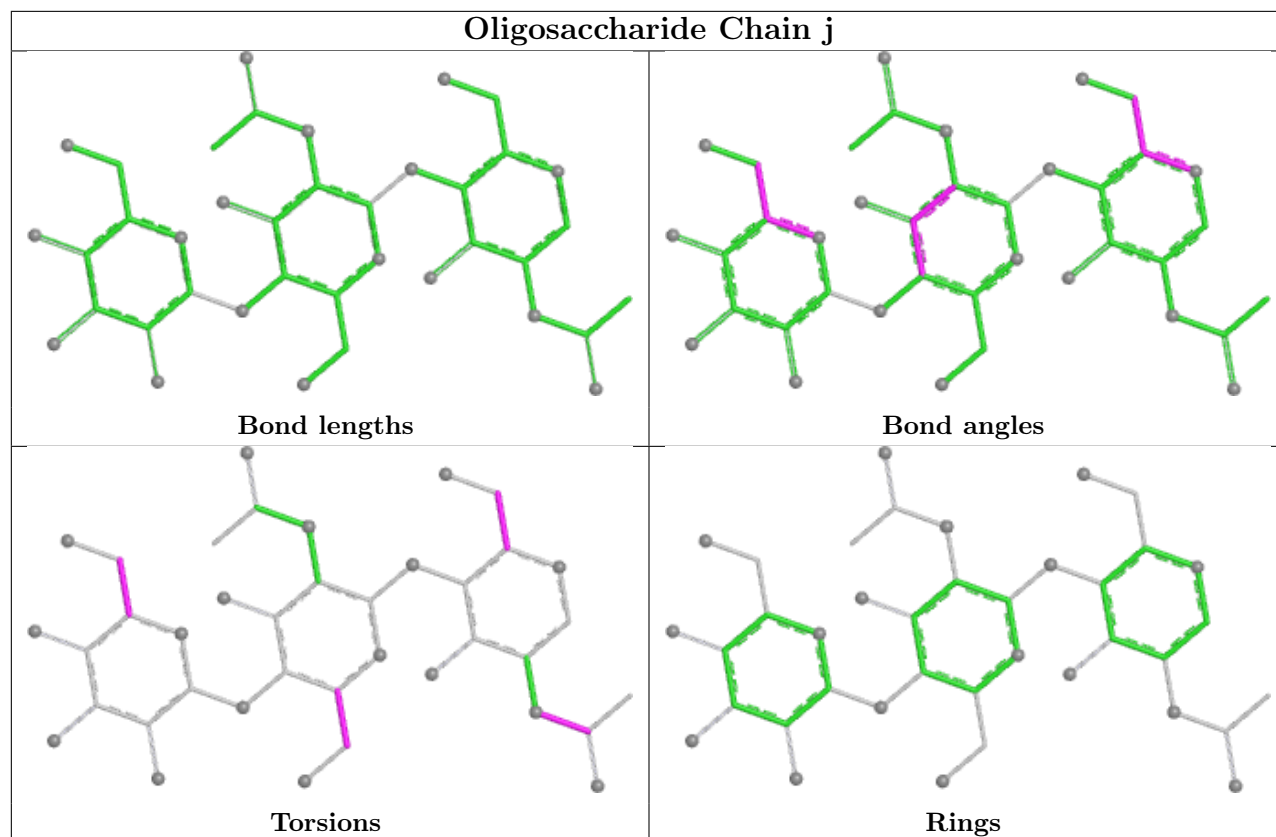
Mol	Chain	Res	Type	Atoms
7	n	5	MAN	C1-C2-C3-C4-C5-O5

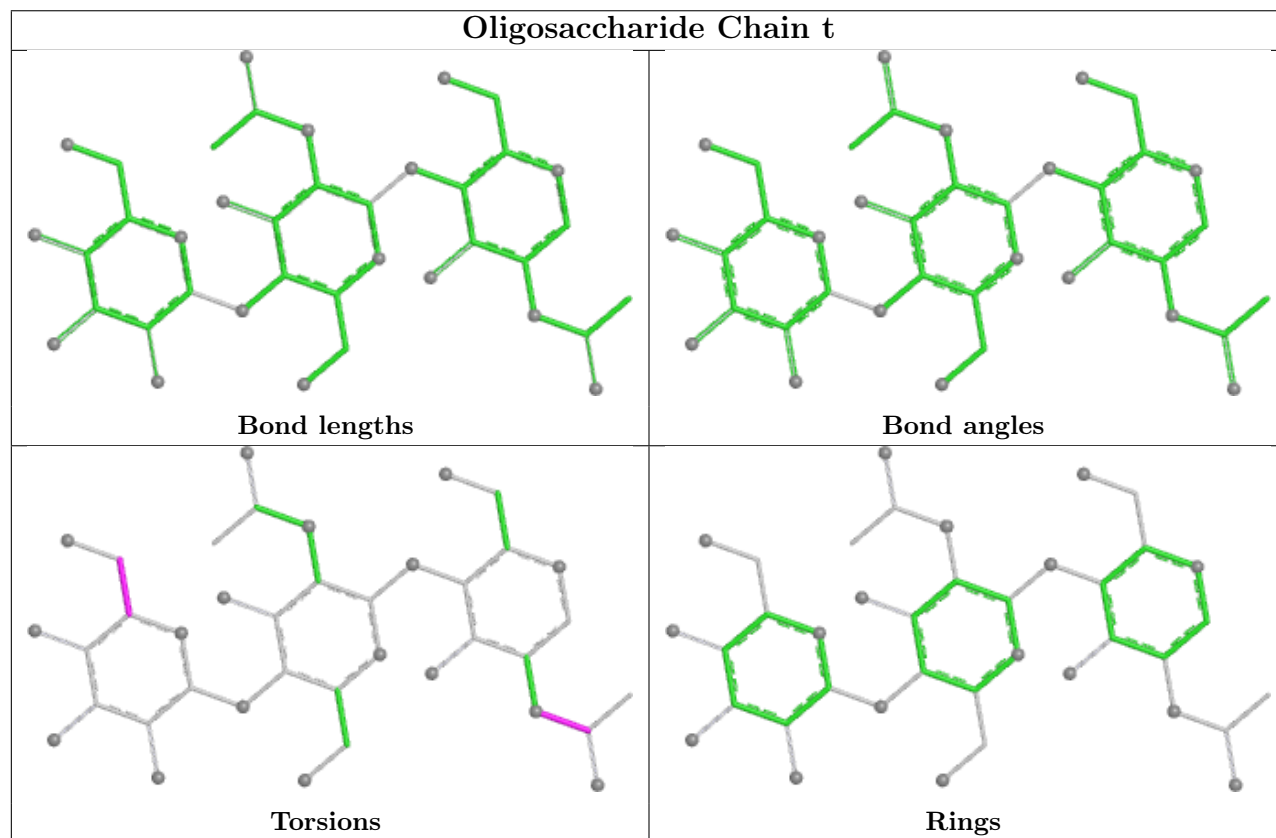
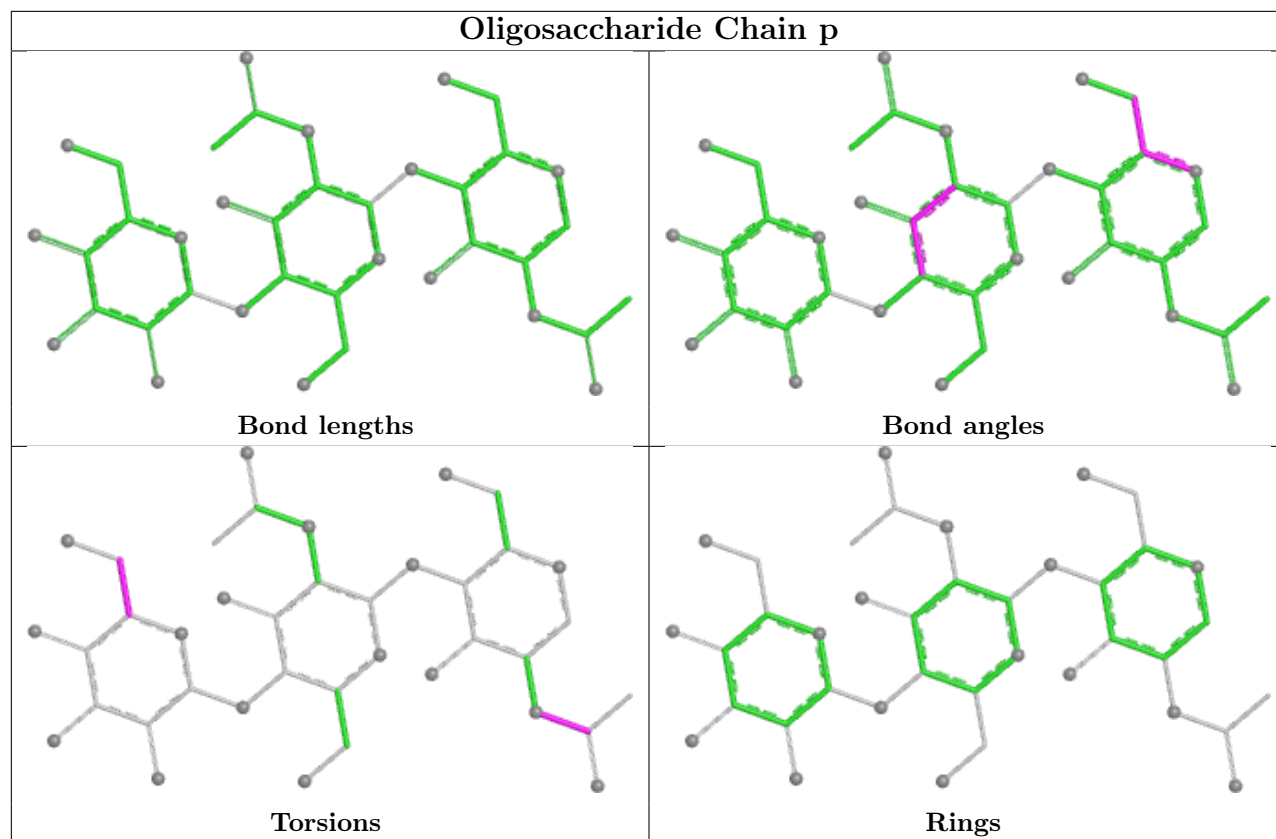
22 monomers are involved in 22 short contacts:

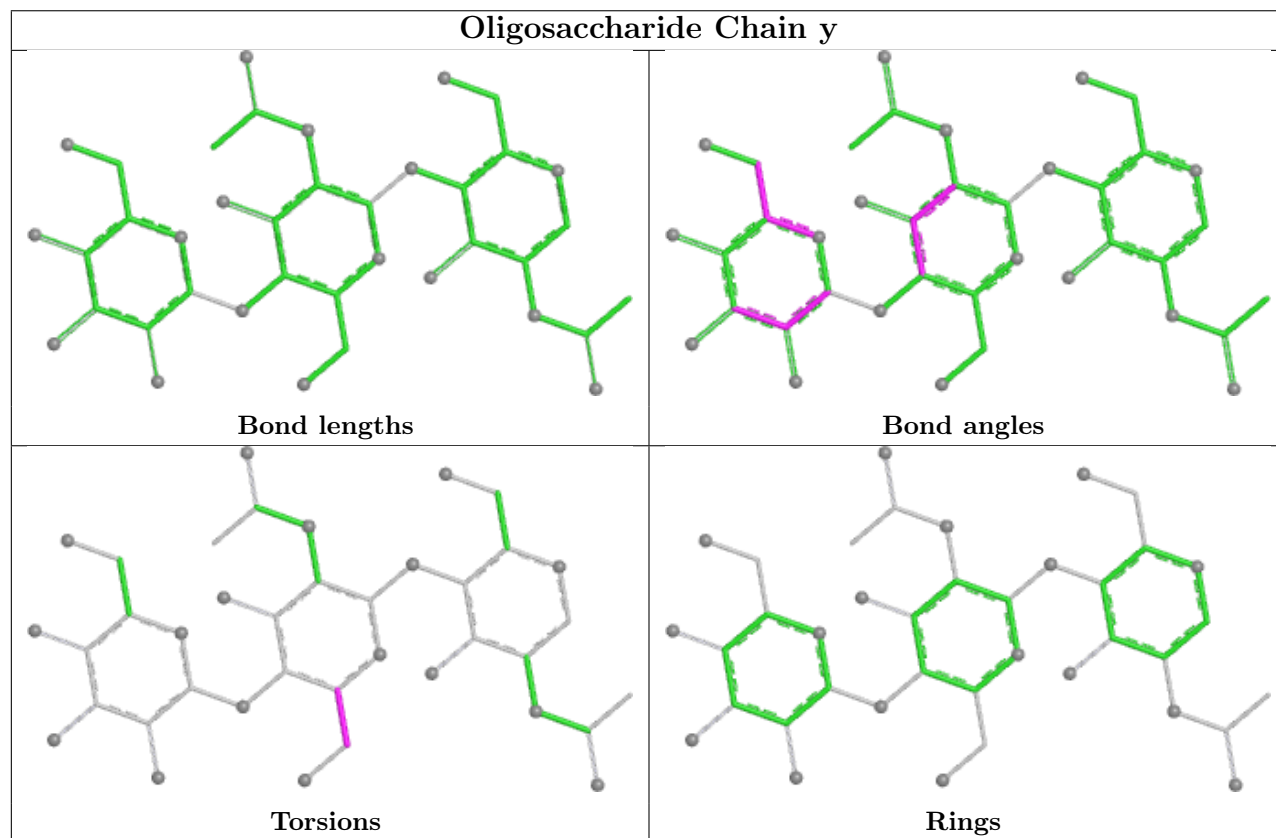
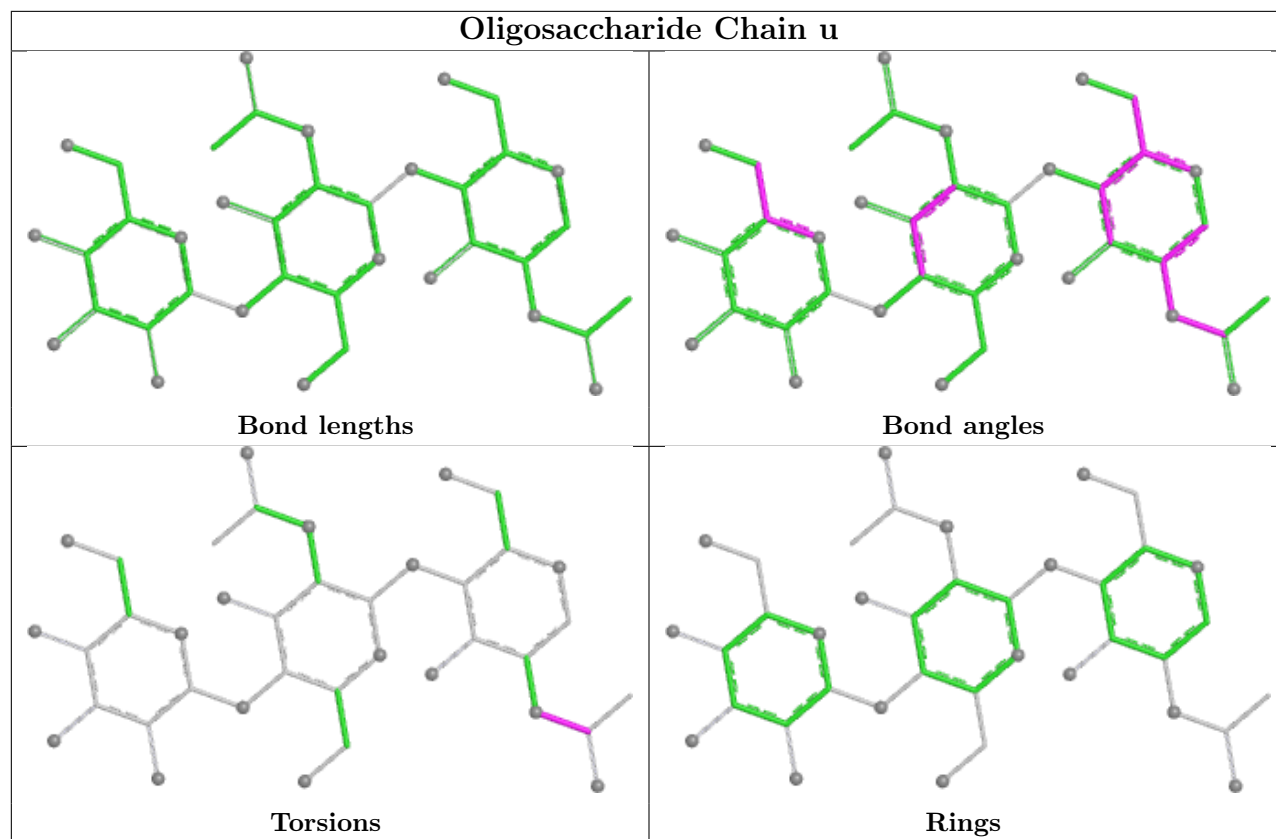
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	c	2	NAG	1	0
7	n	2	NAG	1	0
6	c	1	NAG	1	0
6	w	2	NAG	1	0
6	x	2	NAG	1	0
5	5	2	NAG	1	0
6	d	1	NAG	1	0
5	6	1	NAG	1	0
7	b	1	NAG	1	0
5	j	1	NAG	2	0
5	t	1	NAG	1	0
7	n	1	NAG	2	0
5	5	1	NAG	1	0
7	b	2	NAG	1	0
5	y	1	NAG	2	0
7	h	1	NAG	1	0
5	0	2	NAG	1	0
6	w	1	NAG	1	0
6	s	2	NAG	1	0
6	4	1	NAG	2	0
6	s	1	NAG	3	0
6	x	1	NAG	1	0

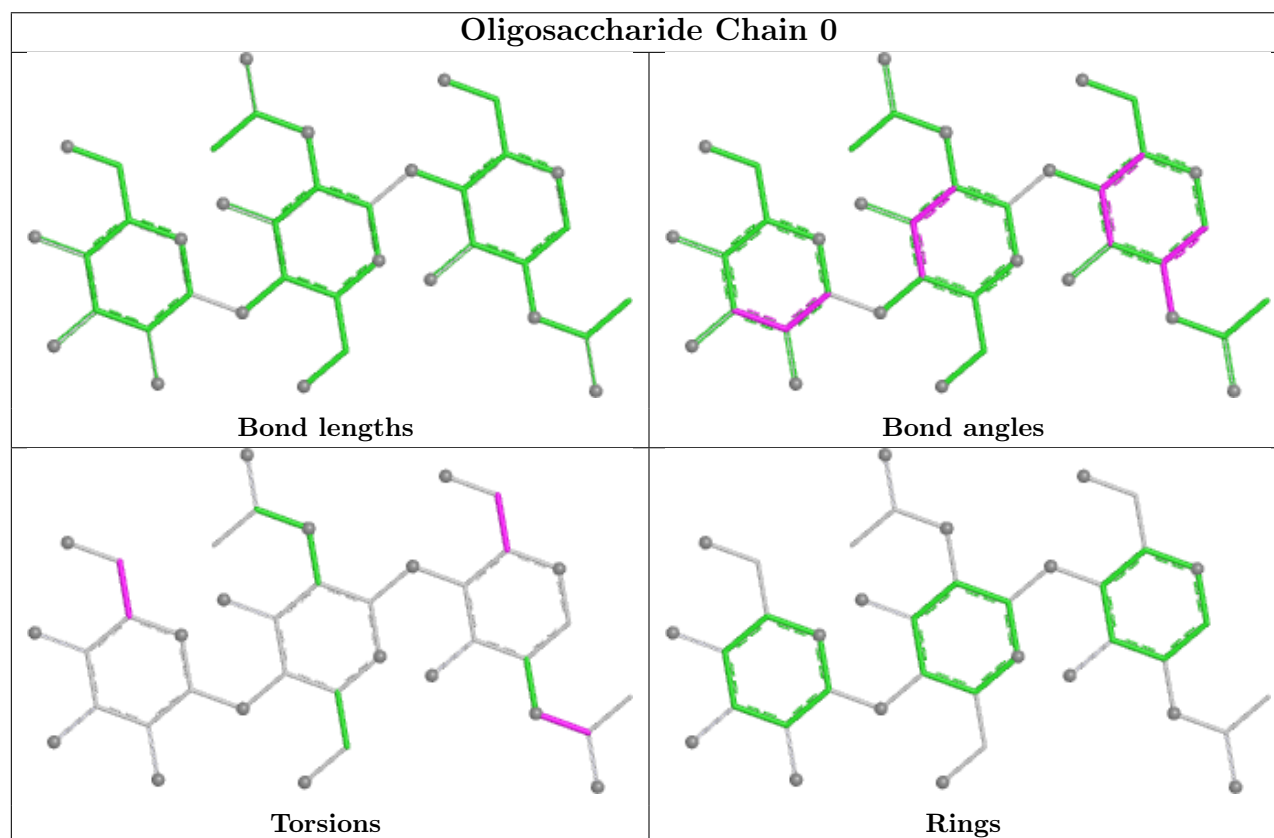
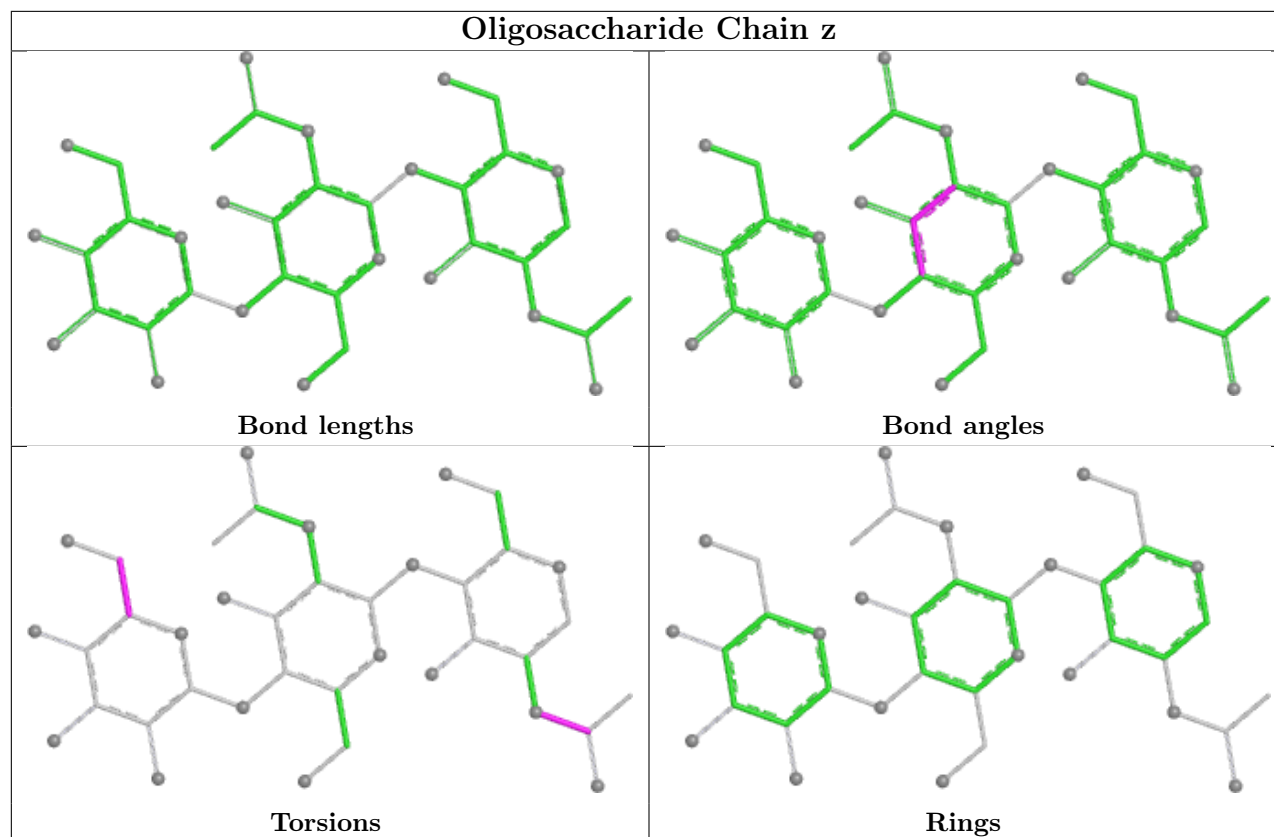
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

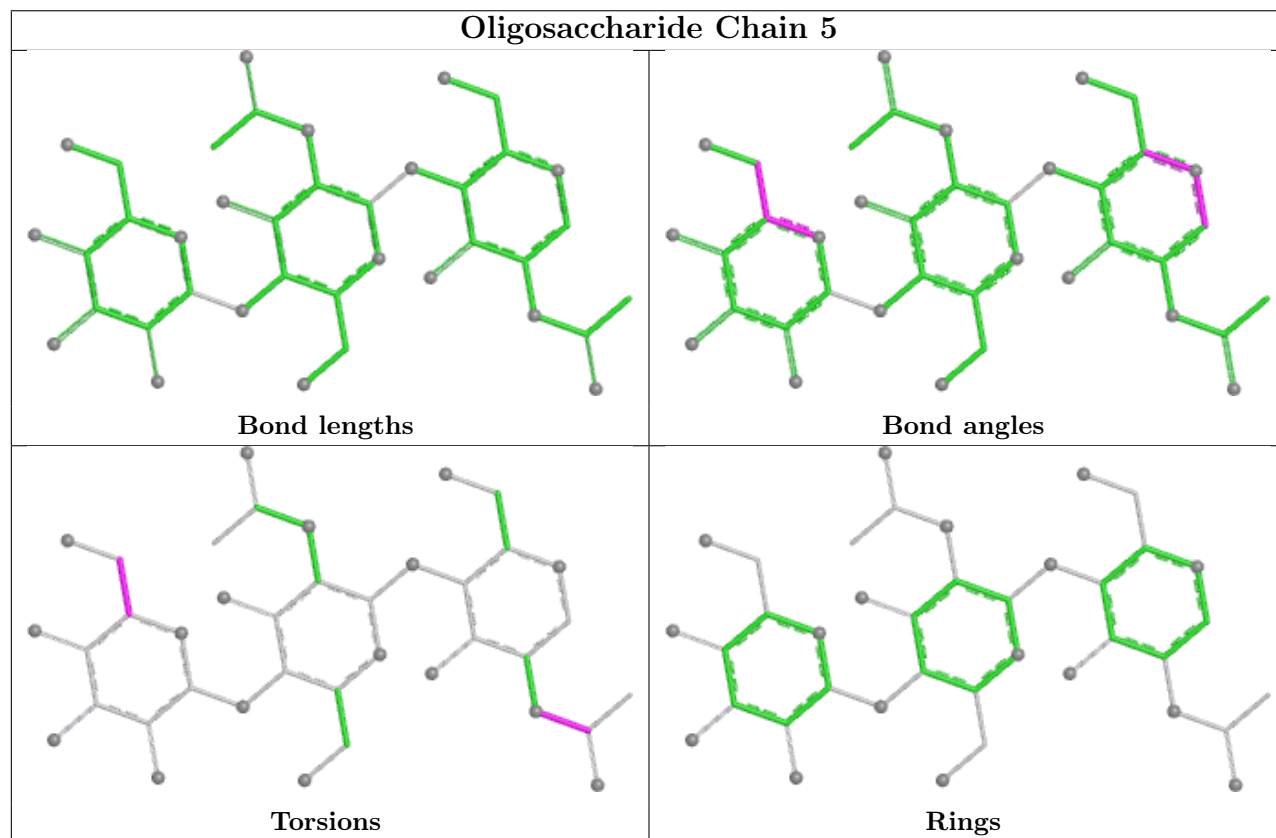
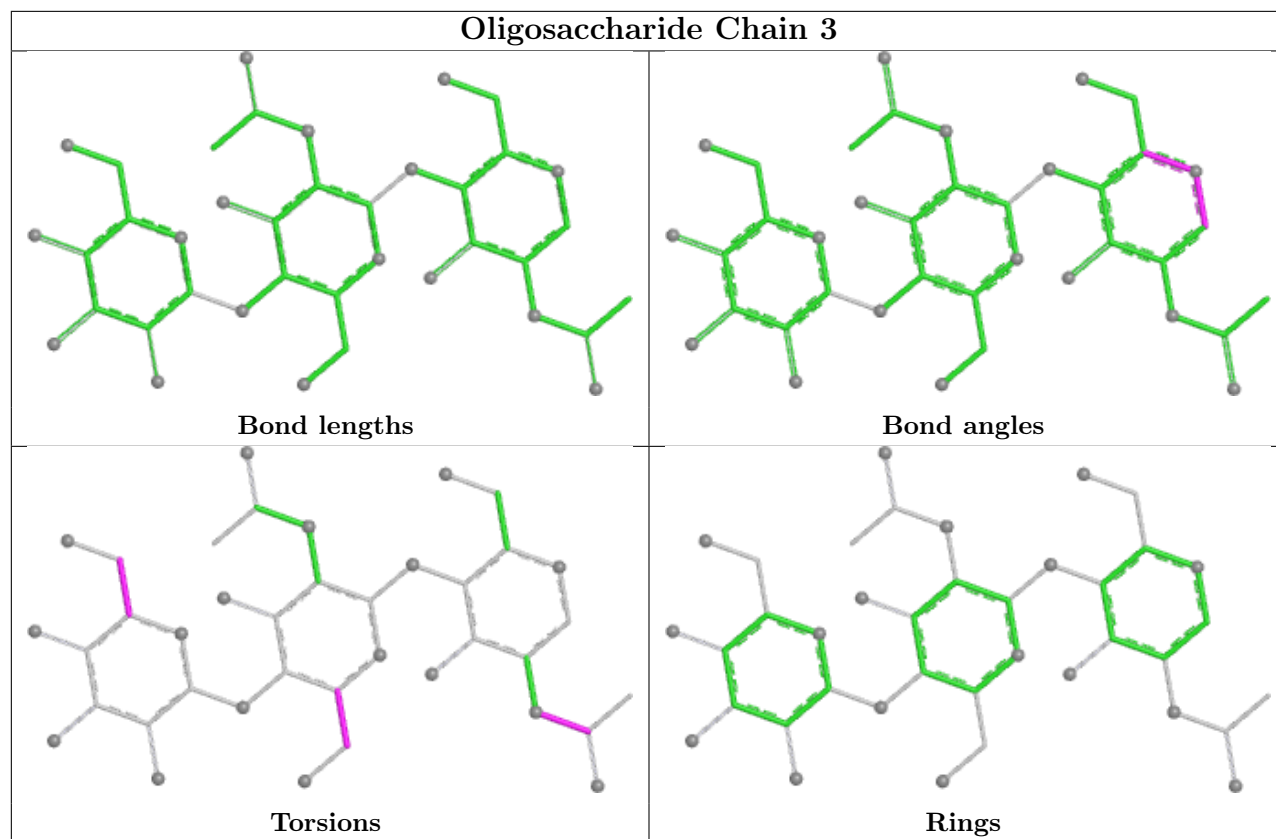


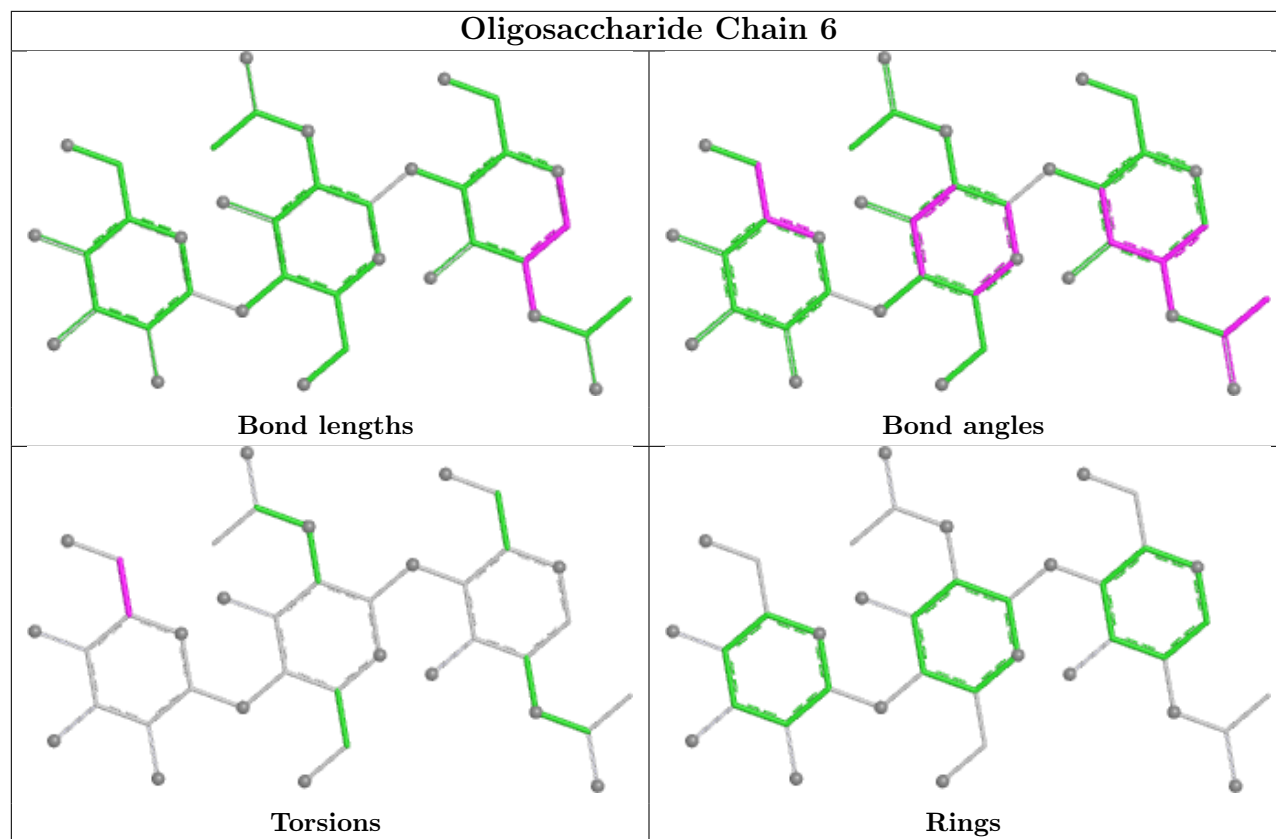


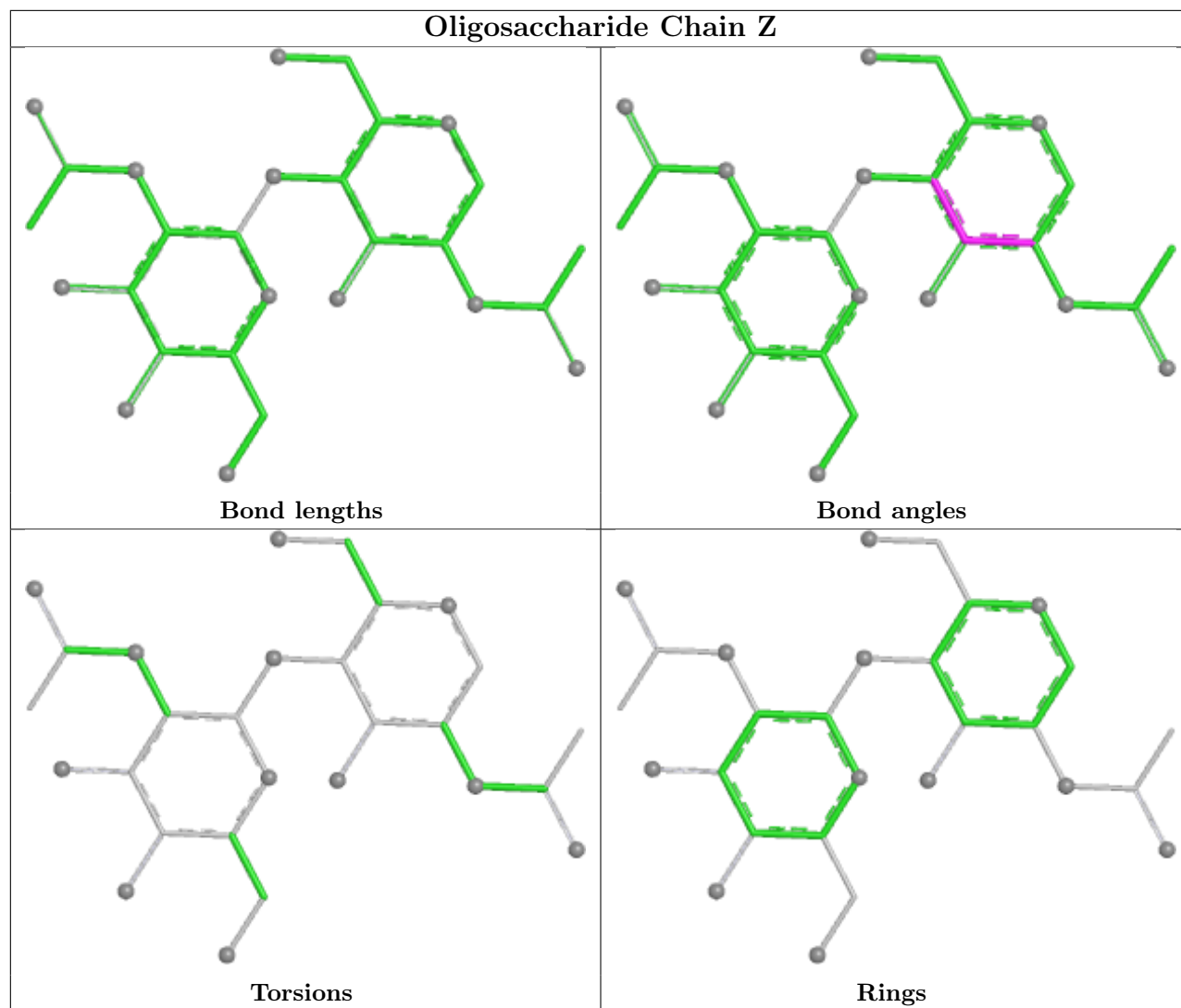


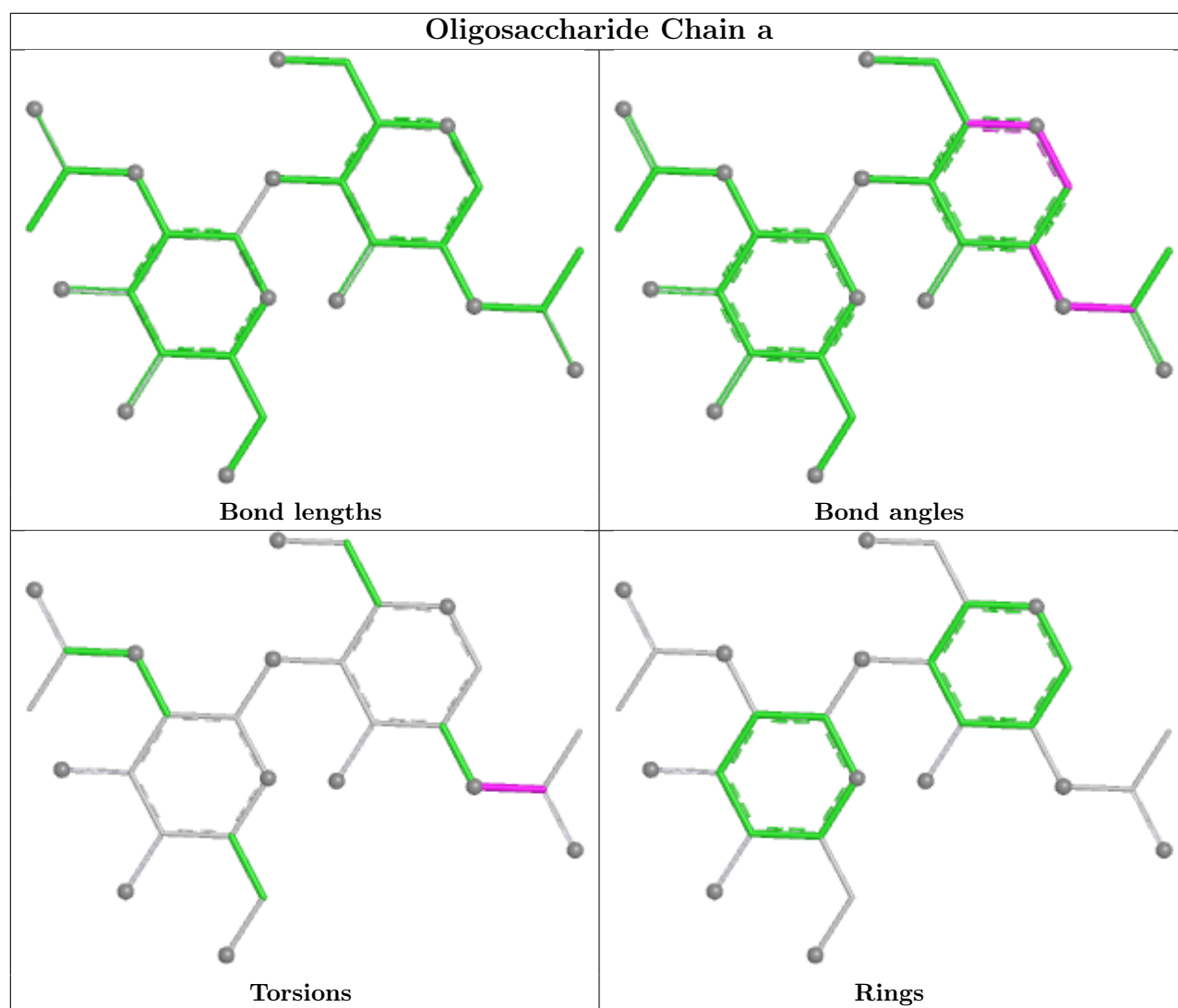


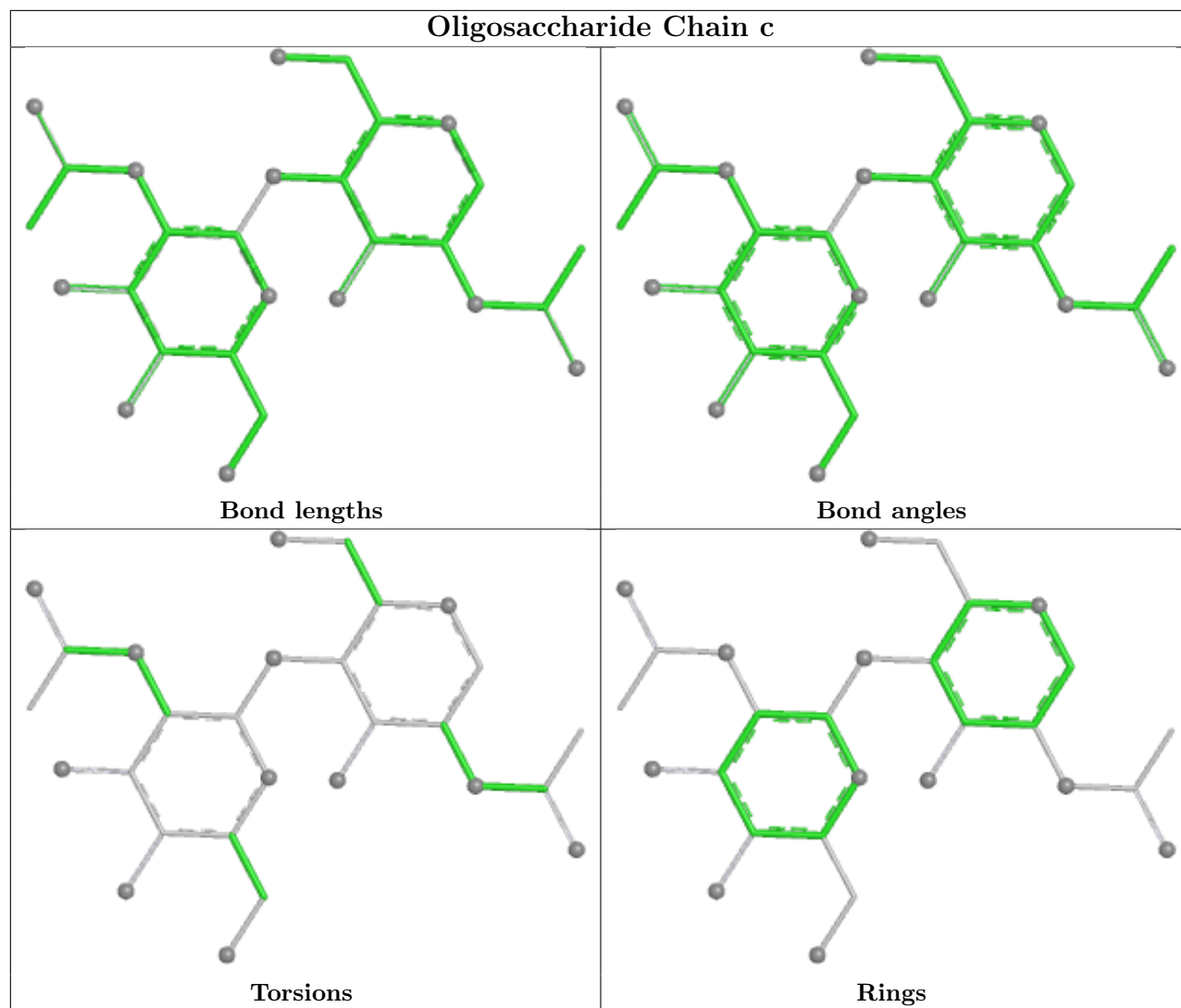


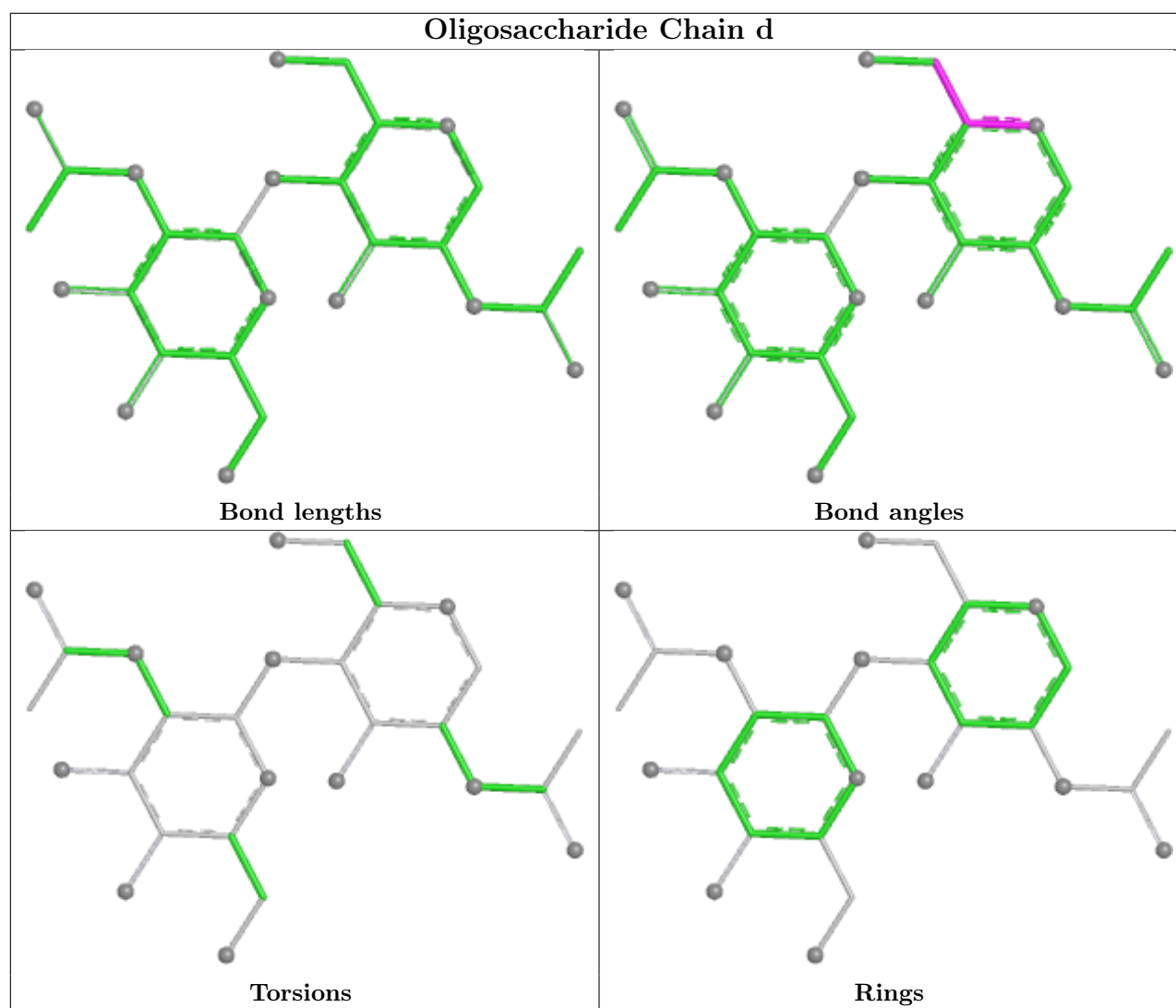


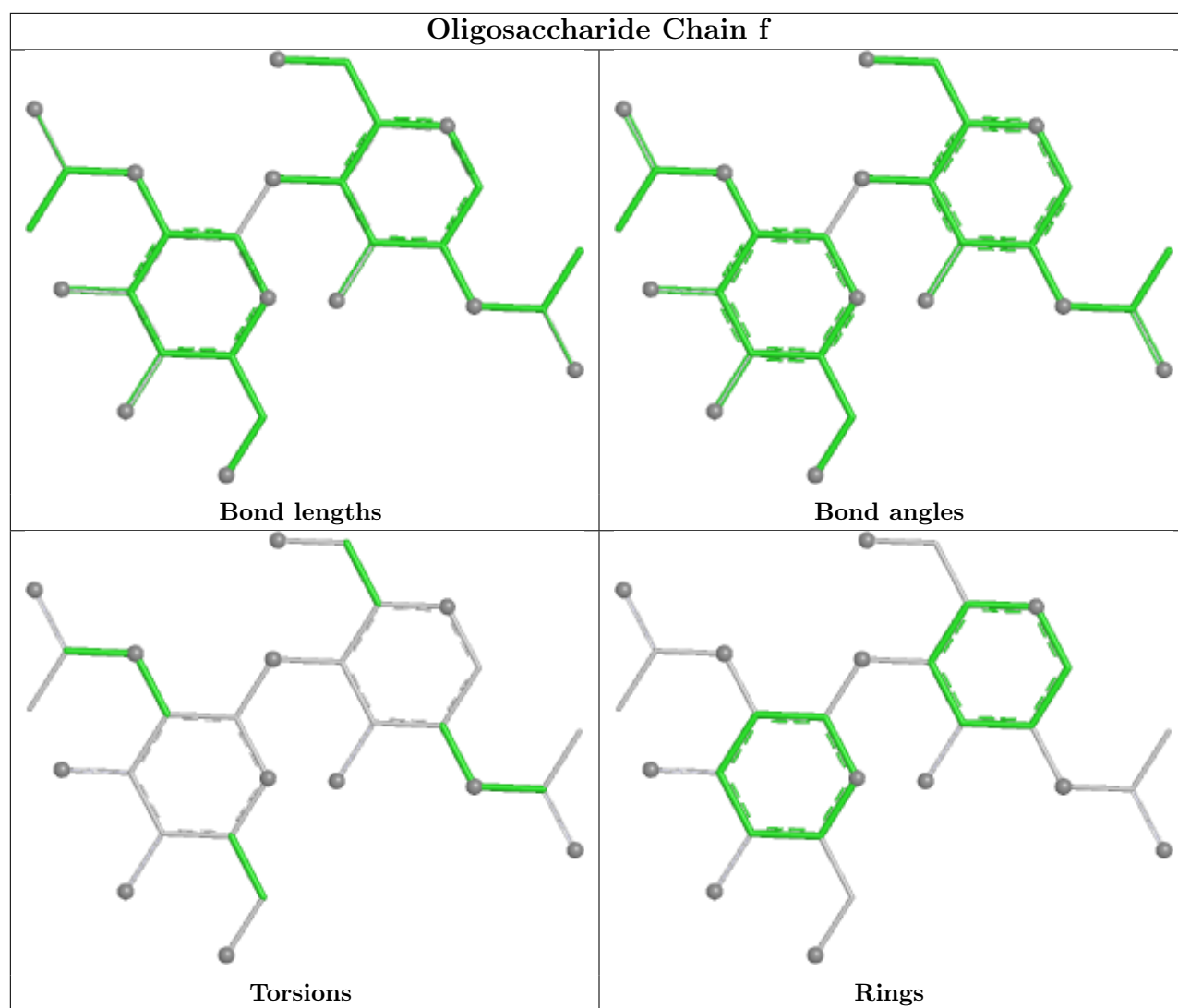


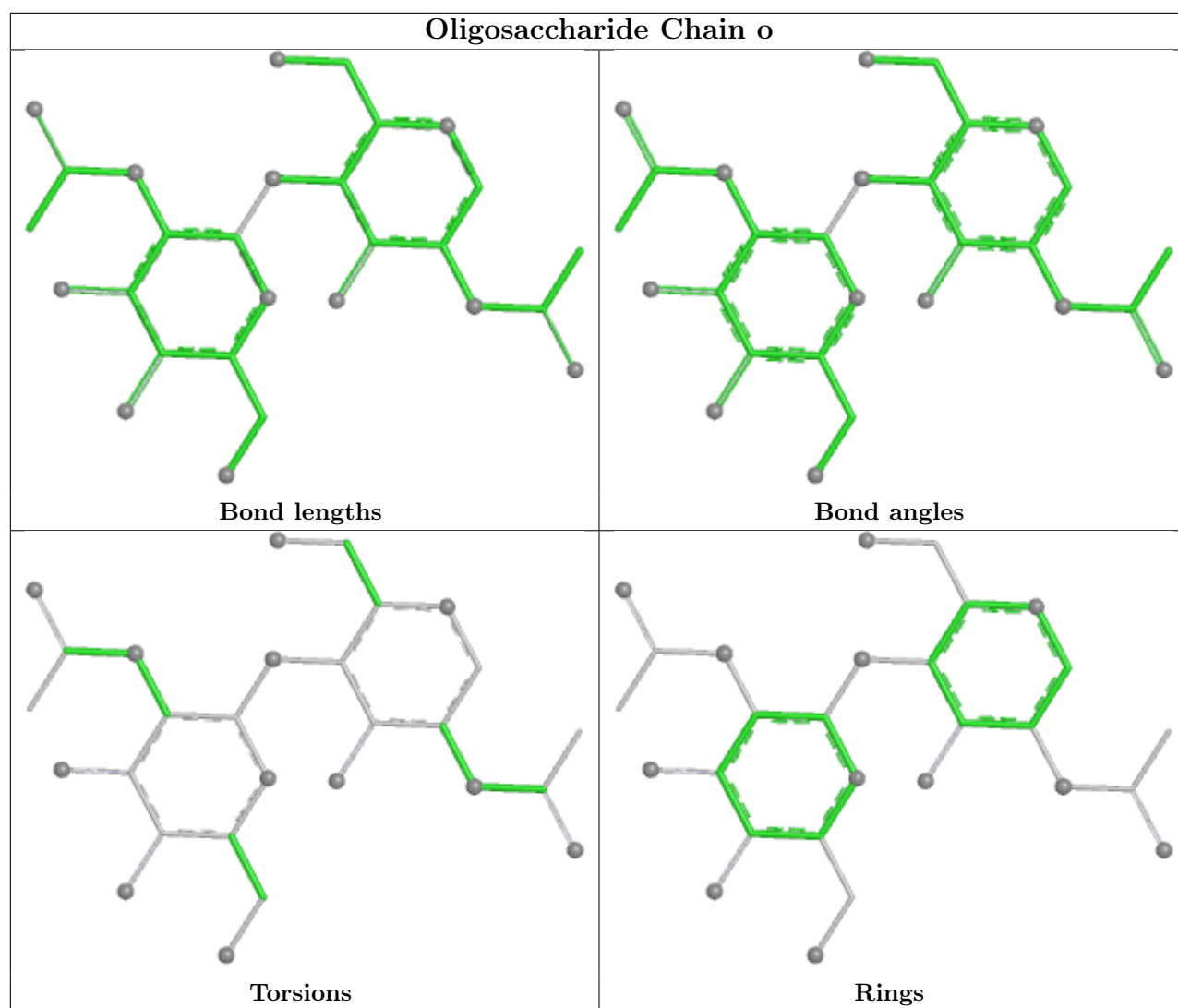


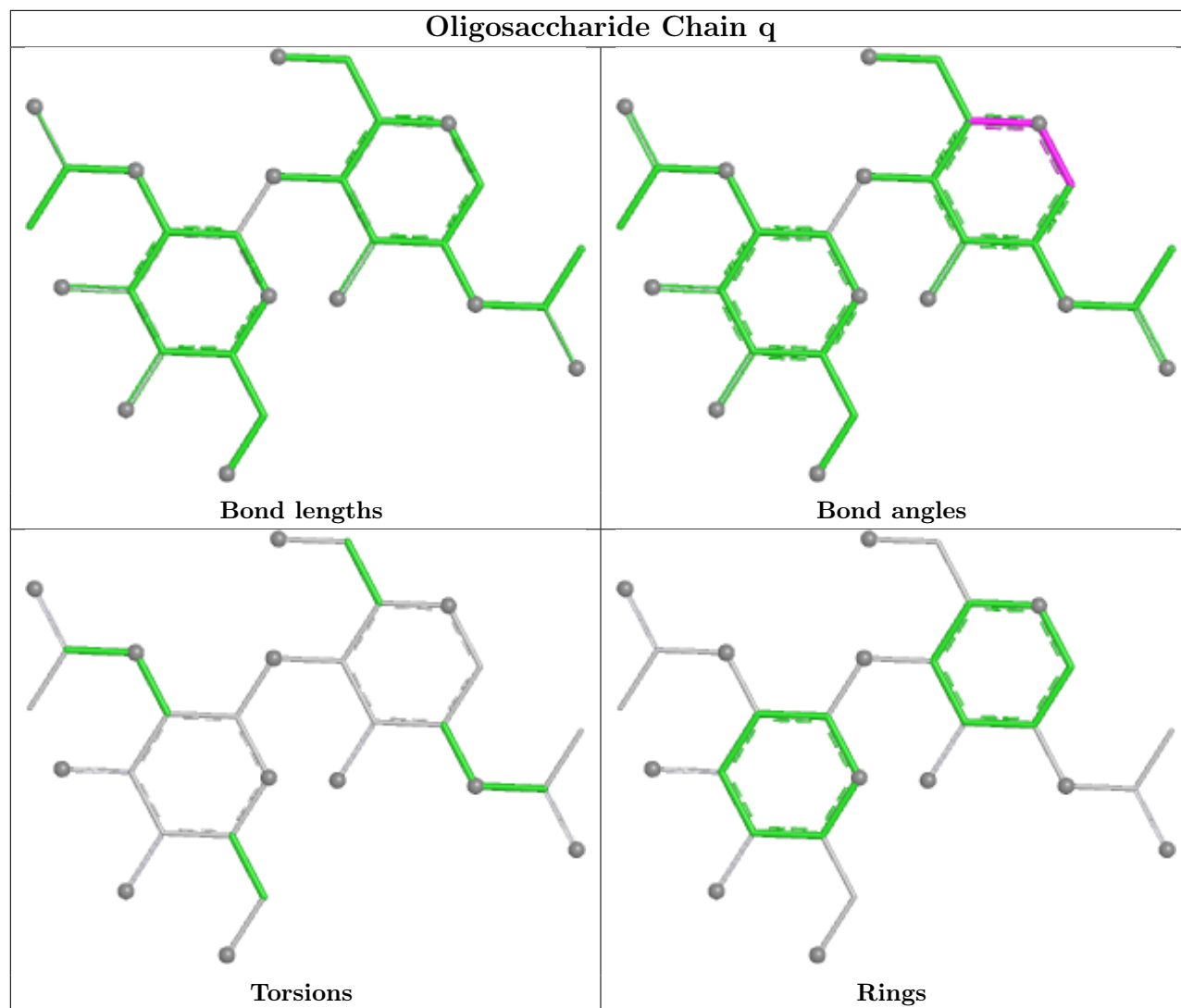


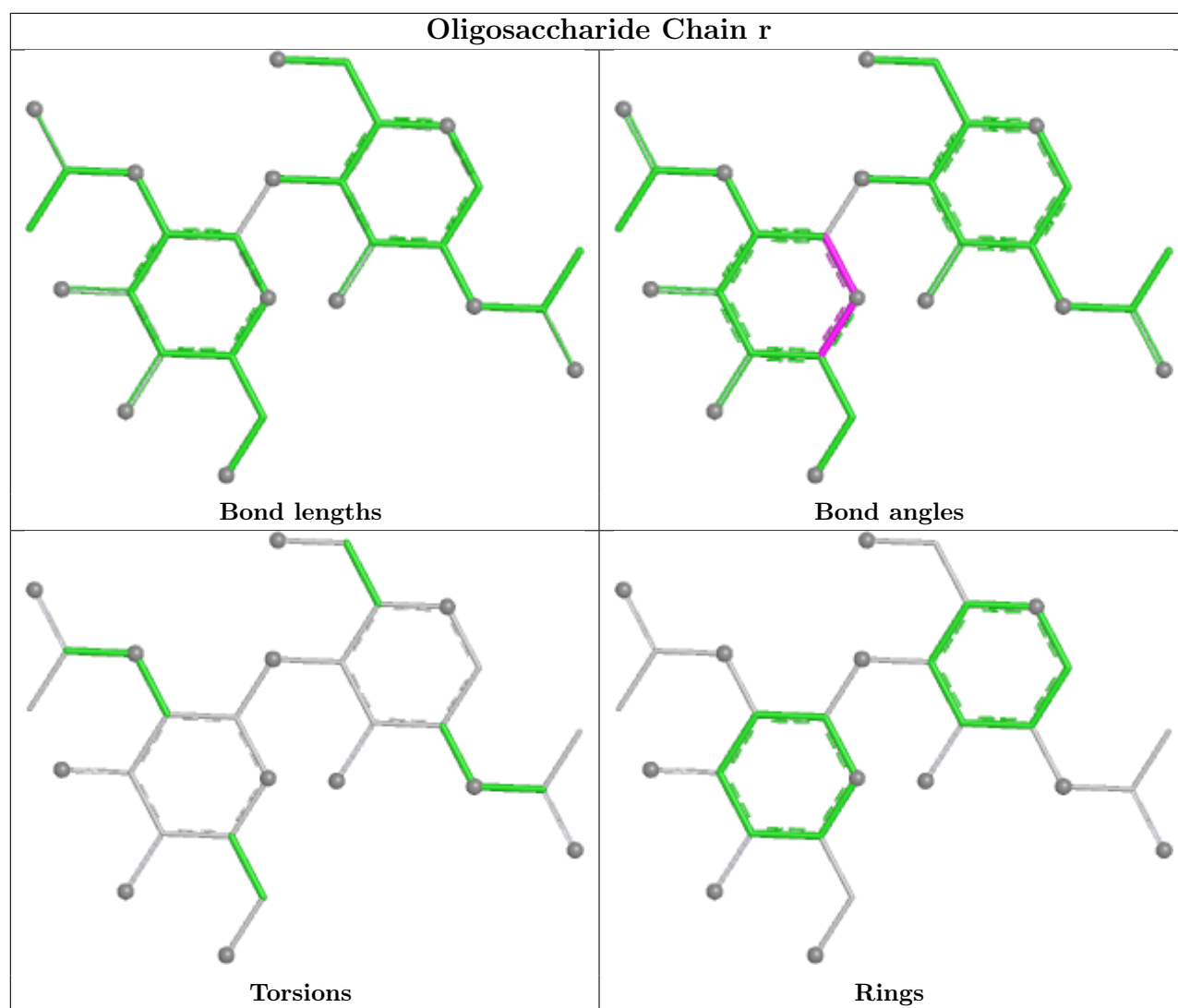


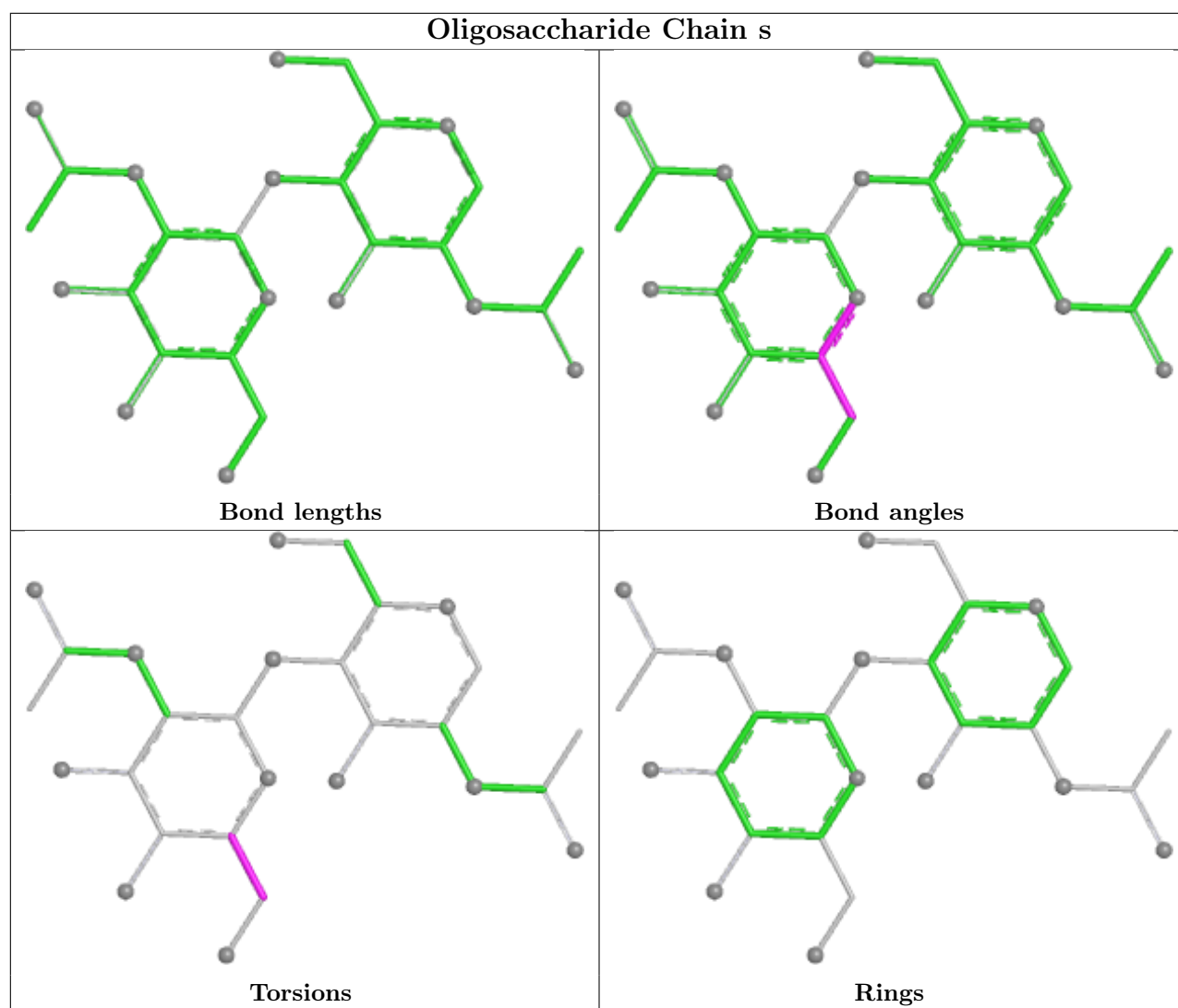


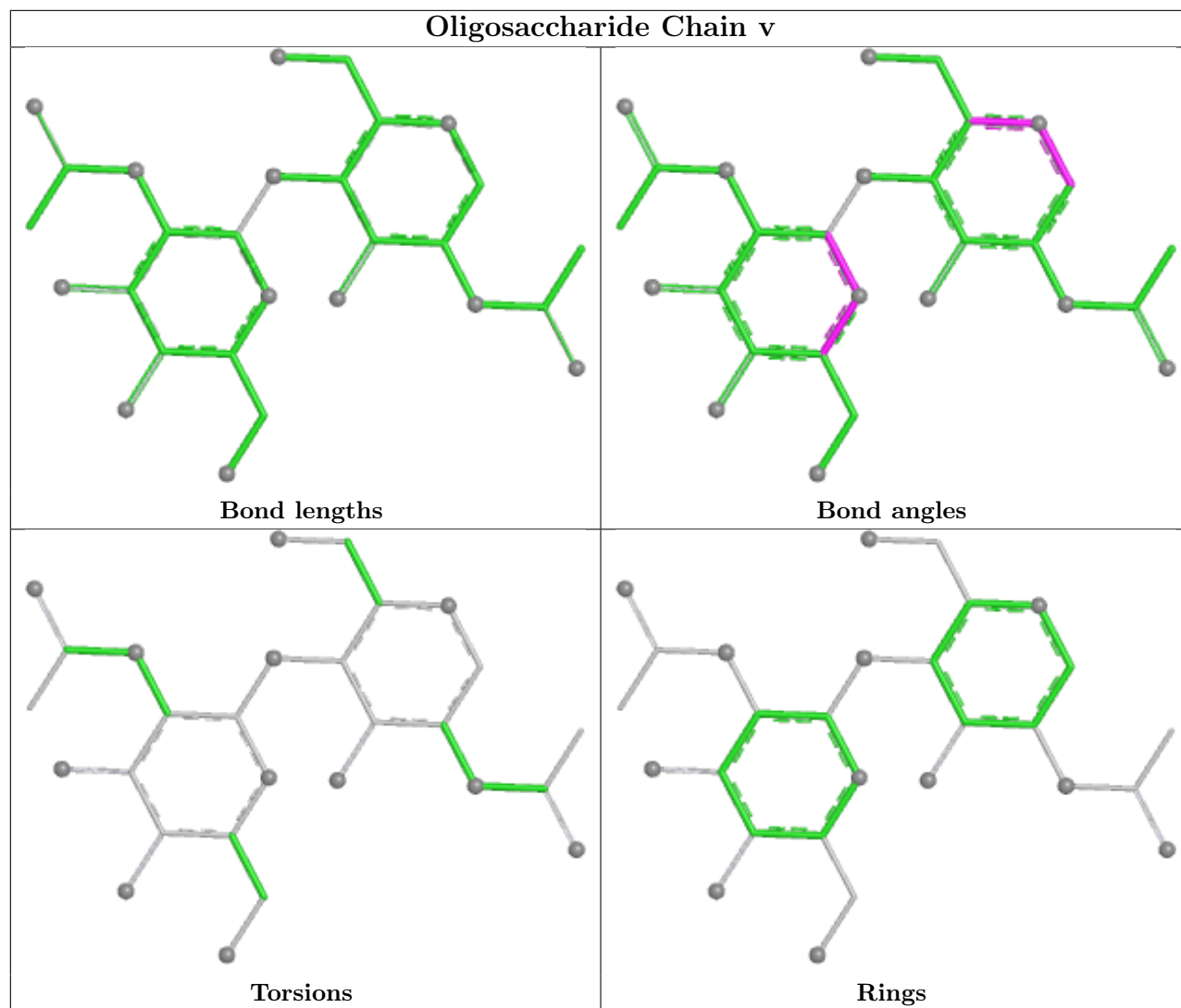


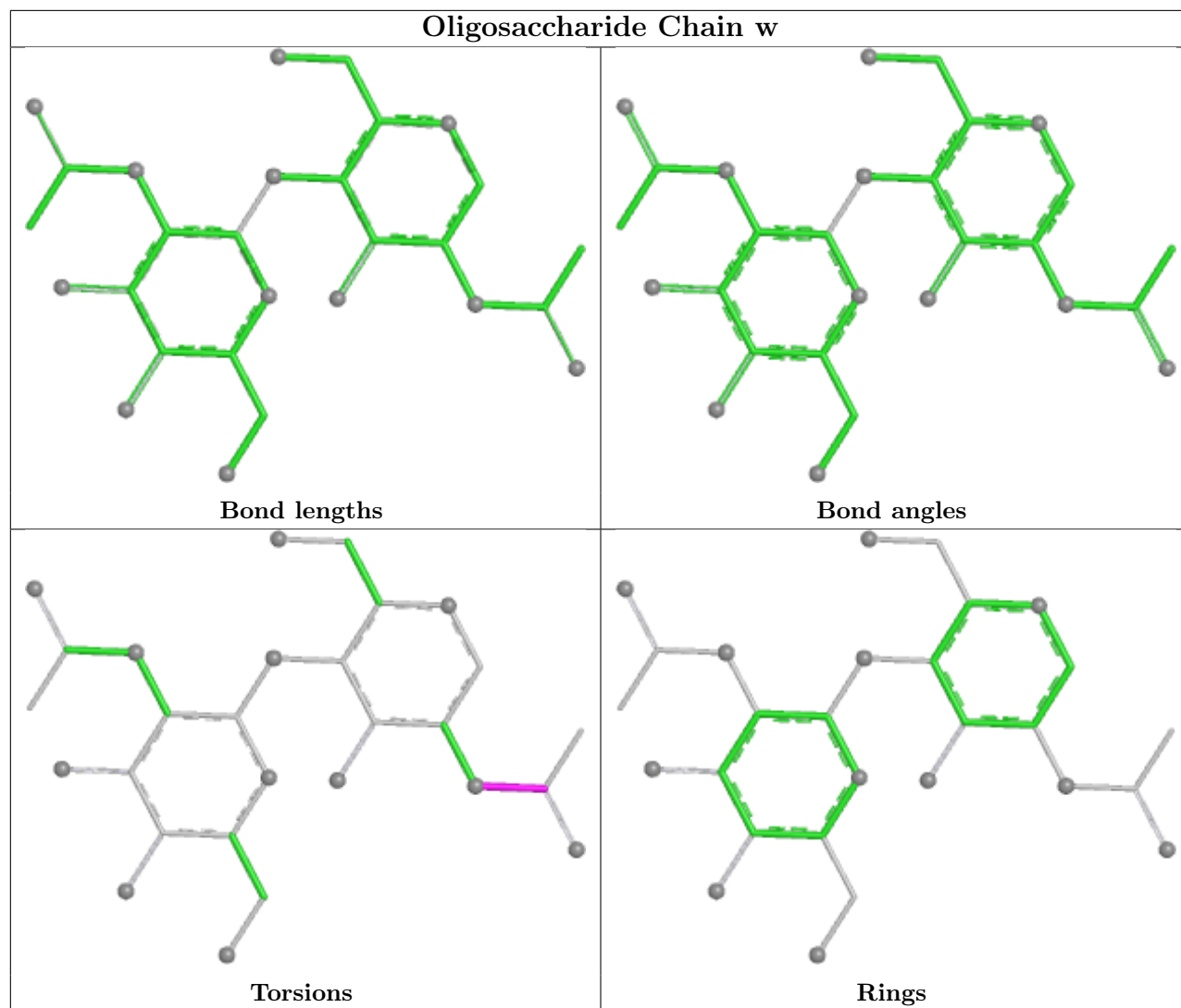


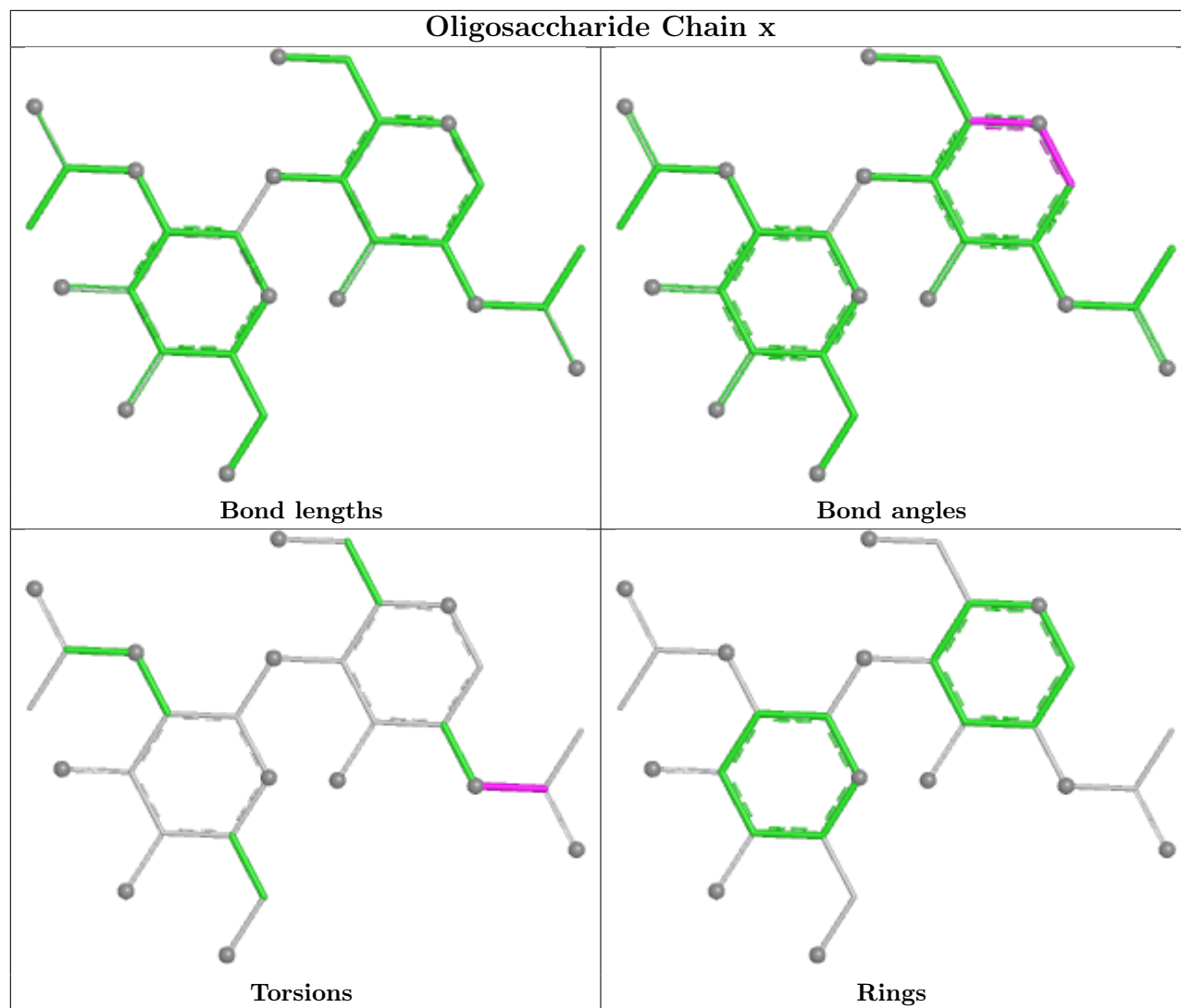


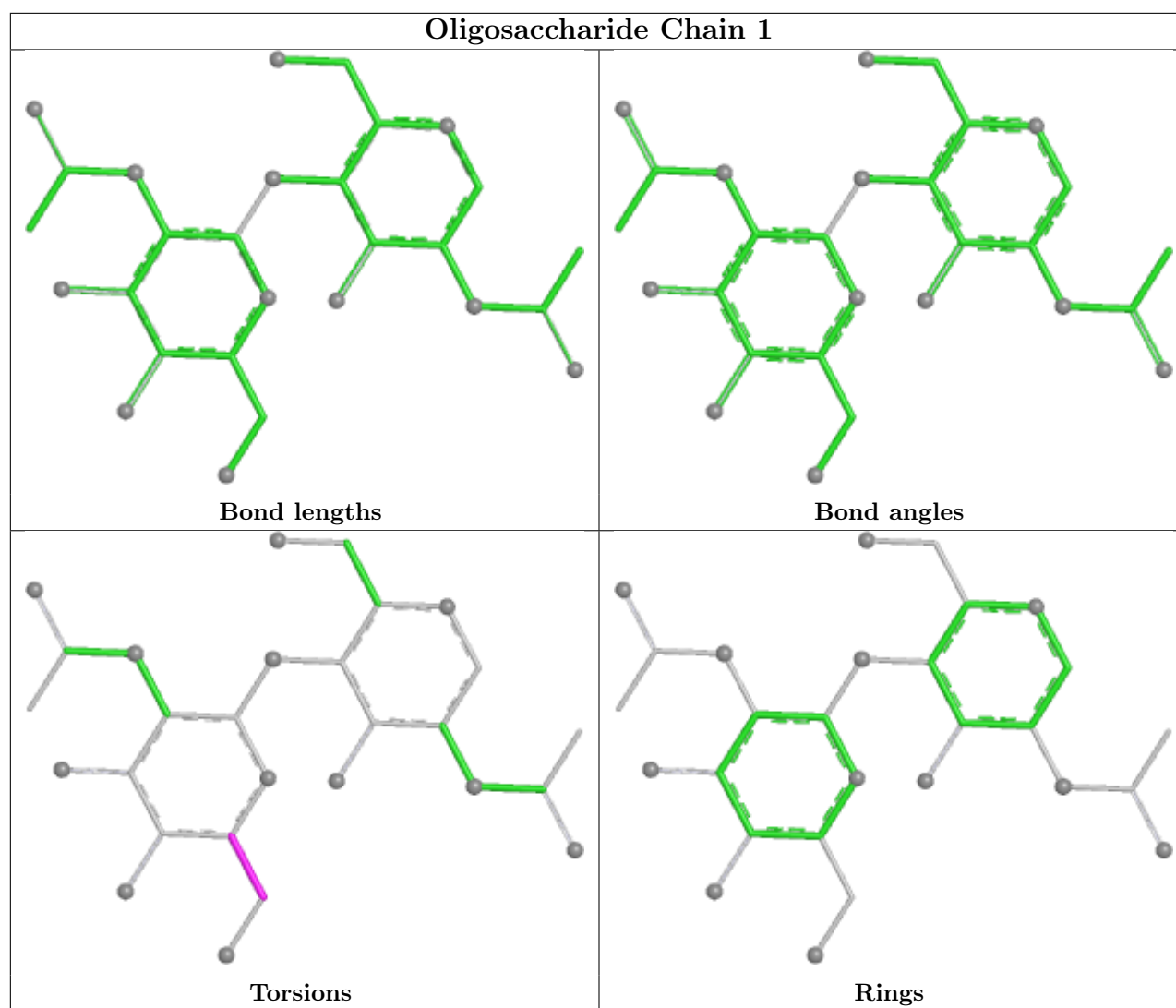


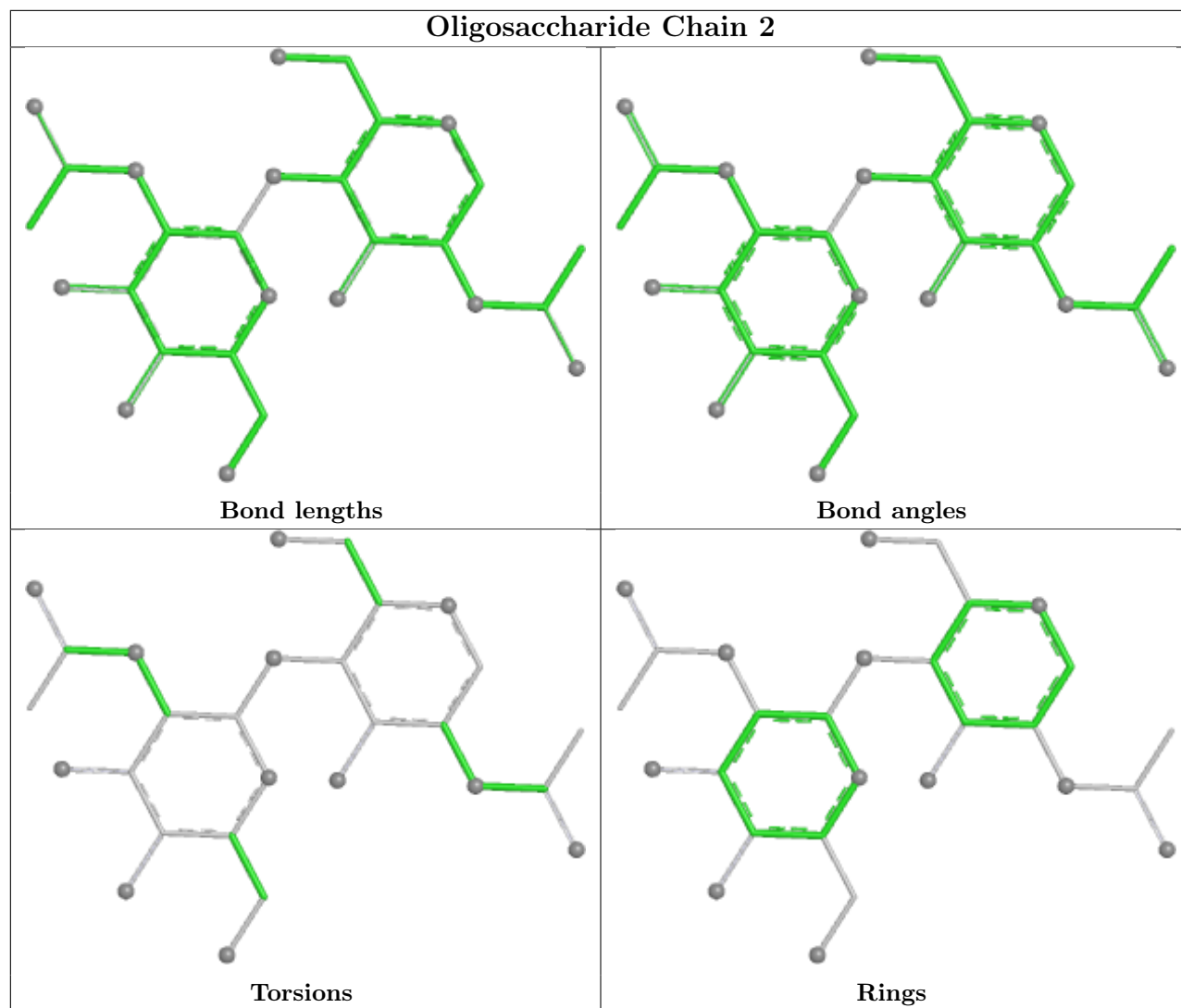


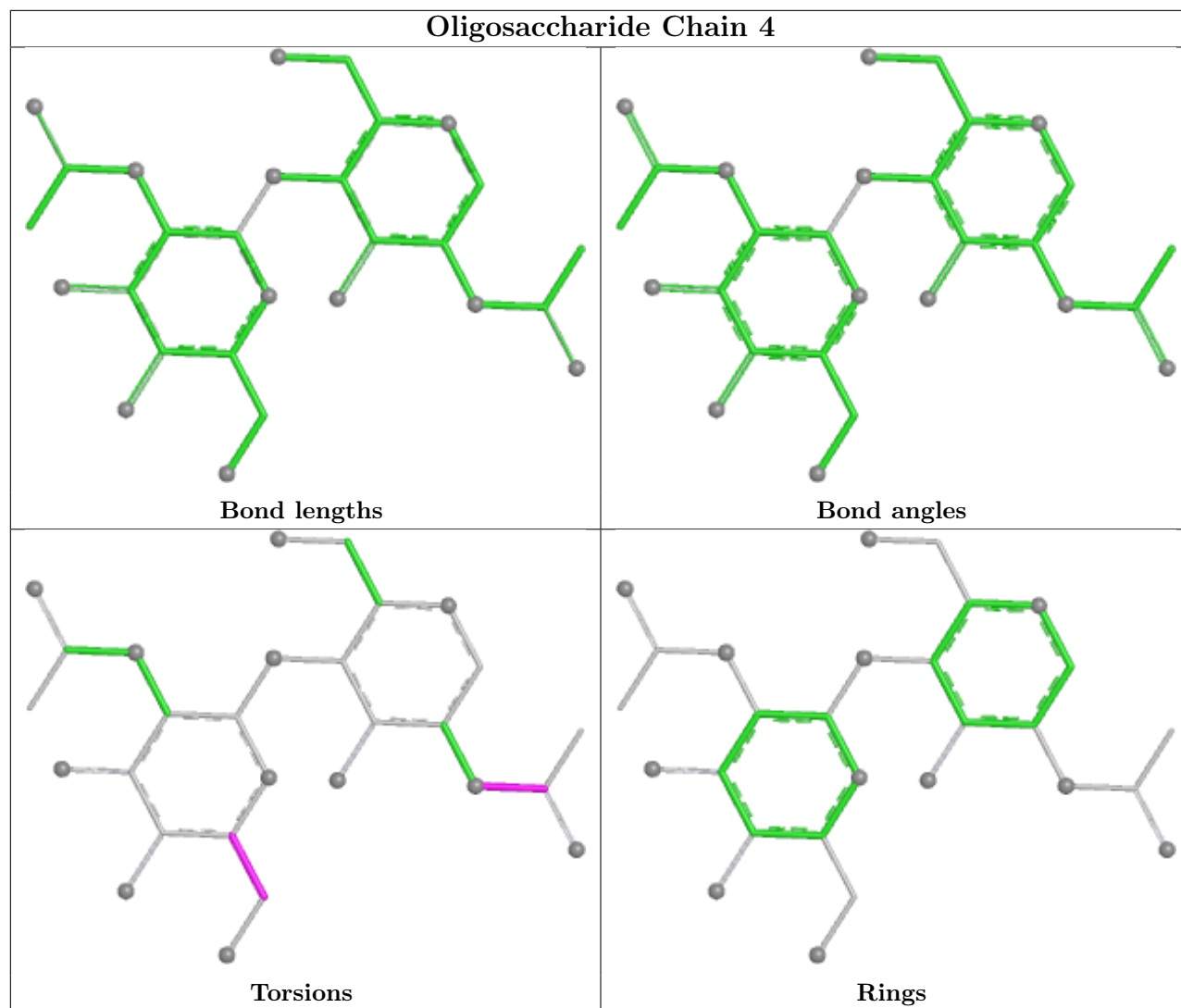


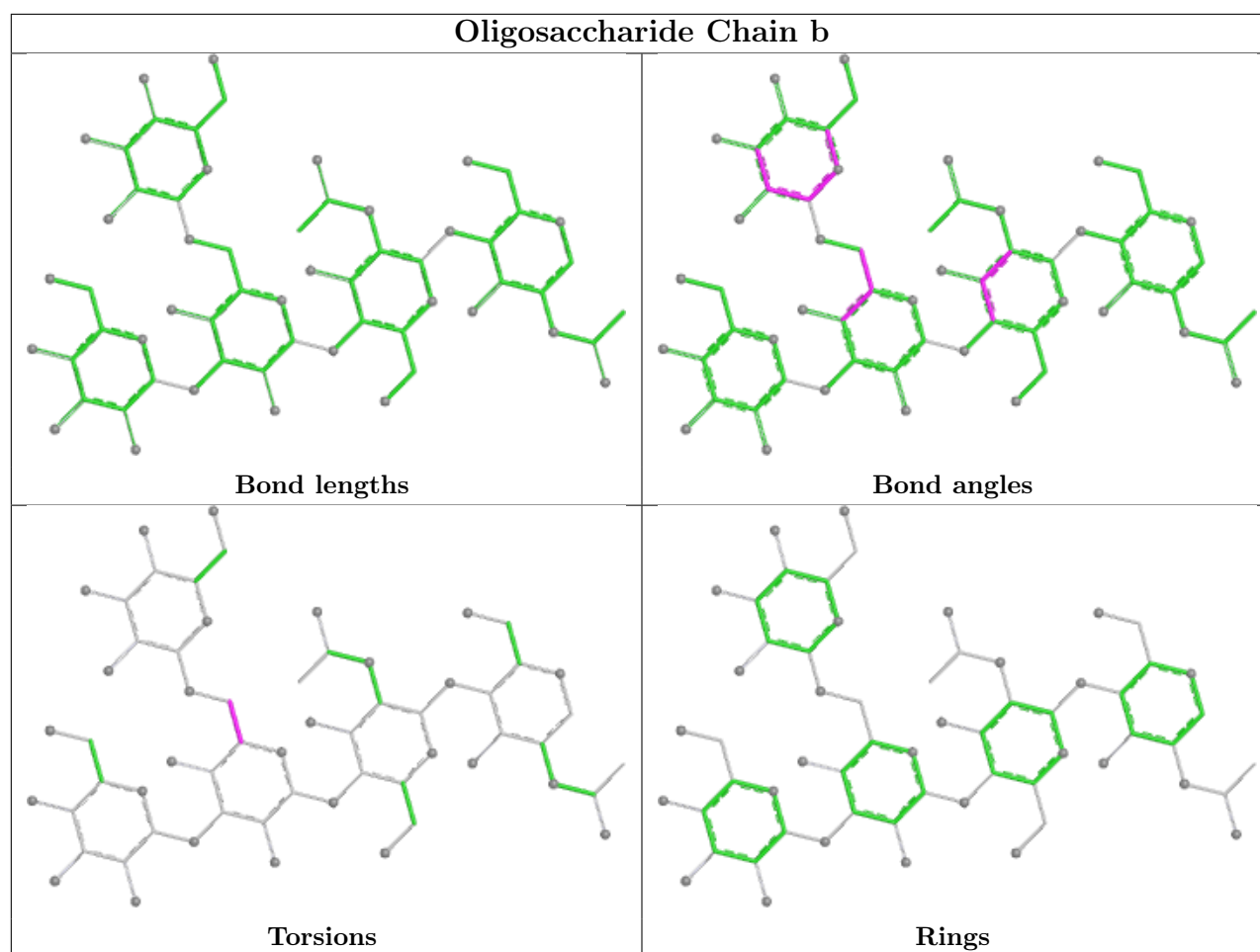


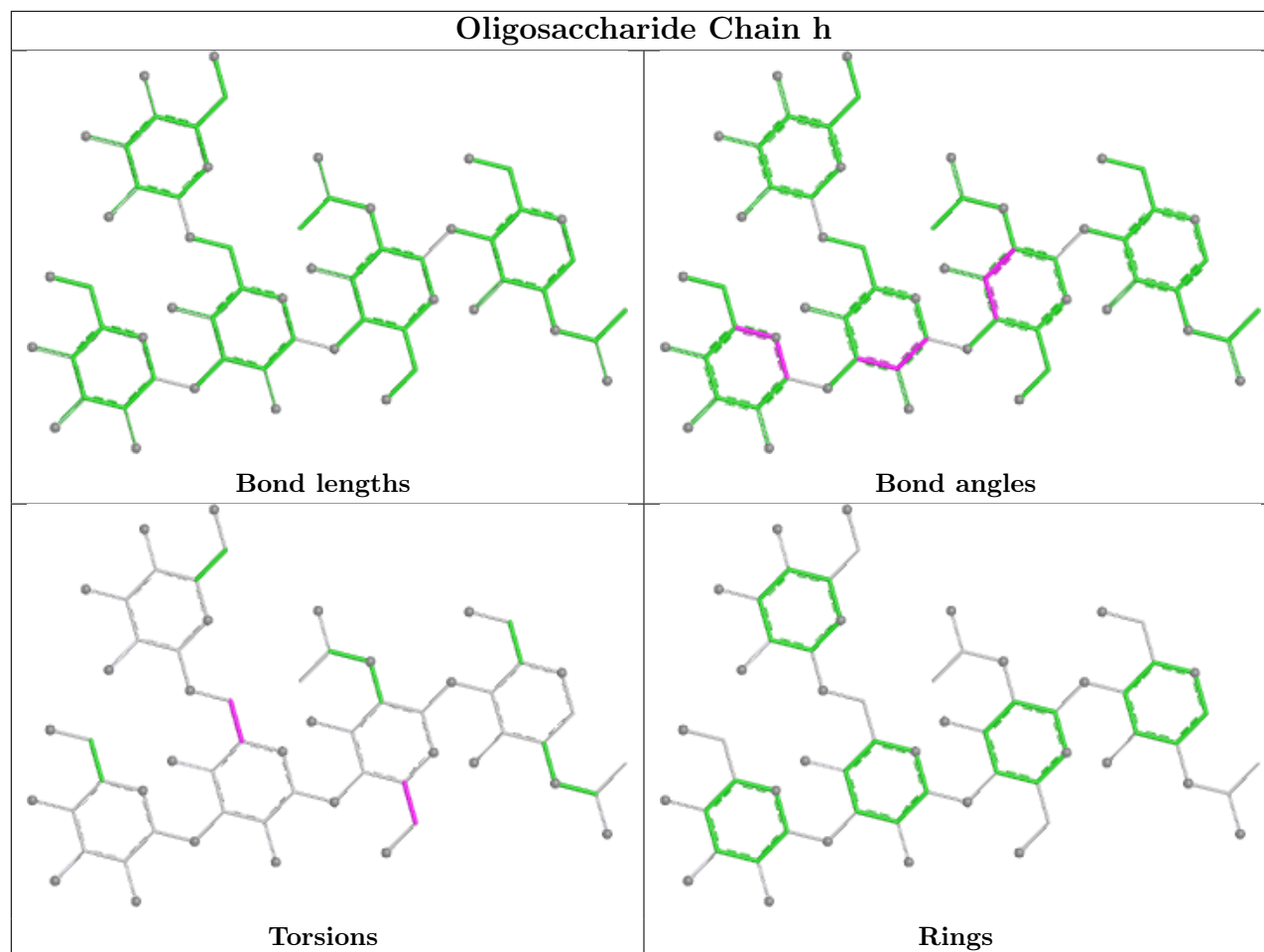


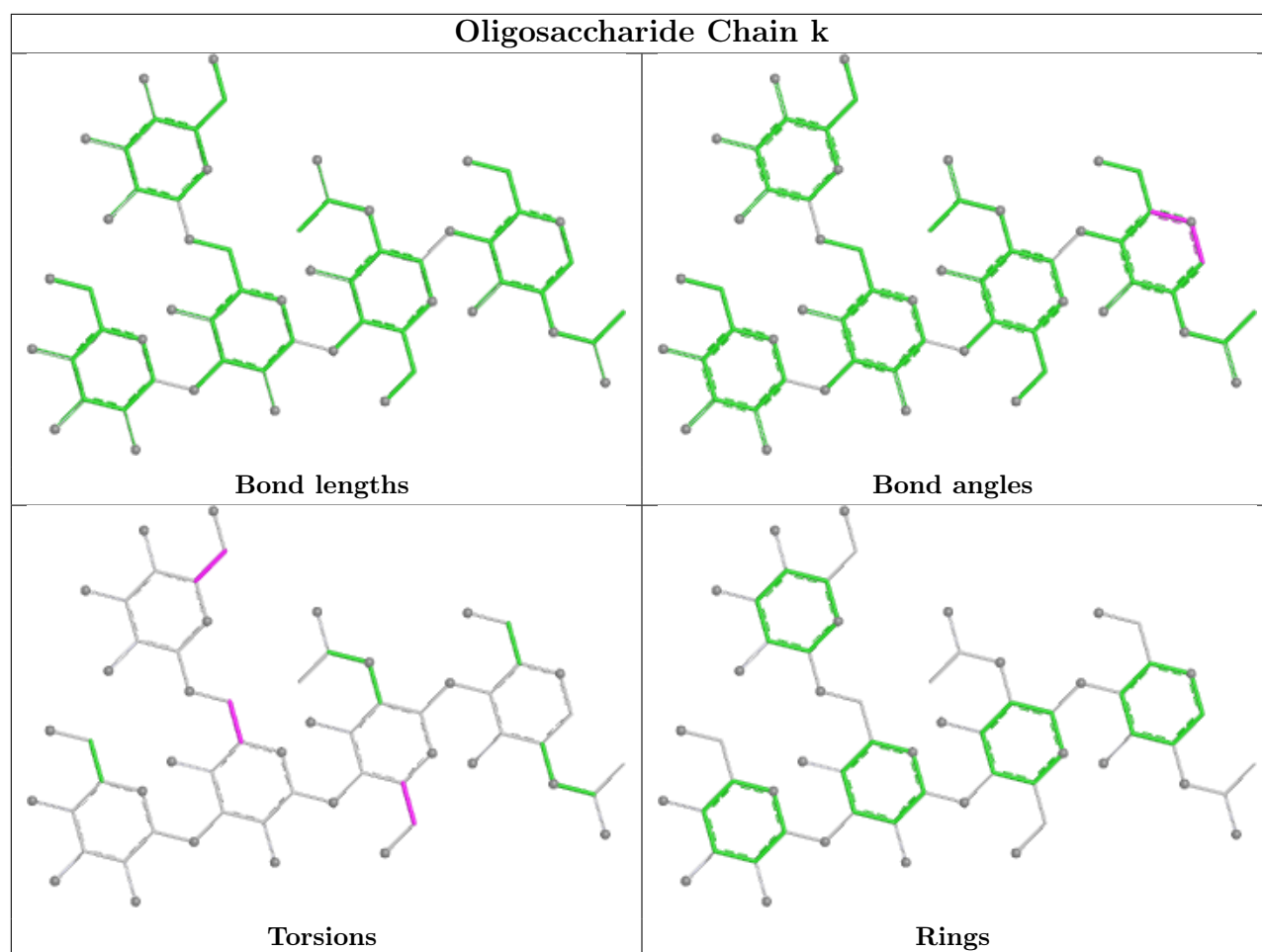


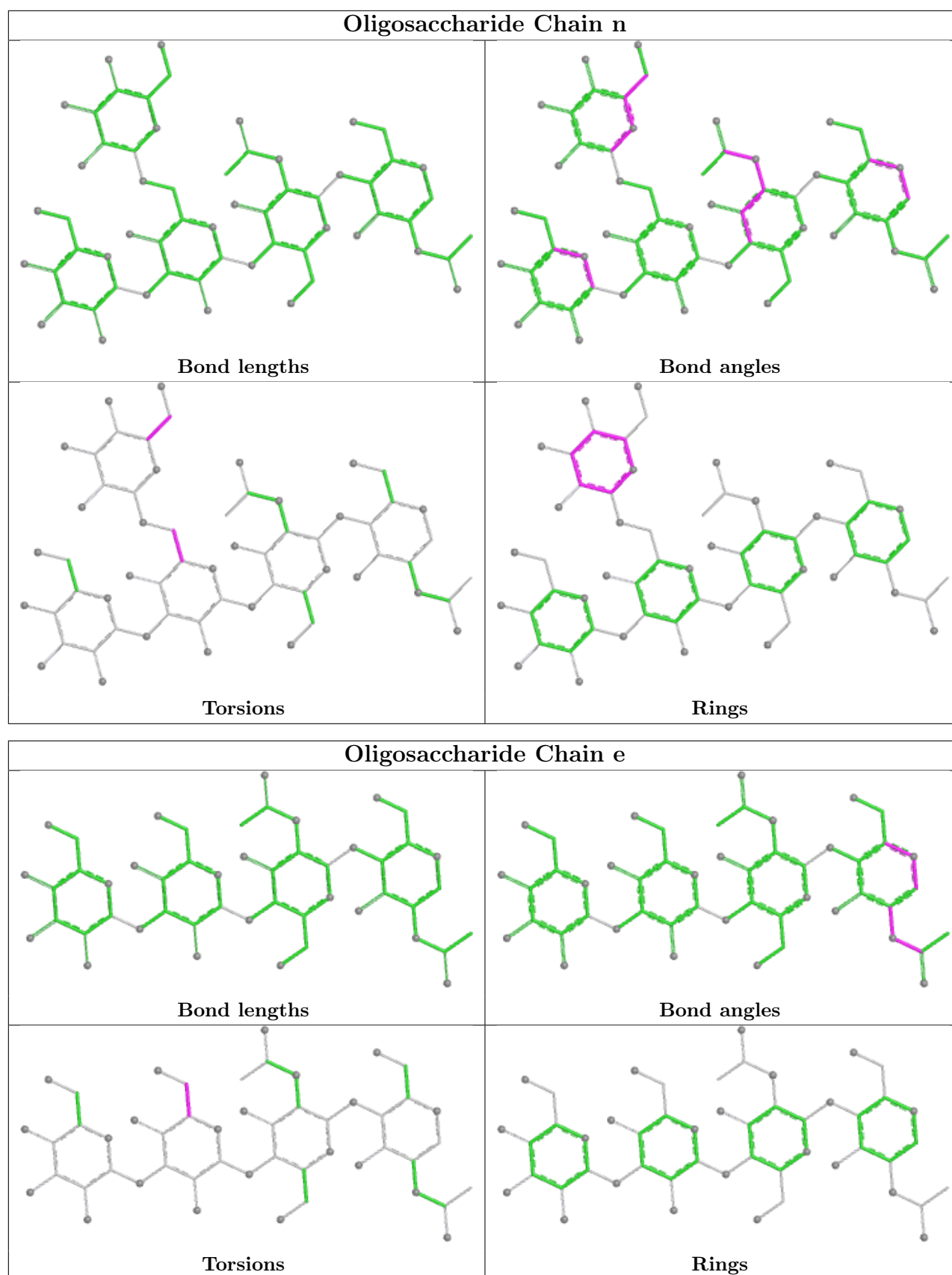


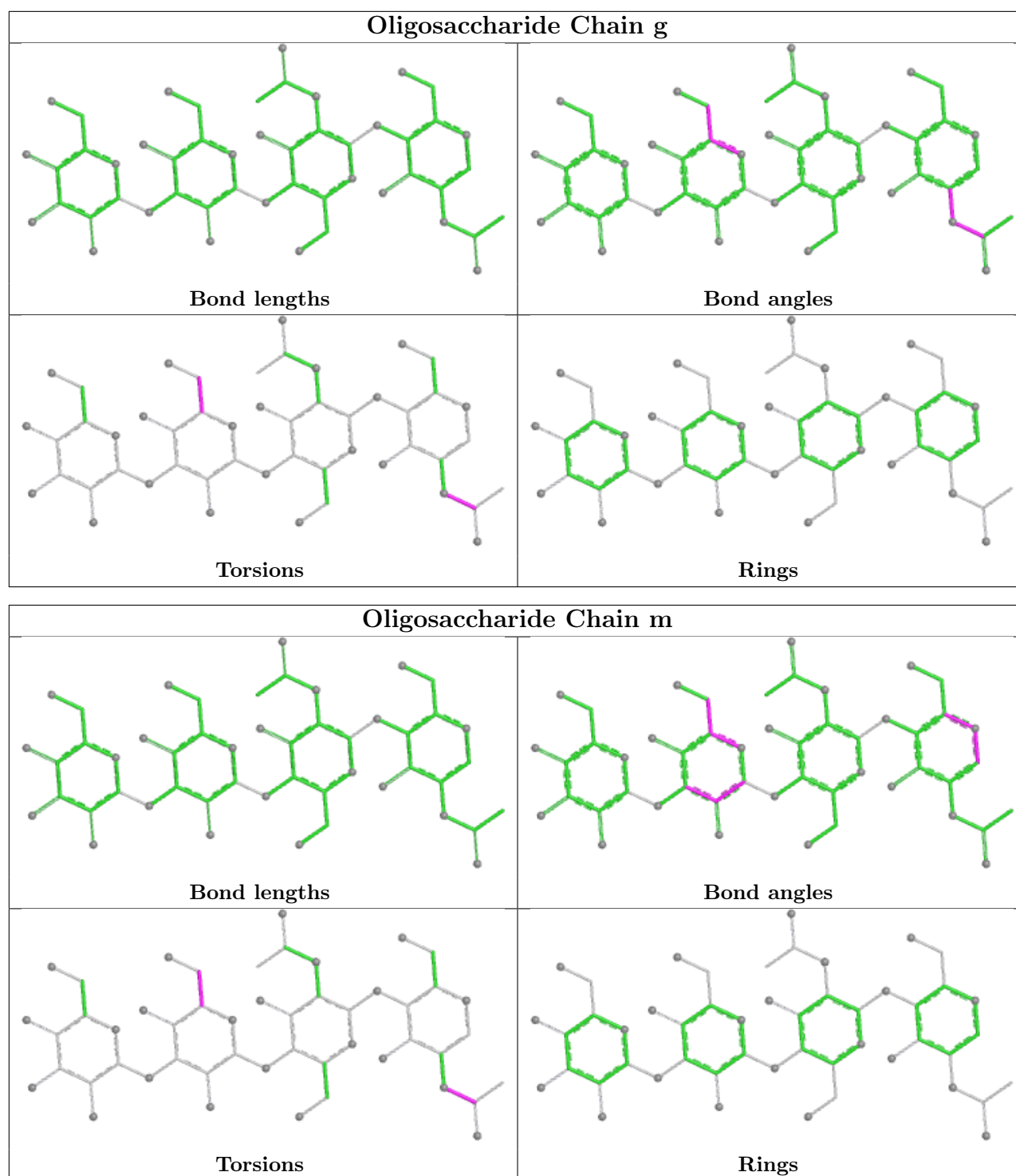












5.6 Ligand geometry [i](#)

12 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
9	NAG	J	201	2	14,14,15	0.51	0	17,19,21	0.71	0
9	NAG	G	411	1	14,14,15	0.50	0	17,19,21	0.74	0
9	NAG	B	201	2	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
9	NAG	H	201	2	14,14,15	0.46	0	17,19,21	0.75	0
9	NAG	F	201	2	14,14,15	0.58	0	17,19,21	0.88	0
9	NAG	C	419	1	14,14,15	0.48	0	17,19,21	0.78	0
9	NAG	I	413	1	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
9	NAG	G	403	1	14,14,15	0.47	0	17,19,21	0.64	0
9	NAG	D	201	2	14,14,15	0.52	0	17,19,21	0.72	0
9	NAG	L	201	2	14,14,15	0.50	0	17,19,21	0.79	0
9	NAG	K	413	1	14,14,15	0.52	0	17,19,21	0.69	0
9	NAG	E	420	1	14,14,15	0.53	0	17,19,21	0.98	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	J	201	2	-	3/6/23/26	0/1/1/1
9	NAG	G	411	1	-	0/6/23/26	0/1/1/1
9	NAG	B	201	2	-	2/6/23/26	0/1/1/1
9	NAG	H	201	2	-	4/6/23/26	0/1/1/1
9	NAG	F	201	2	-	2/6/23/26	0/1/1/1
9	NAG	C	419	1	-	0/6/23/26	0/1/1/1
9	NAG	I	413	1	-	0/6/23/26	0/1/1/1
9	NAG	G	403	1	-	2/6/23/26	0/1/1/1
9	NAG	D	201	2	-	0/6/23/26	0/1/1/1
9	NAG	L	201	2	-	0/6/23/26	0/1/1/1
9	NAG	K	413	1	-	0/6/23/26	0/1/1/1
9	NAG	E	420	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	B	201	NAG	C1-O5-C5	2.95	116.14	112.19
9	E	420	NAG	C1-O5-C5	2.17	115.09	112.19
9	E	420	NAG	O5-C5-C6	2.13	111.81	107.66
9	I	413	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	403	NAG	C8-C7-N2-C2
9	G	403	NAG	O7-C7-N2-C2
9	H	201	NAG	C8-C7-N2-C2
9	B	201	NAG	C8-C7-N2-C2
9	H	201	NAG	O7-C7-N2-C2
9	F	201	NAG	C4-C5-C6-O6
9	B	201	NAG	O7-C7-N2-C2
9	H	201	NAG	C4-C5-C6-O6
9	H	201	NAG	O5-C5-C6-O6
9	F	201	NAG	O5-C5-C6-O6
9	J	201	NAG	C8-C7-N2-C2
9	J	201	NAG	O7-C7-N2-C2
9	J	201	NAG	C4-C5-C6-O6

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/323 (98%)	-0.19	5 (1%) 70 59	51, 102, 190, 323	0
1	C	317/323 (98%)	-0.23	2 (0%) 85 75	48, 101, 201, 288	0
1	E	317/323 (98%)	-0.15	9 (2%) 55 48	49, 99, 202, 331	0
1	G	317/323 (98%)	-0.23	1 (0%) 90 82	65, 133, 251, 354	0
1	I	317/323 (98%)	-0.17	6 (1%) 66 56	66, 131, 245, 350	0
1	K	317/323 (98%)	-0.22	3 (0%) 81 70	62, 132, 248, 379	0
2	B	173/176 (98%)	-0.23	3 (1%) 69 59	48, 99, 198, 361	0
2	D	173/176 (98%)	-0.16	3 (1%) 69 59	47, 92, 202, 320	0
2	F	173/176 (98%)	-0.25	0 100 100	47, 95, 195, 276	0
2	H	173/176 (98%)	-0.17	1 (0%) 85 75	57, 141, 306, 537	0
2	J	173/176 (98%)	-0.01	2 (1%) 76 65	58, 142, 297, 584	0
2	L	173/176 (98%)	-0.18	3 (1%) 69 59	56, 135, 263, 477	0
3	M	226/240 (94%)	-0.12	5 (2%) 62 53	58, 130, 256, 349	0
3	O	226/240 (94%)	-0.09	2 (0%) 81 70	65, 135, 302, 457	0
3	Q	226/240 (94%)	-0.05	7 (3%) 51 46	68, 122, 232, 376	0
3	S	226/240 (94%)	0.01	8 (3%) 47 43	72, 166, 300, 444	0
3	U	226/240 (94%)	0.00	6 (2%) 56 48	106, 170, 303, 521	0
3	W	226/240 (94%)	0.03	5 (2%) 62 53	95, 168, 298, 474	0
4	N	213/216 (98%)	-0.29	1 (0%) 87 77	48, 130, 258, 473	0
4	P	213/216 (98%)	-0.27	3 (1%) 73 62	57, 122, 241, 435	0
4	R	213/216 (98%)	-0.11	0 100 100	60, 118, 243, 365	0
4	T	213/216 (98%)	0.06	6 (2%) 55 48	109, 182, 302, 468	0
4	V	213/216 (98%)	-0.09	2 (0%) 81 70	118, 178, 337, 403	0
4	X	213/216 (98%)	-0.15	3 (1%) 73 62	104, 181, 327, 448	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5574/5730 (97%)	-0.14	86 (1%) 72 60	47, 134, 269, 584	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	127	SER	6.5
1	I	264	LYS	5.8
3	U	34	ASN	5.1
3	S	179	SER	4.8
4	T	133	VAL	4.2
3	U	43	GLN	4.1
3	O	32	ALA	4.1
3	M	44	GLY	3.9
4	T	120	PRO	3.7
4	V	120	PRO	3.7
1	E	264	LYS	3.5
1	K	143	SER	3.4
3	W	113	SER	3.4
1	C	183	HIS	3.3
4	T	134	CYS	3.3
1	G	264	LYS	3.1
3	S	85	GLU	3.1
3	W	7	SER	3.1
4	X	108	GLN	3.0
2	B	74	GLU	3.0
3	Q	92	CYS	3.0
1	E	96	ASN	2.9
1	E	144	ASN	2.9
4	X	67	SER	2.8
3	O	93	ALA	2.8
3	U	94	GLY	2.8
1	I	144	ASN	2.8
1	K	262	SER	2.8
2	J	147	ALA	2.7
3	S	93	ALA	2.7
4	T	116	THR	2.7
1	K	208	ARG	2.7
3	W	118	GLY	2.7
3	U	107	THR	2.7
1	E	173	GLN	2.7
1	A	262	SER	2.7
1	E	263	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	Q	48	MET	2.6
2	B	72	GLU	2.6
1	I	9	PRO	2.6
1	I	274	ILE	2.5
1	I	305	CYS	2.5
3	S	43	GLN	2.5
2	J	87	THR	2.5
2	D	22	TYR	2.5
1	E	211	GLN	2.4
4	P	67	SER	2.4
3	Q	100(M)	TYR	2.4
3	S	178	LEU	2.4
2	L	82	LYS	2.4
4	V	1	GLN	2.4
2	H	36	ALA	2.4
1	A	199	SER	2.4
1	E	181	GLY	2.3
2	D	168	ASN	2.3
3	M	71	ALA	2.3
3	U	180	SER	2.2
4	P	158	GLY	2.2
1	I	290	ASN	2.2
3	Q	104	GLY	2.2
2	B	96	ALA	2.2
2	L	70	PHE	2.2
1	E	262	SER	2.2
2	L	160	ASP	2.2
1	E	269	ARG	2.2
3	Q	97	ILE	2.2
3	M	214	LYS	2.2
3	M	98	THR	2.1
3	U	212	GLU	2.1
1	C	9	PRO	2.1
3	Q	125	ALA	2.1
3	S	212	GLU	2.1
4	X	198	GLU	2.1
3	W	121	VAL	2.1
3	M	76	ASN	2.1
3	S	15	GLY	2.1
1	A	274	ILE	2.1
4	P	120	PRO	2.1
1	A	205	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	82	LYS	2.0
1	A	53	ASP	2.0
3	Q	100(J)	ASP	2.0
4	N	205	THR	2.0
4	T	117	LEU	2.0
4	T	196	THR	2.0
3	S	113	SER	2.0

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
6	NAG	Z	2	14/15	0.97	0.05	153,155,157,157	0
5	NAG	Y	2	14/15	0.98	0.10	245,249,251,251	0
5	BMA	Y	3	11/12	0.98	0.06	184,187,189,189	0
5	NAG	i	1	14/15	-	-	167,169,172,172	0
5	NAG	i	2	14/15	-	-	164,166,168,168	0
5	BMA	i	3	11/12	-	-	224,225,227,229	0
5	NAG	j	1	14/15	-	-	150,156,160,161	0
5	NAG	j	2	14/15	-	-	179,182,185,185	0
5	BMA	j	3	11/12	-	-	176,179,181,184	0
5	NAG	l	1	14/15	-	-	129,135,138,139	0
5	NAG	l	2	14/15	-	-	190,196,198,199	0
5	BMA	l	3	11/12	-	-	215,219,220,221	0
5	NAG	p	1	14/15	-	-	129,135,139,140	0
5	NAG	p	2	14/15	-	-	187,191,193,194	0
5	BMA	p	3	11/12	-	-	229,233,234,237	0
5	NAG	t	1	14/15	-	-	210,212,216,216	0
5	NAG	t	2	14/15	-	-	215,219,221,221	0
5	BMA	t	3	11/12	-	-	216,220,222,223	0
5	NAG	u	1	14/15	-	-	117,121,127,129	0
5	NAG	u	2	14/15	-	-	185,188,191,191	0
5	BMA	u	3	11/12	-	-	212,213,216,220	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	y	1	14/15	-	-	141,147,150,151	0
5	NAG	y	2	14/15	-	-	124,133,133,137	0
5	BMA	y	3	11/12	-	-	174,176,181,182	0
5	NAG	z	1	14/15	-	-	173,177,178,178	0
5	NAG	z	2	14/15	-	-	240,243,245,245	0
5	BMA	z	3	11/12	-	-	201,203,205,206	0
5	NAG	0	1	14/15	-	-	146,151,156,158	0
5	NAG	0	2	14/15	-	-	223,226,228,229	0
5	BMA	0	3	11/12	-	-	207,209,212,215	0
5	NAG	3	1	14/15	-	-	150,154,155,156	0
5	NAG	3	2	14/15	-	-	182,187,189,193	0
5	BMA	3	3	11/12	-	-	185,188,195,197	0
5	NAG	5	1	14/15	-	-	178,181,182,182	0
5	NAG	5	2	14/15	-	-	272,275,277,277	0
5	BMA	5	3	11/12	-	-	271,272,274,275	0
5	NAG	6	1	14/15	-	-	124,133,141,144	0
5	NAG	6	2	14/15	-	-	194,197,203,204	0
5	BMA	6	3	11/12	-	-	187,191,196,202	0
6	NAG	Z	1	14/15	0.98	0.06	113,115,118,119	0
5	NAG	Y	1	14/15	0.98	0.11	108,112,115,115	0
6	NAG	a	1	14/15	-	-	91,93,96,96	0
6	NAG	a	2	14/15	-	-	209,214,215,216	0
6	NAG	c	1	14/15	-	-	175,178,181,182	0
6	NAG	c	2	14/15	-	-	215,217,219,219	0
6	NAG	d	1	14/15	-	-	146,152,156,157	0
6	NAG	d	2	14/15	-	-	208,212,215,215	0
6	NAG	f	1	14/15	-	-	111,117,120,121	0
6	NAG	f	2	14/15	-	-	187,193,195,196	0
6	NAG	o	1	14/15	-	-	172,175,175,176	0
6	NAG	o	2	14/15	-	-	165,166,168,169	0
6	NAG	q	1	14/15	-	-	150,156,159,159	0
6	NAG	q	2	14/15	-	-	136,144,148,148	0
6	NAG	r	1	14/15	-	-	142,148,150,150	0
6	NAG	r	2	14/15	-	-	192,200,207,209	0
6	NAG	s	1	14/15	-	-	131,135,137,137	0
6	NAG	s	2	14/15	-	-	144,150,152,153	0
6	NAG	v	1	14/15	-	-	117,123,125,126	0
6	NAG	v	2	14/15	-	-	171,179,182,183	0
6	NAG	w	1	14/15	-	-	163,168,177,181	0
6	NAG	w	2	14/15	-	-	171,182,186,193	0
6	NAG	x	1	14/15	-	-	161,167,169,170	0
6	NAG	x	2	14/15	-	-	151,163,169,174	0

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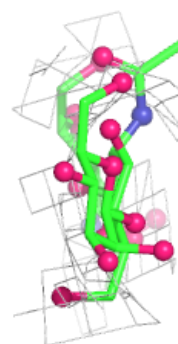
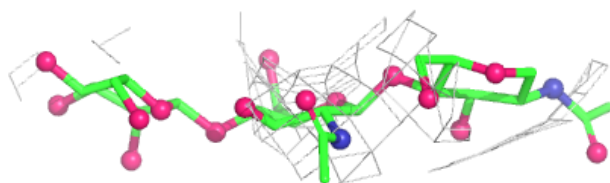
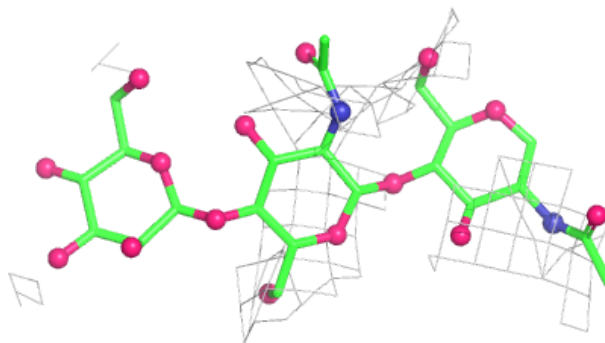
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	1	1	14/15	-	-	122,129,130,131	0
6	NAG	1	2	14/15	-	-	190,196,199,199	0
6	NAG	2	1	14/15	-	-	159,165,171,175	0
6	NAG	2	2	14/15	-	-	177,187,191,198	0
6	NAG	4	1	14/15	-	-	104,107,109,110	0
6	NAG	4	2	14/15	-	-	127,132,134,135	0
7	NAG	b	1	14/15	-	-	78,81,82,84	0
7	NAG	b	2	14/15	-	-	124,128,128,129	0
7	BMA	b	3	11/12	-	-	207,210,212,212	0
7	MAN	b	4	11/12	-	-	161,165,167,168	0
7	MAN	b	5	11/12	-	-	167,171,173,173	0
7	NAG	h	1	14/15	-	-	98,102,104,104	0
7	NAG	h	2	14/15	-	-	97,101,102,103	0
7	BMA	h	3	11/12	-	-	131,134,135,135	0
7	MAN	h	4	11/12	-	-	208,212,213,215	0
7	MAN	h	5	11/12	-	-	186,189,191,191	0
7	NAG	k	1	14/15	-	-	114,119,121,121	0
7	NAG	k	2	14/15	-	-	230,232,234,234	0
7	BMA	k	3	11/12	-	-	234,237,238,239	0
7	MAN	k	4	11/12	-	-	188,190,191,195	0
7	MAN	k	5	11/12	-	-	181,183,186,186	0
7	NAG	n	1	14/15	-	-	81,83,85,85	0
7	NAG	n	2	14/15	-	-	126,131,132,132	0
7	BMA	n	3	11/12	-	-	229,232,234,235	0
7	MAN	n	4	11/12	-	-	140,143,144,146	0
7	MAN	n	5	11/12	-	-	191,195,197,197	0
8	NAG	e	1	14/15	-	-	87,94,97,98	0
8	NAG	e	2	14/15	-	-	263,271,272,273	0
8	BMA	e	3	11/12	-	-	256,260,262,262	0
8	MAN	e	4	11/12	-	-	170,177,180,185	0
8	NAG	g	1	14/15	-	-	84,86,88,88	0
8	NAG	g	2	14/15	-	-	150,155,156,156	0
8	BMA	g	3	11/12	-	-	198,201,203,204	0
8	MAN	g	4	11/12	-	-	149,152,153,155	0
8	NAG	m	1	14/15	-	-	95,99,100,100	0
8	NAG	m	2	14/15	-	-	146,150,151,151	0
8	BMA	m	3	11/12	-	-	197,200,202,202	0
8	MAN	m	4	11/12	-	-	162,166,168,170	0

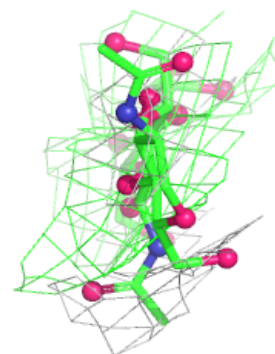
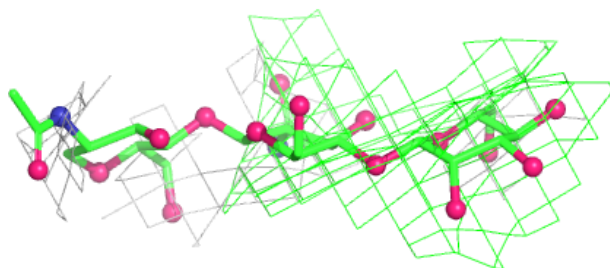
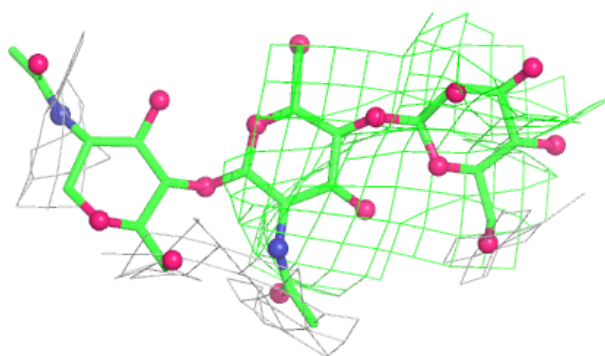
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

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

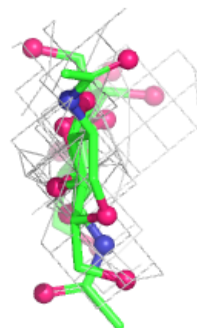
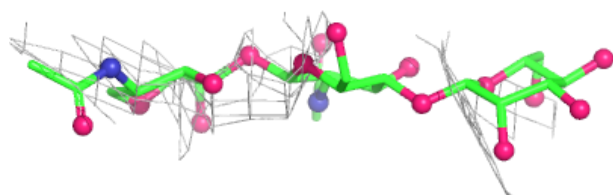
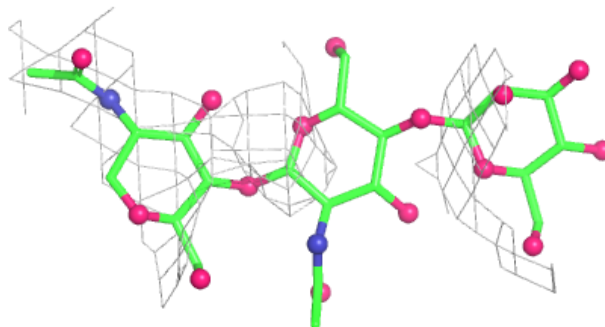
**Electron density around Chain i:**

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

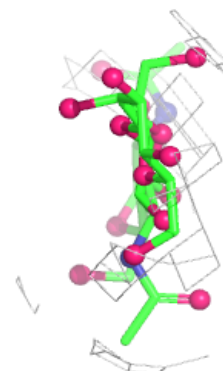
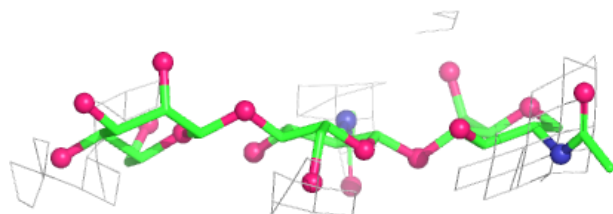
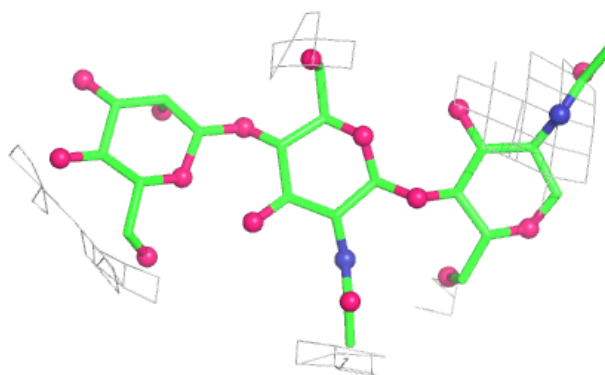


Electron density around Chain j:

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

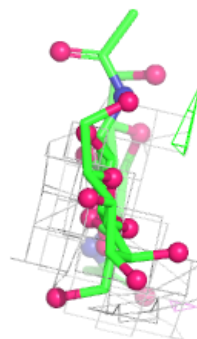
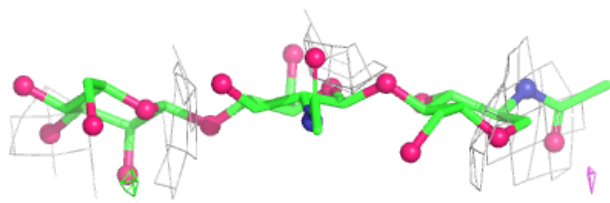
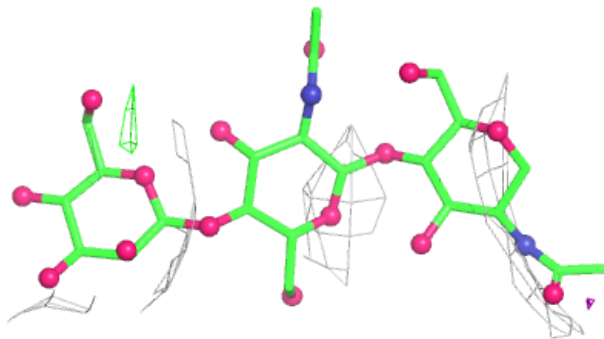
**Electron density around Chain l:**

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

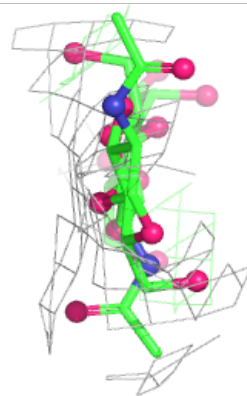
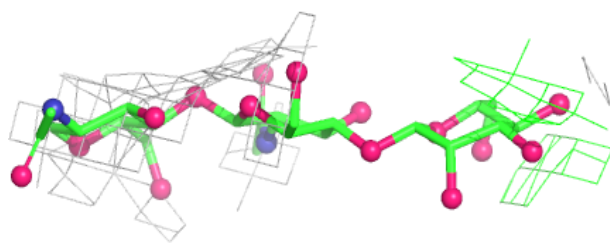
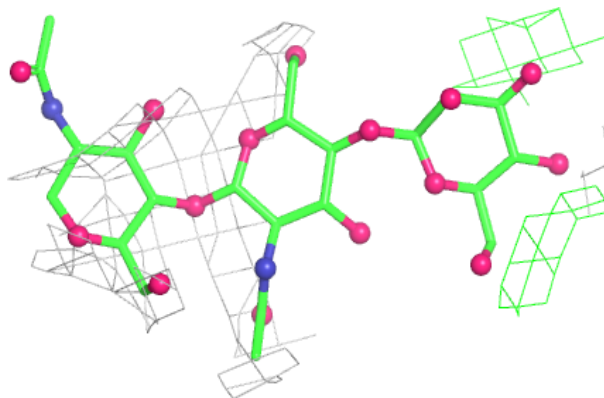


Electron density around Chain p:

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

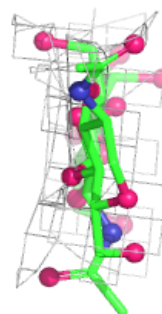
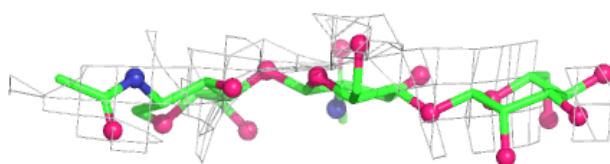
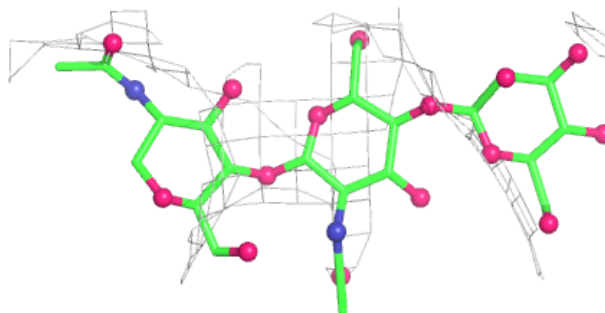
**Electron density around Chain t:**

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

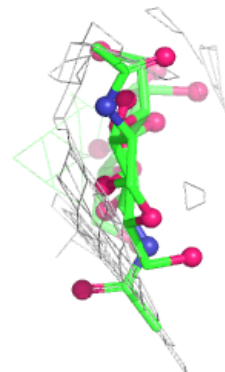
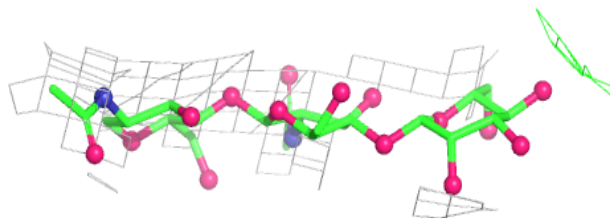
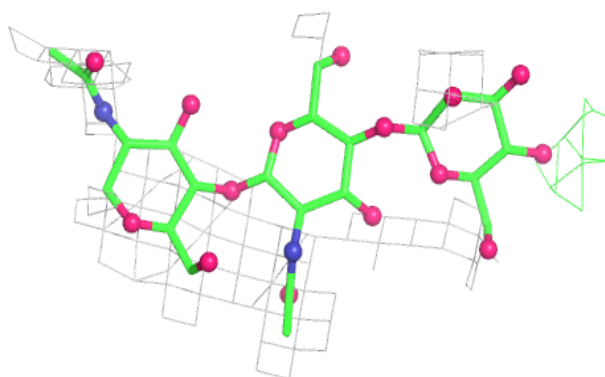


Electron density around Chain u:

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

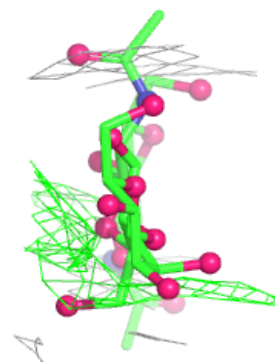
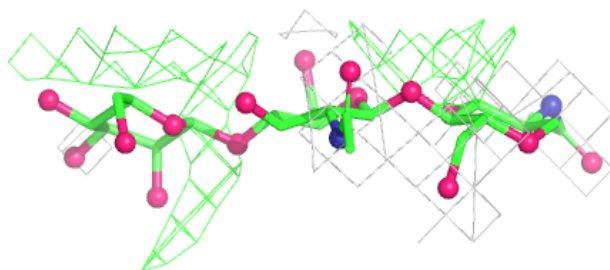
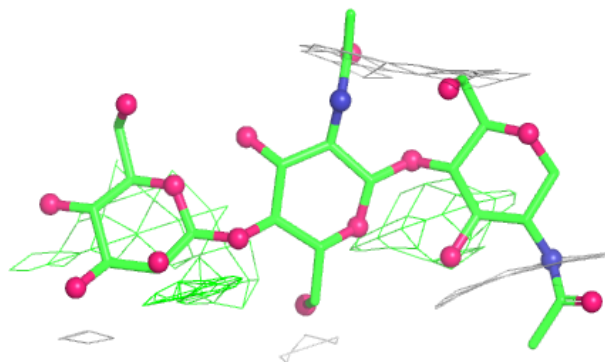
**Electron density around Chain y:**

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

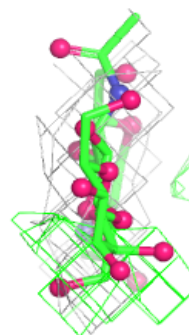
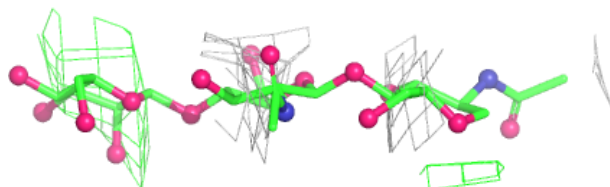
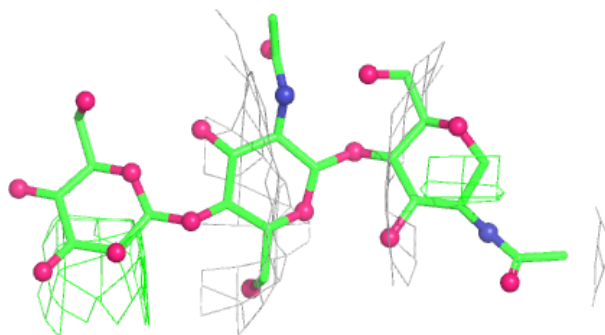


Electron density around Chain z:

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

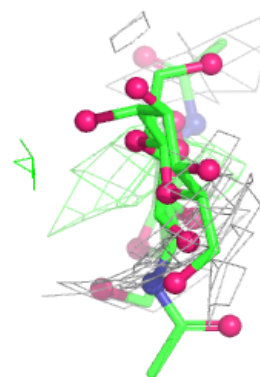
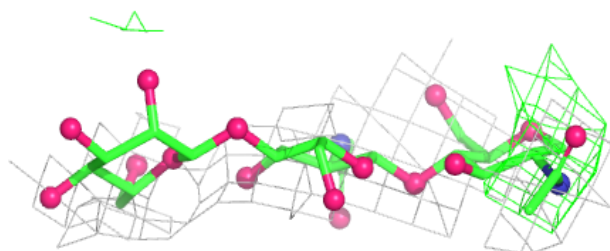
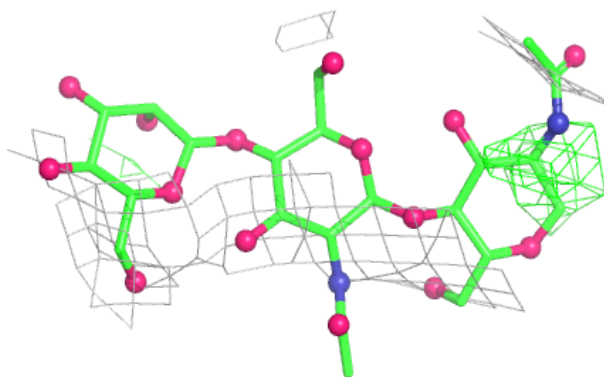
**Electron density around Chain 0:**

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

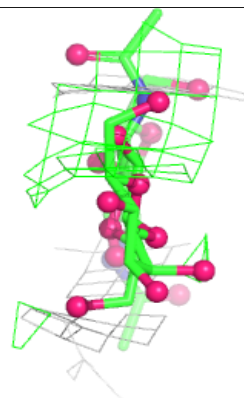
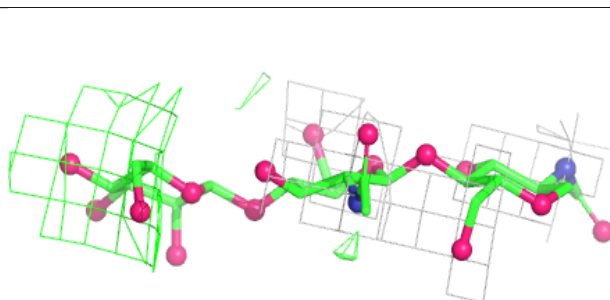
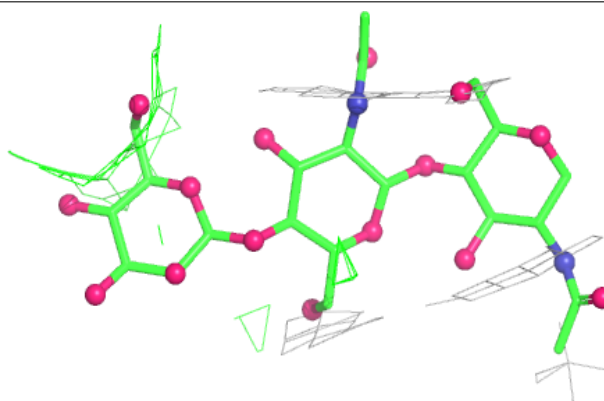


Electron density around Chain 3:

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

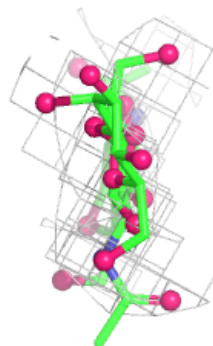
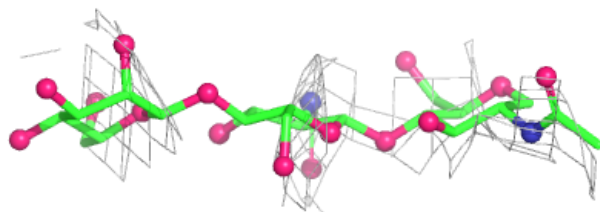
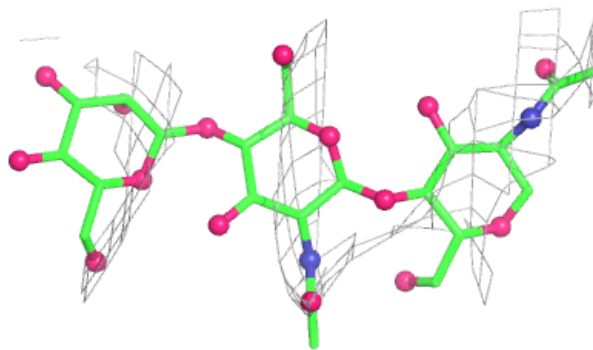
**Electron density around Chain 5:**

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



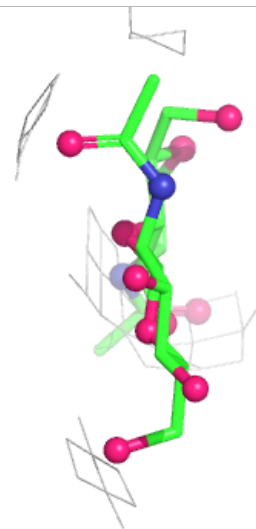
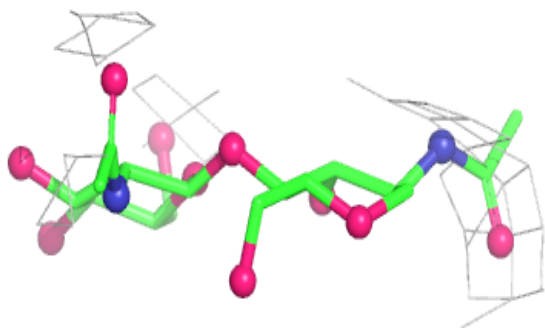
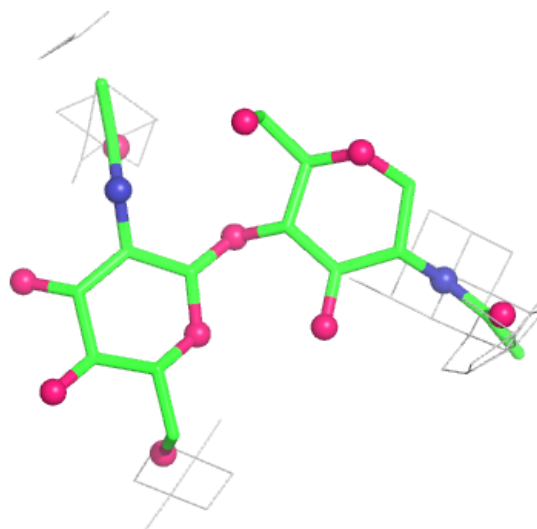
Electron density around Chain 6:

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



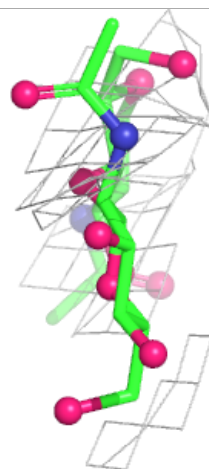
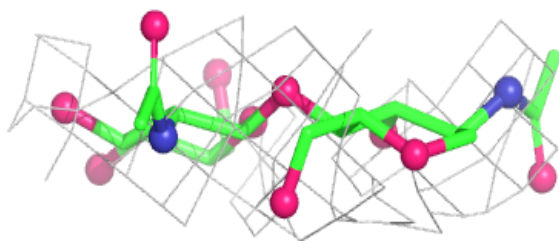
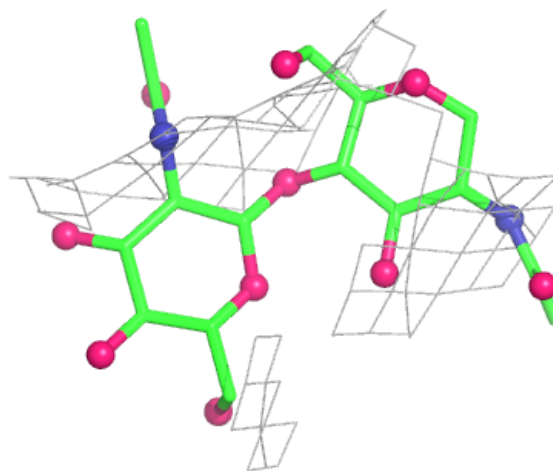
Electron density around Chain Z:

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



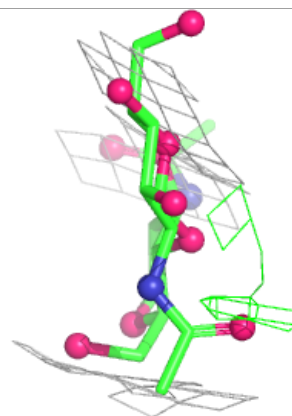
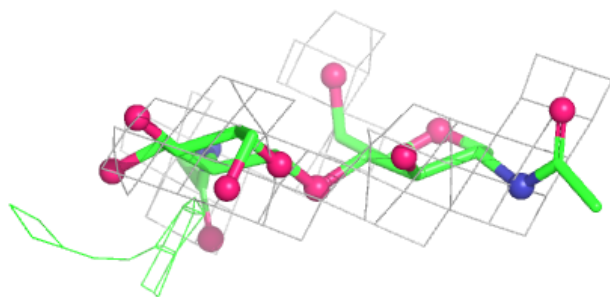
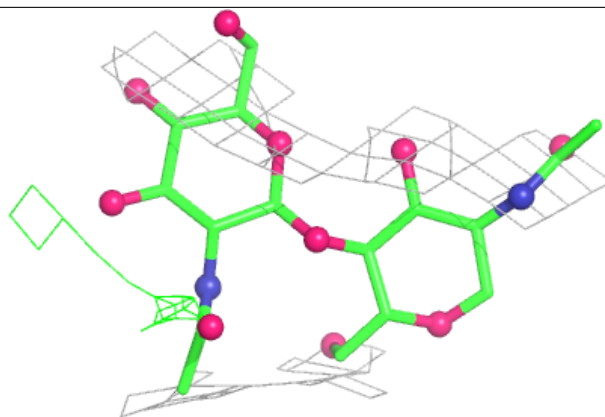
Electron density around Chain a:

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

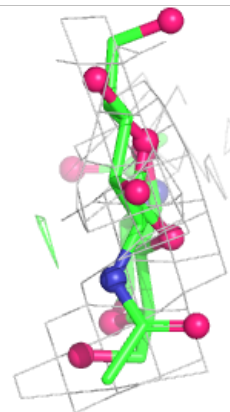
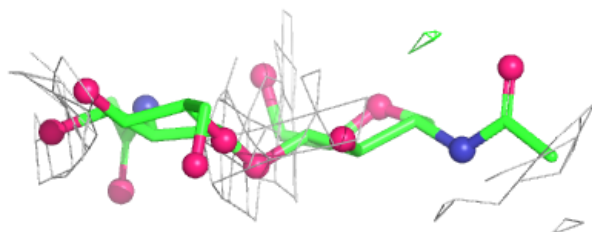
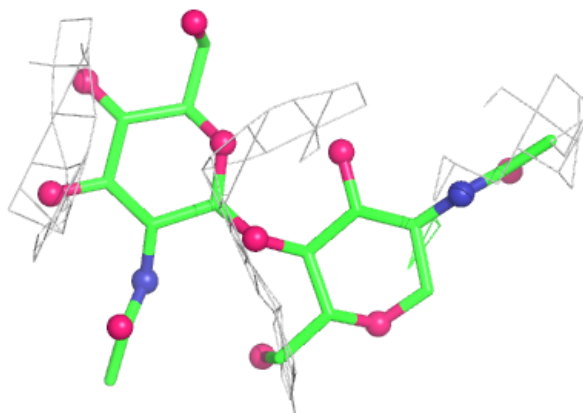


Electron density around Chain c:

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

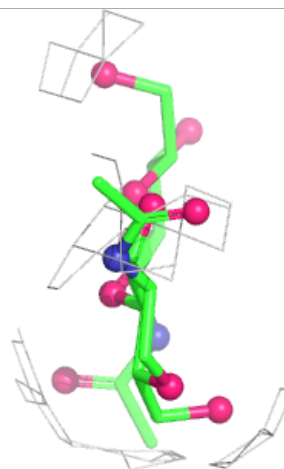
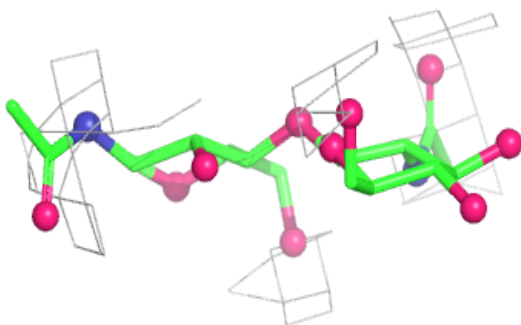
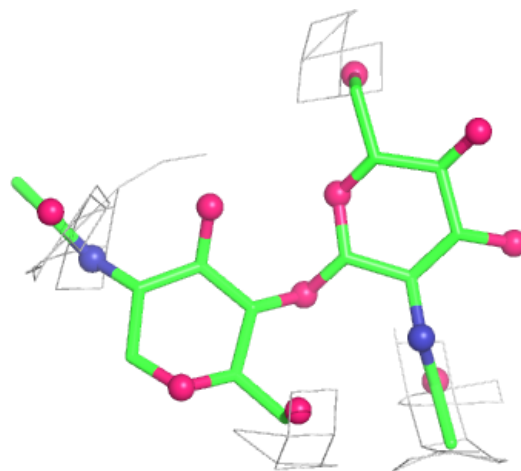
**Electron density around Chain d:**

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



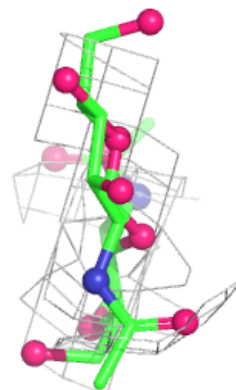
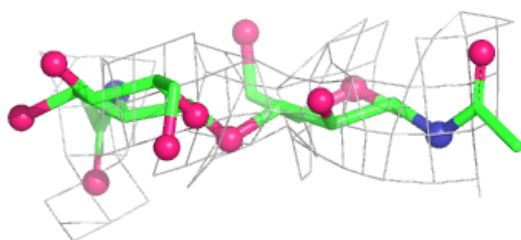
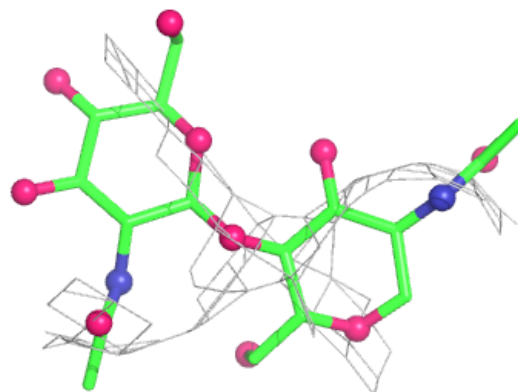
Electron density around Chain f:

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



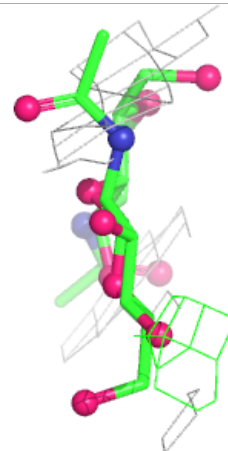
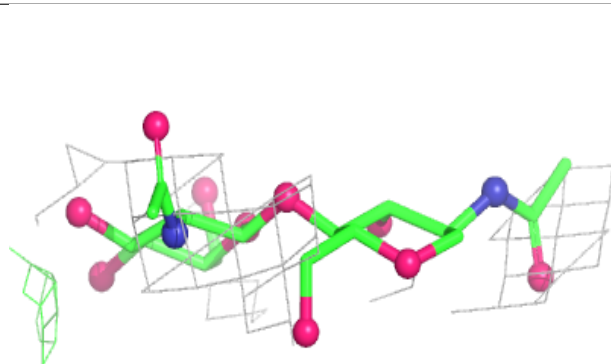
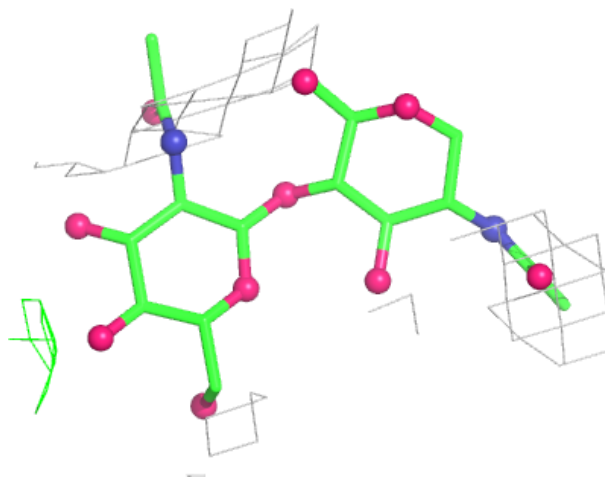
Electron density around Chain o:

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



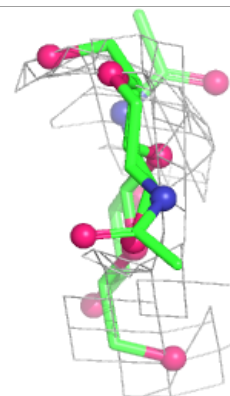
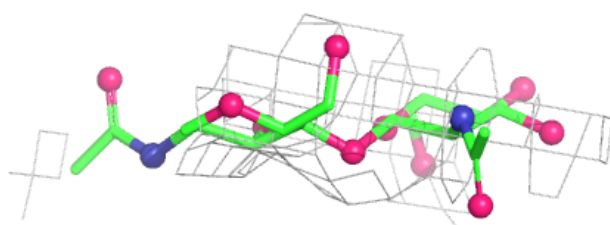
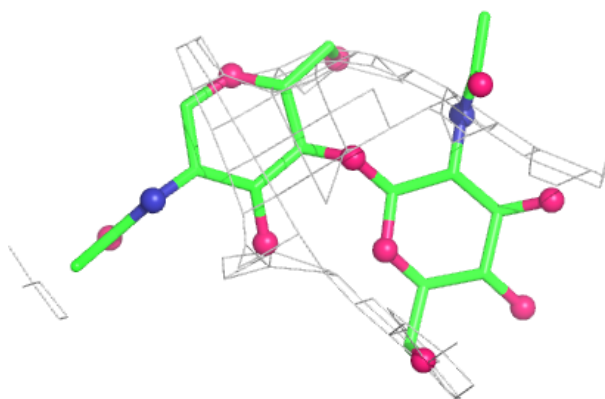
Electron density around Chain q:

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

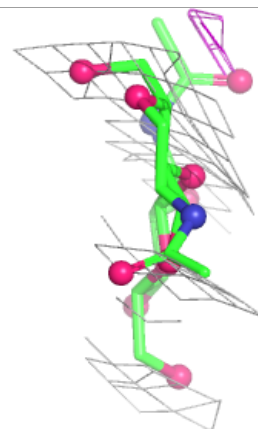
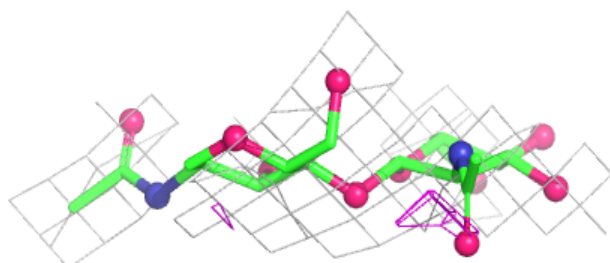
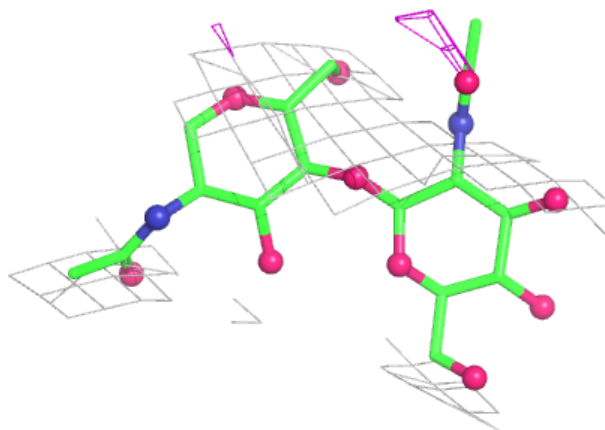


Electron density around Chain r:

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

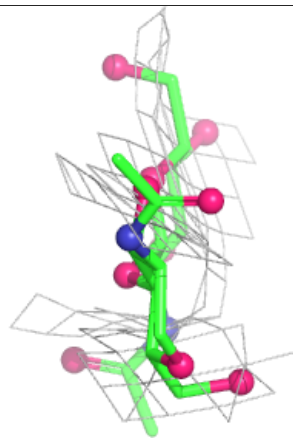
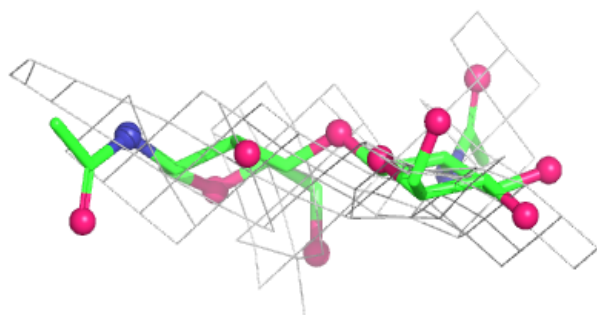
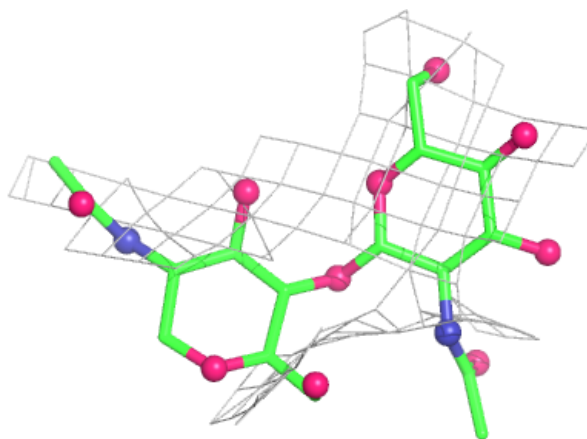
**Electron density around Chain s:**

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



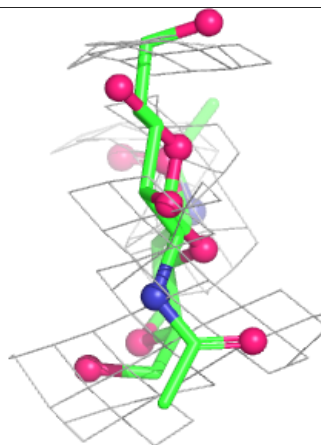
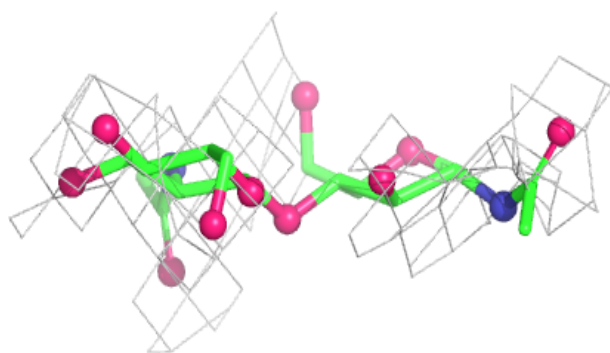
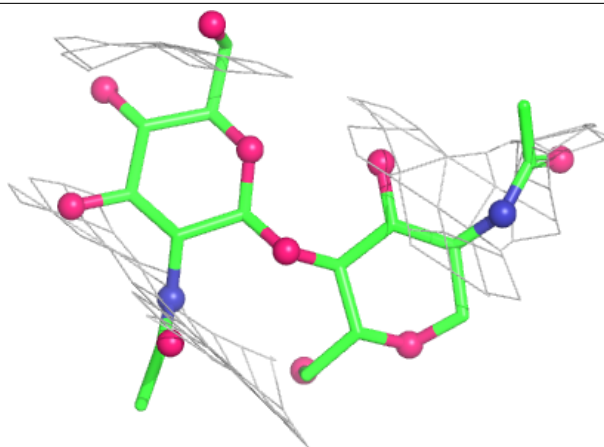
Electron density around Chain v:

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



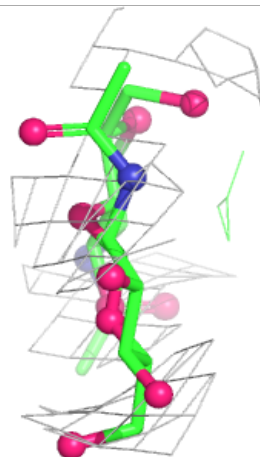
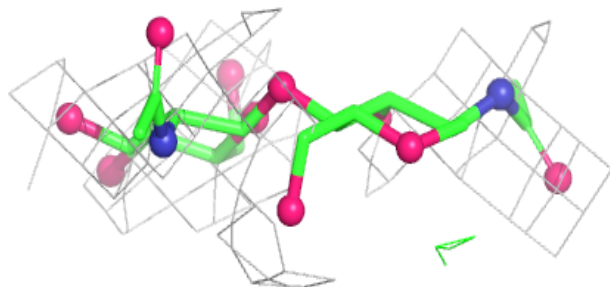
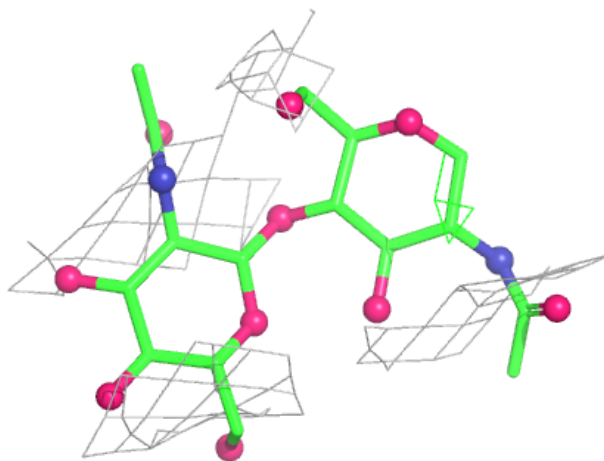
Electron density around Chain w:

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



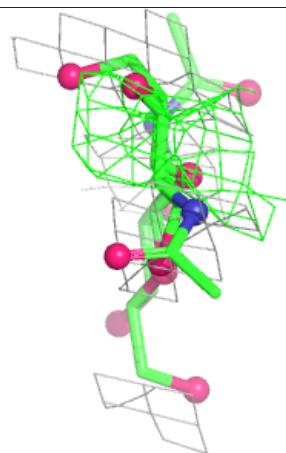
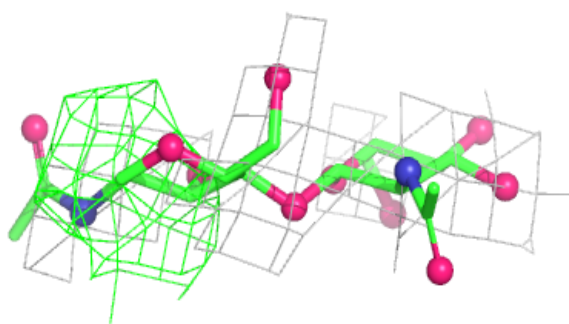
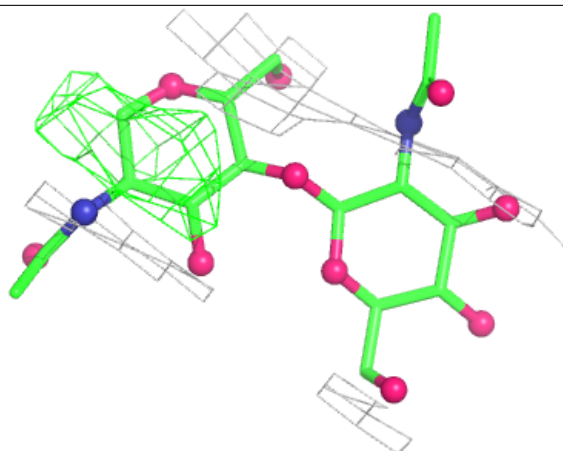
Electron density around Chain x:

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



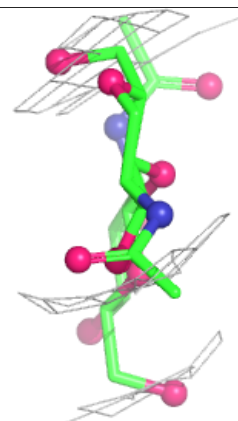
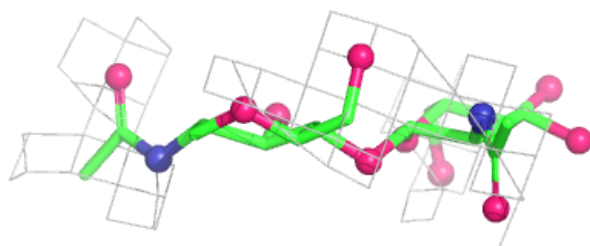
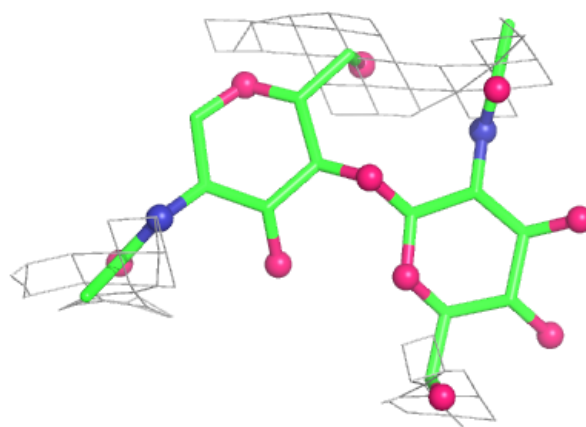
Electron density around Chain 1:

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



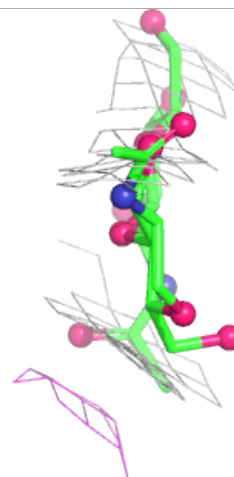
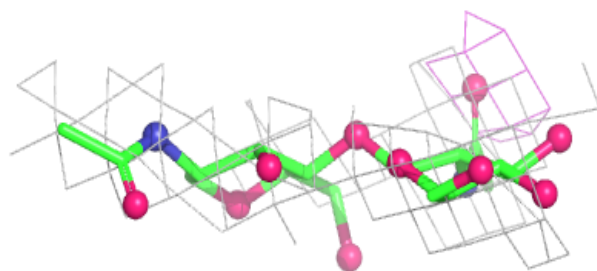
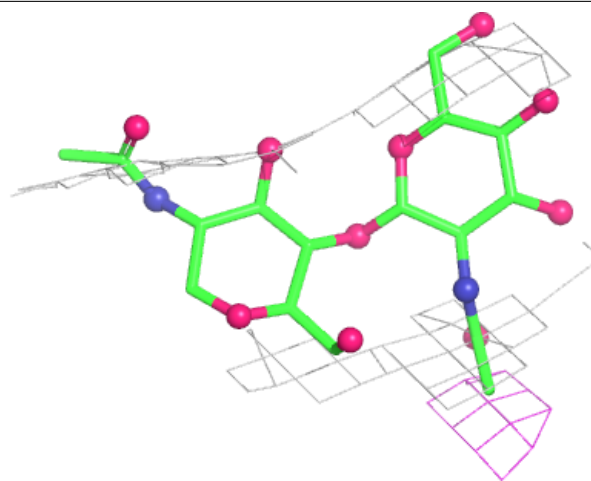
Electron density around Chain 2:

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



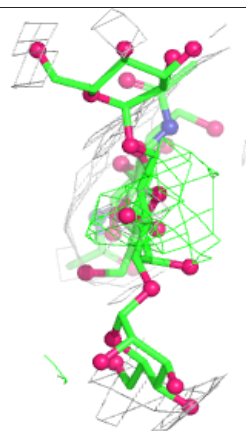
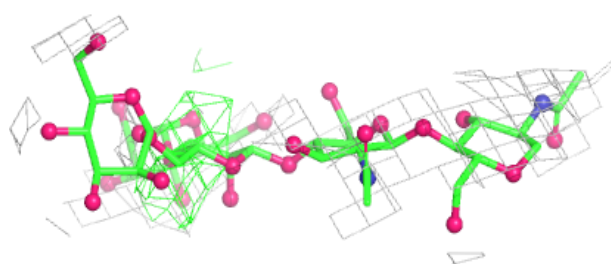
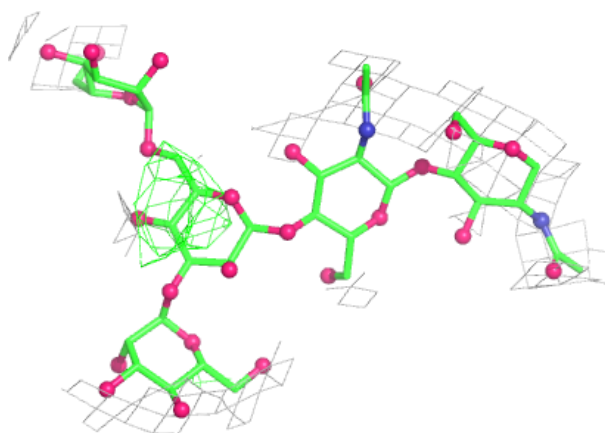
Electron density around Chain 4:

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



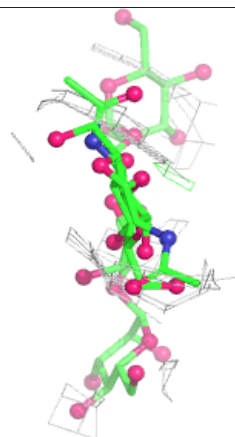
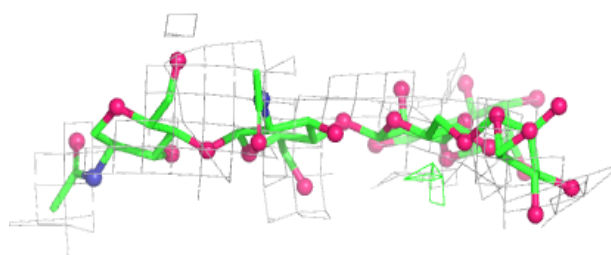
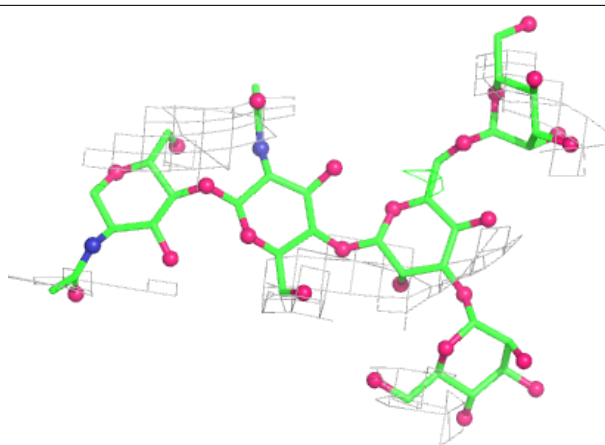
Electron density around Chain b:

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

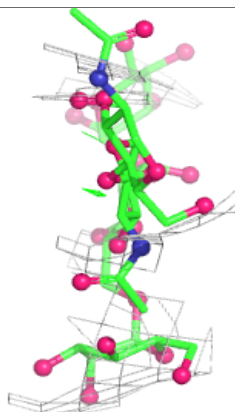
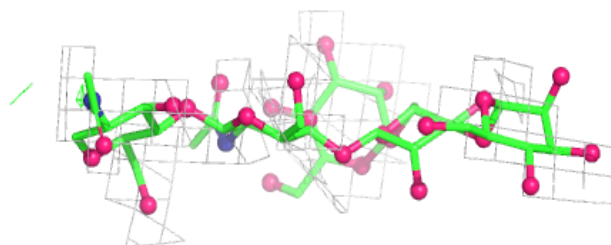
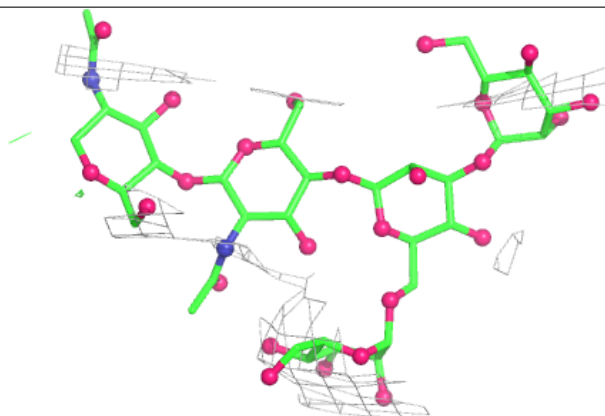


Electron density around Chain h:

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

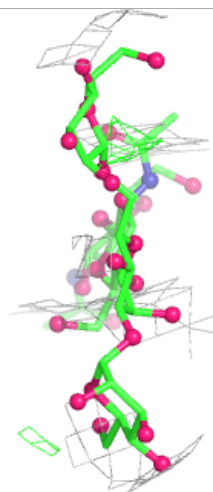
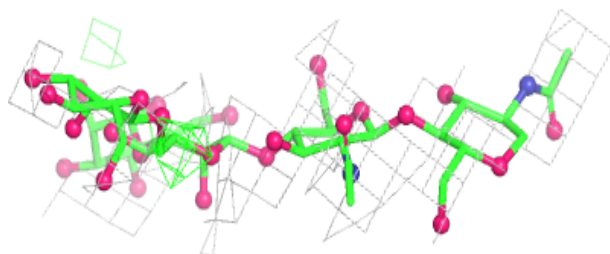
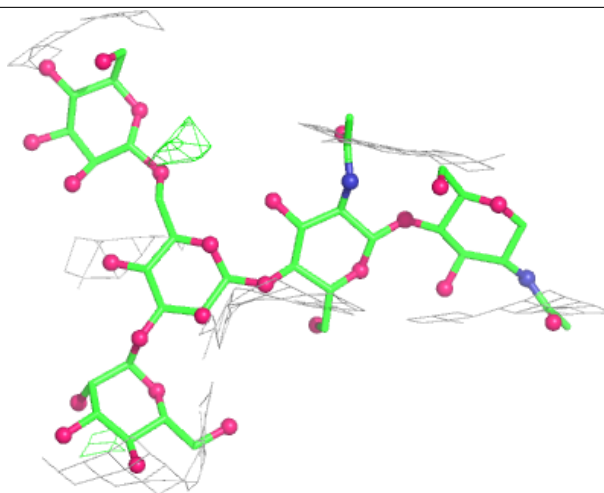
**Electron density around Chain k:**

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



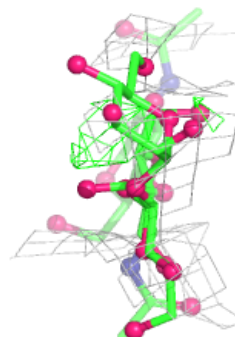
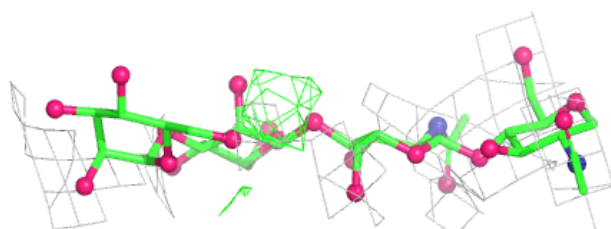
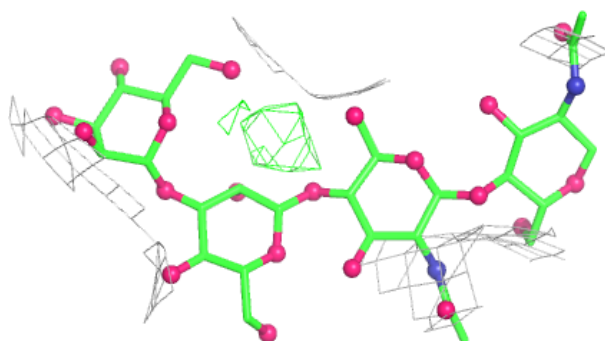
Electron density around Chain n:

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

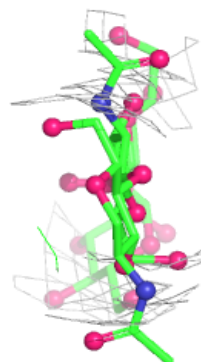
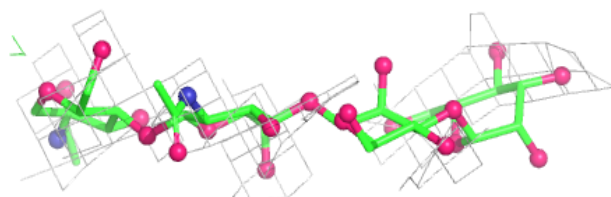
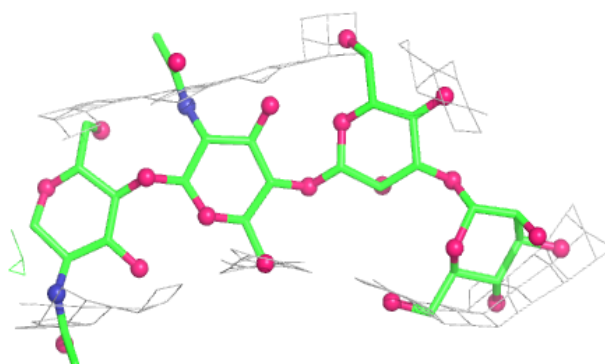


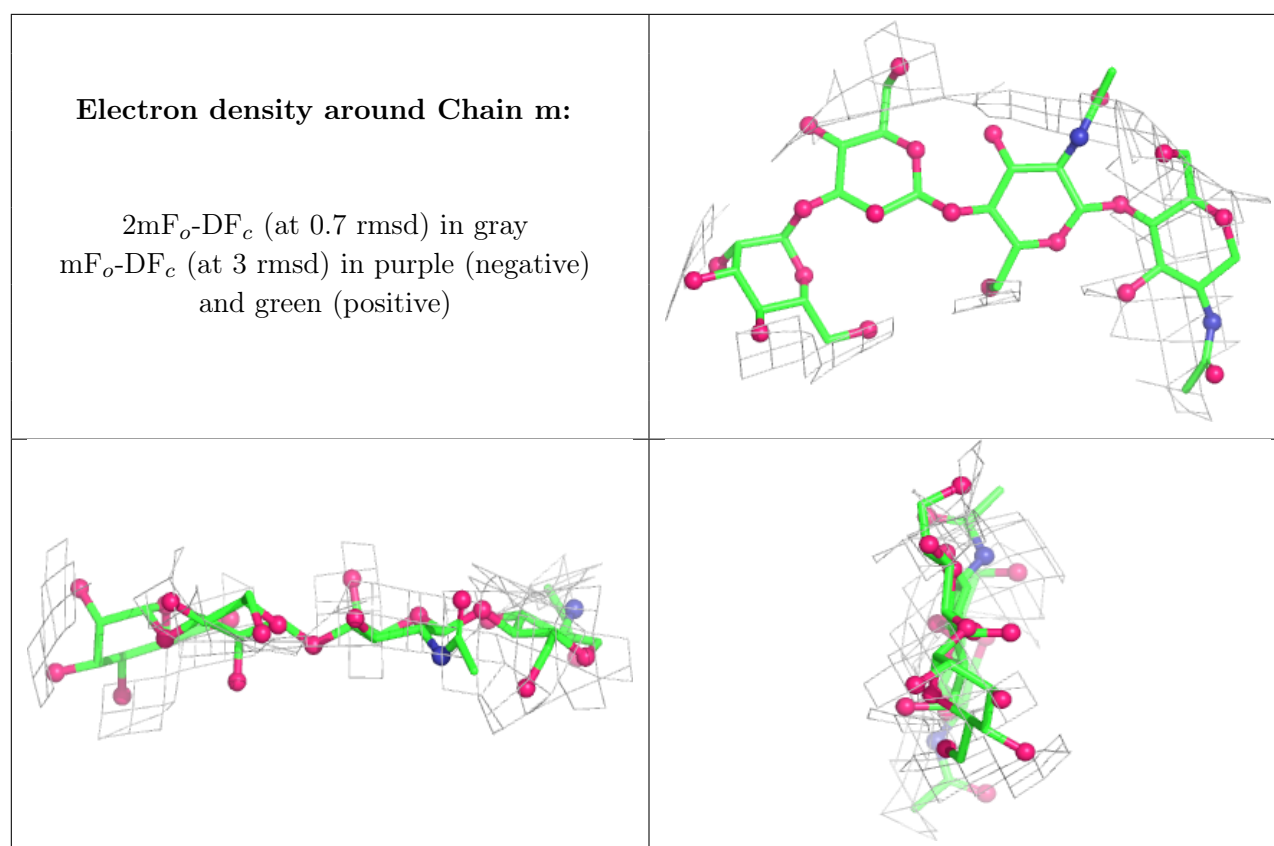
Electron density around Chain e:

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

**Electron density around Chain g:**

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





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
9	NAG	K	413	14/15	0.90	0.17	162,171,175,176	0
9	NAG	J	201	14/15	0.92	0.16	137,145,154,155	0
9	NAG	B	201	14/15	0.94	0.11	99,102,104,105	0
9	NAG	C	419	14/15	0.95	0.11	143,150,153,155	0
9	NAG	H	201	14/15	0.95	0.14	140,145,148,150	0
9	NAG	E	420	14/15	0.96	0.09	130,136,140,141	0
9	NAG	F	201	14/15	0.96	0.15	156,160,162,162	0
9	NAG	G	411	14/15	0.96	0.10	167,178,182,183	0
9	NAG	I	413	14/15	0.97	0.08	129,140,147,147	0
9	NAG	L	201	14/15	0.97	0.15	131,137,145,146	0
9	NAG	D	201	14/15	0.98	0.09	121,124,126,127	0
9	NAG	G	403	14/15	0.98	0.10	116,120,127,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.