



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2023 – 01:37 AM EDT

PDB ID : 5W1X
Title : Crystal Structure of Humanpapillomavirus18 (HPV18) Capsid L1 Pentamers
Bound to Heparin Oligosaccharides
Authors : Chen, X.S.; Dasgupta, J.
Deposited on : 2017-06-05
Resolution : 3.37 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

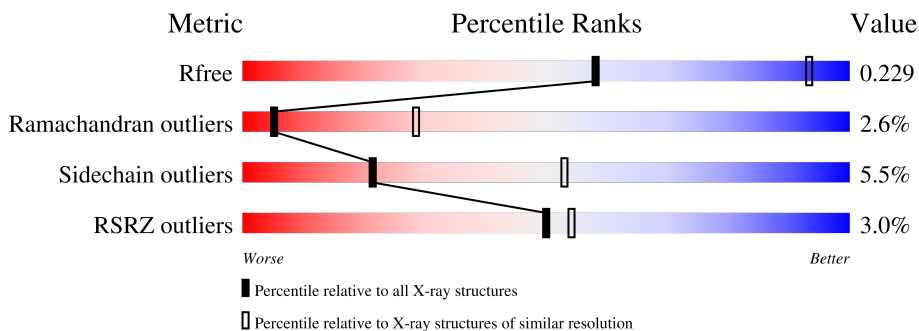
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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}	130704	1691 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	427	 4% 93% 5%
1	B	427	 4% 93% 6%
1	C	427	 3% 92% 6%
1	D	427	 2% 91% 8%
1	E	427	 2% 93% 6%
1	F	427	 2% 93% 5%

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Mol	Chain	Length	Quality of chain
1	G	427	 4% 92% 6% ..
1	H	427	 3% 91% 7% .
1	I	427	 2% 93% 6% .
1	J	427	 2% 94% . .
1	K	427	 3% 91% 7% .
1	L	427	 3% 90% 8% .
1	M	427	 3% 89% 9% ..
1	N	427	 2% 92% 6% ..
1	O	427	 5% 92% 7% .
2	P	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
2	W	2	 100%
2	Y	2	 100%
2	Z	2	 100%
2	a	2	 100%
2	d	2	 100%
2	i	2	 100%
2	j	2	 100%
2	k	2	 100%
2	l	2	 100%
2	m	2	 100%
2	n	2	 100%
2	o	2	 100%

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Mol	Chain	Length	Quality of chain
2	q	2	 100%
2	r	2	 100%
2	s	2	 100%
3	Q	4	 100%
3	R	4	 100%
3	V	4	 100%
3	X	4	 100%
3	b	4	 100%
3	c	4	 100%
3	g	4	 100%
3	h	4	 100%
3	p	4	 100%
4	e	6	 100%
5	f	10	 90%  10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JHM	P	1	-	-	-	X
2	IDS	P	2	-	-	-	X
2	JHM	S	1	-	-	-	X
2	IDS	S	2	-	-	-	X
2	JHM	T	1	-	-	-	X
2	IDS	T	2	-	-	-	X
2	JHM	U	1	-	-	-	X
2	IDS	U	2	-	-	-	X
2	JHM	W	1	-	-	-	X
2	IDS	W	2	-	-	-	X
2	JHM	Y	1	-	-	-	X
2	IDS	Y	2	-	-	-	X
2	JHM	Z	1	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IDS	Z	2	-	-	-	X
2	JHM	a	1	-	-	-	X
2	IDS	a	2	-	-	-	X
2	JHM	d	1	-	-	-	X
2	IDS	d	2	-	-	-	X
2	JHM	i	1	-	-	-	X
2	IDS	i	2	-	-	-	X
2	JHM	j	1	-	-	-	X
2	IDS	j	2	-	-	-	X
2	JHM	k	1	-	-	-	X
2	IDS	k	2	-	-	-	X
2	JHM	l	1	-	-	-	X
2	IDS	l	2	-	-	-	X
2	JHM	m	1	-	-	-	X
2	IDS	m	2	-	-	-	X
2	JHM	n	1	-	-	-	X
2	IDS	n	2	-	-	-	X
2	JHM	o	1	-	-	-	X
2	JHM	q	1	-	-	-	X
2	IDS	q	2	-	-	-	X
2	JHM	r	1	-	-	-	X
2	IDS	r	2	-	-	-	X
2	JHM	s	1	-	-	-	X
2	IDS	s	2	-	-	-	X
3	JHM	Q	1	-	-	-	X
3	IDS	Q	2	-	-	-	X
3	JHM	Q	3	-	-	-	X
3	IDS	Q	4	-	-	-	X
3	JHM	R	1	-	-	-	X
3	IDS	R	2	-	-	-	X
3	JHM	R	3	-	-	-	X
3	IDS	R	4	-	-	-	X
3	JHM	V	1	-	-	-	X
3	IDS	V	2	-	-	-	X
3	JHM	V	3	-	-	-	X
3	JHM	X	1	-	-	-	X
3	IDS	X	2	-	-	-	X
3	JHM	X	3	-	-	-	X
3	IDS	X	4	-	-	-	X
3	JHM	b	1	-	-	-	X
3	IDS	b	2	-	-	-	X
3	IDS	b	4	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JHM	c	1	-	-	-	X
3	IDS	c	2	-	-	-	X
3	JHM	c	3	-	-	-	X
3	IDS	c	4	-	-	-	X
3	JHM	g	1	-	-	-	X
3	IDS	g	2	-	-	-	X
3	JHM	g	3	-	-	-	X
3	IDS	g	4	-	-	-	X
3	JHM	h	1	-	-	-	X
3	IDS	h	2	-	-	-	X
3	JHM	h	3	-	-	-	X
3	IDS	h	4	-	-	-	X
3	JHM	p	1	-	-	-	X
3	IDS	p	2	-	-	-	X
3	JHM	p	3	-	-	-	X
3	IDS	p	4	-	-	-	X
4	JHM	e	1	-	-	-	X
4	IDS	e	2	-	-	-	X
4	IDS	e	4	-	-	-	X
4	JHM	e	5	-	-	-	X
4	IDS	e	6	-	-	-	X
5	JHM	f	1	-	-	-	X
5	IDS	f	10	-	-	-	X
5	IDS	f	2	-	-	-	X
5	JHM	f	3	-	-	-	X
5	IDS	f	4	-	-	-	X
5	JHM	f	5	-	-	-	X
5	IDS	f	6	-	-	-	X
5	JHM	f	7	-	-	-	X
5	IDS	f	8	-	-	-	X
5	JHM	f	9	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 51075 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3315	2092	561	642	20	0	0	0
1	B	422	3315	2092	561	642	20	0	0	0
1	C	422	3315	2092	561	642	20	0	0	0
1	D	422	3315	2092	561	642	20	0	0	0
1	E	422	3315	2092	561	642	20	0	0	0
1	F	422	3315	2092	561	642	20	0	0	0
1	G	422	3315	2092	561	642	20	0	0	0
1	H	422	3315	2092	561	642	20	0	0	0
1	I	422	3315	2092	561	642	20	0	0	0
1	J	422	3315	2092	561	642	20	0	0	0
1	K	422	3315	2092	561	642	20	0	0	0
1	L	422	3315	2092	561	642	20	0	0	0
1	M	422	3315	2092	561	642	20	0	0	0
1	N	422	3315	2092	561	642	20	0	0	0
1	O	422	3315	2092	561	642	20	0	0	0

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q5G244
A	47	ASP	ASN	engineered mutation	UNP Q5G244
A	175	SER	CYS	engineered mutation	UNP Q5G244
A	393	GLN	HIS	engineered mutation	UNP Q5G244
A	433	GLY	-	linker	UNP Q5G244
A	434	GLY	-	linker	UNP Q5G244
A	435	SER	-	linker	UNP Q5G244
A	436	GLY	-	linker	UNP Q5G244
A	437	GLY	-	linker	UNP Q5G244
B	20	ALA	-	expression tag	UNP Q5G244
B	47	ASP	ASN	engineered mutation	UNP Q5G244
B	175	SER	CYS	engineered mutation	UNP Q5G244
B	393	GLN	HIS	engineered mutation	UNP Q5G244
B	433	GLY	-	linker	UNP Q5G244
B	434	GLY	-	linker	UNP Q5G244
B	435	SER	-	linker	UNP Q5G244
B	436	GLY	-	linker	UNP Q5G244
B	437	GLY	-	linker	UNP Q5G244
C	20	ALA	-	expression tag	UNP Q5G244
C	47	ASP	ASN	engineered mutation	UNP Q5G244
C	175	SER	CYS	engineered mutation	UNP Q5G244
C	393	GLN	HIS	engineered mutation	UNP Q5G244
C	433	GLY	-	linker	UNP Q5G244
C	434	GLY	-	linker	UNP Q5G244
C	435	SER	-	linker	UNP Q5G244
C	436	GLY	-	linker	UNP Q5G244
C	437	GLY	-	linker	UNP Q5G244
D	20	ALA	-	expression tag	UNP Q5G244
D	47	ASP	ASN	engineered mutation	UNP Q5G244
D	175	SER	CYS	engineered mutation	UNP Q5G244
D	393	GLN	HIS	engineered mutation	UNP Q5G244
D	433	GLY	-	linker	UNP Q5G244
D	434	GLY	-	linker	UNP Q5G244
D	435	SER	-	linker	UNP Q5G244
D	436	GLY	-	linker	UNP Q5G244
D	437	GLY	-	linker	UNP Q5G244
E	20	ALA	-	expression tag	UNP Q5G244
E	47	ASP	ASN	engineered mutation	UNP Q5G244
E	175	SER	CYS	engineered mutation	UNP Q5G244
E	393	GLN	HIS	engineered mutation	UNP Q5G244
E	433	GLY	-	linker	UNP Q5G244
E	434	GLY	-	linker	UNP Q5G244
E	435	SER	-	linker	UNP Q5G244

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	linker	UNP Q5G244
E	437	GLY	-	linker	UNP Q5G244
F	20	ALA	-	expression tag	UNP Q5G244
F	47	ASP	ASN	engineered mutation	UNP Q5G244
F	175	SER	CYS	engineered mutation	UNP Q5G244
F	393	GLN	HIS	engineered mutation	UNP Q5G244
F	433	GLY	-	linker	UNP Q5G244
F	434	GLY	-	linker	UNP Q5G244
F	435	SER	-	linker	UNP Q5G244
F	436	GLY	-	linker	UNP Q5G244
F	437	GLY	-	linker	UNP Q5G244
G	20	ALA	-	expression tag	UNP Q5G244
G	47	ASP	ASN	engineered mutation	UNP Q5G244
G	175	SER	CYS	engineered mutation	UNP Q5G244
G	393	GLN	HIS	engineered mutation	UNP Q5G244
G	433	GLY	-	linker	UNP Q5G244
G	434	GLY	-	linker	UNP Q5G244
G	435	SER	-	linker	UNP Q5G244
G	436	GLY	-	linker	UNP Q5G244
G	437	GLY	-	linker	UNP Q5G244
H	20	ALA	-	expression tag	UNP Q5G244
H	47	ASP	ASN	engineered mutation	UNP Q5G244
H	175	SER	CYS	engineered mutation	UNP Q5G244
H	393	GLN	HIS	engineered mutation	UNP Q5G244
H	433	GLY	-	linker	UNP Q5G244
H	434	GLY	-	linker	UNP Q5G244
H	435	SER	-	linker	UNP Q5G244
H	436	GLY	-	linker	UNP Q5G244
H	437	GLY	-	linker	UNP Q5G244
I	20	ALA	-	expression tag	UNP Q5G244
I	47	ASP	ASN	engineered mutation	UNP Q5G244
I	175	SER	CYS	engineered mutation	UNP Q5G244
I	393	GLN	HIS	engineered mutation	UNP Q5G244
I	433	GLY	-	linker	UNP Q5G244
I	434	GLY	-	linker	UNP Q5G244
I	435	SER	-	linker	UNP Q5G244
I	436	GLY	-	linker	UNP Q5G244
I	437	GLY	-	linker	UNP Q5G244
J	20	ALA	-	expression tag	UNP Q5G244
J	47	ASP	ASN	engineered mutation	UNP Q5G244
J	175	SER	CYS	engineered mutation	UNP Q5G244
J	393	GLN	HIS	engineered mutation	UNP Q5G244

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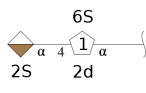
Chain	Residue	Modelled	Actual	Comment	Reference
J	433	GLY	-	linker	UNP Q5G244
J	434	GLY	-	linker	UNP Q5G244
J	435	SER	-	linker	UNP Q5G244
J	436	GLY	-	linker	UNP Q5G244
J	437	GLY	-	linker	UNP Q5G244
K	20	ALA	-	expression tag	UNP Q5G244
K	47	ASP	ASN	engineered mutation	UNP Q5G244
K	175	SER	CYS	engineered mutation	UNP Q5G244
K	393	GLN	HIS	engineered mutation	UNP Q5G244
K	433	GLY	-	linker	UNP Q5G244
K	434	GLY	-	linker	UNP Q5G244
K	435	SER	-	linker	UNP Q5G244
K	436	GLY	-	linker	UNP Q5G244
K	437	GLY	-	linker	UNP Q5G244
L	20	ALA	-	expression tag	UNP Q5G244
L	47	ASP	ASN	engineered mutation	UNP Q5G244
L	175	SER	CYS	engineered mutation	UNP Q5G244
L	393	GLN	HIS	engineered mutation	UNP Q5G244
L	433	GLY	-	linker	UNP Q5G244
L	434	GLY	-	linker	UNP Q5G244
L	435	SER	-	linker	UNP Q5G244
L	436	GLY	-	linker	UNP Q5G244
L	437	GLY	-	linker	UNP Q5G244
M	20	ALA	-	expression tag	UNP Q5G244
M	47	ASP	ASN	engineered mutation	UNP Q5G244
M	175	SER	CYS	engineered mutation	UNP Q5G244
M	393	GLN	HIS	engineered mutation	UNP Q5G244
M	433	GLY	-	linker	UNP Q5G244
M	434	GLY	-	linker	UNP Q5G244
M	435	SER	-	linker	UNP Q5G244
M	436	GLY	-	linker	UNP Q5G244
M	437	GLY	-	linker	UNP Q5G244
N	20	ALA	-	expression tag	UNP Q5G244
N	47	ASP	ASN	engineered mutation	UNP Q5G244
N	175	SER	CYS	engineered mutation	UNP Q5G244
N	393	GLN	HIS	engineered mutation	UNP Q5G244
N	433	GLY	-	linker	UNP Q5G244
N	434	GLY	-	linker	UNP Q5G244
N	435	SER	-	linker	UNP Q5G244
N	436	GLY	-	linker	UNP Q5G244
N	437	GLY	-	linker	UNP Q5G244
O	20	ALA	-	expression tag	UNP Q5G244

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Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	engineered mutation	UNP Q5G244
O	175	SER	CYS	engineered mutation	UNP Q5G244
O	393	GLN	HIS	engineered mutation	UNP Q5G244
O	433	GLY	-	linker	UNP Q5G244
O	434	GLY	-	linker	UNP Q5G244
O	435	SER	-	linker	UNP Q5G244
O	436	GLY	-	linker	UNP Q5G244
O	437	GLY	-	linker	UNP Q5G244

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



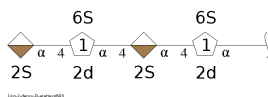
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	P	2	30	12	16	2	0	0	0
2	S	2	30	12	16	2	0	0	0
2	T	2	30	12	16	2	0	0	0
2	U	2	30	12	16	2	0	0	0
2	W	2	30	12	16	2	0	0	0
2	Y	2	30	12	16	2	0	0	0
2	Z	2	30	12	16	2	0	0	0
2	a	2	30	12	16	2	0	0	0
2	d	2	30	12	16	2	0	0	0
2	i	2	30	12	16	2	0	0	0
2	j	2	30	12	16	2	0	0	0
2	k	2	30	12	16	2	0	0	0

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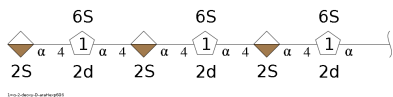
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	l	2	Total 30	C 12	O 16	S 2	0	0	0
2	m	2	Total 30	C 12	O 16	S 2	0	0	0
2	n	2	Total 30	C 12	O 16	S 2	0	0	0
2	o	2	Total 30	C 12	O 16	S 2	0	0	0
2	q	2	Total 30	C 12	O 16	S 2	0	0	0
2	r	2	Total 30	C 12	O 16	S 2	0	0	0
2	s	2	Total 30	C 12	O 16	S 2	0	0	0

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



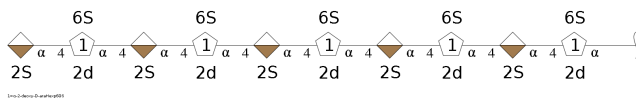
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
3	Q	4	Total 60	C 24	O 32	S 4	0	0	0
3	R	4	Total 60	C 24	O 32	S 4	0	0	0
3	V	4	Total 60	C 24	O 32	S 4	0	0	0
3	X	4	Total 60	C 24	O 32	S 4	0	0	0
3	b	4	Total 60	C 24	O 32	S 4	0	0	0
3	c	4	Total 60	C 24	O 32	S 4	0	0	0
3	g	4	Total 60	C 24	O 32	S 4	0	0	0
3	h	4	Total 60	C 24	O 32	S 4	0	0	0
3	p	4	Total 60	C 24	O 32	S 4	0	0	0

- Molecule 4 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
4	e	6	90	36	48	6	0	0	0

- Molecule 5 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.

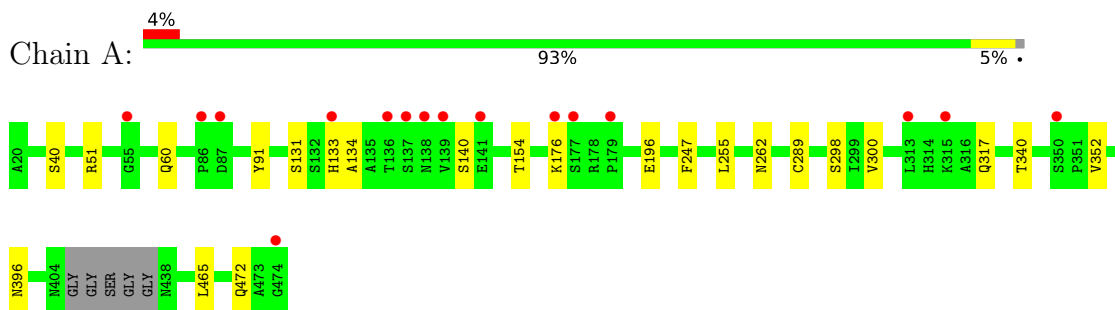


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
5	f	10	150	60	80	10	0	0	0

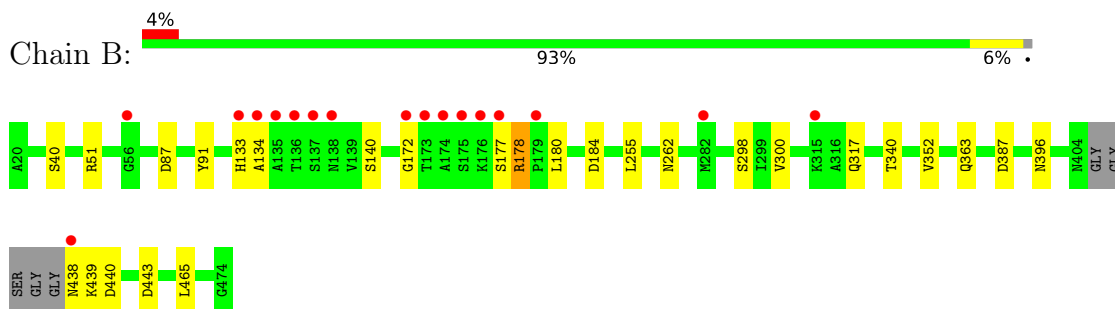
3 Residue-property plots [i](#)

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.

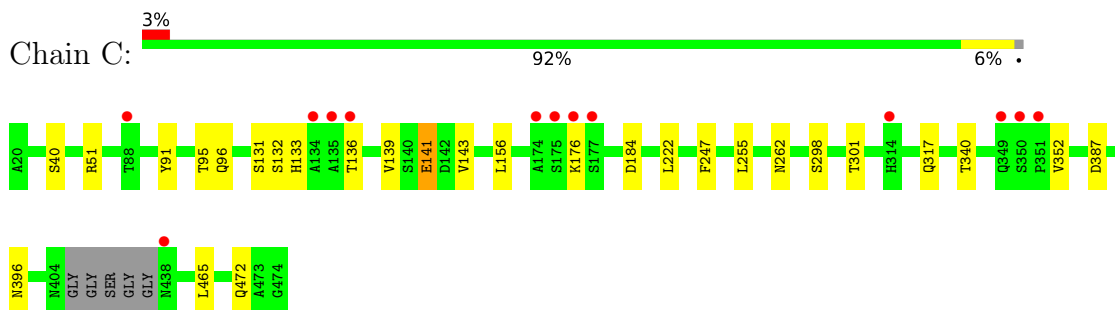
- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1

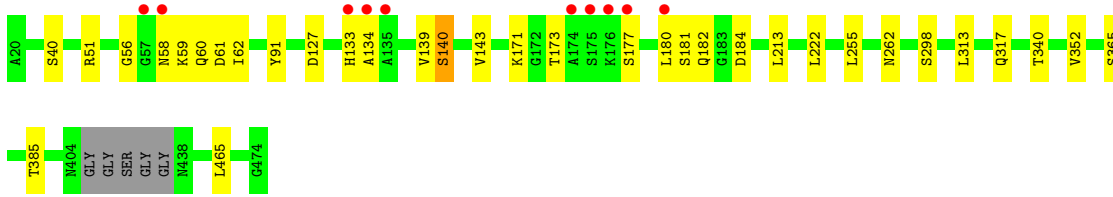


- Molecule 1: Major capsid protein L1

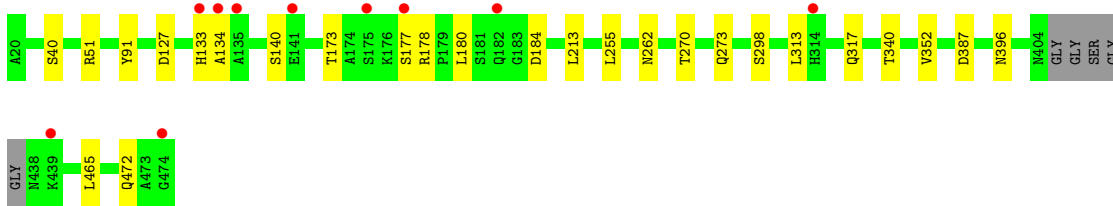


- Molecule 1: Major capsid protein L1

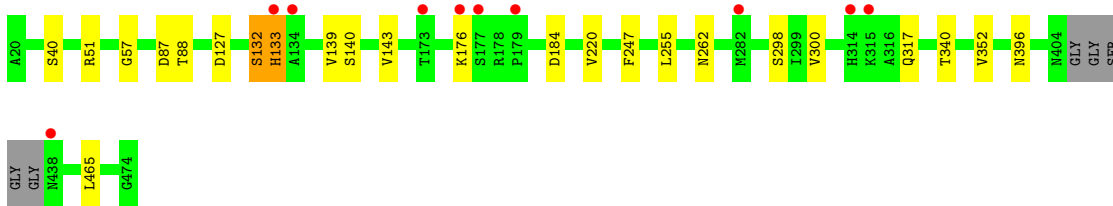
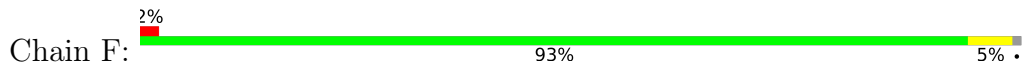




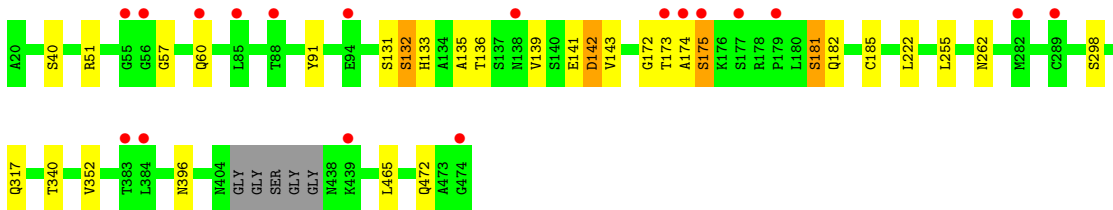
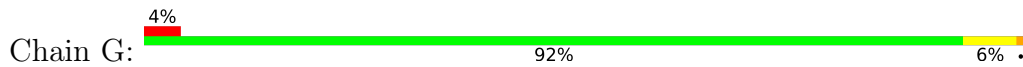
- Molecule 1: Major capsid protein L1



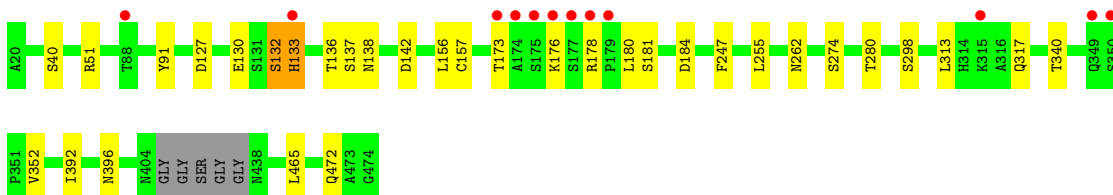
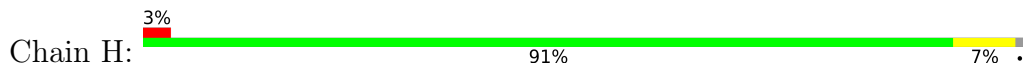
- Molecule 1: Major capsid protein L1



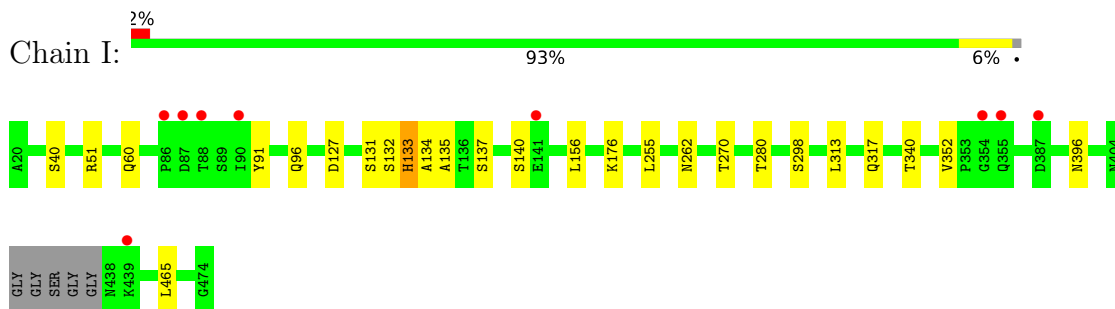
- Molecule 1: Major capsid protein L1



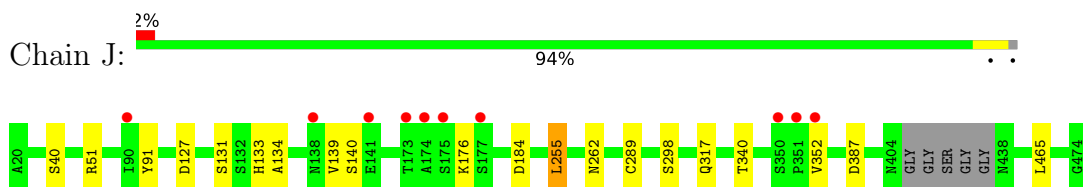
- Molecule 1: Major capsid protein L1



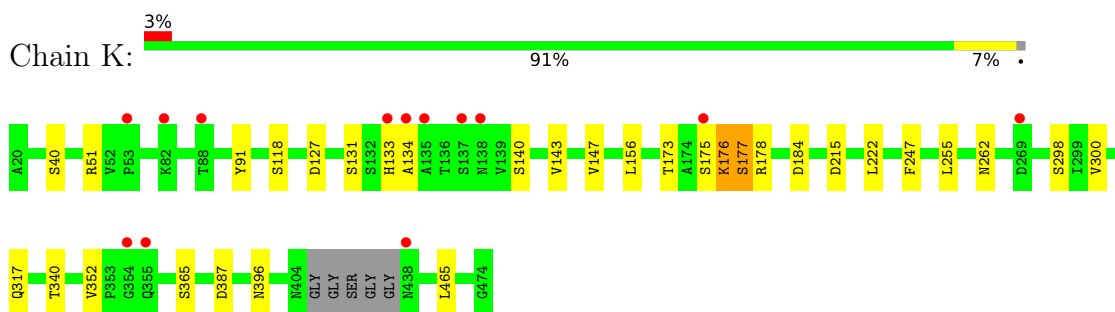
- Molecule 1: Major capsid protein L1



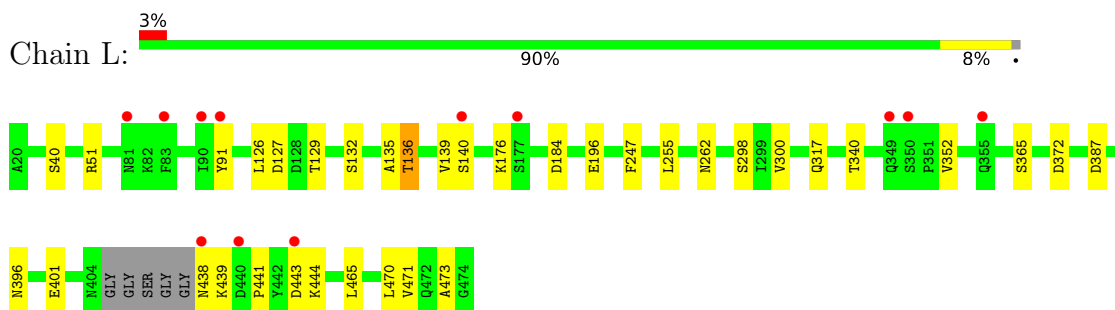
- Molecule 1: Major capsid protein L1



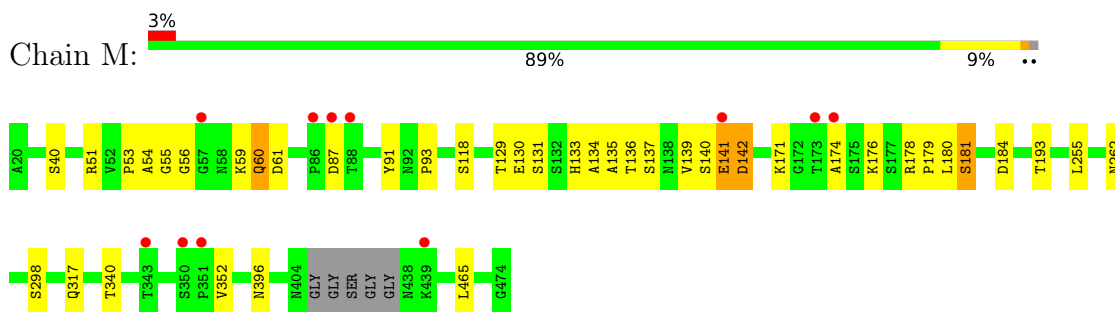
- Molecule 1: Major capsid protein L1



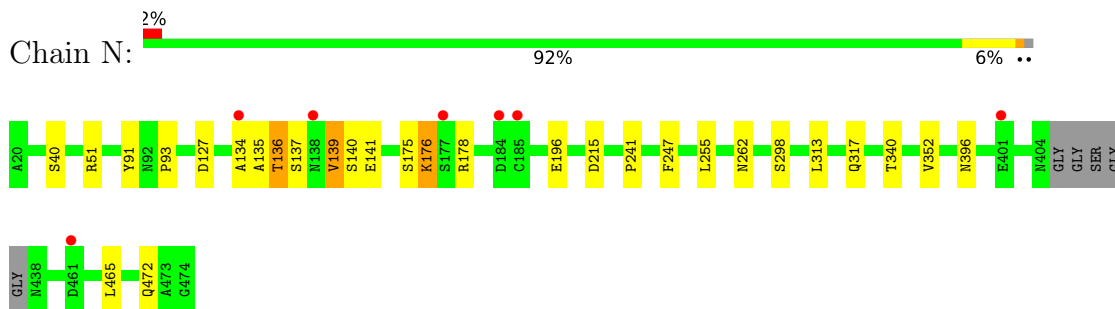
- Molecule 1: Major capsid protein L1



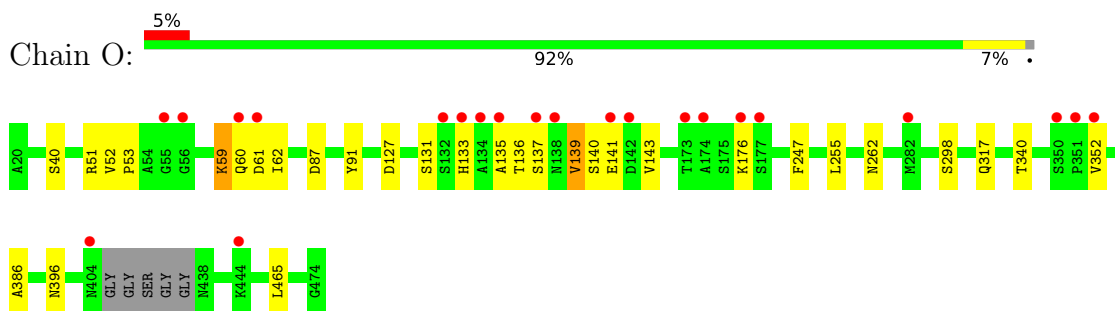
- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1



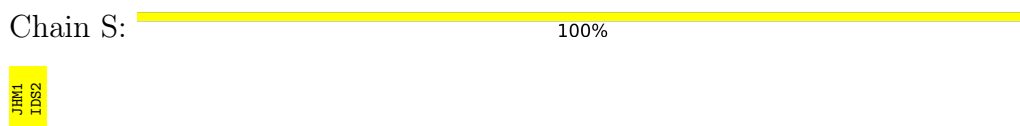
- Molecule 1: Major capsid protein L1



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose



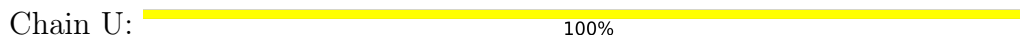
- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose



JHM1
IDS2

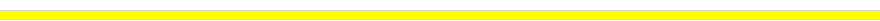
- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain W:  100%JHM1
IDS2

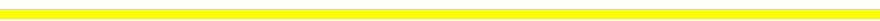
- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Y:  100%JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Z:  100%JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain a:  100%JHM1
IDS2


- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain d:  100%JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

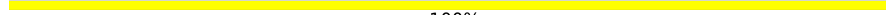
Chain i:  100%JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain j:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain k:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain l:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain m:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain n:  100%


JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain o:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain q:  100%


JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain r:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain s:  100%


JHM1
IDS2

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Q:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain R:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain V:  100%


JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain X:  100%


JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain b:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain c:  100%


JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain g:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain h:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain p:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 4: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain e:  100%

JHM1
IDS2
JHM3
IDS4
JHM5
IDS6

- Molecule 5: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain f:

90%

10%

JHM1
IDS2
JHM3
IDS4
JHM5
IDS6
JHM7
IDS8
JHM9
IDS10

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.99Å 106.49Å 237.66Å 88.46° 85.75° 69.02°	Depositor
Resolution (Å)	42.79 – 3.37 42.79 – 3.37	Depositor EDS
% Data completeness (in resolution range)	89.3 (42.79-3.37) 84.3 (42.79-3.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.171 , 0.234 0.171 , 0.229	Depositor DCC
R_{free} test set	4610 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for -h,-h+k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	51075	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JHM, IDS

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	0.25	0/3400	0.42	0/4622
1	B	0.26	0/3400	0.45	1/4622 (0.0%)
1	C	0.25	0/3400	0.44	0/4622
1	D	0.28	0/3400	0.46	0/4622
1	E	0.25	0/3400	0.44	0/4622
1	F	0.25	0/3400	0.43	0/4622
1	G	0.24	0/3400	0.44	0/4622
1	H	0.25	0/3400	0.45	0/4622
1	I	0.25	0/3400	0.44	0/4622
1	J	0.24	0/3400	0.42	1/4622 (0.0%)
1	K	0.24	0/3400	0.43	0/4622
1	L	0.27	0/3400	0.48	0/4622
1	M	0.29	0/3400	0.46	0/4622
1	N	0.25	0/3400	0.46	0/4622
1	O	0.27	0/3400	0.46	0/4622
All	All	0.26	0/51000	0.45	2/69330 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ARG	NE-CZ-NH1	5.73	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	255	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	133	HIS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	418/427 (98%)	383 (92%)	28 (7%)	7 (2%)	9	36
1	B	418/427 (98%)	380 (91%)	30 (7%)	8 (2%)	8	34
1	C	418/427 (98%)	379 (91%)	31 (7%)	8 (2%)	8	34
1	D	418/427 (98%)	376 (90%)	32 (8%)	10 (2%)	6	30
1	E	418/427 (98%)	382 (91%)	31 (7%)	5 (1%)	13	44
1	F	418/427 (98%)	382 (91%)	28 (7%)	8 (2%)	8	34
1	G	418/427 (98%)	372 (89%)	30 (7%)	16 (4%)	3	21
1	H	418/427 (98%)	371 (89%)	37 (9%)	10 (2%)	6	30
1	I	418/427 (98%)	378 (90%)	29 (7%)	11 (3%)	5	28
1	J	418/427 (98%)	383 (92%)	28 (7%)	7 (2%)	9	36
1	K	418/427 (98%)	382 (91%)	28 (7%)	8 (2%)	8	34
1	L	418/427 (98%)	372 (89%)	31 (7%)	15 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	418/427 (98%)	374 (90%)	23 (6%)	21 (5%)	2	15
1	N	418/427 (98%)	377 (90%)	27 (6%)	14 (3%)	4	24
1	O	418/427 (98%)	372 (89%)	34 (8%)	12 (3%)	4	26
All	All	6270/6405 (98%)	5663 (90%)	447 (7%)	160 (3%)	5	28

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	SER
1	B	177	SER
1	C	132	SER
1	C	133	HIS
1	C	139	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/370 (100%)	353 (96%)	16 (4%)	29	60
1	B	369/370 (100%)	350 (95%)	19 (5%)	24	55
1	C	369/370 (100%)	348 (94%)	21 (6%)	20	52
1	D	369/370 (100%)	344 (93%)	25 (7%)	16	46
1	E	369/370 (100%)	348 (94%)	21 (6%)	20	52
1	F	369/370 (100%)	351 (95%)	18 (5%)	25	57
1	G	369/370 (100%)	350 (95%)	19 (5%)	24	55
1	H	369/370 (100%)	345 (94%)	24 (6%)	17	48
1	I	369/370 (100%)	353 (96%)	16 (4%)	29	60
1	J	369/370 (100%)	356 (96%)	13 (4%)	36	65
1	K	369/370 (100%)	343 (93%)	26 (7%)	15	45
1	L	369/370 (100%)	347 (94%)	22 (6%)	19	50
1	M	369/370 (100%)	345 (94%)	24 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	369/370 (100%)	351 (95%)	18 (5%)	25	57
1	O	369/370 (100%)	348 (94%)	21 (6%)	20	52
All	All	5535/5550 (100%)	5232 (94%)	303 (6%)	21	53

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	340	THR
1	O	62	ILE
1	L	444	LYS
1	M	317	GLN
1	O	340	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 220 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	226	GLN
1	J	462	GLN
1	O	462	GLN
1	N	317	GLN
1	I	308	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

90 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	JHM	P	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	P	2	2	15,15,17	1.95	1 (6%)	15,22,26	2.32	4 (26%)
3	JHM	Q	1	3	15,15,15	1.10	2 (13%)	18,22,22	1.27	2 (11%)
3	IDS	Q	2	3	16,16,17	2.16	3 (18%)	17,24,26	5.21	5 (29%)
3	JHM	Q	3	3	14,14,15	0.95	1 (7%)	18,20,22	1.42	3 (16%)
3	IDS	Q	4	3	15,15,17	1.98	2 (13%)	15,22,26	2.35	4 (26%)
3	JHM	R	1	3	15,15,15	1.09	2 (13%)	18,22,22	1.25	2 (11%)
3	IDS	R	2	3	16,16,17	2.11	2 (12%)	17,24,26	4.08	5 (29%)
3	JHM	R	3	3	14,14,15	0.97	1 (7%)	18,20,22	1.43	3 (16%)
3	IDS	R	4	3	15,15,17	1.97	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	S	1	2	15,15,15	1.10	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	S	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.34	4 (26%)
2	JHM	T	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	T	2	2	15,15,17	1.95	2 (13%)	15,22,26	2.35	4 (26%)
2	JHM	U	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	U	2	2	15,15,17	1.96	2 (13%)	15,22,26	2.33	4 (26%)
3	JHM	V	1	3	15,15,15	1.07	2 (13%)	18,22,22	1.24	2 (11%)
3	IDS	V	2	3	16,16,17	2.04	2 (12%)	17,24,26	3.30	5 (29%)
3	JHM	V	3	3	14,14,15	0.94	1 (7%)	18,20,22	1.42	3 (16%)
3	IDS	V	4	3	15,15,17	1.97	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	W	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	W	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.34	4 (26%)
3	JHM	X	1	3	15,15,15	1.08	2 (13%)	18,22,22	1.26	2 (11%)
3	IDS	X	2	3	16,16,17	1.91	2 (12%)	17,24,26	3.90	5 (29%)
3	JHM	X	3	3	14,14,15	0.95	1 (7%)	18,20,22	1.41	3 (16%)
3	IDS	X	4	3	15,15,17	1.96	2 (13%)	15,22,26	2.35	4 (26%)
2	JHM	Y	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.24	2 (11%)
2	IDS	Y	2	2	15,15,17	1.93	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	Z	1	2	15,15,15	1.10	2 (13%)	18,22,22	1.27	2 (11%)
2	IDS	Z	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.35	4 (26%)
2	JHM	a	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	a	2	2	15,15,17	1.96	1 (6%)	15,22,26	2.33	4 (26%)
3	JHM	b	1	3	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IDS	b	2	3	16,16,17	1.89	1 (6%)	17,24,26	3.08	4 (23%)
3	JHM	b	3	3	14,14,15	0.98	1 (7%)	18,20,22	1.42	3 (16%)
3	IDS	b	4	3	15,15,17	1.96	1 (6%)	15,22,26	2.31	4 (26%)
3	JHM	c	1	3	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
3	IDS	c	2	3	16,16,17	2.26	3 (18%)	17,24,26	5.62	5 (29%)
3	JHM	c	3	3	14,14,15	0.95	1 (7%)	18,20,22	1.43	3 (16%)
3	IDS	c	4	3	15,15,17	1.96	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	d	1	2	15,15,15	1.06	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	d	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.31	4 (26%)
4	JHM	e	1	4	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
4	IDS	e	2	4	16,16,17	2.27	3 (18%)	17,24,26	3.24	6 (35%)
4	JHM	e	3	4	14,14,15	0.95	1 (7%)	18,20,22	1.41	3 (16%)
4	IDS	e	4	4	16,16,17	1.94	2 (12%)	17,24,26	3.11	6 (35%)
4	JHM	e	5	4	14,14,15	0.95	1 (7%)	18,20,22	1.42	3 (16%)
4	IDS	e	6	4	15,15,17	1.98	2 (13%)	15,22,26	2.34	4 (26%)
5	JHM	f	1	5	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
5	IDS	f	10	5	15,15,17	1.94	1 (6%)	15,22,26	2.33	4 (26%)
5	IDS	f	2	5	16,16,17	2.26	2 (12%)	17,24,26	3.59	4 (23%)
5	JHM	f	3	5	14,14,15	0.97	1 (7%)	18,20,22	1.41	3 (16%)
5	IDS	f	4	5	16,16,17	2.21	2 (12%)	17,24,26	3.30	4 (23%)
5	JHM	f	5	5	14,14,15	0.95	1 (7%)	18,20,22	1.43	3 (16%)
5	IDS	f	6	5	16,16,17	1.88	1 (6%)	17,24,26	3.66	4 (23%)
5	JHM	f	7	5	14,14,15	0.96	1 (7%)	18,20,22	1.41	3 (16%)
5	IDS	f	8	5	16,16,17	2.04	2 (12%)	17,24,26	3.63	4 (23%)
5	JHM	f	9	5	14,14,15	0.95	1 (7%)	18,20,22	1.42	3 (16%)
3	JHM	g	1	3	15,15,15	1.07	2 (13%)	18,22,22	1.24	2 (11%)
3	IDS	g	2	3	16,16,17	1.89	1 (6%)	17,24,26	4.15	5 (29%)
3	JHM	g	3	3	14,14,15	0.96	1 (7%)	18,20,22	1.42	3 (16%)
3	IDS	g	4	3	15,15,17	1.94	1 (6%)	15,22,26	2.32	4 (26%)
3	JHM	h	1	3	15,15,15	1.08	2 (13%)	18,22,22	1.24	2 (11%)
3	IDS	h	2	3	16,16,17	1.88	1 (6%)	17,24,26	2.87	5 (29%)
3	JHM	h	3	3	14,14,15	0.96	1 (7%)	18,20,22	1.43	3 (16%)
3	IDS	h	4	3	15,15,17	1.94	1 (6%)	15,22,26	2.33	4 (26%)
2	JHM	i	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	i	2	2	15,15,17	1.99	2 (13%)	15,22,26	2.35	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JHM	j	1	2	15,15,15	1.06	2 (13%)	18,22,22	1.24	2 (11%)
2	IDS	j	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.33	4 (26%)
2	JHM	k	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	k	2	2	15,15,17	1.93	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	l	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	l	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.31	4 (26%)
2	JHM	m	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	m	2	2	15,15,17	1.95	1 (6%)	15,22,26	2.32	4 (26%)
2	JHM	n	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	n	2	2	15,15,17	1.93	1 (6%)	15,22,26	2.33	4 (26%)
2	JHM	o	1	2	15,15,15	1.09	2 (13%)	18,22,22	1.24	2 (11%)
2	IDS	o	2	2	15,15,17	1.94	1 (6%)	15,22,26	2.32	4 (26%)
3	JHM	p	1	3	15,15,15	1.07	2 (13%)	18,22,22	1.25	2 (11%)
3	IDS	p	2	3	16,16,17	1.96	2 (12%)	17,24,26	3.04	5 (29%)
3	JHM	p	3	3	14,14,15	0.94	1 (7%)	18,20,22	1.42	3 (16%)
3	IDS	p	4	3	15,15,17	1.96	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	q	1	2	15,15,15	1.07	2 (13%)	18,22,22	1.26	2 (11%)
2	IDS	q	2	2	15,15,17	1.96	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	r	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	r	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.33	4 (26%)
2	JHM	s	1	2	15,15,15	1.08	2 (13%)	18,22,22	1.25	2 (11%)
2	IDS	s	2	2	15,15,17	1.97	2 (13%)	15,22,26	2.33	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JHM	P	1	2	-	2/6/22/22	0/1/1/1
2	IDS	P	2	2	-	1/9/22/29	0/1/1/1
3	JHM	Q	1	3	-	0/6/22/22	0/1/1/1
3	IDS	Q	2	3	-	0/9/26/29	0/1/1/1
3	JHM	Q	3	3	-	0/6/20/22	0/1/1/1
3	IDS	Q	4	3	-	0/9/22/29	0/1/1/1
3	JHM	R	1	3	-	2/6/22/22	0/1/1/1
3	IDS	R	2	3	-	0/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JHM	R	3	3	-	0/6/20/22	0/1/1/1
3	IDS	R	4	3	-	0/9/22/29	0/1/1/1
2	JHM	S	1	2	-	0/6/22/22	0/1/1/1
2	IDS	S	2	2	-	0/9/22/29	0/1/1/1
2	JHM	T	1	2	-	0/6/22/22	0/1/1/1
2	IDS	T	2	2	-	0/9/22/29	0/1/1/1
2	JHM	U	1	2	-	1/6/22/22	0/1/1/1
2	IDS	U	2	2	-	0/9/22/29	0/1/1/1
3	JHM	V	1	3	-	2/6/22/22	0/1/1/1
3	IDS	V	2	3	-	0/9/26/29	0/1/1/1
3	JHM	V	3	3	-	0/6/20/22	0/1/1/1
3	IDS	V	4	3	-	0/9/22/29	0/1/1/1
2	JHM	W	1	2	-	1/6/22/22	0/1/1/1
2	IDS	W	2	2	-	0/9/22/29	0/1/1/1
3	JHM	X	1	3	-	0/6/22/22	0/1/1/1
3	IDS	X	2	3	-	0/9/26/29	0/1/1/1
3	JHM	X	3	3	-	2/6/20/22	0/1/1/1
3	IDS	X	4	3	-	0/9/22/29	0/1/1/1
2	JHM	Y	1	2	-	2/6/22/22	0/1/1/1
2	IDS	Y	2	2	-	1/9/22/29	0/1/1/1
2	JHM	Z	1	2	-	0/6/22/22	0/1/1/1
2	IDS	Z	2	2	-	0/9/22/29	0/1/1/1
2	JHM	a	1	2	-	2/6/22/22	0/1/1/1
2	IDS	a	2	2	-	1/9/22/29	0/1/1/1
3	JHM	b	1	3	-	2/6/22/22	0/1/1/1
3	IDS	b	2	3	-	0/9/26/29	0/1/1/1
3	JHM	b	3	3	-	2/6/20/22	0/1/1/1
3	IDS	b	4	3	-	1/9/22/29	0/1/1/1
3	JHM	c	1	3	-	0/6/22/22	0/1/1/1
3	IDS	c	2	3	-	0/9/26/29	0/1/1/1
3	JHM	c	3	3	-	1/6/20/22	0/1/1/1
3	IDS	c	4	3	-	0/9/22/29	0/1/1/1
2	JHM	d	1	2	-	2/6/22/22	0/1/1/1
2	IDS	d	2	2	-	1/9/22/29	0/1/1/1
4	JHM	e	1	4	-	1/6/22/22	0/1/1/1
4	IDS	e	2	4	-	0/9/26/29	0/1/1/1
4	JHM	e	3	4	-	1/6/20/22	0/1/1/1
4	IDS	e	4	4	-	0/9/26/29	0/1/1/1
4	JHM	e	5	4	-	1/6/20/22	0/1/1/1
4	IDS	e	6	4	-	0/9/22/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JHM	f	1	5	-	2/6/22/22	0/1/1/1
5	IDS	f	10	5	-	1/9/22/29	0/1/1/1
5	IDS	f	2	5	-	0/9/26/29	0/1/1/1
5	JHM	f	3	5	-	2/6/20/22	0/1/1/1
5	IDS	f	4	5	-	0/9/26/29	0/1/1/1
5	JHM	f	5	5	-	0/6/20/22	0/1/1/1
5	IDS	f	6	5	-	0/9/26/29	0/1/1/1
5	JHM	f	7	5	-	2/6/20/22	0/1/1/1
5	IDS	f	8	5	-	0/9/26/29	0/1/1/1
5	JHM	f	9	5	-	2/6/20/22	0/1/1/1
3	JHM	g	1	3	-	2/6/22/22	0/1/1/1
3	IDS	g	2	3	-	0/9/26/29	0/1/1/1
3	JHM	g	3	3	-	0/6/20/22	0/1/1/1
3	IDS	g	4	3	-	1/9/22/29	0/1/1/1
3	JHM	h	1	3	-	2/6/22/22	0/1/1/1
3	IDS	h	2	3	-	0/9/26/29	0/1/1/1
3	JHM	h	3	3	-	0/6/20/22	0/1/1/1
3	IDS	h	4	3	-	1/9/22/29	0/1/1/1
2	JHM	i	1	2	-	0/6/22/22	0/1/1/1
2	IDS	i	2	2	-	0/9/22/29	0/1/1/1
2	JHM	j	1	2	-	1/6/22/22	0/1/1/1
2	IDS	j	2	2	-	1/9/22/29	0/1/1/1
2	JHM	k	1	2	-	1/6/22/22	0/1/1/1
2	IDS	k	2	2	-	1/9/22/29	0/1/1/1
2	JHM	l	1	2	-	1/6/22/22	0/1/1/1
2	IDS	l	2	2	-	1/9/22/29	0/1/1/1
2	JHM	m	1	2	-	0/6/22/22	0/1/1/1
2	IDS	m	2	2	-	1/9/22/29	0/1/1/1
2	JHM	n	1	2	-	0/6/22/22	0/1/1/1
2	IDS	n	2	2	-	1/9/22/29	0/1/1/1
2	JHM	o	1	2	-	2/6/22/22	0/1/1/1
2	IDS	o	2	2	-	1/9/22/29	0/1/1/1
3	JHM	p	1	3	-	1/6/22/22	0/1/1/1
3	IDS	p	2	3	-	0/9/26/29	0/1/1/1
3	JHM	p	3	3	-	1/6/20/22	0/1/1/1
3	IDS	p	4	3	-	0/9/22/29	0/1/1/1
2	JHM	q	1	2	-	1/6/22/22	0/1/1/1
2	IDS	q	2	2	-	0/9/22/29	0/1/1/1
2	JHM	r	1	2	-	1/6/22/22	0/1/1/1
2	IDS	r	2	2	-	0/9/22/29	0/1/1/1
2	JHM	s	1	2	-	1/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDS	s	2	2	-	0/9/22/29	0/1/1/1

The worst 5 of 150 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	IDS	O2-C2	-6.59	1.37	1.47
2	i	2	IDS	O2-C2	-6.59	1.37	1.47
3	Q	4	IDS	O2-C2	-6.57	1.37	1.47
2	m	2	IDS	O2-C2	-6.56	1.37	1.47
3	b	4	IDS	O2-C2	-6.55	1.37	1.47

The worst 5 of 297 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	2	IDS	O4-C4-C5	20.18	155.01	109.74
3	Q	2	IDS	O4-C4-C5	18.11	150.35	109.74
3	R	2	IDS	O4-C4-C3	14.12	143.00	110.35
3	g	2	IDS	O4-C4-C5	13.52	140.07	109.74
3	X	2	IDS	O4-C4-C3	13.36	141.24	110.35

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

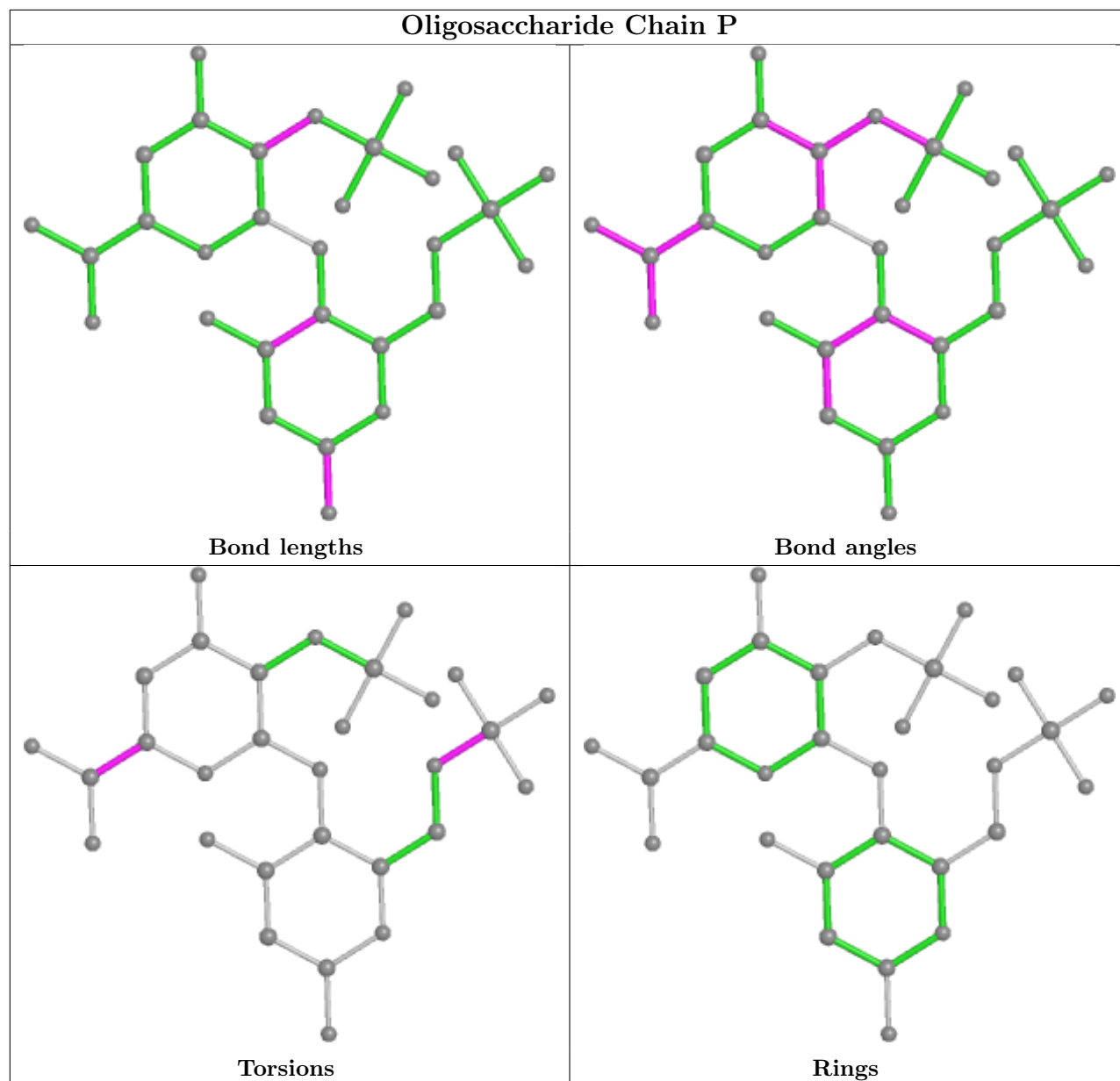
Mol	Chain	Res	Type	Atoms
2	P	1	JHM	C6-O6-S-O8
2	Y	1	JHM	C6-O6-S-O8
2	a	1	JHM	C6-O6-S-O8
2	d	1	JHM	C6-O6-S-O8
2	o	1	JHM	C6-O6-S-O8

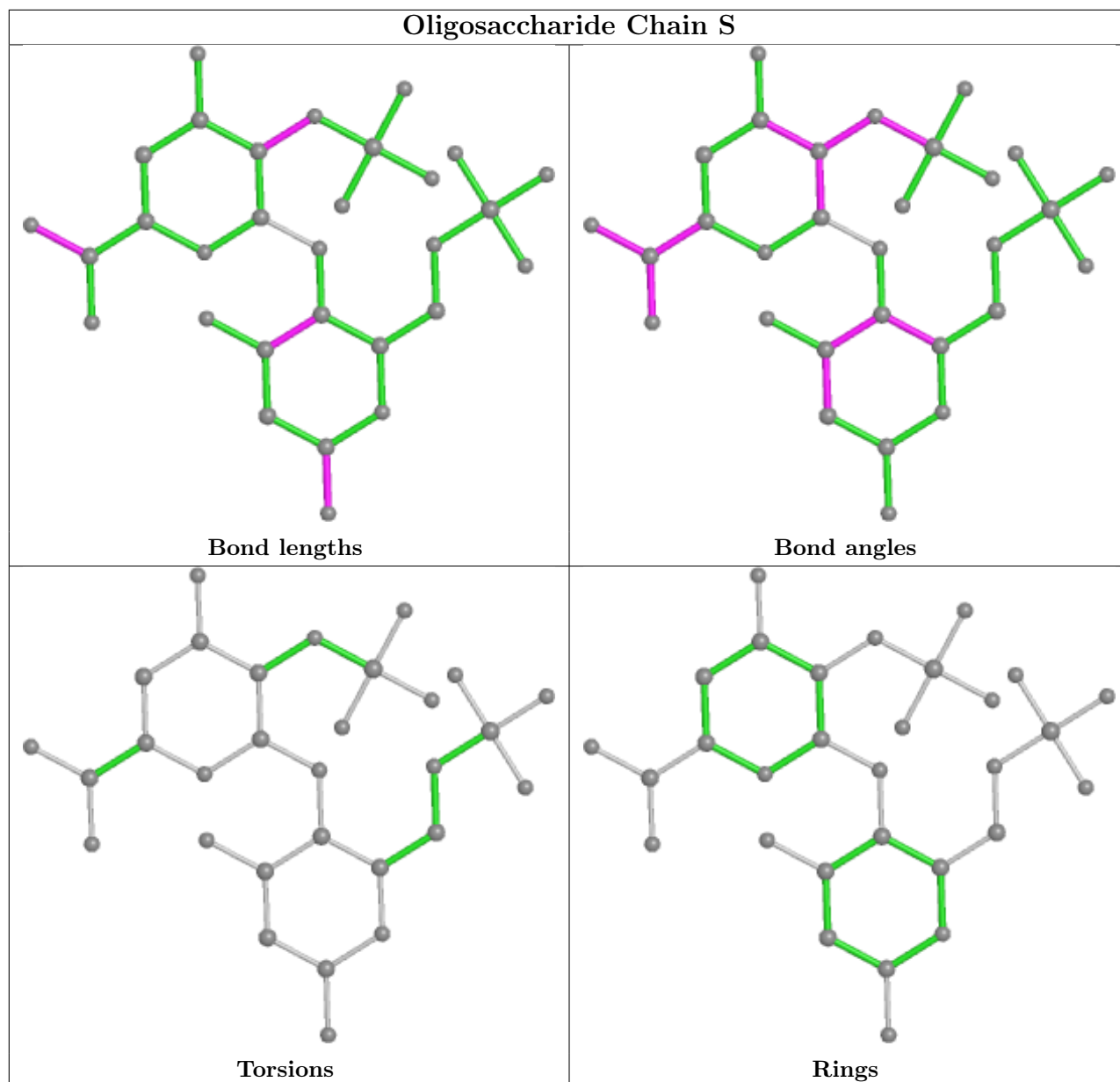
There are no ring outliers.

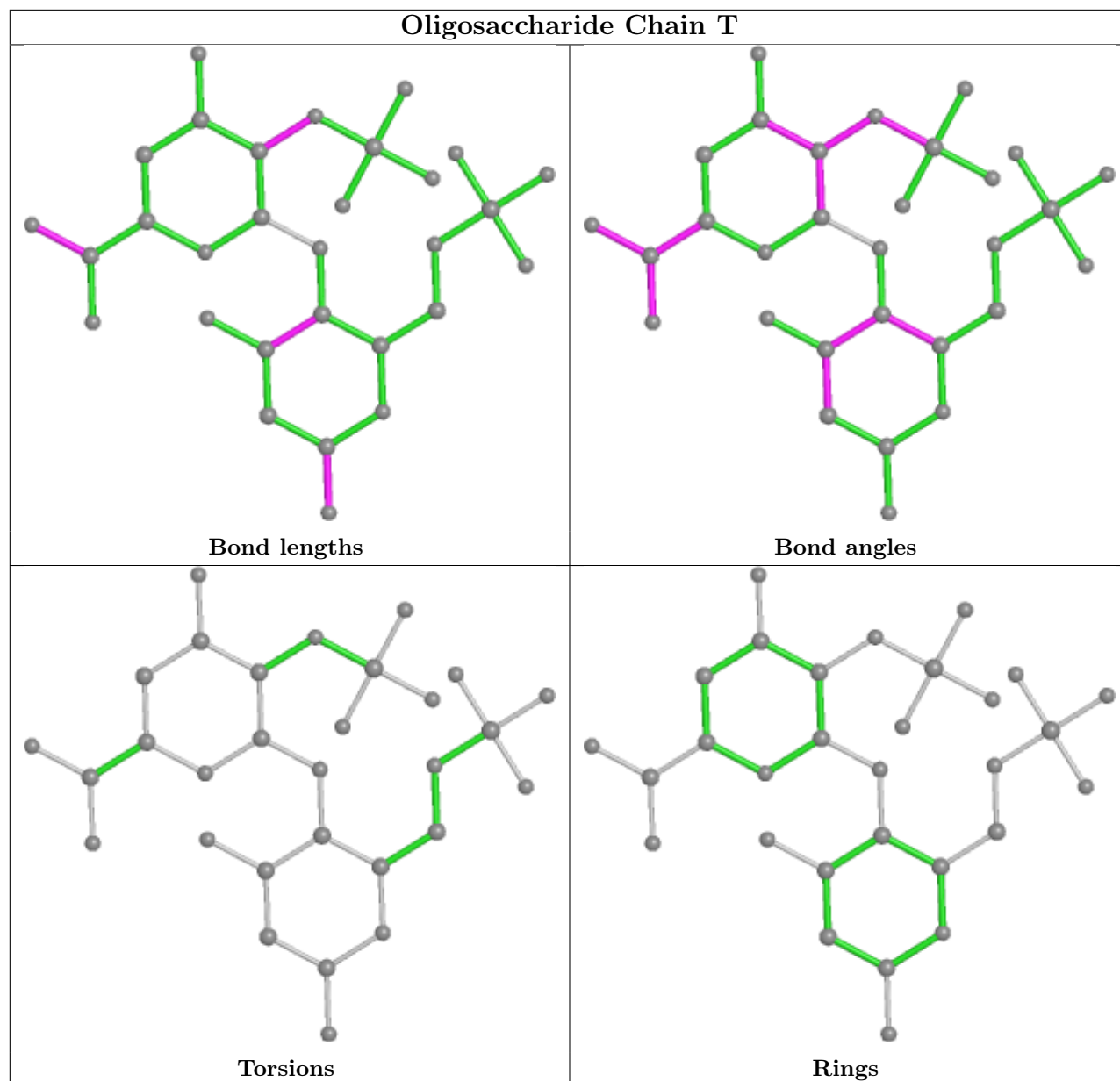
1 monomer is involved in 1 short contact:

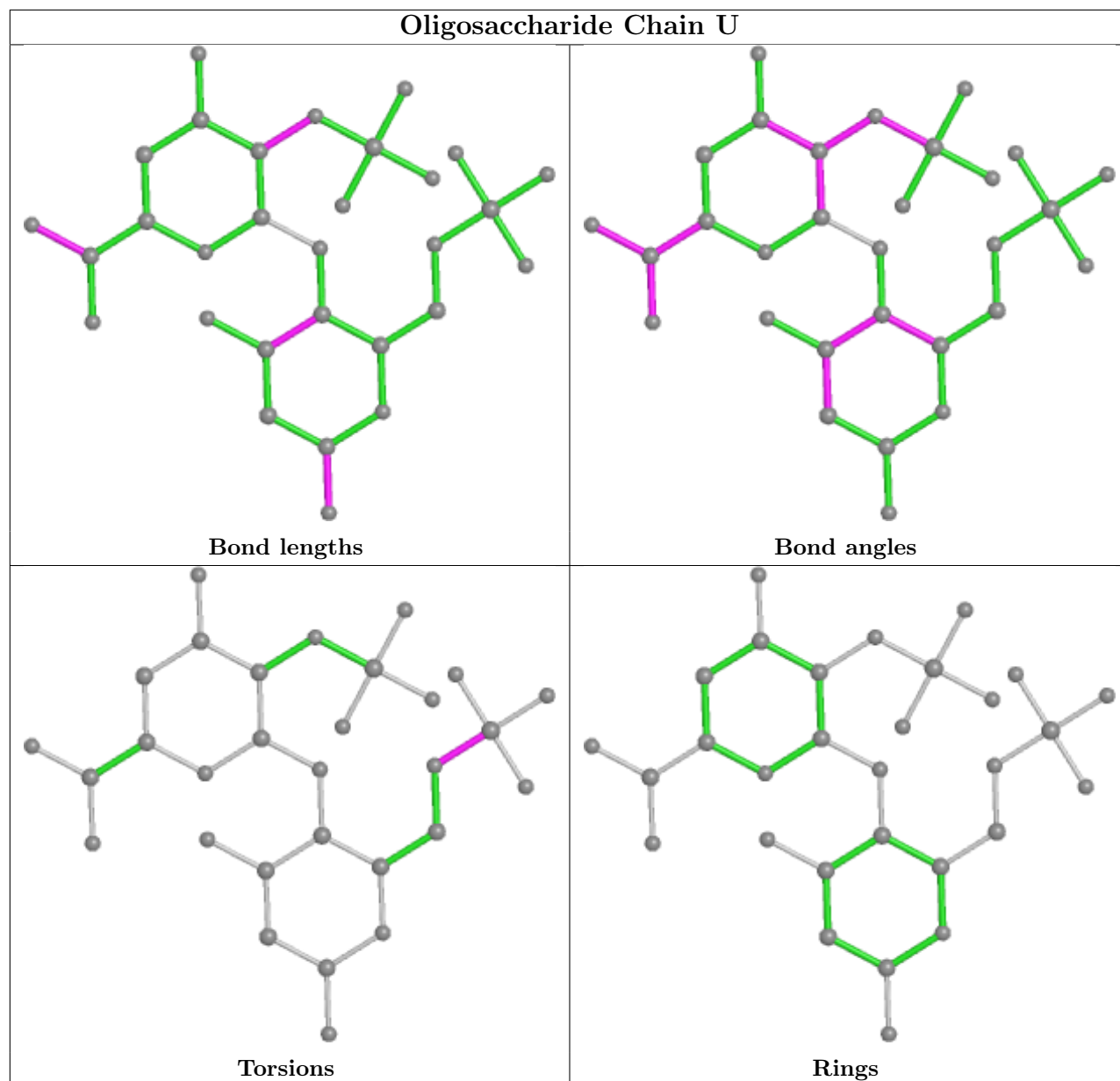
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	f	3	JHM	0	1

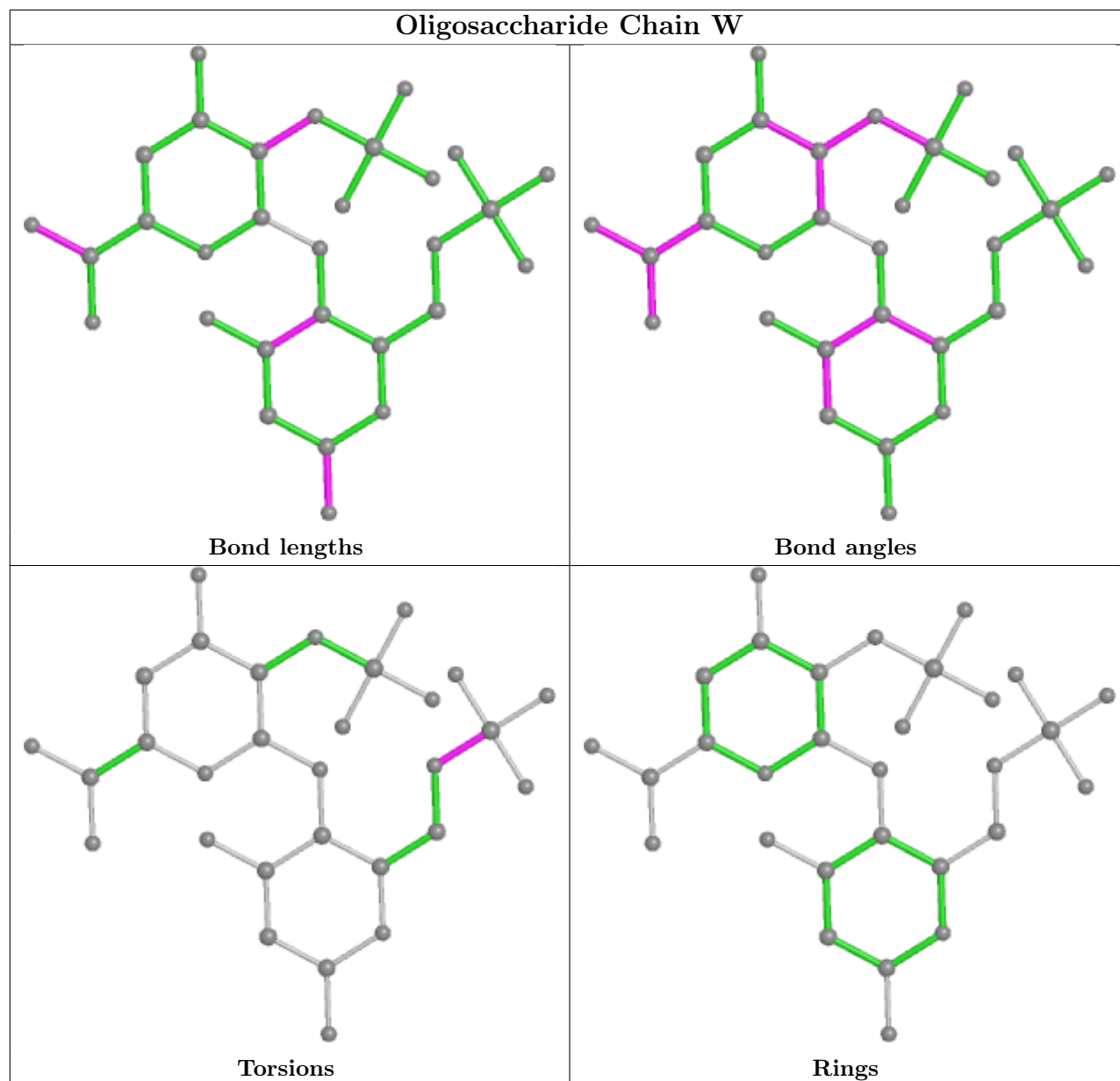
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

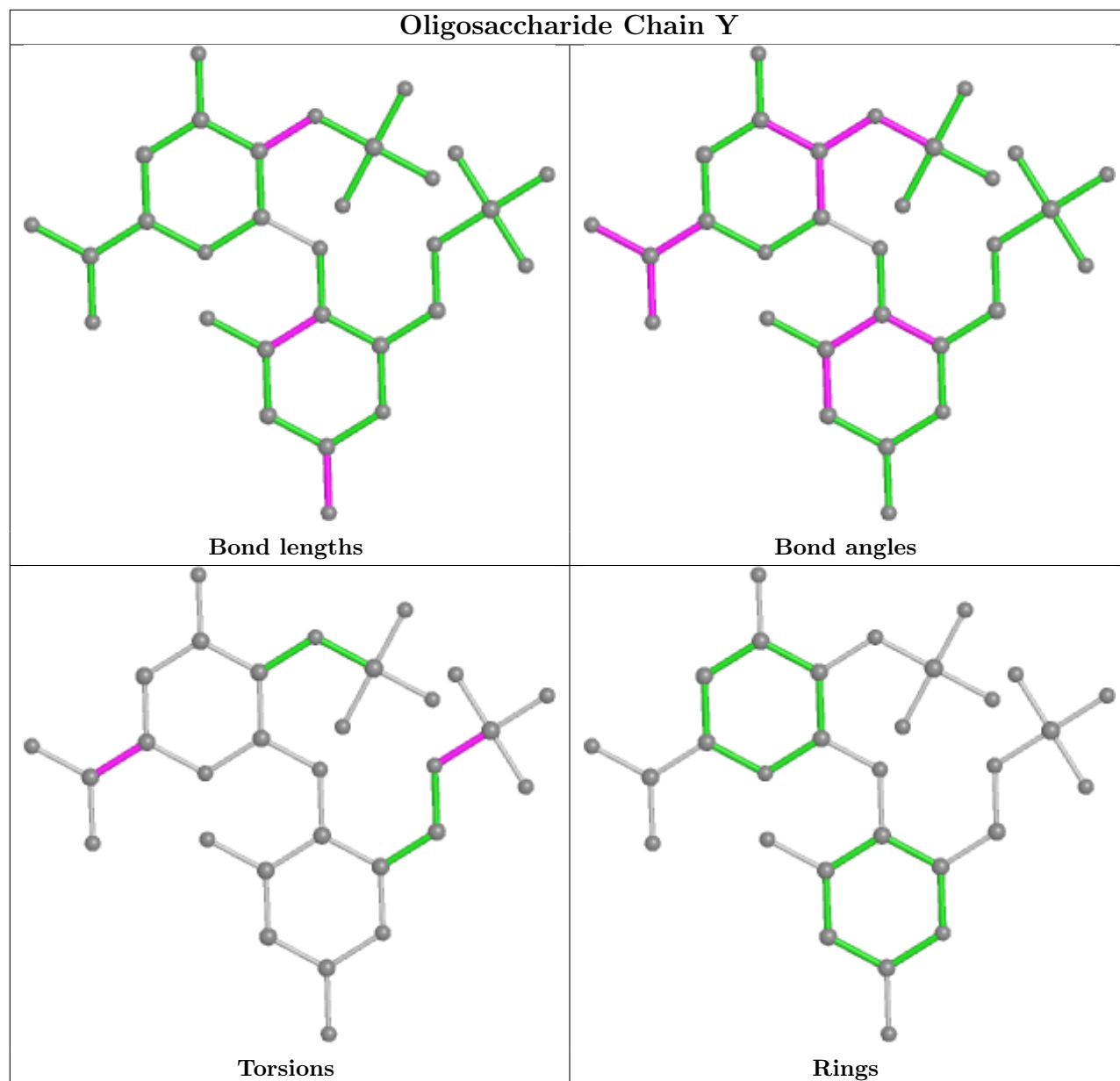


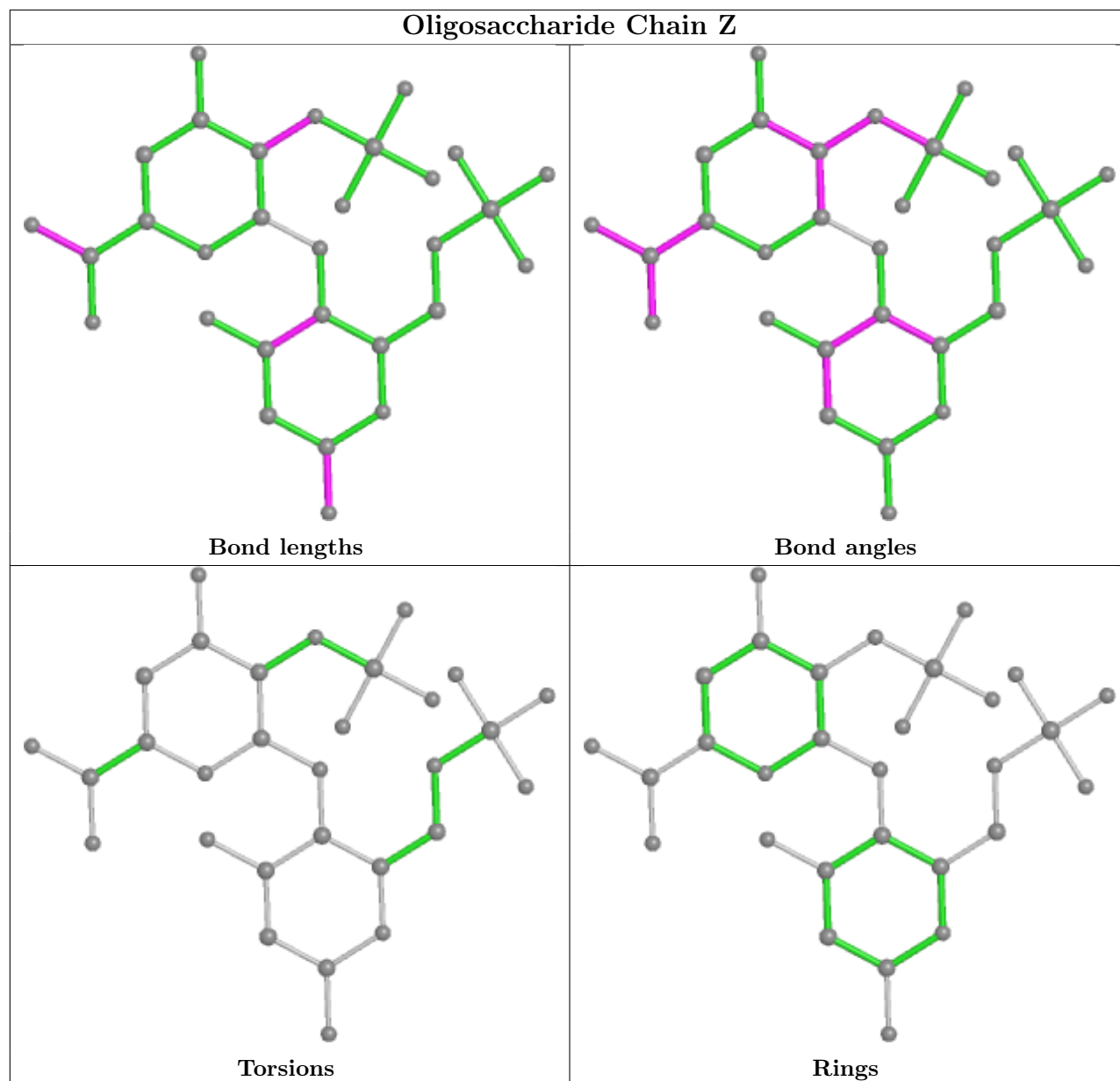


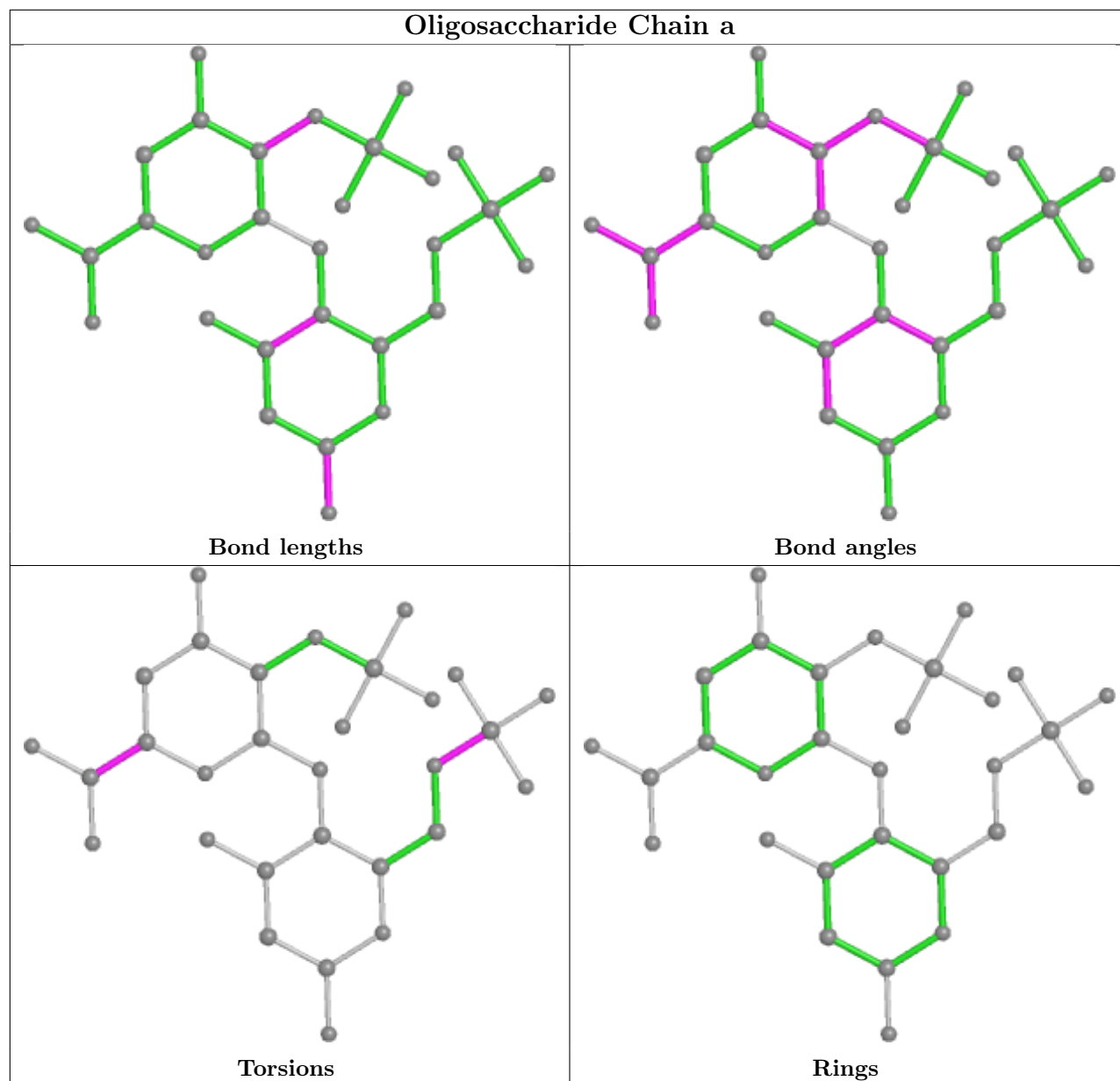


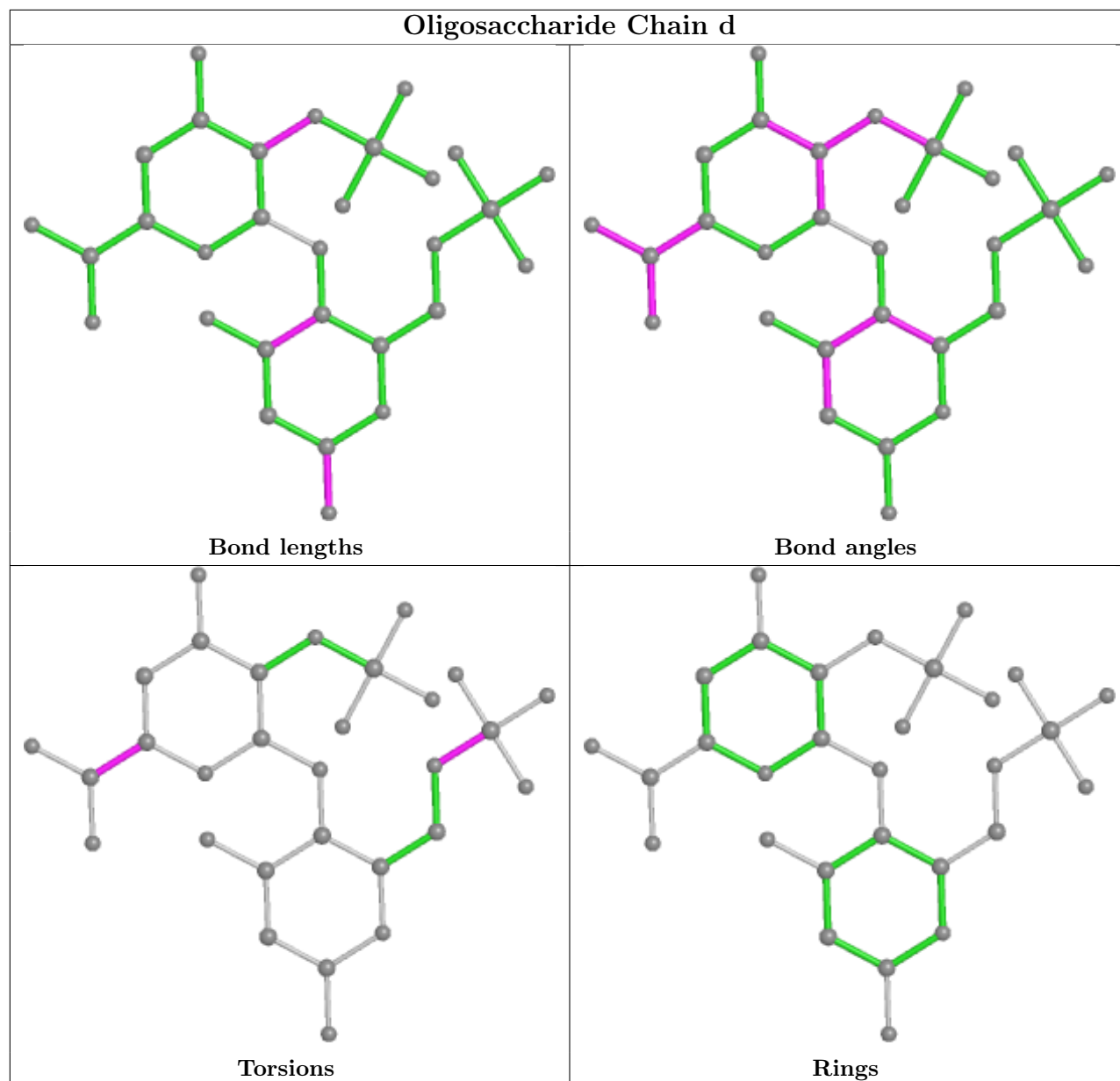


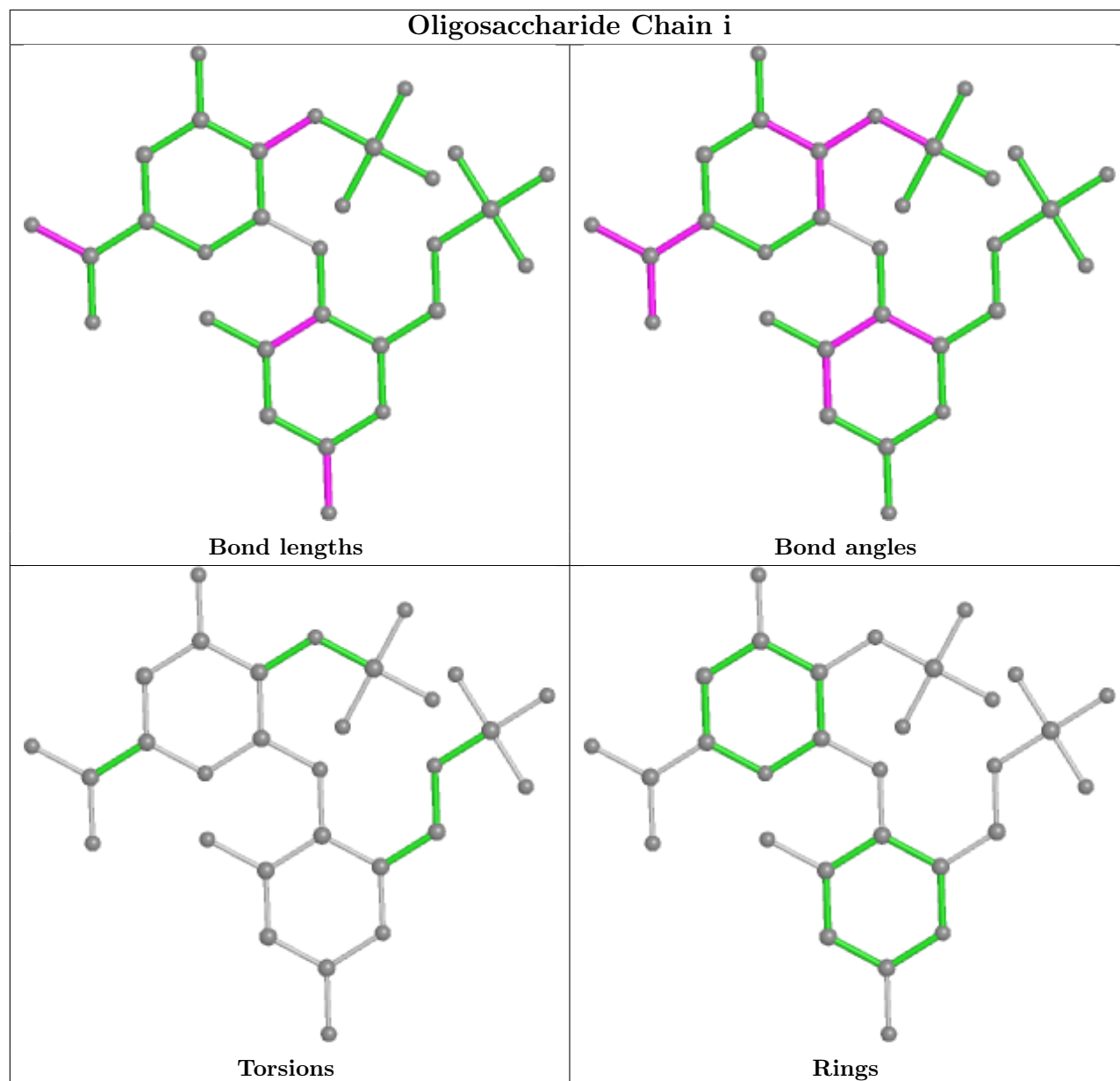


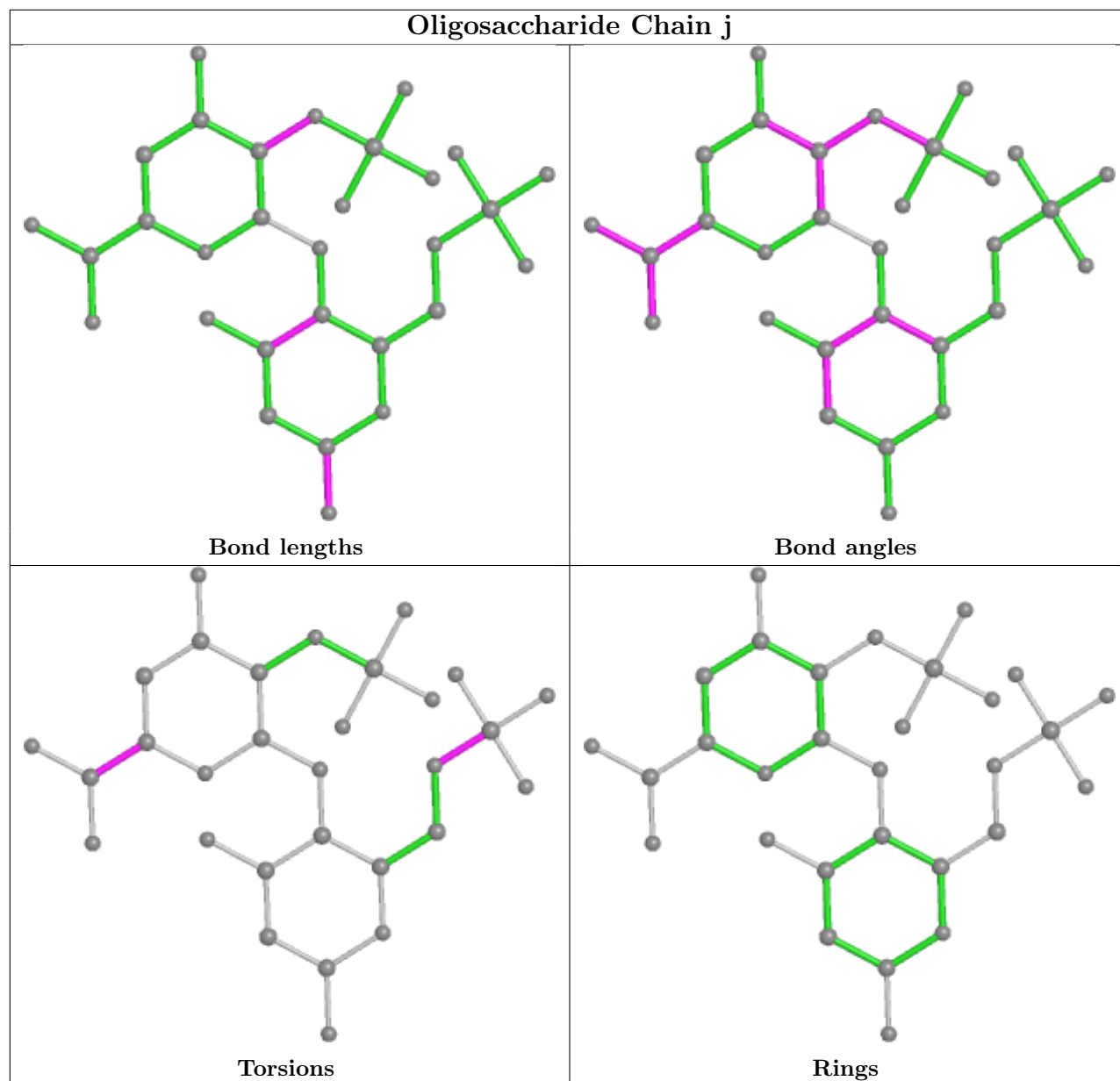


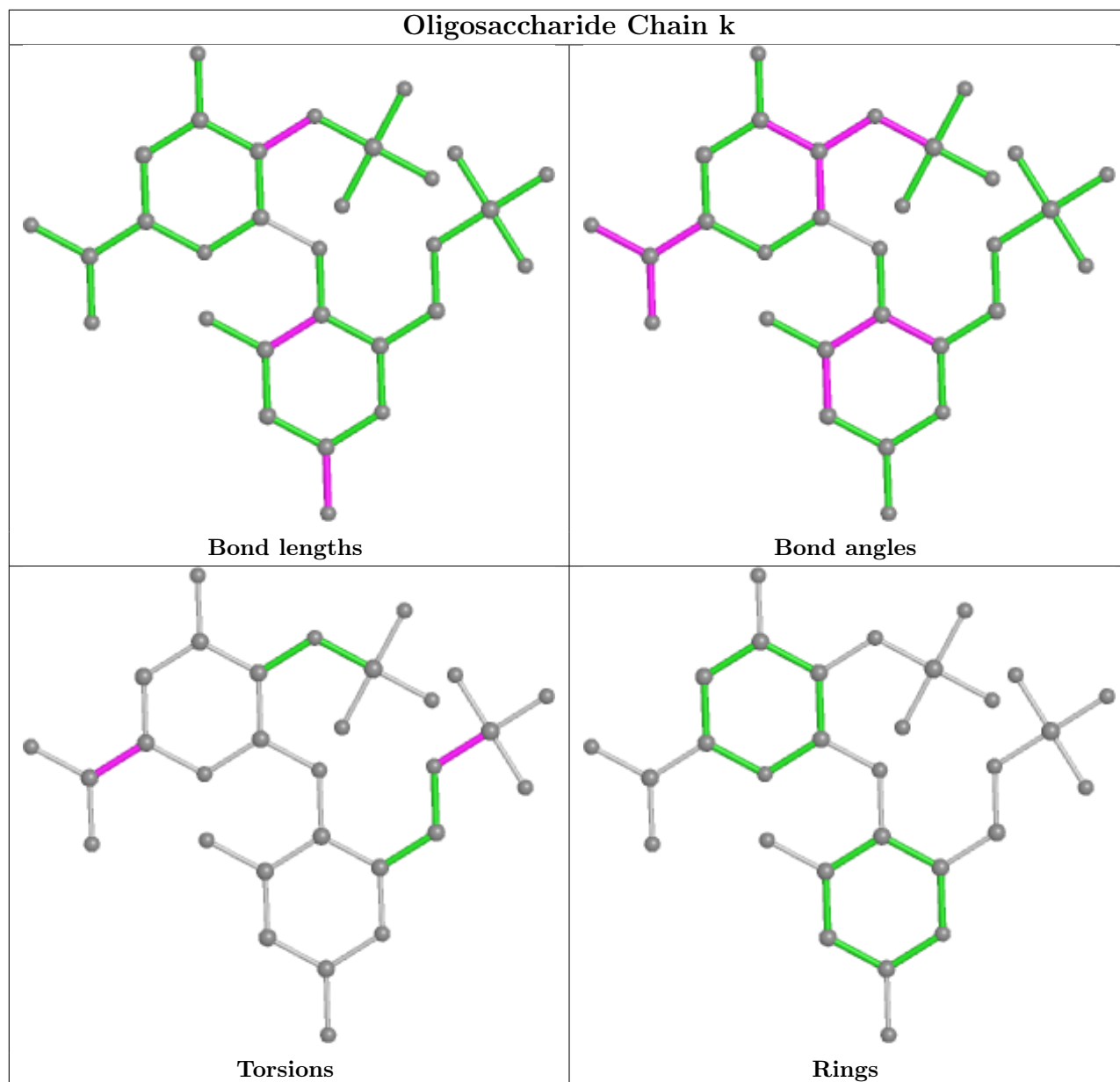


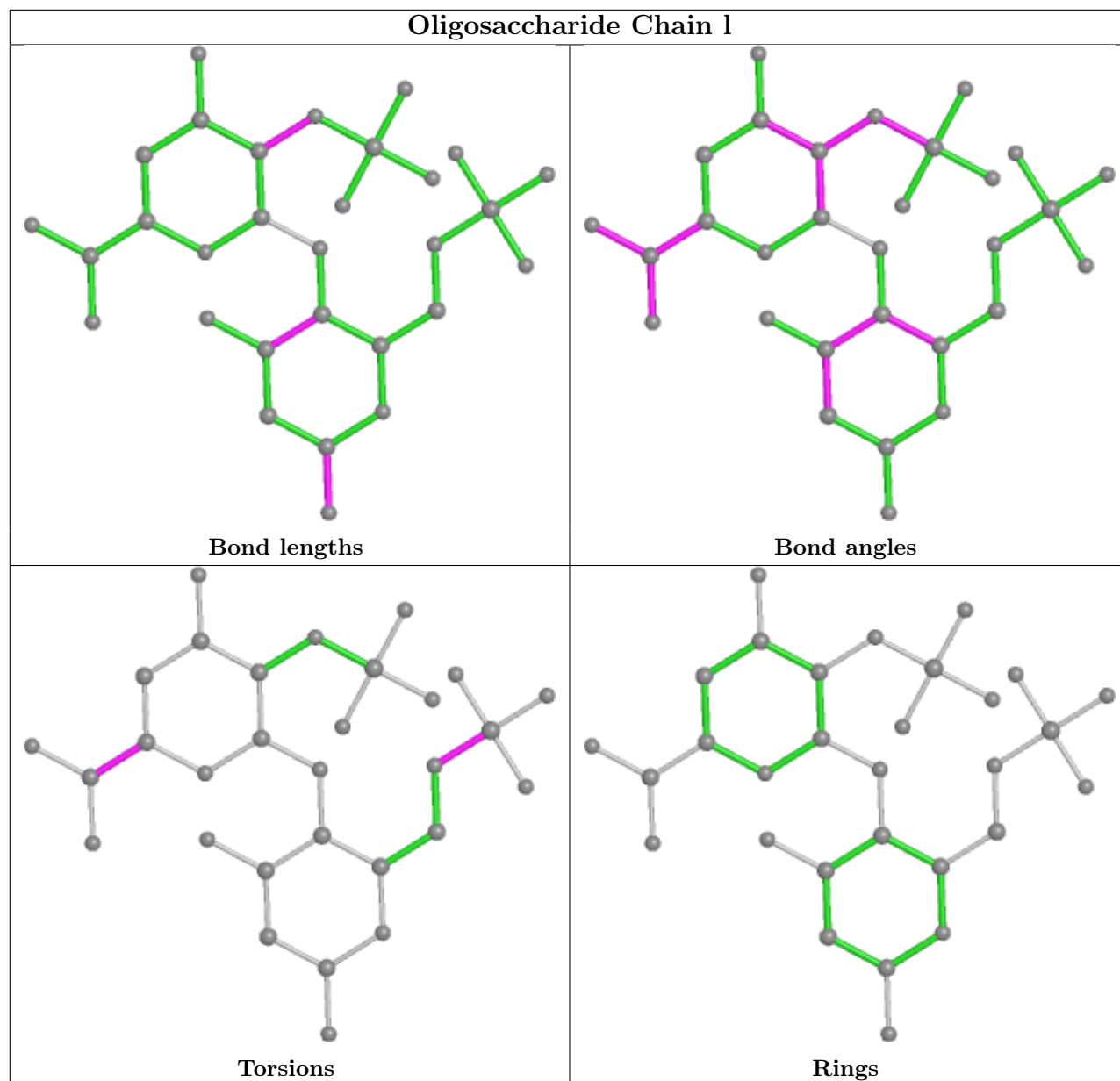


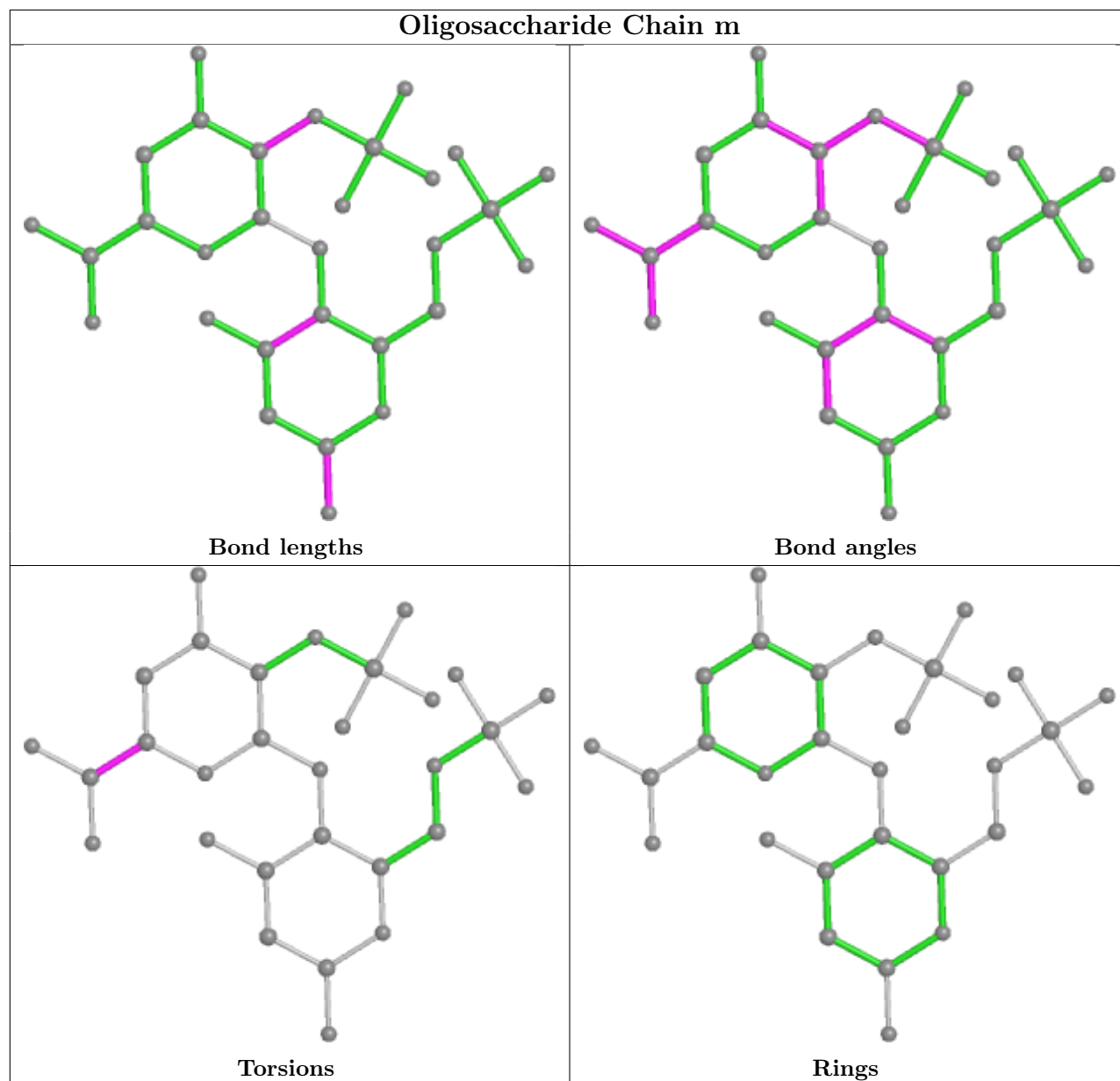


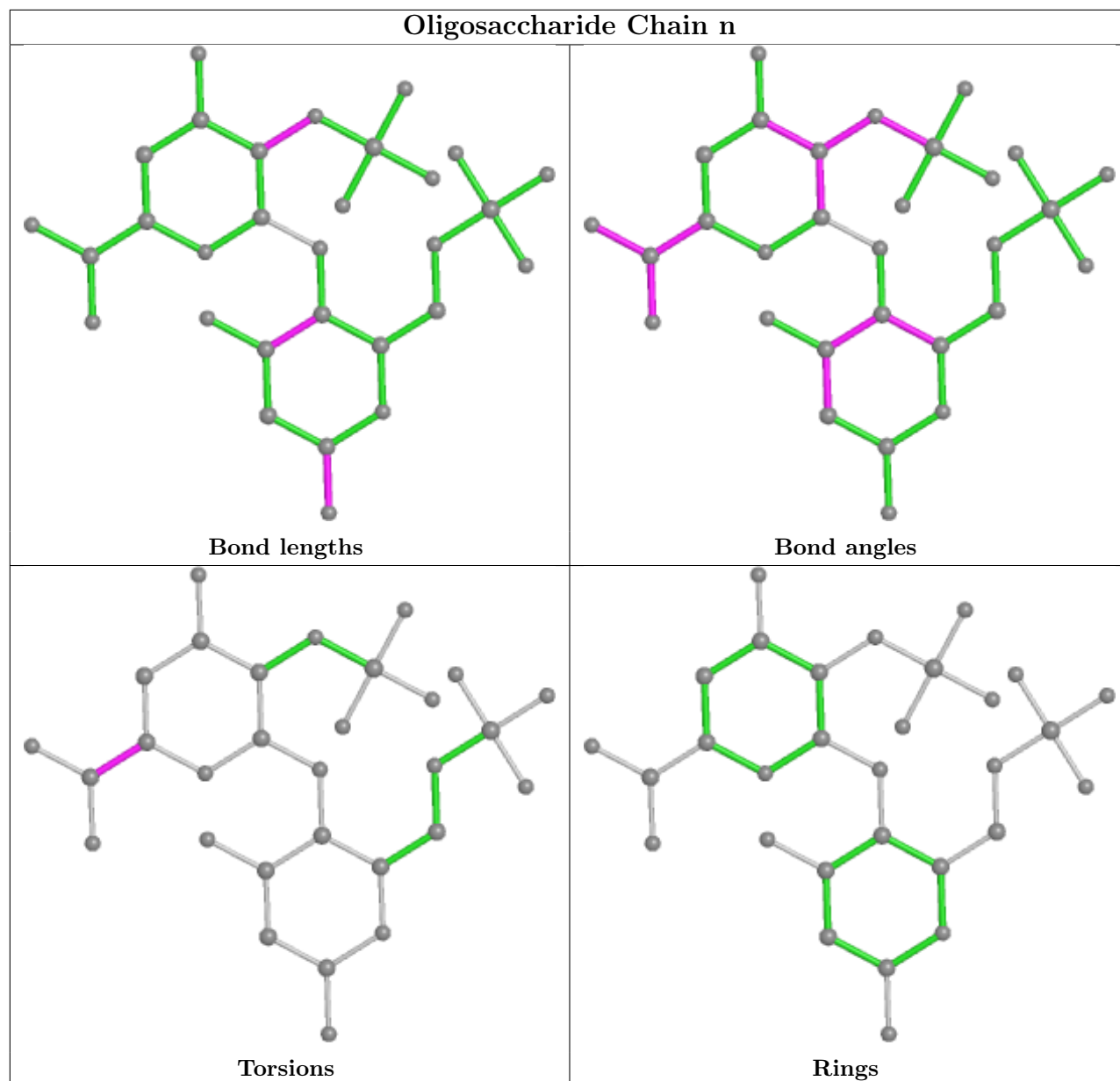


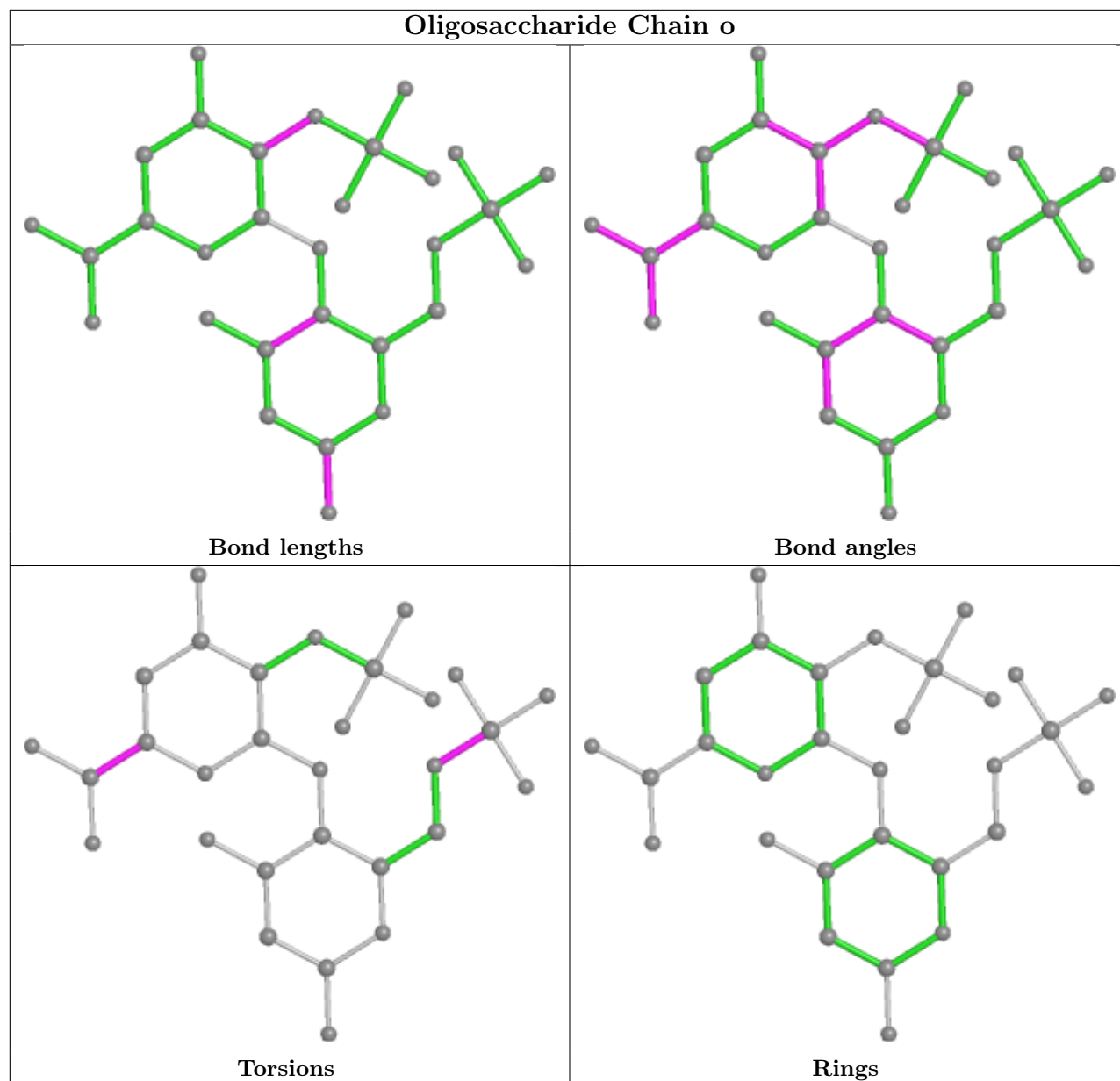


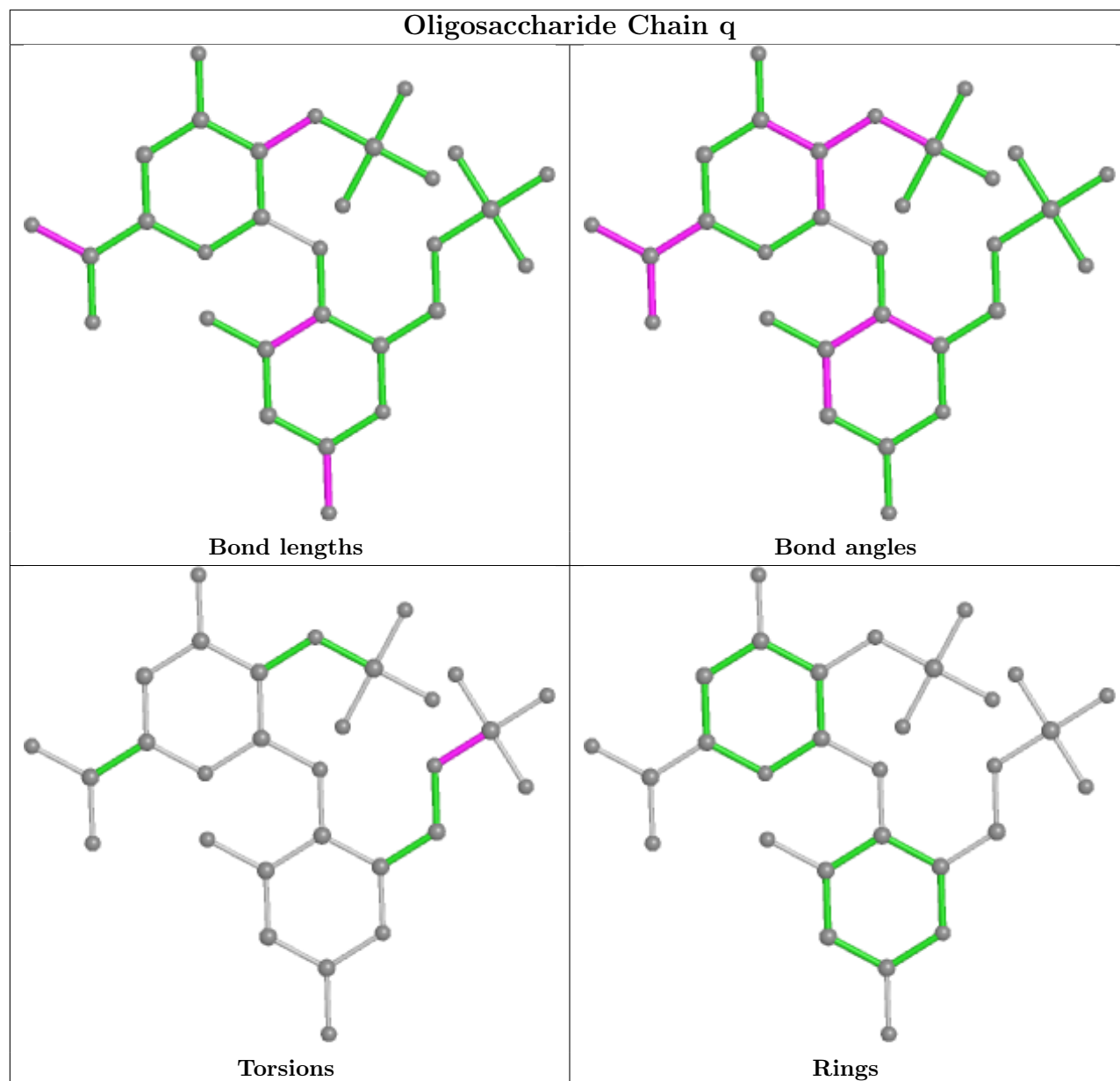


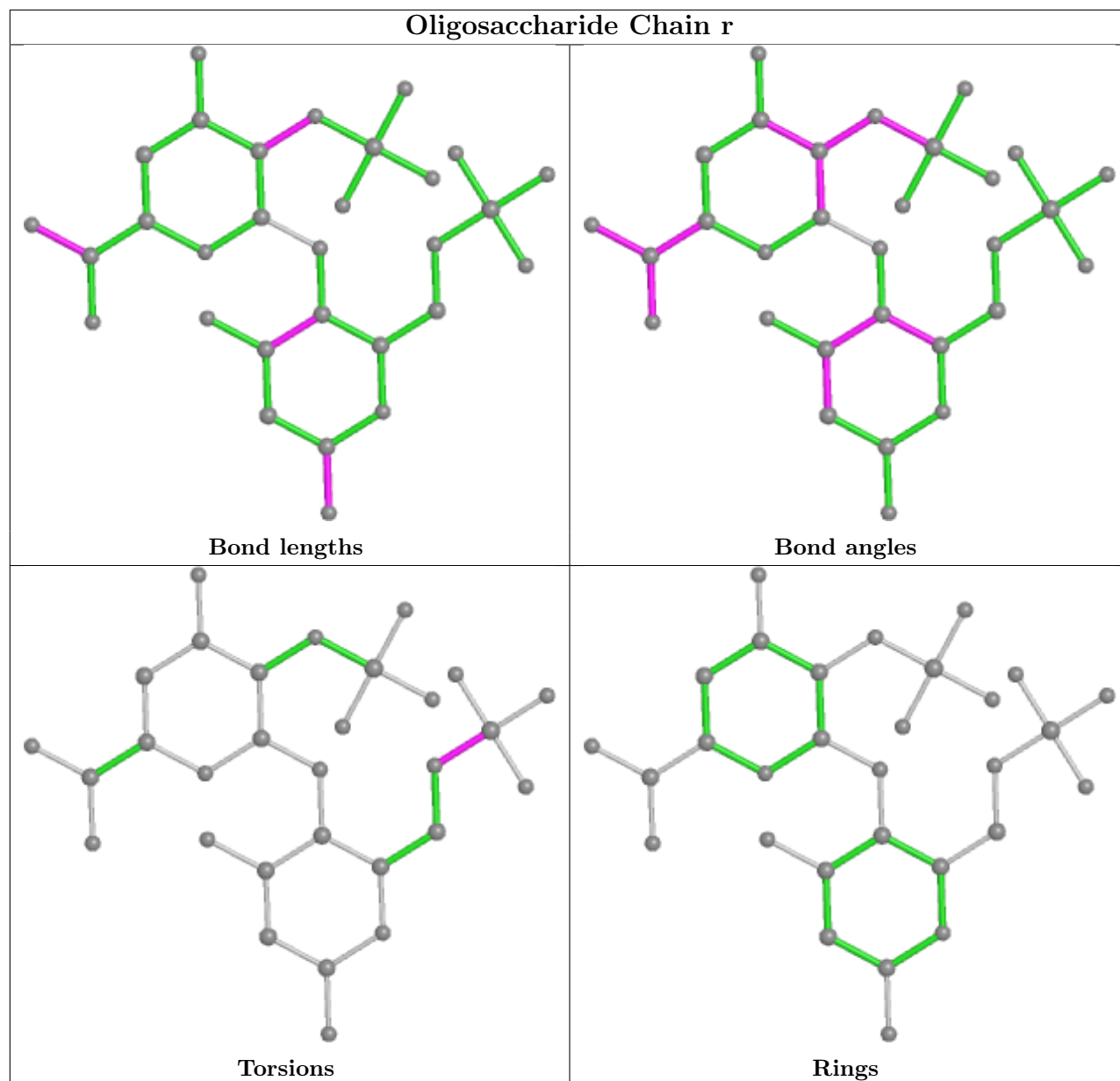


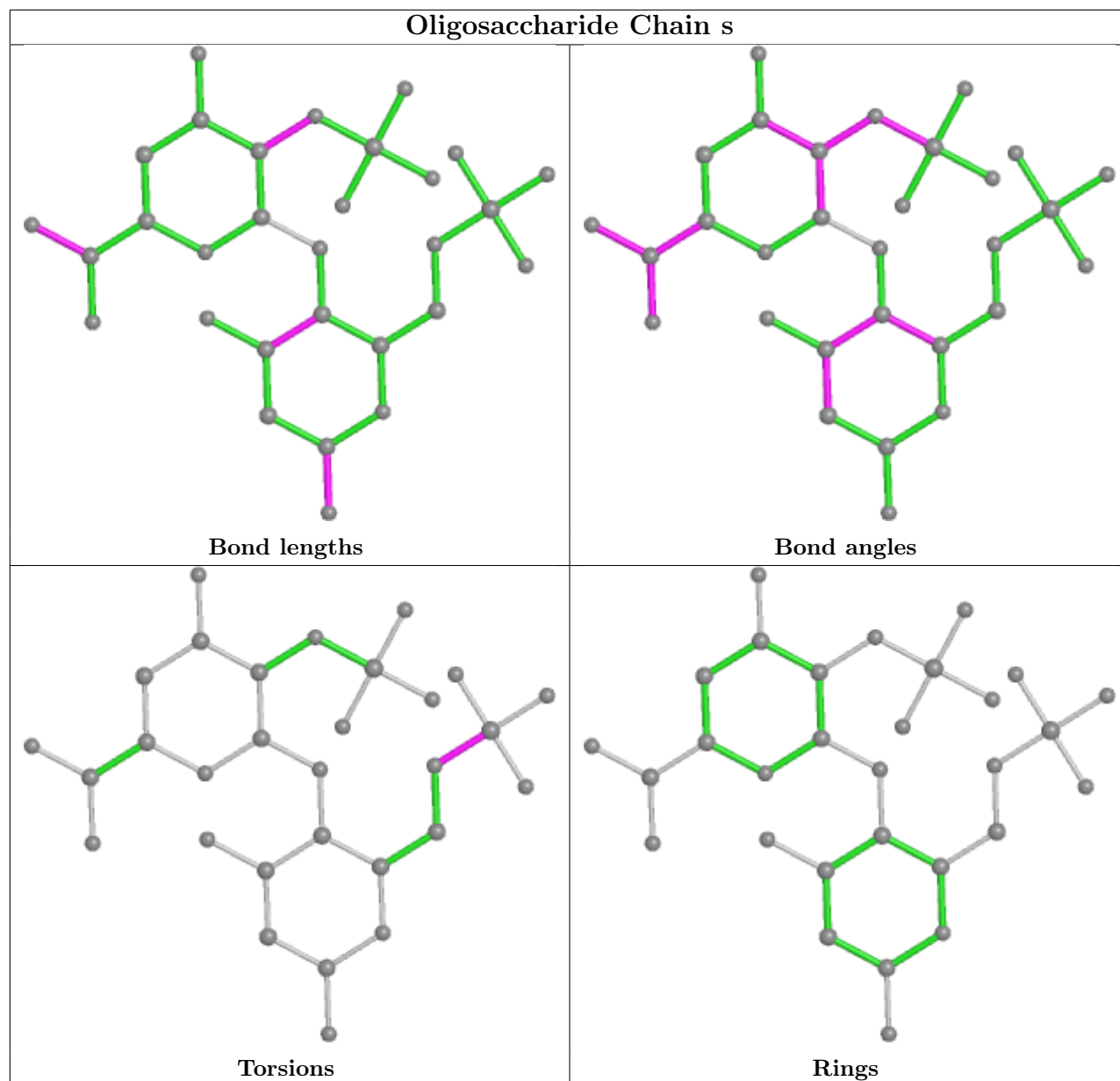


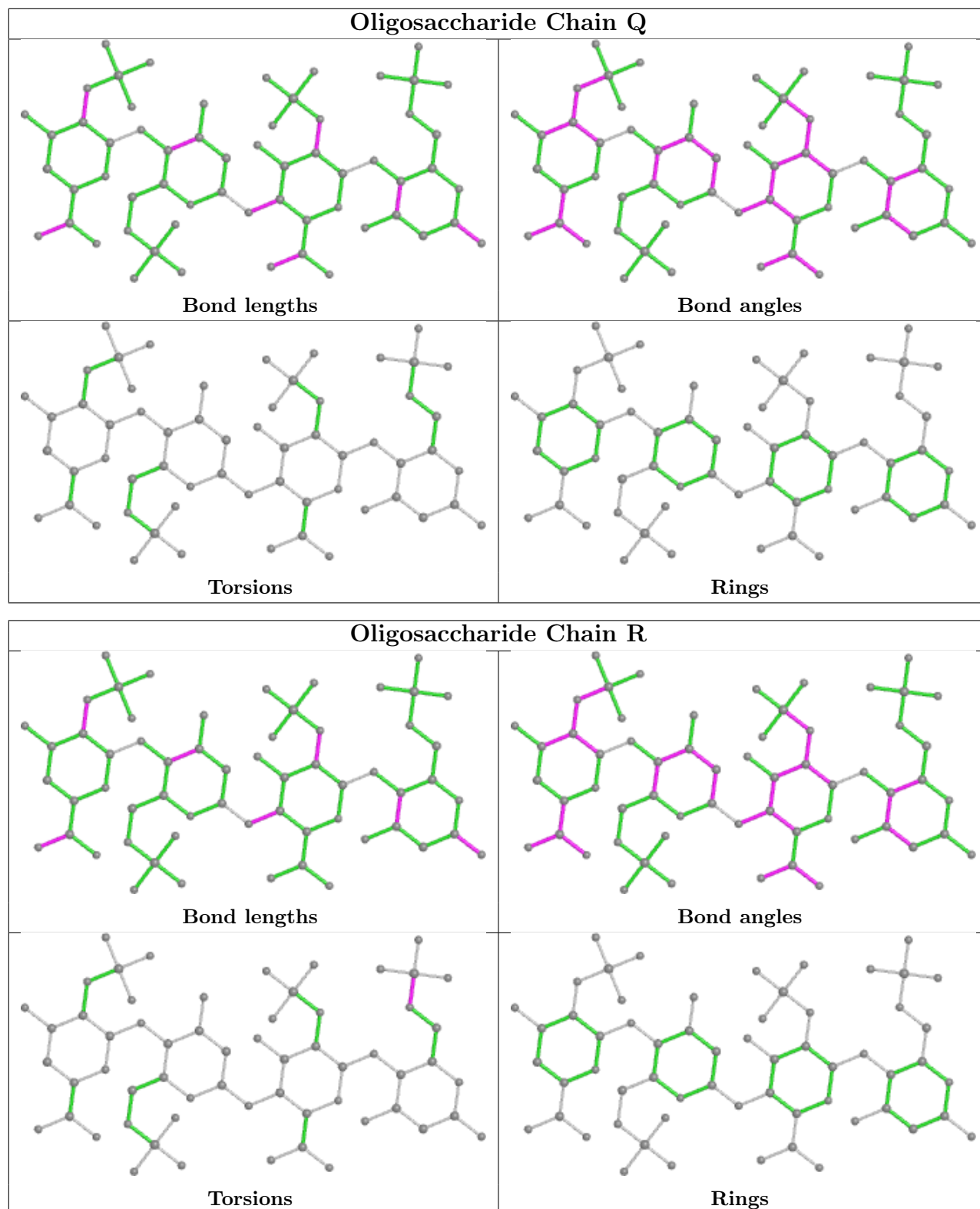


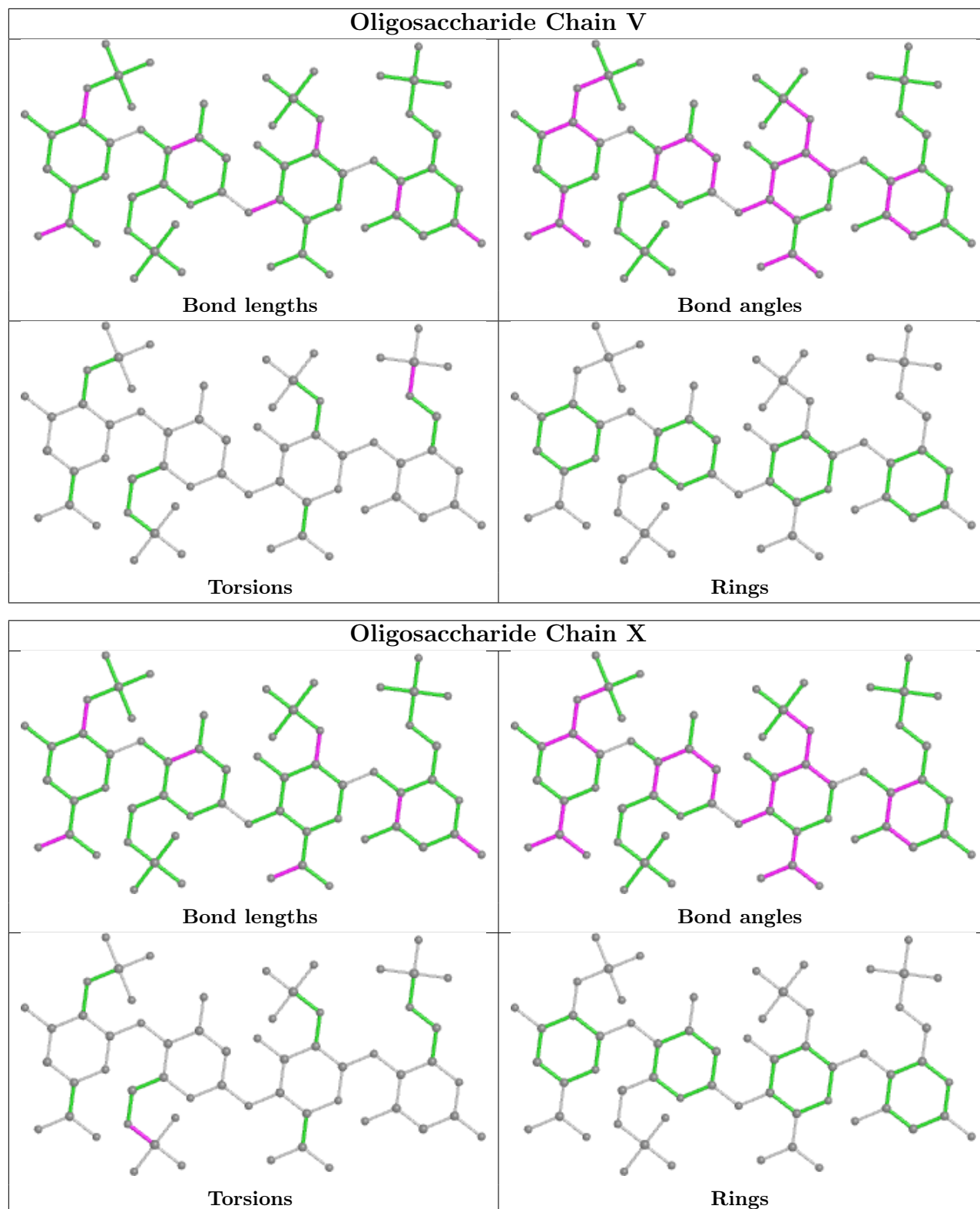


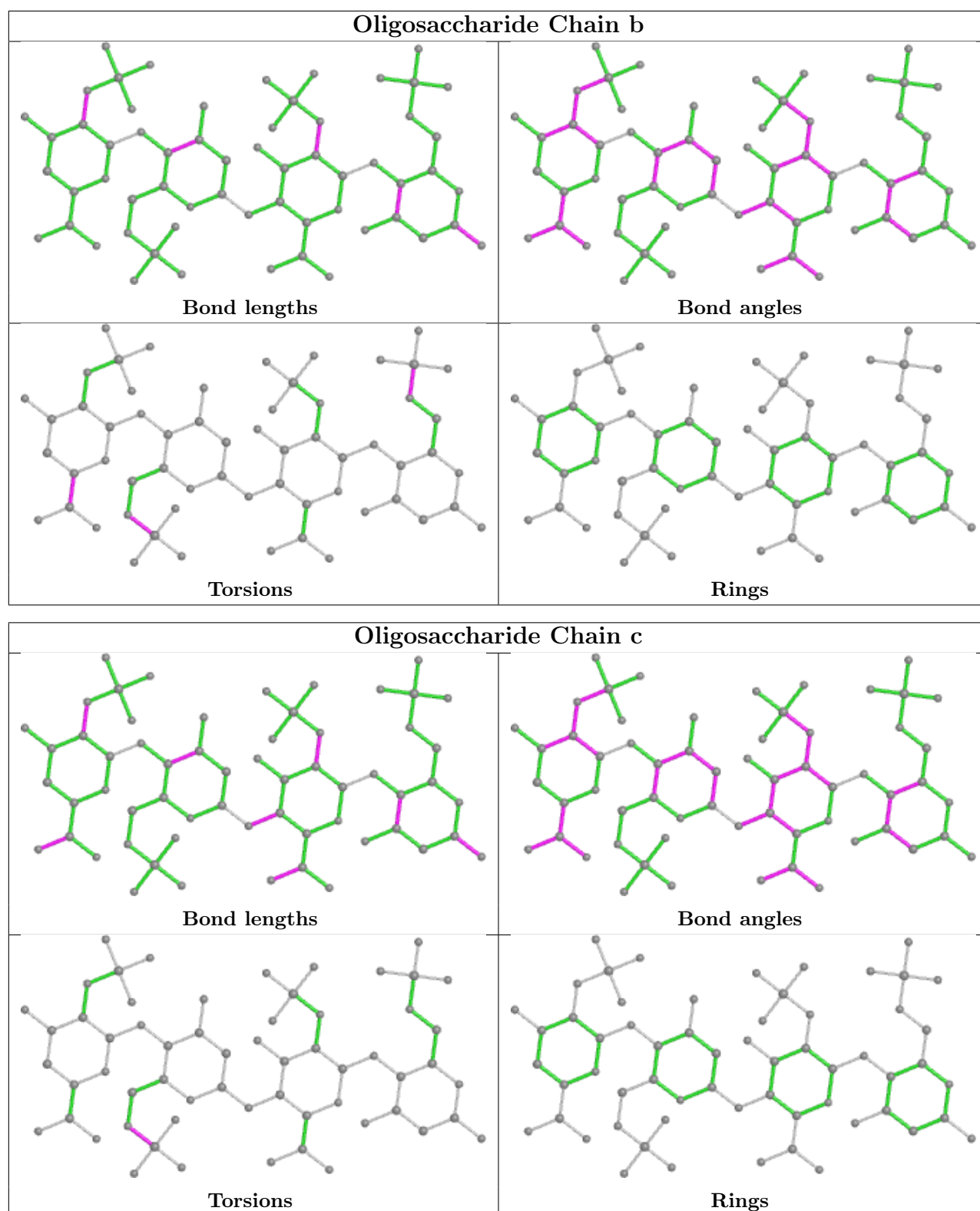


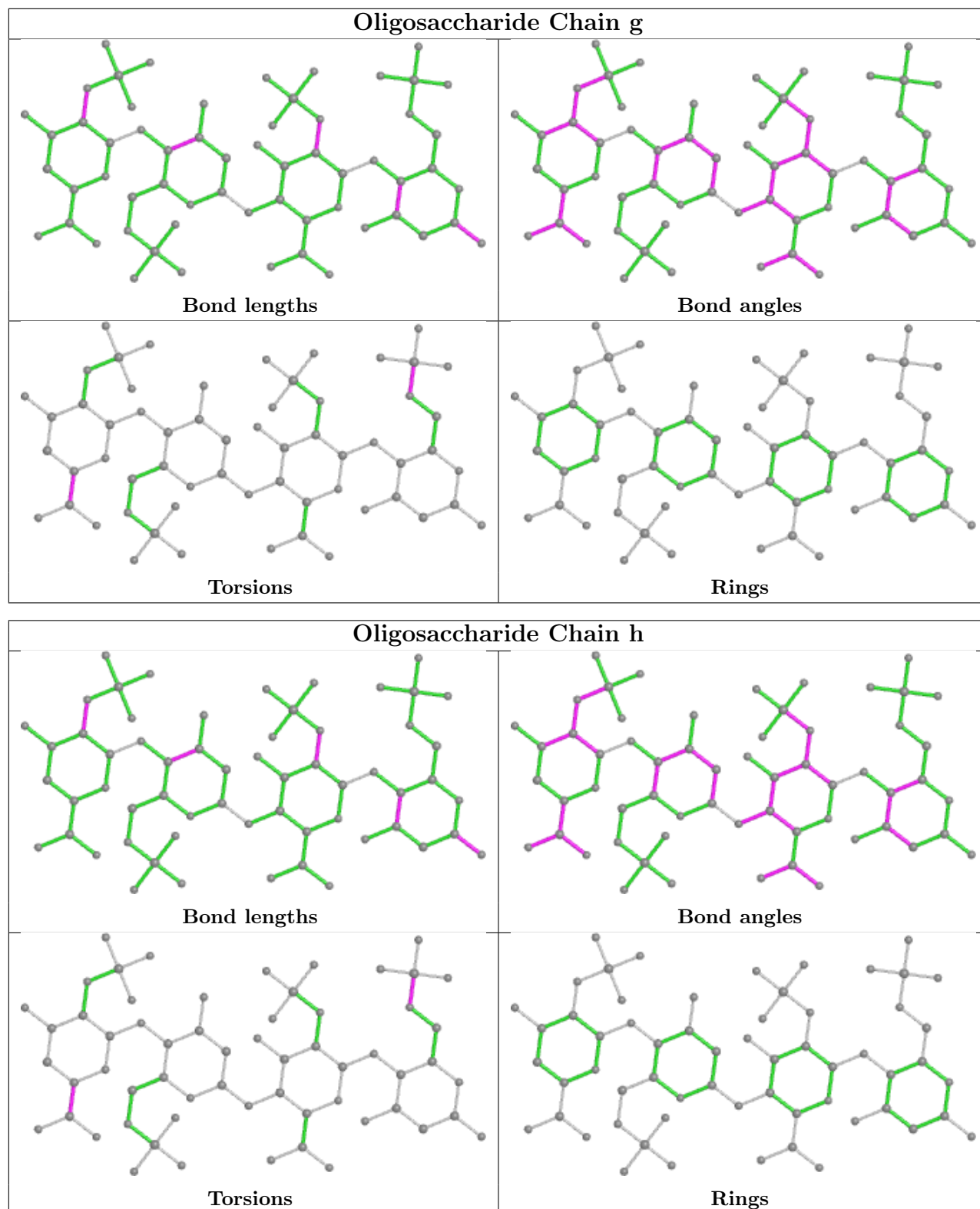


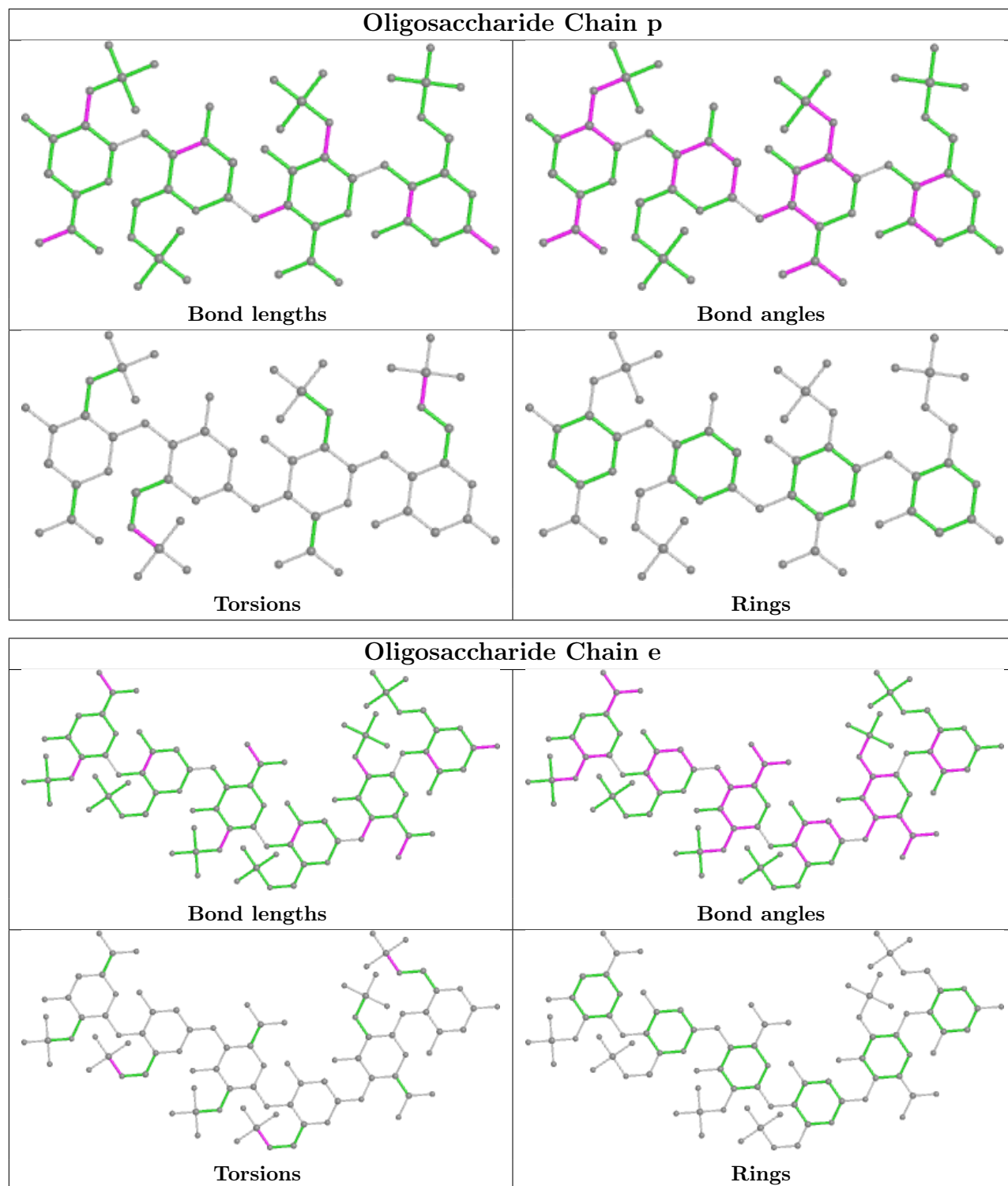


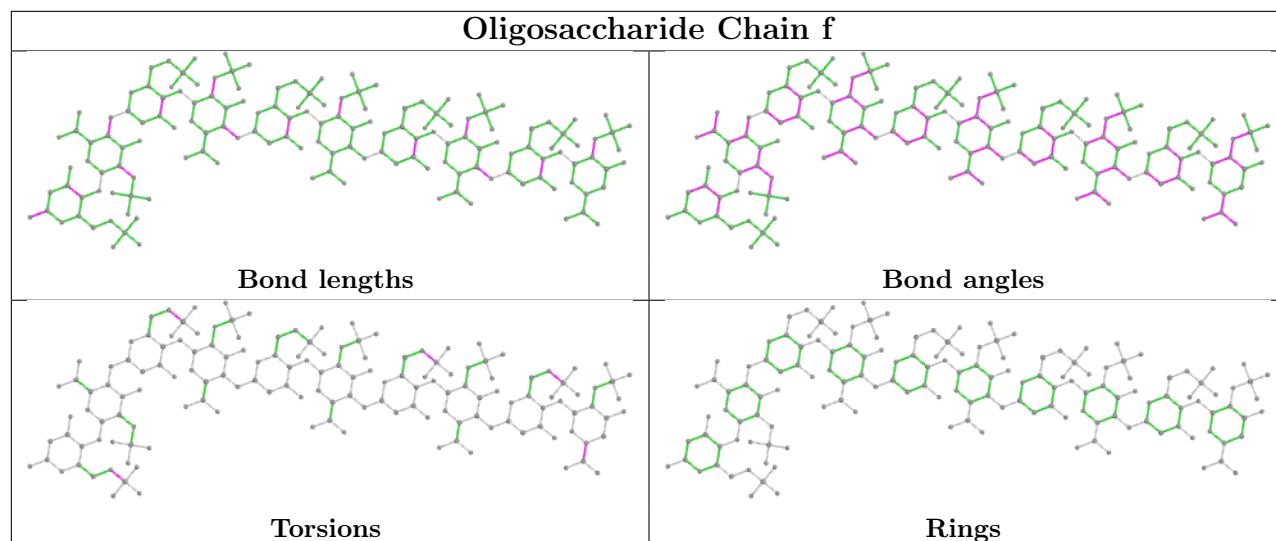












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	422/427 (98%)	-0.11	16 (3%) 40 43	37, 75, 133, 159	0
1	B	422/427 (98%)	-0.14	17 (4%) 38 41	34, 72, 130, 174	0
1	C	422/427 (98%)	-0.20	13 (3%) 49 53	26, 63, 122, 162	0
1	D	422/427 (98%)	-0.27	10 (2%) 59 62	30, 64, 129, 174	0
1	E	422/427 (98%)	-0.27	10 (2%) 59 62	30, 66, 125, 160	0
1	F	422/427 (98%)	-0.22	10 (2%) 59 62	34, 75, 131, 166	0
1	G	422/427 (98%)	-0.02	18 (4%) 35 39	36, 77, 134, 203	0
1	H	422/427 (98%)	-0.19	12 (2%) 53 57	31, 64, 118, 150	0
1	I	422/427 (98%)	-0.25	9 (2%) 63 67	30, 64, 122, 143	0
1	J	422/427 (98%)	-0.08	10 (2%) 59 62	33, 70, 137, 164	0
1	K	422/427 (98%)	-0.10	13 (3%) 49 53	38, 74, 129, 168	0
1	L	422/427 (98%)	-0.09	12 (2%) 53 57	43, 72, 128, 157	0
1	M	422/427 (98%)	-0.10	11 (2%) 56 59	44, 76, 128, 147	0
1	N	422/427 (98%)	-0.16	7 (1%) 70 74	43, 79, 128, 151	0
1	O	422/427 (98%)	-0.03	22 (5%) 27 30	40, 77, 136, 169	0
All	All	6330/6405 (98%)	-0.15	190 (3%) 50 54	26, 71, 129, 203	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	SER	6.6
1	D	135	ALA	6.0
1	H	177	SER	5.9
1	O	141	GLU	5.8
1	H	174	ALA	5.6

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
2	JHM	j	1	15/15	-0.13	1.04	212,232,254,254	0
2	IDS	m	2	15/17	-0.10	0.75	249,251,259,263	0
3	JHM	h	3	14/15	-0.03	0.86	271,292,314,314	0
2	JHM	Y	1	15/15	0.09	0.89	235,255,276,277	0
2	JHM	i	1	15/15	0.12	0.89	228,247,270,272	0
2	IDS	U	2	15/17	0.16	1.19	260,261,269,273	0
2	JHM	U	1	15/15	0.19	0.68	235,256,278,278	0
2	IDS	a	2	15/17	0.20	0.66	211,213,221,225	0
5	IDS	f	4	16/17	0.21	0.86	238,318,323,327	0
3	IDS	p	4	15/17	0.22	0.69	221,222,230,234	0
3	JHM	R	1	15/15	0.24	0.59	224,245,267,269	0
2	JHM	T	1	15/15	0.24	0.64	203,225,247,247	0
3	IDS	h	4	15/17	0.26	0.68	261,263,270,274	0
2	JHM	a	1	15/15	0.28	0.90	193,214,235,235	0
4	IDS	e	2	16/17	0.28	0.57	251,281,287,291	0
2	IDS	d	2	15/17	0.28	0.57	223,225,232,236	0
3	JHM	R	3	14/15	0.29	0.68	232,253,274,274	0
2	JHM	S	1	15/15	0.29	0.64	258,278,299,300	0
2	JHM	m	1	15/15	0.29	0.83	207,227,248,249	0
3	JHM	b	3	14/15	0.30	0.40	217,237,258,259	0
2	IDS	T	2	15/17	0.30	0.88	255,256,264,268	0
3	JHM	h	1	15/15	0.31	0.97	245,266,287,288	0
3	JHM	V	1	15/15	0.31	0.82	233,254,275,276	0
5	JHM	f	9	14/15	0.31	0.90	238,259,280,282	0
2	IDS	Y	2	15/17	0.32	0.56	226,227,235,239	0
2	JHM	r	1	15/15	0.32	0.73	198,219,240,240	0
2	IDS	r	2	15/17	0.32	0.91	270,272,280,283	0
3	JHM	X	3	14/15	0.32	0.56	200,219,242,243	0
2	JHM	n	1	15/15	0.33	0.62	185,205,226,227	0
2	JHM	q	1	15/15	0.33	0.81	235,255,277,278	0
3	IDS	Q	4	15/17	0.33	0.67	264,265,274,278	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	JHM	b	1	15/15	0.34	0.68	254,274,294,296	0
3	IDS	b	2	16/17	0.34	0.55	241,271,279,282	0
5	JHM	f	7	14/15	0.34	0.56	216,237,260,261	0
3	IDS	h	2	16/17	0.34	1.16	293,295,301,305	0
3	IDS	p	2	16/17	0.35	0.87	227,266,274,278	0
3	JHM	c	1	15/15	0.36	0.58	204,224,246,247	0
2	IDS	S	2	15/17	0.37	0.49	281,283,290,294	0
3	IDS	R	4	15/17	0.38	0.54	238,240,249,252	0
2	JHM	s	1	15/15	0.39	0.85	210,231,252,253	0
3	JHM	p	1	15/15	0.40	1.00	222,243,265,265	0
2	IDS	j	2	15/17	0.41	1.03	247,248,256,260	0
3	IDS	c	2	16/17	0.41	0.63	221,223,233,237	0
5	JHM	f	1	15/15	0.41	0.95	234,255,276,277	0
3	IDS	c	4	15/17	0.43	0.90	231,233,240,244	0
2	IDS	Z	2	15/17	0.43	0.57	252,254,262,266	0
2	IDS	i	2	15/17	0.43	0.49	261,264,269,273	0
4	IDS	e	4	16/17	0.43	0.60	249,286,292,296	0
3	JHM	p	3	14/15	0.45	0.73	204,224,246,246	0
3	JHM	c	3	14/15	0.45	0.59	214,234,257,257	0
2	IDS	l	2	15/17	0.45	0.63	260,261,269,274	0
3	JHM	g	1	15/15	0.45	0.86	217,238,258,259	0
3	JHM	g	3	14/15	0.46	0.42	228,248,270,270	0
2	JHM	Z	1	15/15	0.47	0.74	206,227,248,249	0
3	IDS	R	2	16/17	0.48	0.74	255,258,263,267	0
2	IDS	k	2	15/17	0.48	0.60	226,227,235,239	0
3	JHM	X	1	15/15	0.49	0.50	206,226,248,249	0
5	IDS	f	10	15/17	0.49	0.62	227,229,236,239	0
2	IDS	q	2	15/17	0.50	0.76	261,263,271,275	0
2	IDS	n	2	15/17	0.51	0.71	245,247,254,258	0
4	JHM	e	1	15/15	0.51	0.50	264,284,305,307	0
2	JHM	k	1	15/15	0.51	0.71	218,238,261,261	0
3	JHM	Q	3	14/15	0.52	0.50	213,233,255,255	0
2	IDS	W	2	15/17	0.52	0.64	219,221,228,231	0
2	JHM	l	1	15/15	0.52	0.51	224,244,266,266	0
5	JHM	f	3	14/15	0.52	0.70	225,245,267,268	0
5	JHM	f	5	14/15	0.53	0.60	214,234,255,256	0
2	JHM	o	1	15/15	0.53	0.70	220,240,261,262	0
2	JHM	W	1	15/15	0.55	0.69	223,243,265,266	0
5	IDS	f	8	16/17	0.56	0.54	186,189,199,262	0
3	JHM	V	3	14/15	0.56	0.56	210,231,253,254	0
3	IDS	Q	2	16/17	0.56	0.56	219,222,234,236	0

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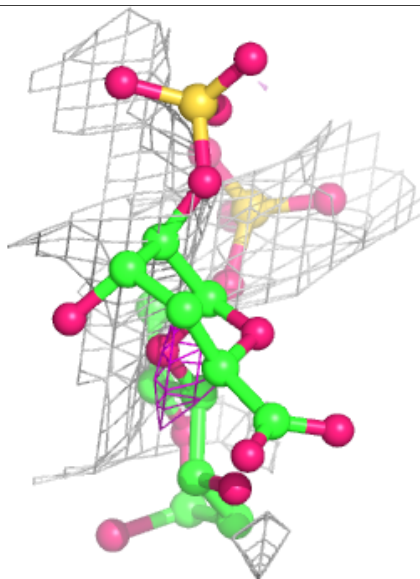
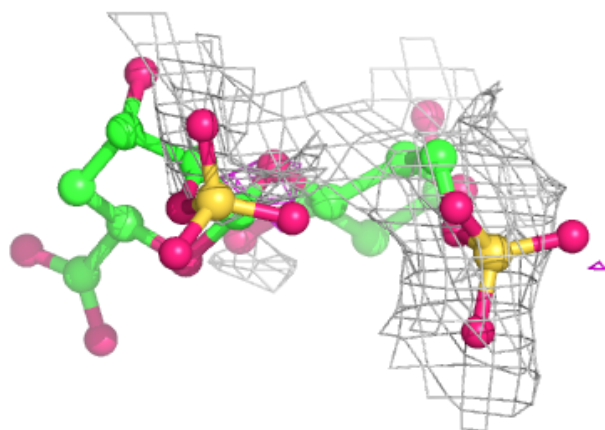
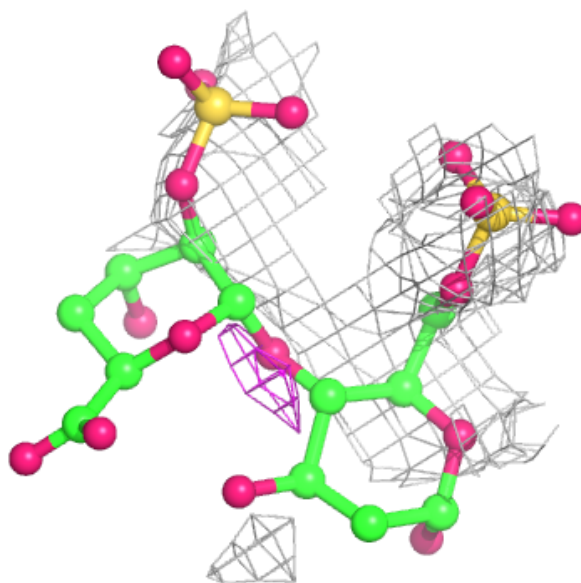
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	JHM	e	3	14/15	0.57	0.34	227,248,268,270	0
4	IDS	e	6	15/17	0.57	0.68	239,241,247,251	0
3	IDS	b	4	15/17	0.59	0.41	235,237,245,248	0
2	JHM	d	1	15/15	0.60	0.58	201,221,243,244	0
2	IDS	s	2	15/17	0.60	0.72	227,229,237,241	0
5	IDS	f	2	16/17	0.61	0.67	248,255,262,265	0
4	JHM	e	5	14/15	0.62	0.66	226,246,268,269	0
5	IDS	f	6	16/17	0.62	0.51	209,212,222,240	0
3	IDS	X	2	16/17	0.63	0.50	222,227,235,239	0
3	IDS	g	2	16/17	0.63	0.62	251,264,272,276	0
2	JHM	P	1	15/15	0.63	0.52	192,212,234,235	0
3	JHM	Q	1	15/15	0.64	0.70	194,215,236,236	0
3	IDS	X	4	15/17	0.68	0.85	230,232,239,243	0
2	IDS	P	2	15/17	0.68	0.66	267,270,276,279	0
3	IDS	V	2	16/17	0.68	0.62	234,267,274,278	0
3	IDS	g	4	15/17	0.69	0.55	238,240,248,252	0
3	IDS	V	4	15/17	0.79	0.34	273,275,282,286	0
2	IDS	o	2	15/17	0.80	0.36	214,215,224,228	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.

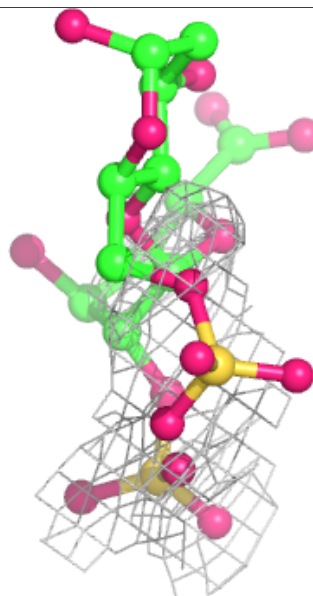
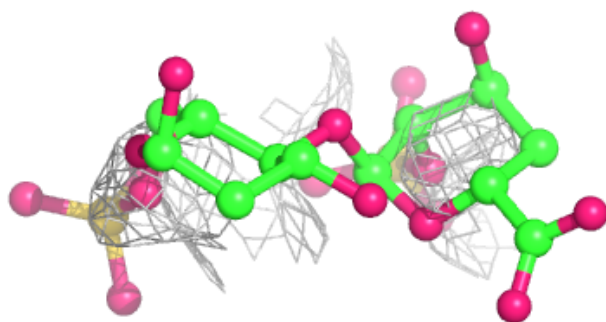
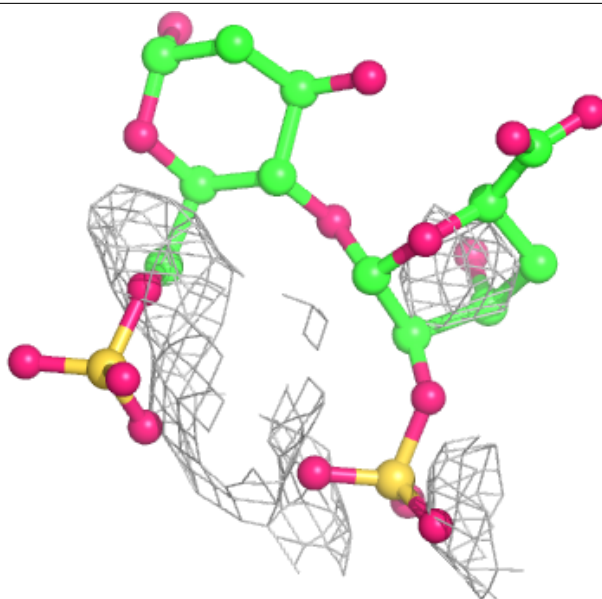
Electron density around Chain P:

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



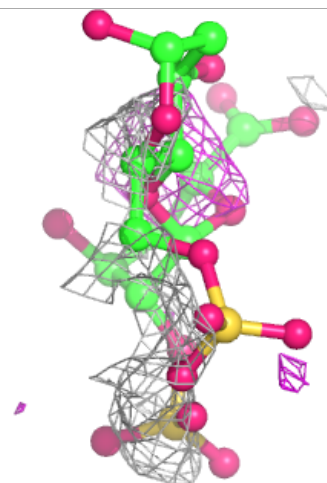
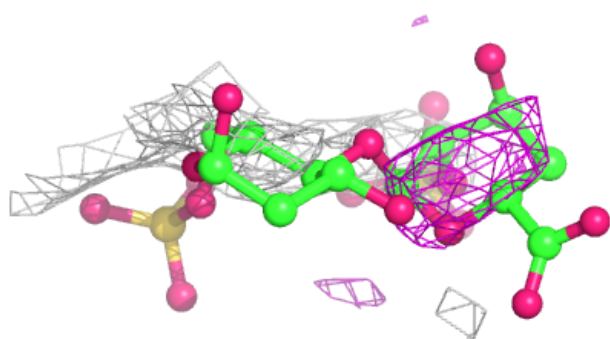
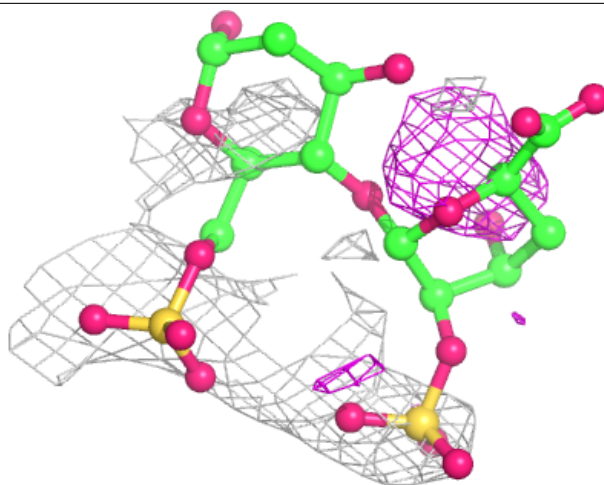
Electron density around Chain S:

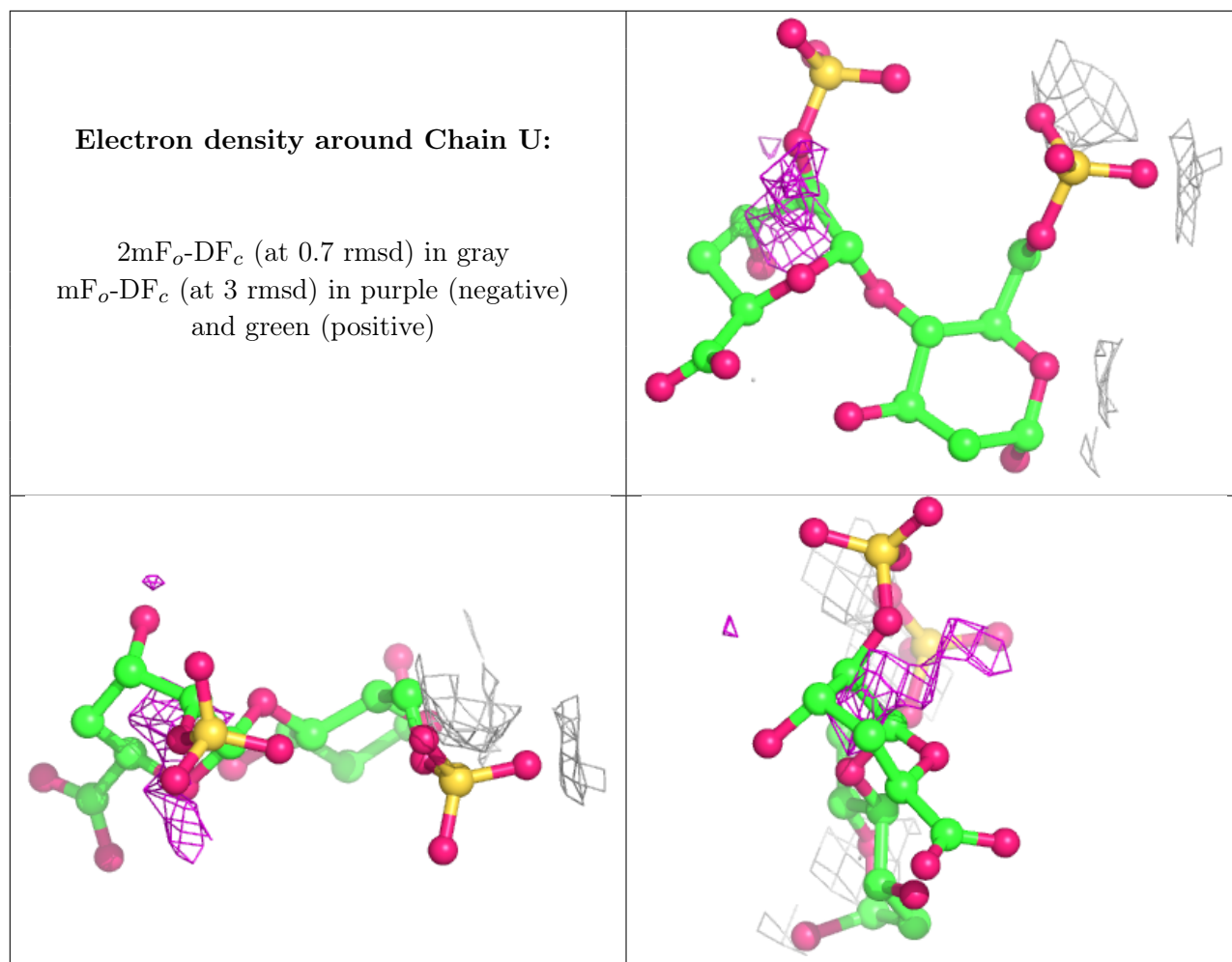
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

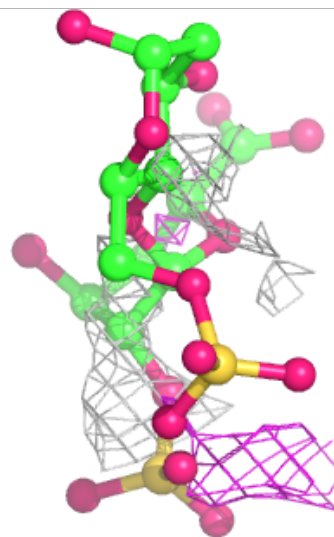
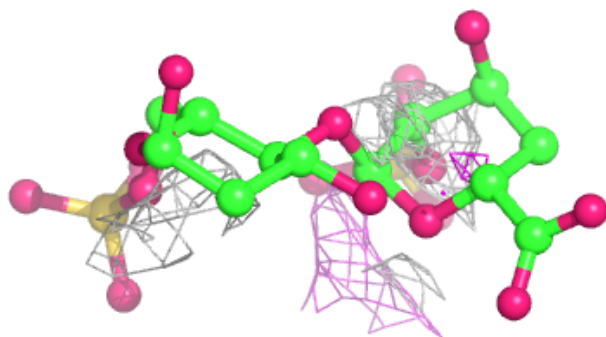
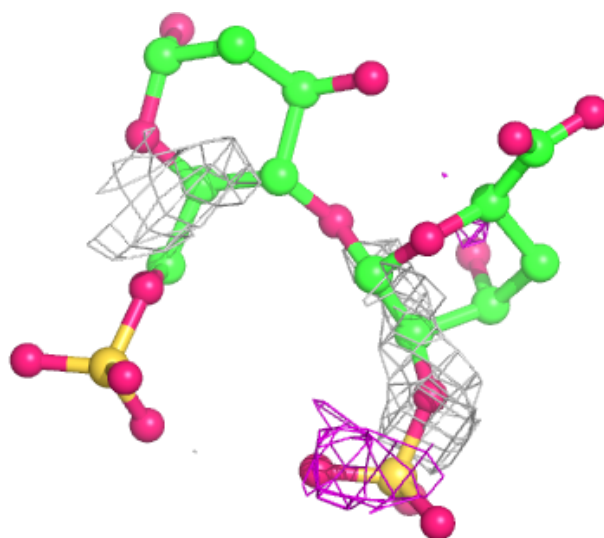
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





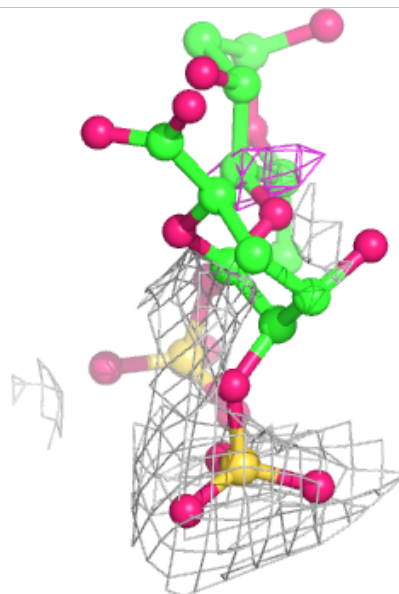
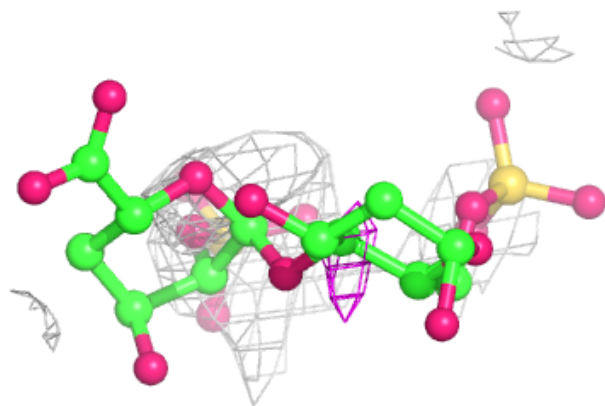
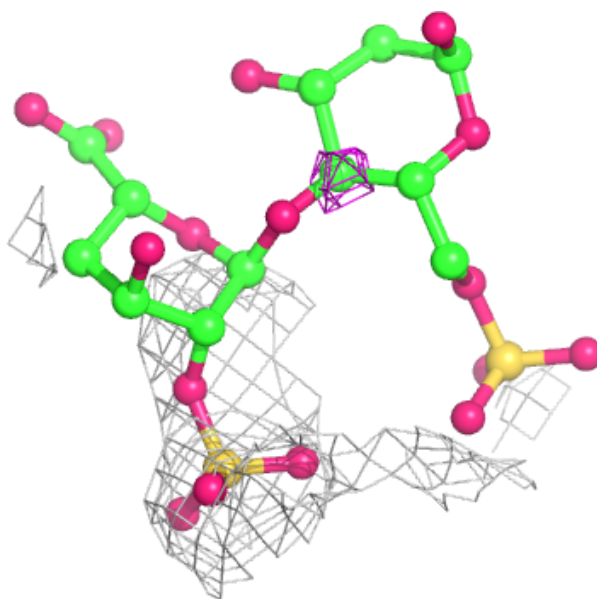
Electron density around Chain W:

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



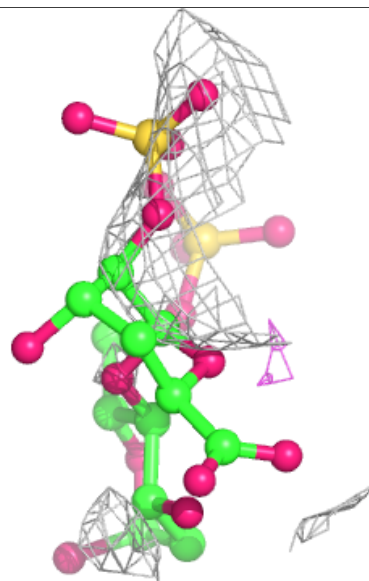
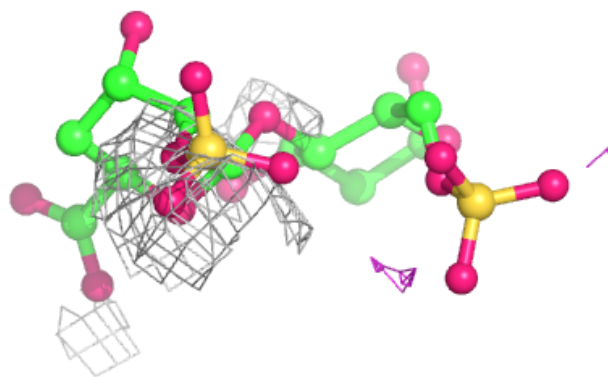
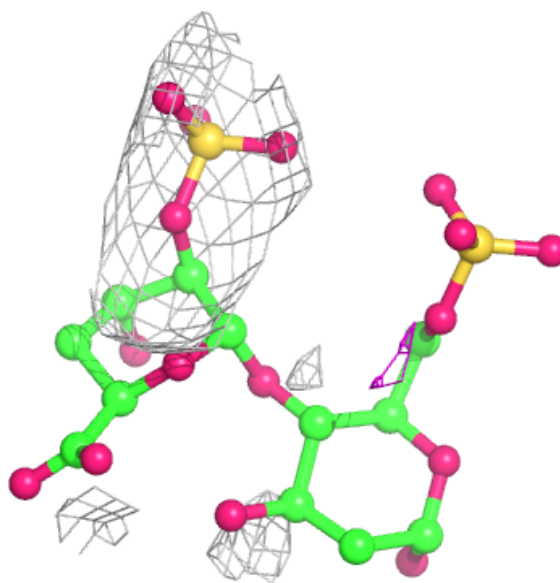
Electron density around Chain Y:

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



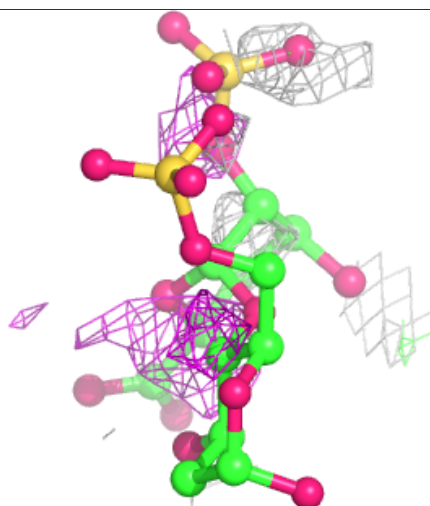
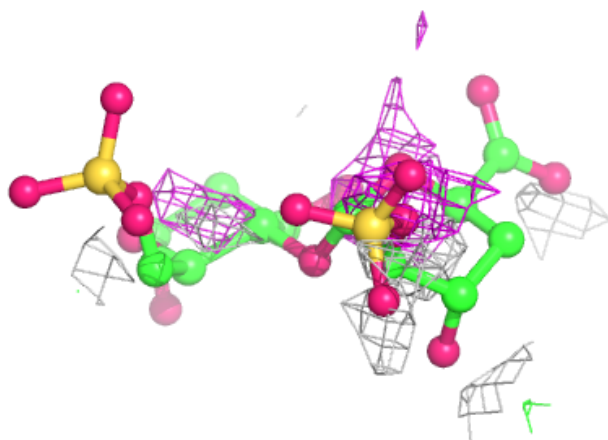
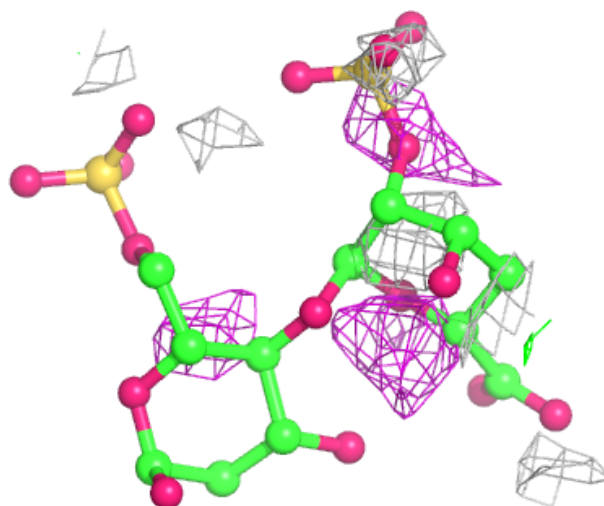
Electron density around Chain Z:

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



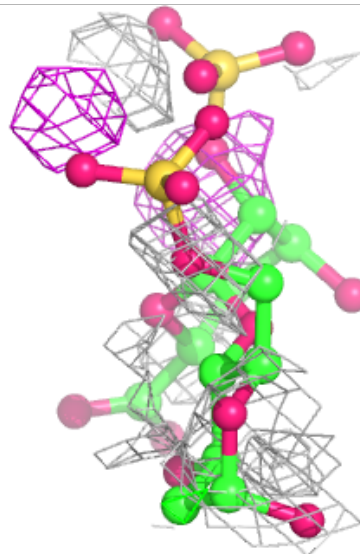
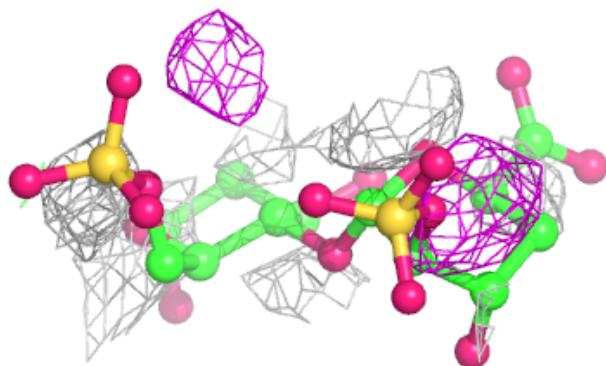
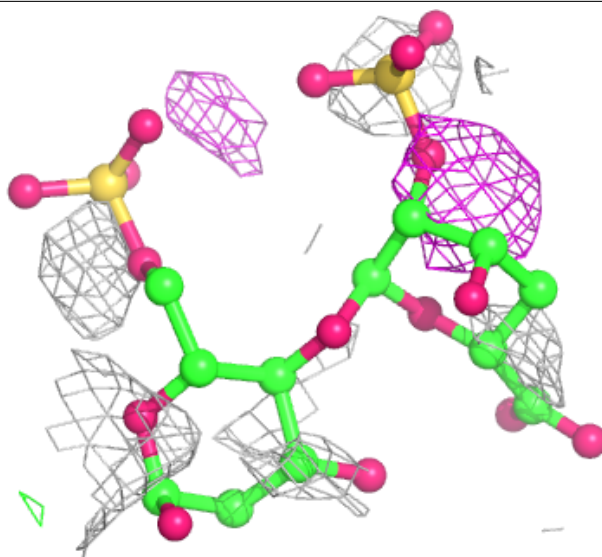
Electron density around Chain a:

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



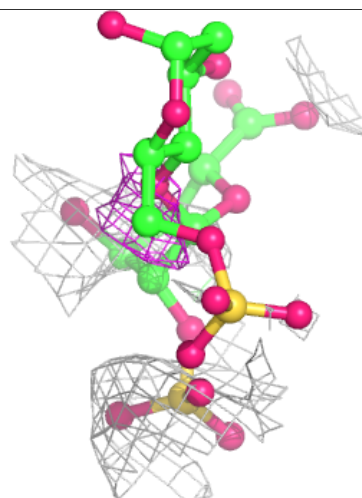
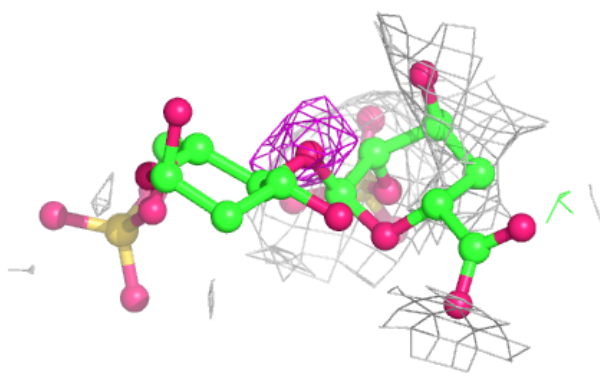
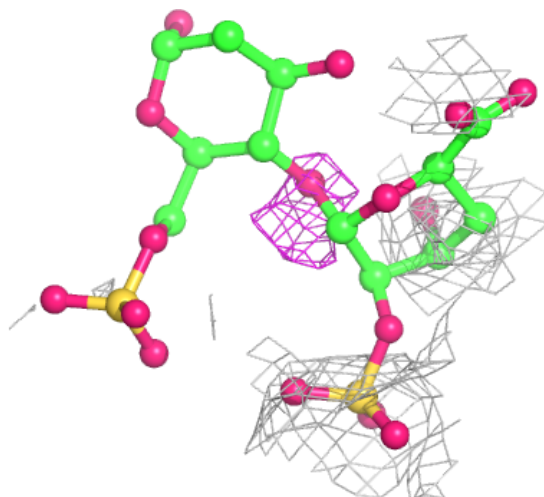
Electron density around Chain d:

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



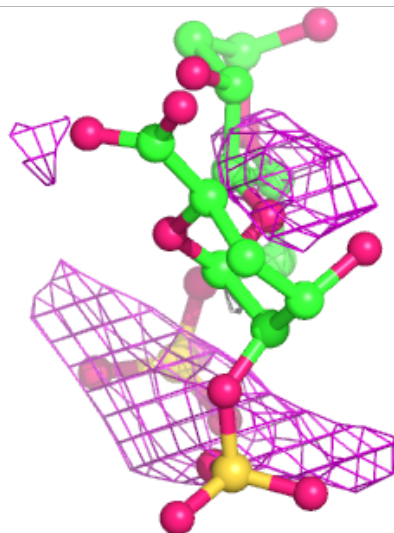
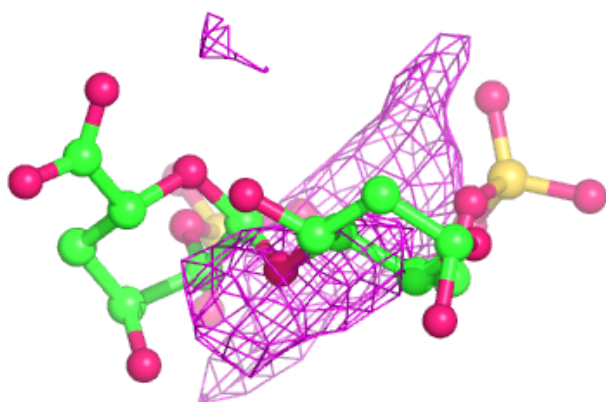
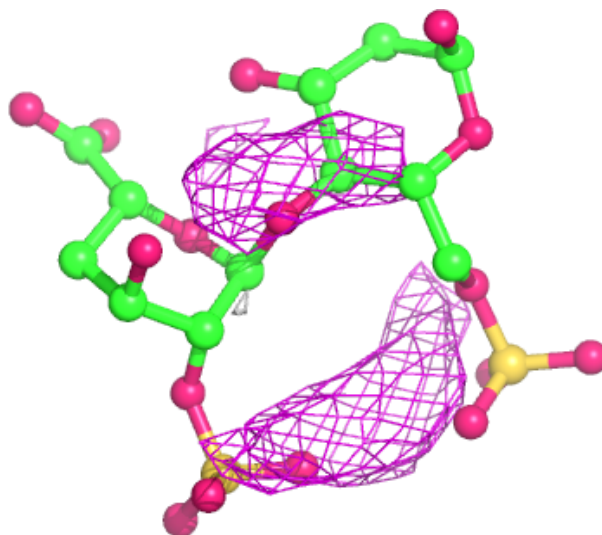
Electron density around Chain i:

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



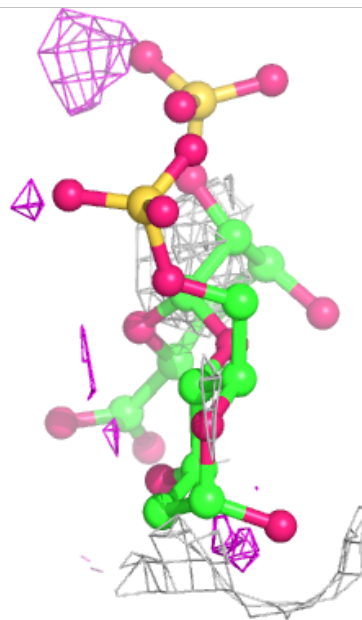
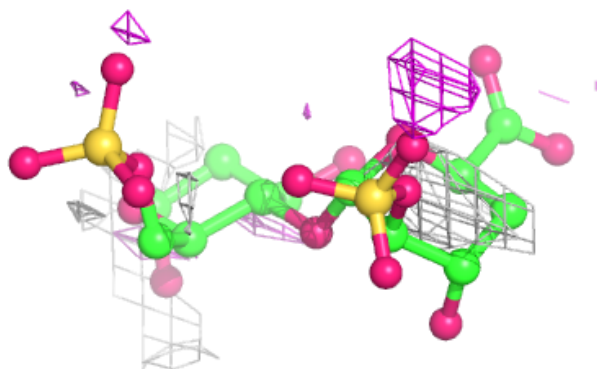
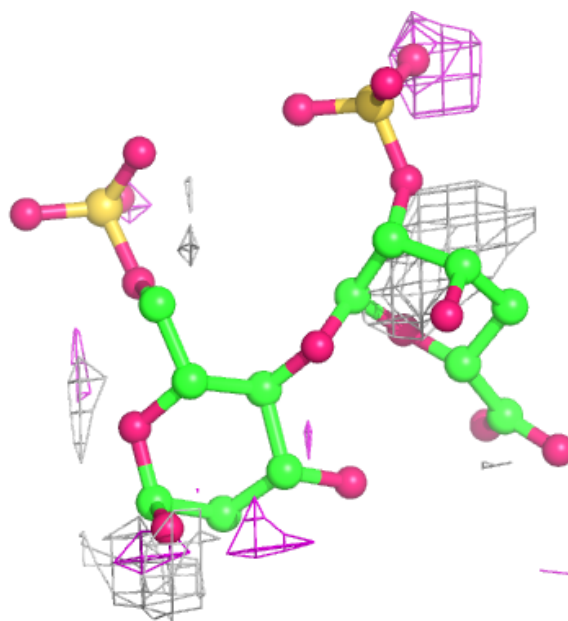
Electron density around Chain j:

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



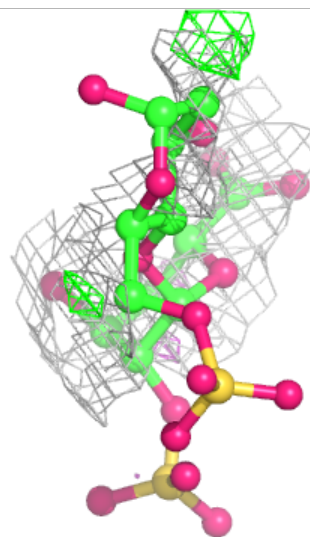
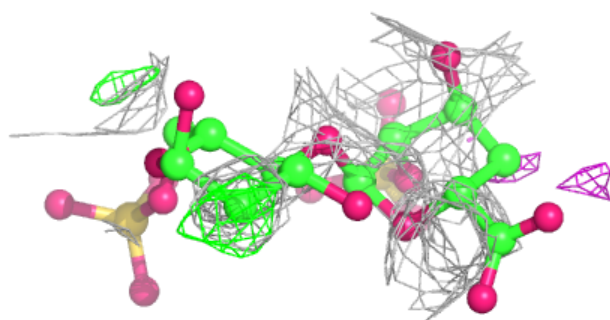
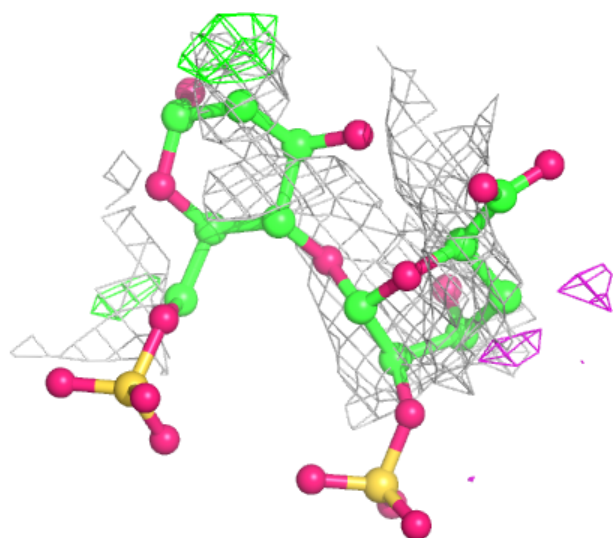
Electron density around Chain k:

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



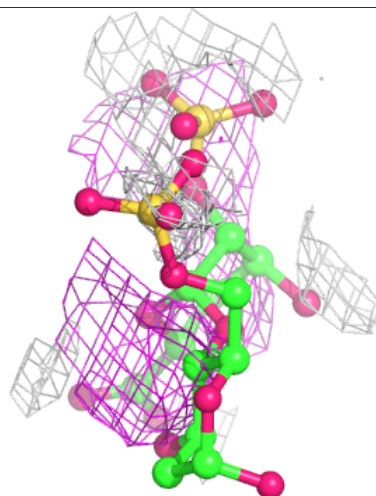
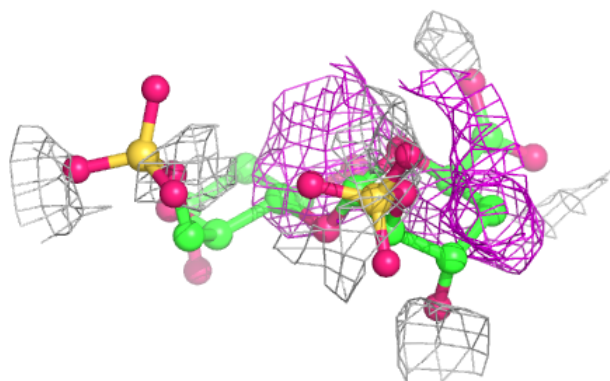
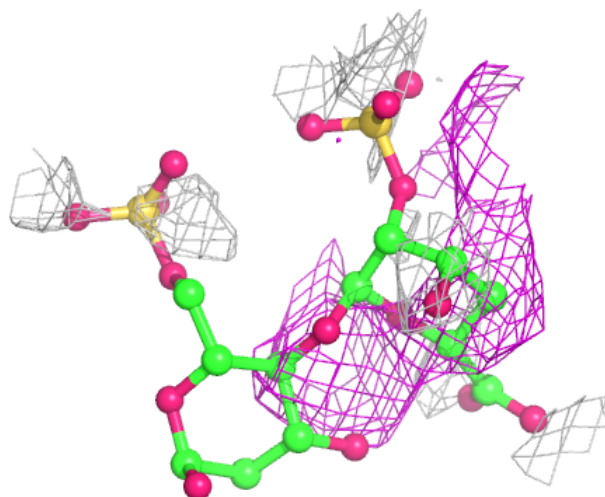
Electron density around Chain 1:

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



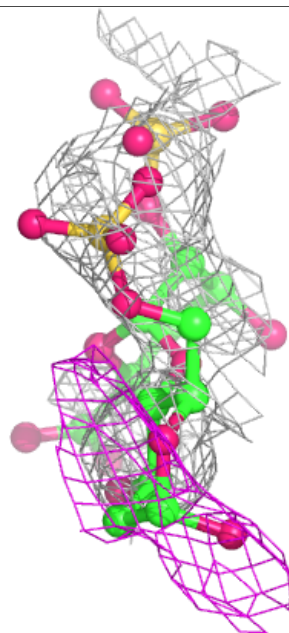
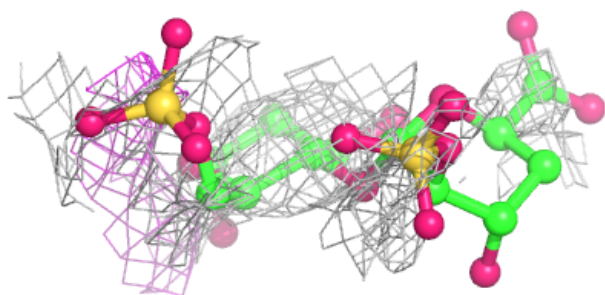
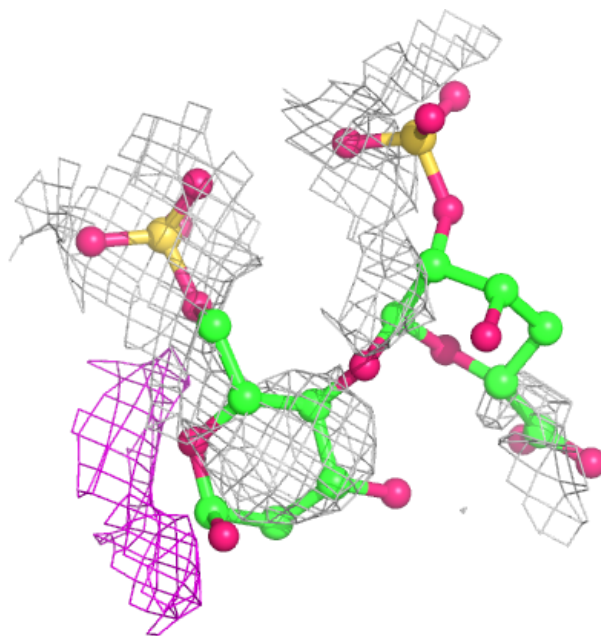
Electron density around Chain m:

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



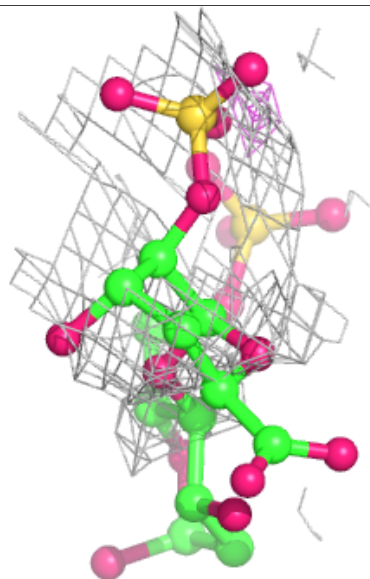
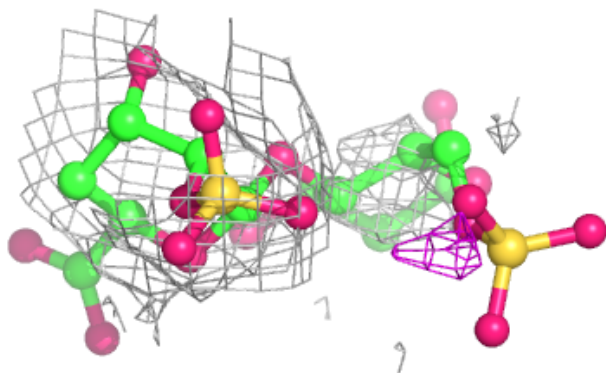
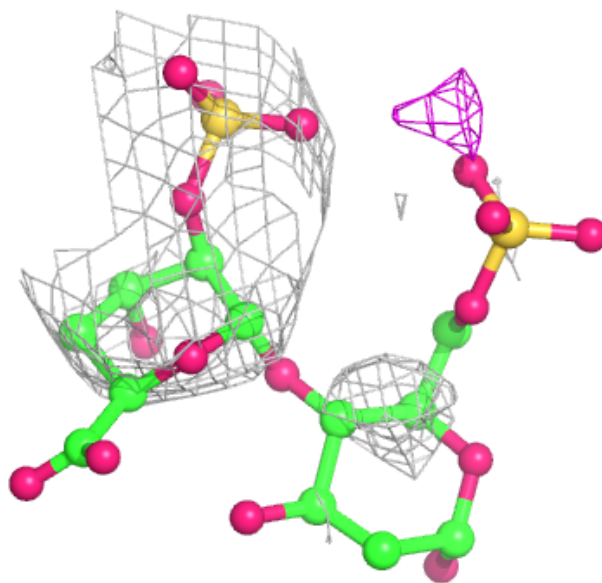
Electron density around Chain n:

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



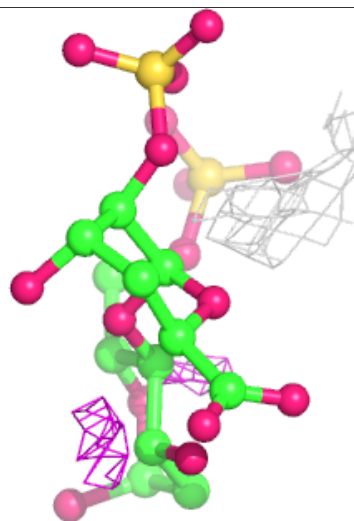
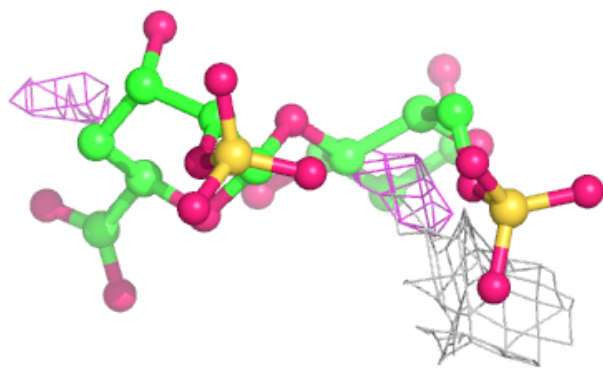
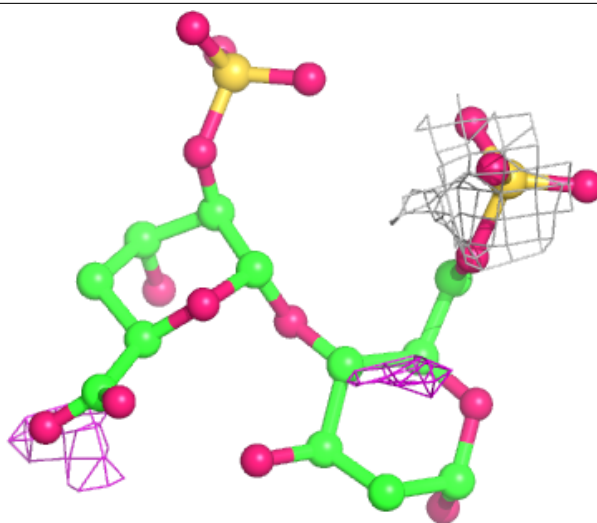
Electron density around Chain o:

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



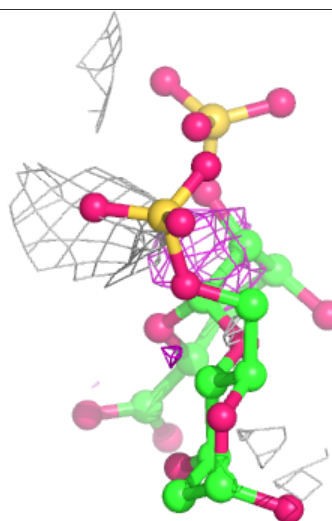
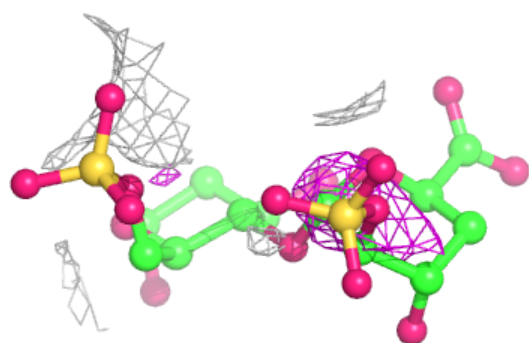
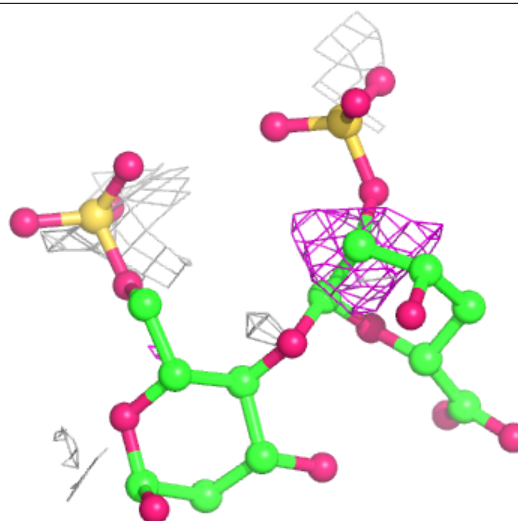
Electron density around Chain q:

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



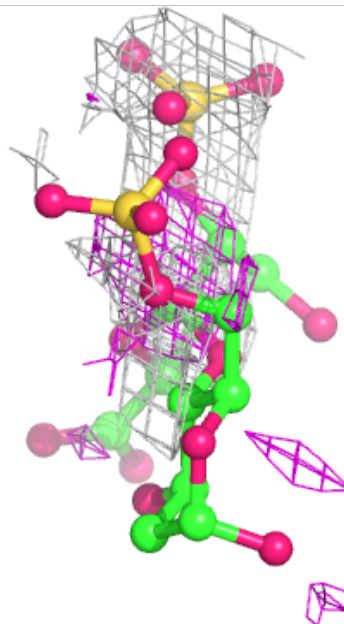
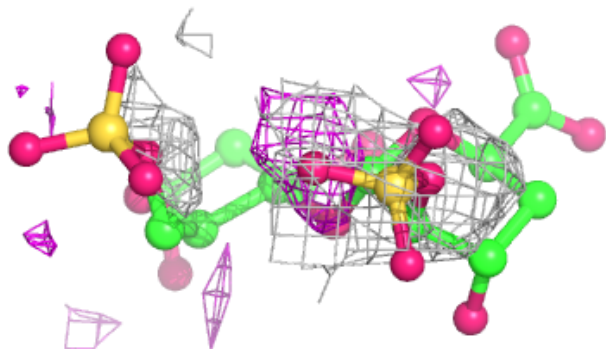
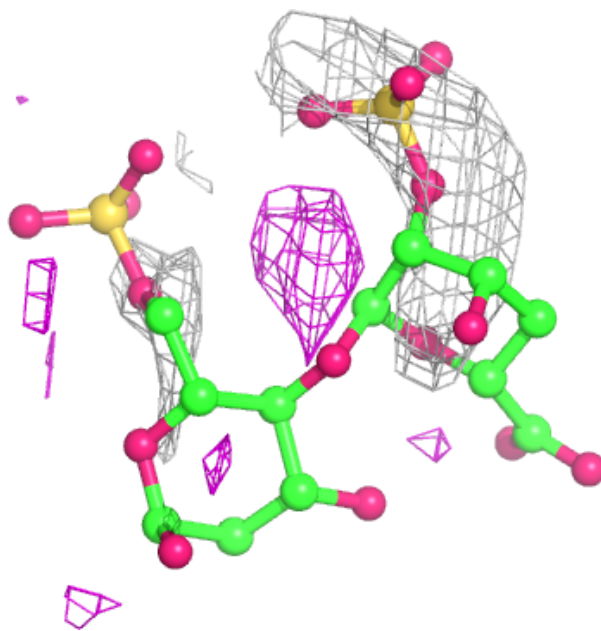
Electron density around Chain r:

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



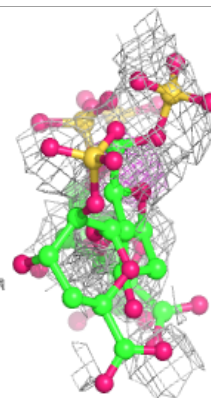
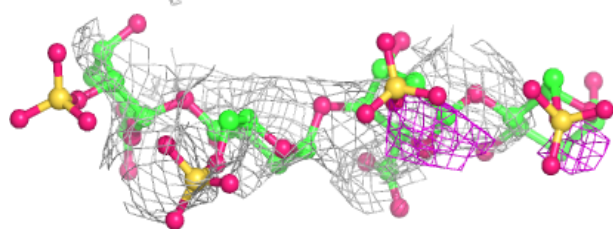
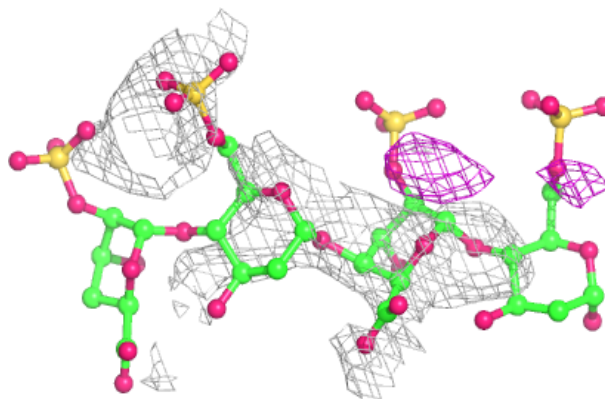
Electron density around Chain s:

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

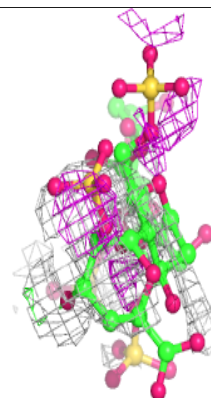
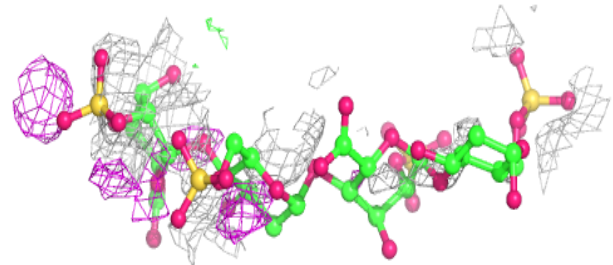
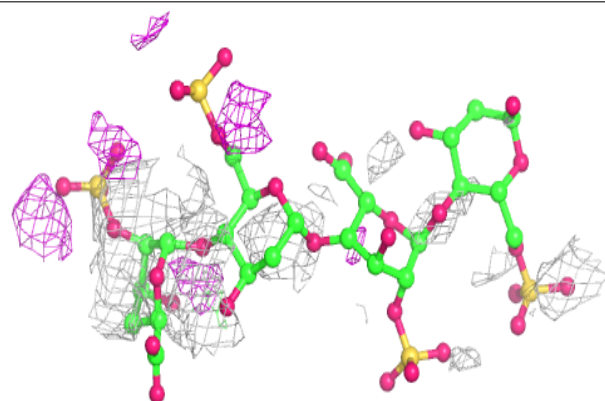


Electron density around Chain Q:

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

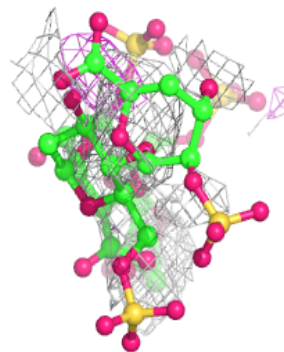
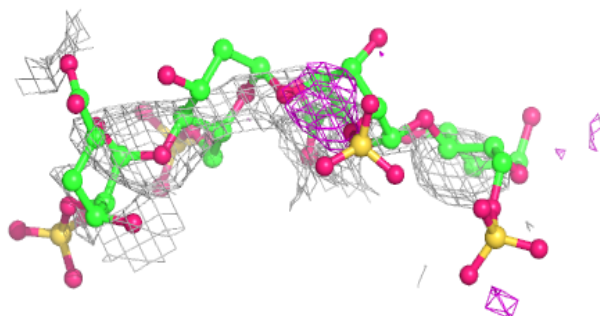
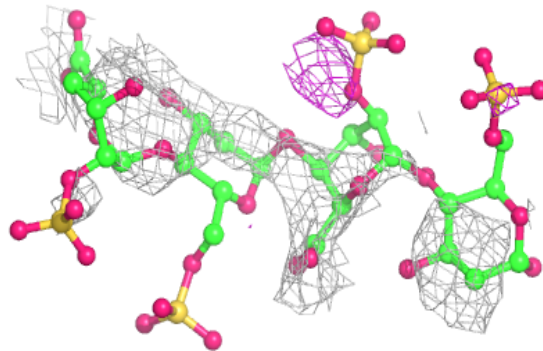
**Electron density around Chain R:**

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

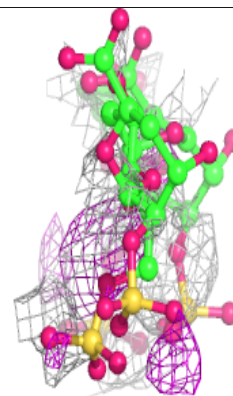
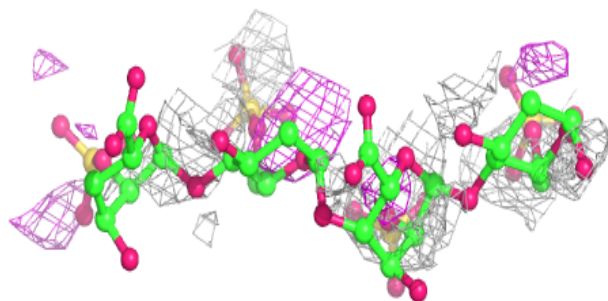
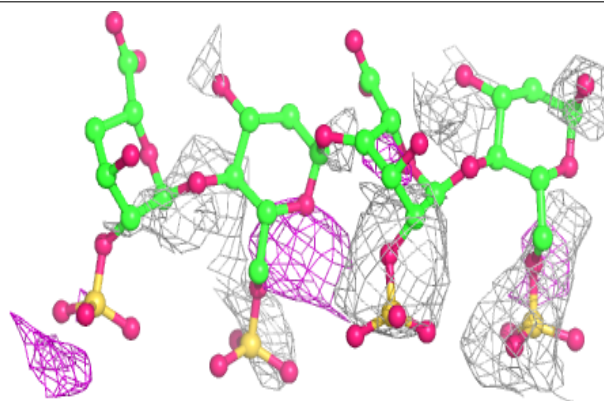


Electron density around Chain V:

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

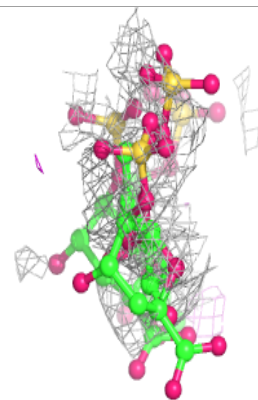
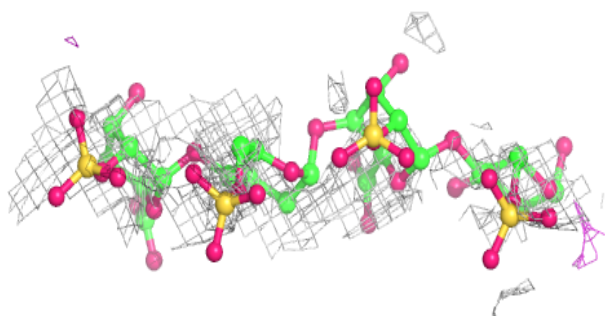
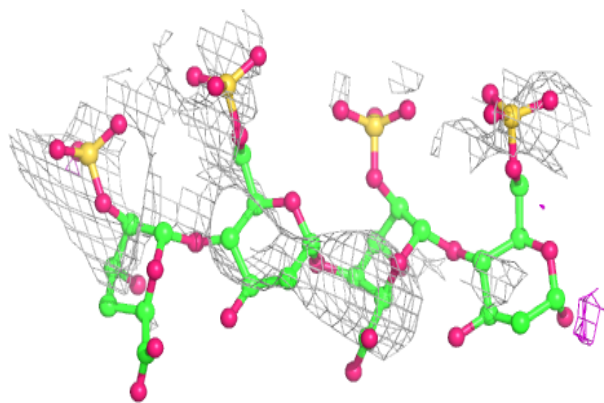
**Electron density around Chain X:**

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

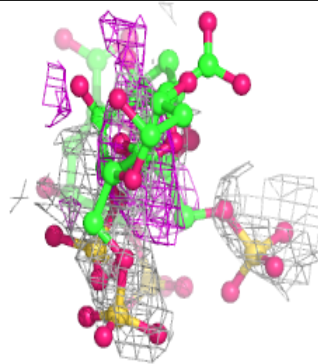
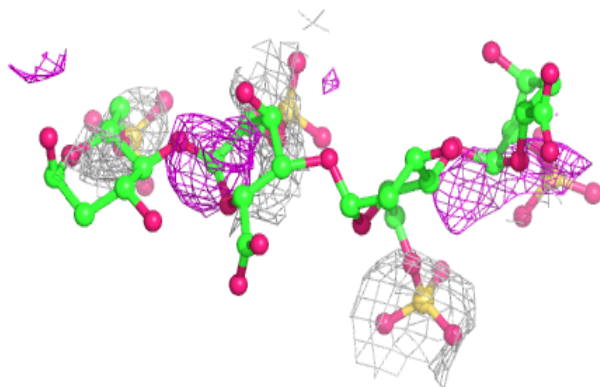
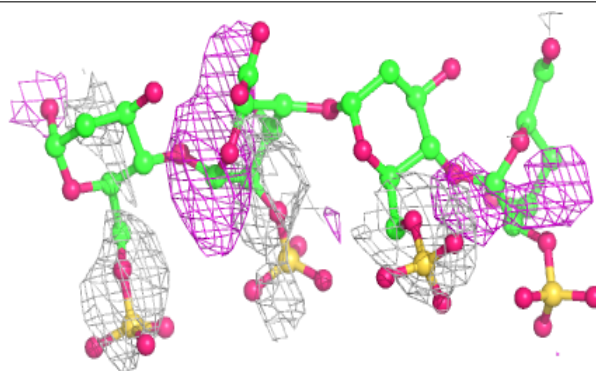


Electron density around Chain b:

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

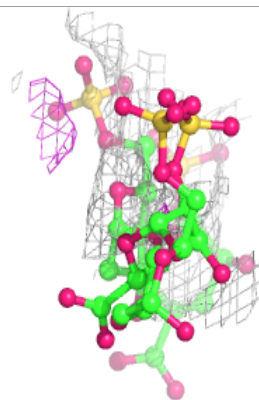
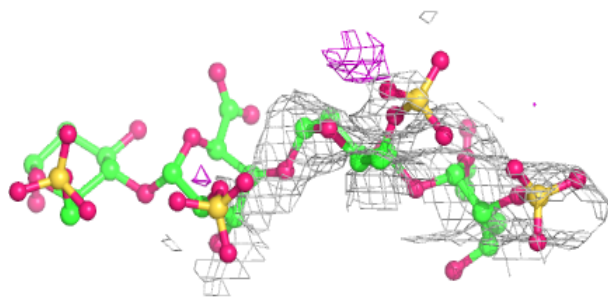
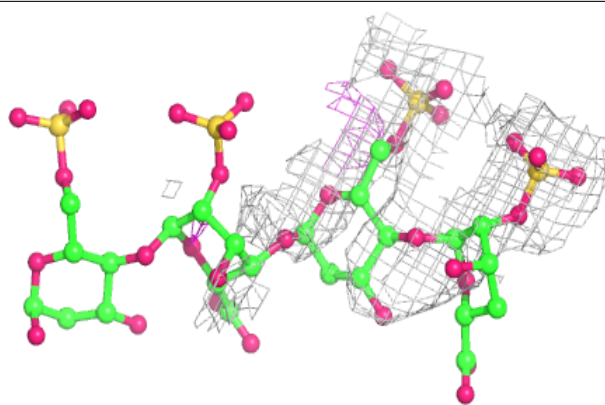
**Electron density around Chain c:**

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

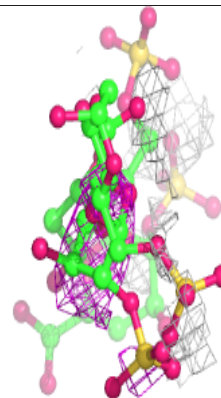
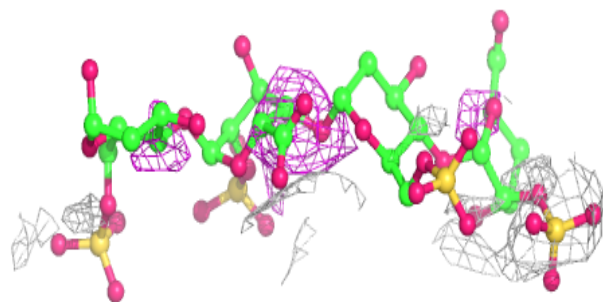
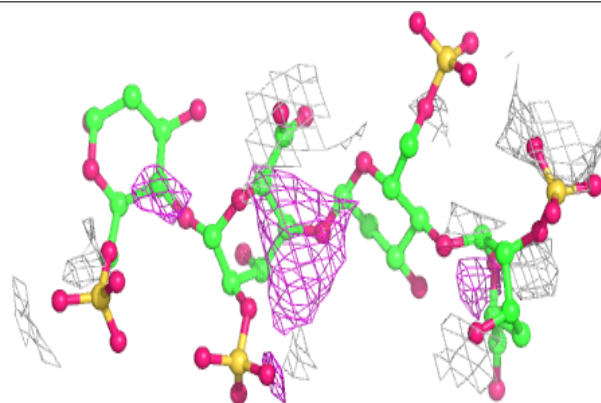


Electron density around Chain g:

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

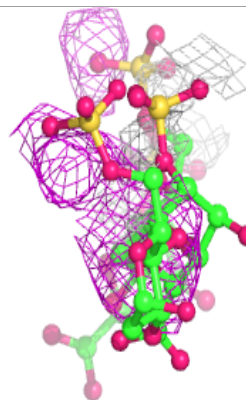
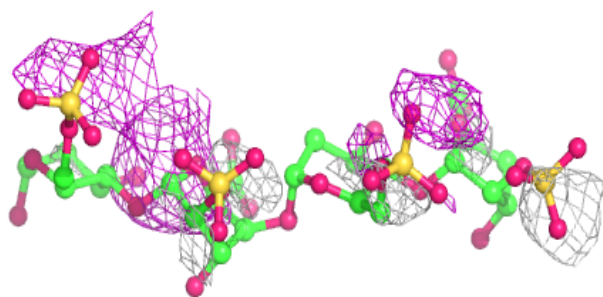
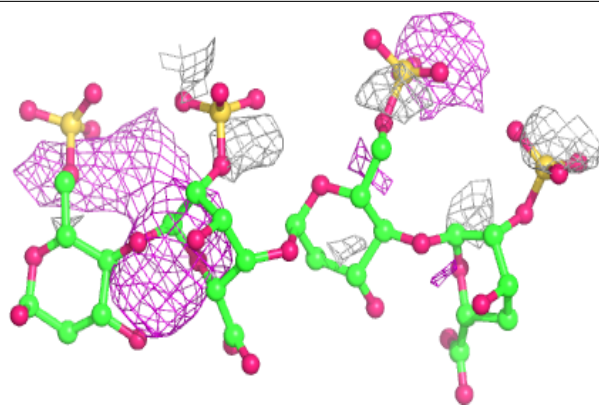
**Electron density around Chain h:**

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

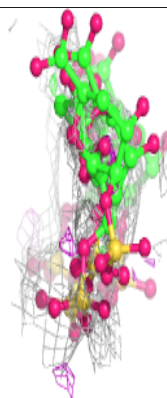
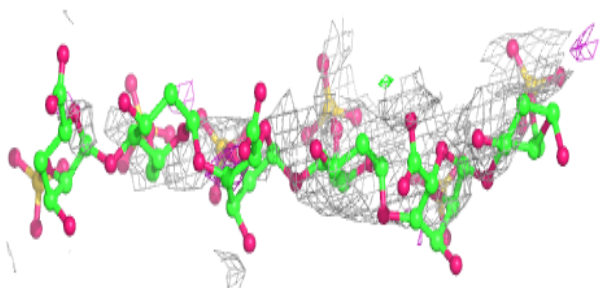
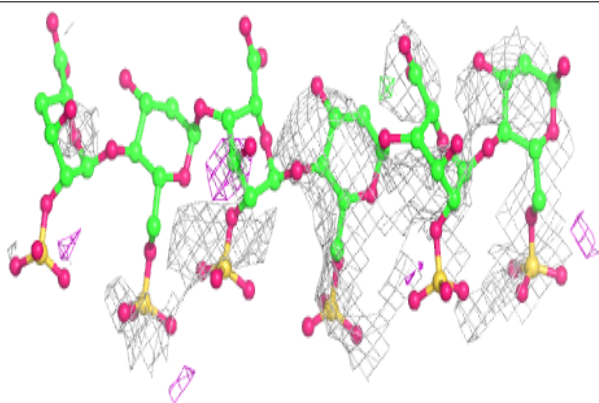


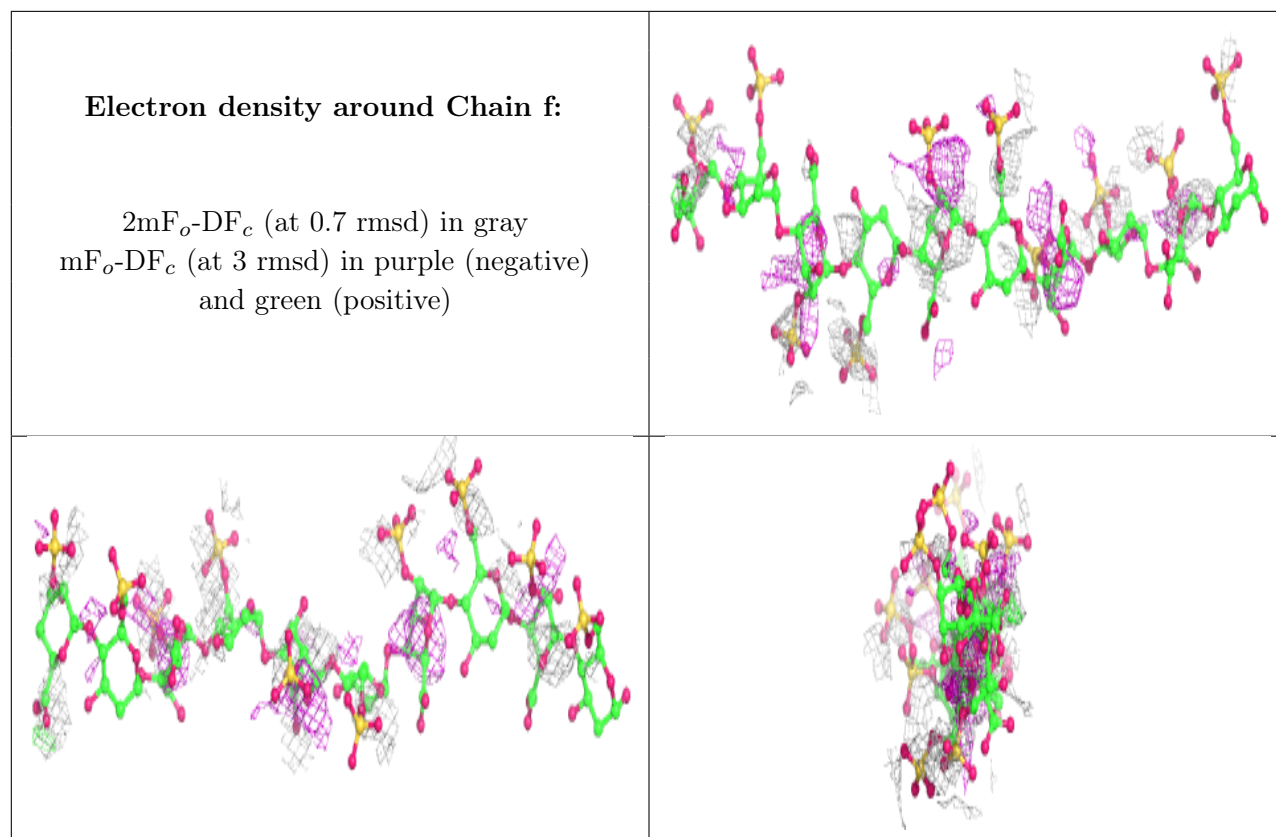
Electron density around Chain p:

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

**Electron density around Chain e:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.