



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:18 PM UTC

PDB ID : 4N5Y / pdb_00004n5y
Title : Crystal structure of H5 hemagglutinin mutant (N158D, N224K and Q226L)
from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-10-10
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

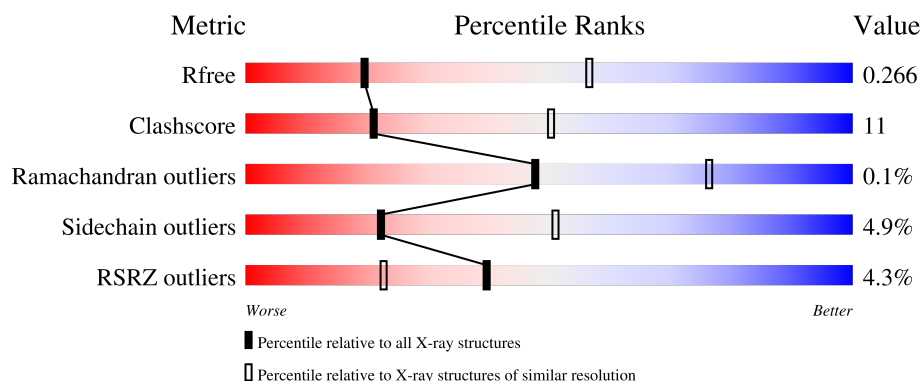
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	334	% 65% 27% 5% .
1	C	334	% 68% 26% . .
1	E	334	2% 64% 29% . .
1	G	334	61% 31% . .
1	I	334	67% 24% 6% .

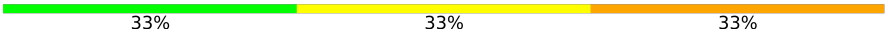
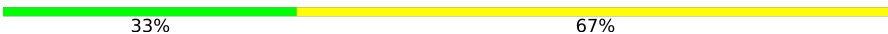
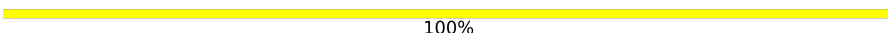
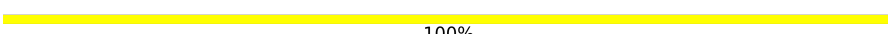
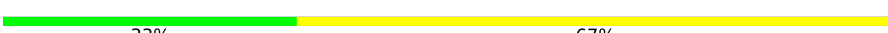
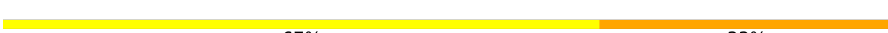
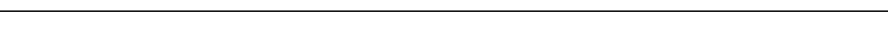
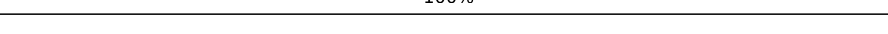
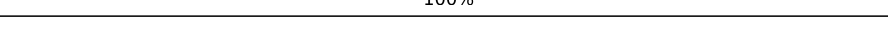
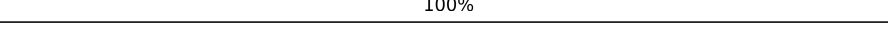
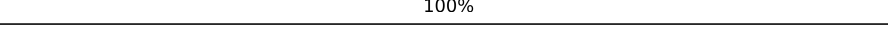
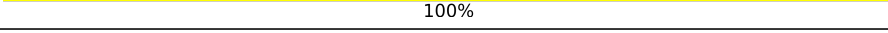
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	334	
1	M	334	
1	O	334	
1	Q	334	
1	S	334	
1	U	334	
1	W	334	
1	Y	334	
1	a	334	
1	c	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
2	T	181	
2	V	181	
2	X	181	
2	Z	181	
2	b	181	
2	d	181	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	e	3	 33% 33% 33%
3	g	3	 33% 67%
3	h	3	 100%
3	j	3	 67% 33%
3	l	3	 100%
3	n	3	 33% 67%
3	o	3	 67% 33%
3	q	3	 33% 33% 33%
3	w	3	 67% 33%
3	y	3	 33% 67%
4	0	2	 50% 50%
4	1	2	 50% 50%
4	f	2	 100%
4	i	2	 100%
4	k	2	 100%
4	m	2	 100%
4	p	2	 50% 50%
4	r	2	 100%
4	t	2	 100%
4	u	2	 50% 50%
4	v	2	 100%
4	x	2	 50% 50%
4	z	2	 100%
5	s	4	 25% 75%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60964 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	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	C	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	E	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	G	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	I	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	K	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	M	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	O	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	S	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	U	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	W	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	a	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	c	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q6DQ33
A	8	ASP	-	expression tag	UNP Q6DQ33
A	9	PRO	-	expression tag	UNP Q6DQ33
A	10	GLY	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	7	ALA	-	expression tag	UNP Q6DQ33
C	8	ASP	-	expression tag	UNP Q6DQ33
C	9	PRO	-	expression tag	UNP Q6DQ33
C	10	GLY	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	7	ALA	-	expression tag	UNP Q6DQ33
E	8	ASP	-	expression tag	UNP Q6DQ33
E	9	PRO	-	expression tag	UNP Q6DQ33
E	10	GLY	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
G	7	ALA	-	expression tag	UNP Q6DQ33
G	8	ASP	-	expression tag	UNP Q6DQ33
G	9	PRO	-	expression tag	UNP Q6DQ33
G	10	GLY	-	expression tag	UNP Q6DQ33
G	158	ASP	ASN	engineered mutation	UNP Q6DQ33
G	224	LYS	ASN	engineered mutation	UNP Q6DQ33
G	226	LEU	GLN	engineered mutation	UNP Q6DQ33
I	7	ALA	-	expression tag	UNP Q6DQ33
I	8	ASP	-	expression tag	UNP Q6DQ33
I	9	PRO	-	expression tag	UNP Q6DQ33
I	10	GLY	-	expression tag	UNP Q6DQ33
I	158	ASP	ASN	engineered mutation	UNP Q6DQ33
I	224	LYS	ASN	engineered mutation	UNP Q6DQ33
I	226	LEU	GLN	engineered mutation	UNP Q6DQ33
K	7	ALA	-	expression tag	UNP Q6DQ33
K	8	ASP	-	expression tag	UNP Q6DQ33
K	9	PRO	-	expression tag	UNP Q6DQ33
K	10	GLY	-	expression tag	UNP Q6DQ33
K	158	ASP	ASN	engineered mutation	UNP Q6DQ33
K	224	LYS	ASN	engineered mutation	UNP Q6DQ33
K	226	LEU	GLN	engineered mutation	UNP Q6DQ33
M	7	ALA	-	expression tag	UNP Q6DQ33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	ASP	-	expression tag	UNP Q6DQ33
M	9	PRO	-	expression tag	UNP Q6DQ33
M	10	GLY	-	expression tag	UNP Q6DQ33
M	158	ASP	ASN	engineered mutation	UNP Q6DQ33
M	224	LYS	ASN	engineered mutation	UNP Q6DQ33
M	226	LEU	GLN	engineered mutation	UNP Q6DQ33
O	7	ALA	-	expression tag	UNP Q6DQ33
O	8	ASP	-	expression tag	UNP Q6DQ33
O	9	PRO	-	expression tag	UNP Q6DQ33
O	10	GLY	-	expression tag	UNP Q6DQ33
O	158	ASP	ASN	engineered mutation	UNP Q6DQ33
O	224	LYS	ASN	engineered mutation	UNP Q6DQ33
O	226	LEU	GLN	engineered mutation	UNP Q6DQ33
Q	7	ALA	-	expression tag	UNP Q6DQ33
Q	8	ASP	-	expression tag	UNP Q6DQ33
Q	9	PRO	-	expression tag	UNP Q6DQ33
Q	10	GLY	-	expression tag	UNP Q6DQ33
Q	158	ASP	ASN	engineered mutation	UNP Q6DQ33
Q	224	LYS	ASN	engineered mutation	UNP Q6DQ33
Q	226	LEU	GLN	engineered mutation	UNP Q6DQ33
S	7	ALA	-	expression tag	UNP Q6DQ33
S	8	ASP	-	expression tag	UNP Q6DQ33
S	9	PRO	-	expression tag	UNP Q6DQ33
S	10	GLY	-	expression tag	UNP Q6DQ33
S	158	ASP	ASN	engineered mutation	UNP Q6DQ33
S	224	LYS	ASN	engineered mutation	UNP Q6DQ33
S	226	LEU	GLN	engineered mutation	UNP Q6DQ33
U	7	ALA	-	expression tag	UNP Q6DQ33
U	8	ASP	-	expression tag	UNP Q6DQ33
U	9	PRO	-	expression tag	UNP Q6DQ33
U	10	GLY	-	expression tag	UNP Q6DQ33
U	158	ASP	ASN	engineered mutation	UNP Q6DQ33
U	224	LYS	ASN	engineered mutation	UNP Q6DQ33
U	226	LEU	GLN	engineered mutation	UNP Q6DQ33
W	7	ALA	-	expression tag	UNP Q6DQ33
W	8	ASP	-	expression tag	UNP Q6DQ33
W	9	PRO	-	expression tag	UNP Q6DQ33
W	10	GLY	-	expression tag	UNP Q6DQ33
W	158	ASP	ASN	engineered mutation	UNP Q6DQ33
W	224	LYS	ASN	engineered mutation	UNP Q6DQ33
W	226	LEU	GLN	engineered mutation	UNP Q6DQ33
Y	7	ALA	-	expression tag	UNP Q6DQ33

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	8	ASP	-	expression tag	UNP Q6DQ33
Y	9	PRO	-	expression tag	UNP Q6DQ33
Y	10	GLY	-	expression tag	UNP Q6DQ33
Y	158	ASP	ASN	engineered mutation	UNP Q6DQ33
Y	224	LYS	ASN	engineered mutation	UNP Q6DQ33
Y	226	LEU	GLN	engineered mutation	UNP Q6DQ33
a	7	ALA	-	expression tag	UNP Q6DQ33
a	8	ASP	-	expression tag	UNP Q6DQ33
a	9	PRO	-	expression tag	UNP Q6DQ33
a	10	GLY	-	expression tag	UNP Q6DQ33
a	158	ASP	ASN	engineered mutation	UNP Q6DQ33
a	224	LYS	ASN	engineered mutation	UNP Q6DQ33
a	226	LEU	GLN	engineered mutation	UNP Q6DQ33
c	7	ALA	-	expression tag	UNP Q6DQ33
c	8	ASP	-	expression tag	UNP Q6DQ33
c	9	PRO	-	expression tag	UNP Q6DQ33
c	10	GLY	-	expression tag	UNP Q6DQ33
c	158	ASP	ASN	engineered mutation	UNP Q6DQ33
c	224	LYS	ASN	engineered mutation	UNP Q6DQ33
c	226	LEU	GLN	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	D	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	F	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	H	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	J	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	L	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	N	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	P	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	R	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	V	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	X	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	Z	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	b	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	d	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6DQ33
B	176	GLY	-	expression tag	UNP Q6DQ33
B	177	ARG	-	expression tag	UNP Q6DQ33
B	178	LEU	-	expression tag	UNP Q6DQ33
B	179	VAL	-	expression tag	UNP Q6DQ33
B	180	PRO	-	expression tag	UNP Q6DQ33
B	181	ARG	-	expression tag	UNP Q6DQ33
D	175	SER	-	expression tag	UNP Q6DQ33
D	176	GLY	-	expression tag	UNP Q6DQ33
D	177	ARG	-	expression tag	UNP Q6DQ33
D	178	LEU	-	expression tag	UNP Q6DQ33
D	179	VAL	-	expression tag	UNP Q6DQ33
D	180	PRO	-	expression tag	UNP Q6DQ33
D	181	ARG	-	expression tag	UNP Q6DQ33
F	175	SER	-	expression tag	UNP Q6DQ33
F	176	GLY	-	expression tag	UNP Q6DQ33
F	177	ARG	-	expression tag	UNP Q6DQ33
F	178	LEU	-	expression tag	UNP Q6DQ33
F	179	VAL	-	expression tag	UNP Q6DQ33
F	180	PRO	-	expression tag	UNP Q6DQ33
F	181	ARG	-	expression tag	UNP Q6DQ33
H	175	SER	-	expression tag	UNP Q6DQ33
H	176	GLY	-	expression tag	UNP Q6DQ33
H	177	ARG	-	expression tag	UNP Q6DQ33
H	178	LEU	-	expression tag	UNP Q6DQ33
H	179	VAL	-	expression tag	UNP Q6DQ33
H	180	PRO	-	expression tag	UNP Q6DQ33

Continued on next page...

Continued from previous page...

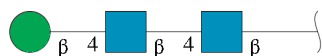
Chain	Residue	Modelled	Actual	Comment	Reference
H	181	ARG	-	expression tag	UNP Q6DQ33
J	175	SER	-	expression tag	UNP Q6DQ33
J	176	GLY	-	expression tag	UNP Q6DQ33
J	177	ARG	-	expression tag	UNP Q6DQ33
J	178	LEU	-	expression tag	UNP Q6DQ33
J	179	VAL	-	expression tag	UNP Q6DQ33
J	180	PRO	-	expression tag	UNP Q6DQ33
J	181	ARG	-	expression tag	UNP Q6DQ33
L	175	SER	-	expression tag	UNP Q6DQ33
L	176	GLY	-	expression tag	UNP Q6DQ33
L	177	ARG	-	expression tag	UNP Q6DQ33
L	178	LEU	-	expression tag	UNP Q6DQ33
L	179	VAL	-	expression tag	UNP Q6DQ33
L	180	PRO	-	expression tag	UNP Q6DQ33
L	181	ARG	-	expression tag	UNP Q6DQ33
N	175	SER	-	expression tag	UNP Q6DQ33
N	176	GLY	-	expression tag	UNP Q6DQ33
N	177	ARG	-	expression tag	UNP Q6DQ33
N	178	LEU	-	expression tag	UNP Q6DQ33
N	179	VAL	-	expression tag	UNP Q6DQ33
N	180	PRO	-	expression tag	UNP Q6DQ33
N	181	ARG	-	expression tag	UNP Q6DQ33
P	175	SER	-	expression tag	UNP Q6DQ33
P	176	GLY	-	expression tag	UNP Q6DQ33
P	177	ARG	-	expression tag	UNP Q6DQ33
P	178	LEU	-	expression tag	UNP Q6DQ33
P	179	VAL	-	expression tag	UNP Q6DQ33
P	180	PRO	-	expression tag	UNP Q6DQ33
P	181	ARG	-	expression tag	UNP Q6DQ33
R	175	SER	-	expression tag	UNP Q6DQ33
R	176	GLY	-	expression tag	UNP Q6DQ33
R	177	ARG	-	expression tag	UNP Q6DQ33
R	178	LEU	-	expression tag	UNP Q6DQ33
R	179	VAL	-	expression tag	UNP Q6DQ33
R	180	PRO	-	expression tag	UNP Q6DQ33
R	181	ARG	-	expression tag	UNP Q6DQ33
T	175	SER	-	expression tag	UNP Q6DQ33
T	176	GLY	-	expression tag	UNP Q6DQ33
T	177	ARG	-	expression tag	UNP Q6DQ33
T	178	LEU	-	expression tag	UNP Q6DQ33
T	179	VAL	-	expression tag	UNP Q6DQ33
T	180	PRO	-	expression tag	UNP Q6DQ33

Continued on next page...

Continued from previous page...

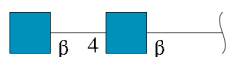
Chain	Residue	Modelled	Actual	Comment	Reference
T	181	ARG	-	expression tag	UNP Q6DQ33
V	175	SER	-	expression tag	UNP Q6DQ33
V	176	GLY	-	expression tag	UNP Q6DQ33
V	177	ARG	-	expression tag	UNP Q6DQ33
V	178	LEU	-	expression tag	UNP Q6DQ33
V	179	VAL	-	expression tag	UNP Q6DQ33
V	180	PRO	-	expression tag	UNP Q6DQ33
V	181	ARG	-	expression tag	UNP Q6DQ33
X	175	SER	-	expression tag	UNP Q6DQ33
X	176	GLY	-	expression tag	UNP Q6DQ33
X	177	ARG	-	expression tag	UNP Q6DQ33
X	178	LEU	-	expression tag	UNP Q6DQ33
X	179	VAL	-	expression tag	UNP Q6DQ33
X	180	PRO	-	expression tag	UNP Q6DQ33
X	181	ARG	-	expression tag	UNP Q6DQ33
Z	175	SER	-	expression tag	UNP Q6DQ33
Z	176	GLY	-	expression tag	UNP Q6DQ33
Z	177	ARG	-	expression tag	UNP Q6DQ33
Z	178	LEU	-	expression tag	UNP Q6DQ33
Z	179	VAL	-	expression tag	UNP Q6DQ33
Z	180	PRO	-	expression tag	UNP Q6DQ33
Z	181	ARG	-	expression tag	UNP Q6DQ33
b	175	SER	-	expression tag	UNP Q6DQ33
b	176	GLY	-	expression tag	UNP Q6DQ33
b	177	ARG	-	expression tag	UNP Q6DQ33
b	178	LEU	-	expression tag	UNP Q6DQ33
b	179	VAL	-	expression tag	UNP Q6DQ33
b	180	PRO	-	expression tag	UNP Q6DQ33
b	181	ARG	-	expression tag	UNP Q6DQ33
d	175	SER	-	expression tag	UNP Q6DQ33
d	176	GLY	-	expression tag	UNP Q6DQ33
d	177	ARG	-	expression tag	UNP Q6DQ33
d	178	LEU	-	expression tag	UNP Q6DQ33
d	179	VAL	-	expression tag	UNP Q6DQ33
d	180	PRO	-	expression tag	UNP Q6DQ33
d	181	ARG	-	expression tag	UNP Q6DQ33

- Molecule 3 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
3	e	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	g	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	n	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	o	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	w	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	y	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	i	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	k	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	m	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	p	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

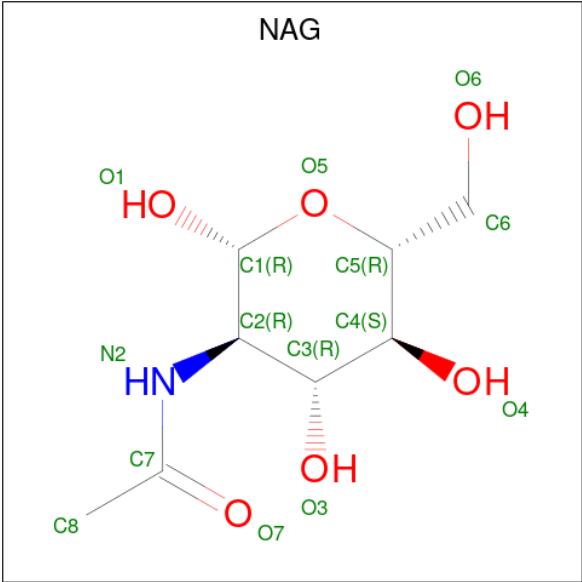
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	r	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	t	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	u	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	v	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	x	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	z	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	0	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	1	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	s	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

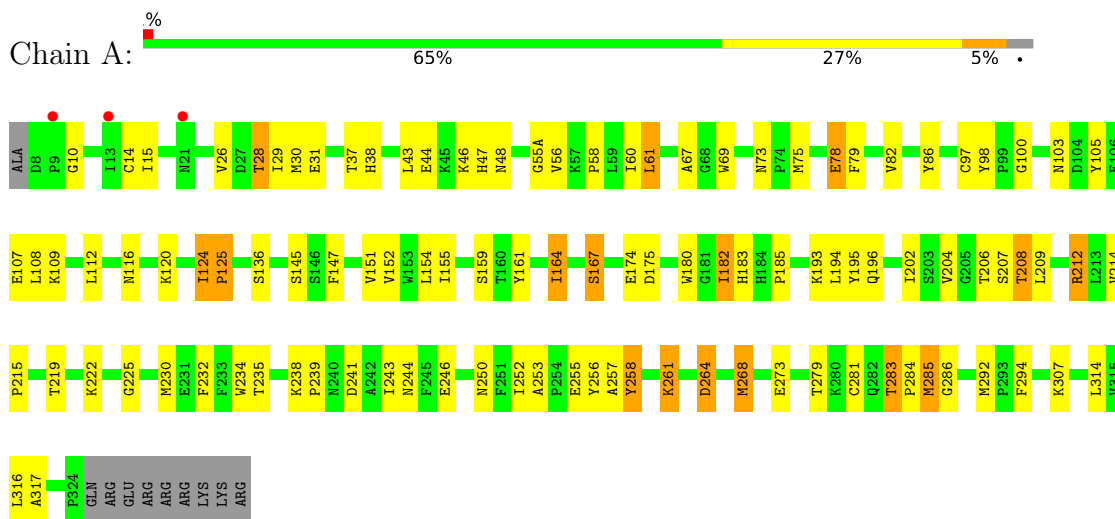


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	O	1	Total	C	N	O	0	0
			14	8	1	5		
6	Y	1	Total	C	N	O	0	0
			14	8	1	5		
6	c	1	Total	C	N	O	0	0
			14	8	1	5		
6	c	1	Total	C	N	O	0	0
			14	8	1	5		

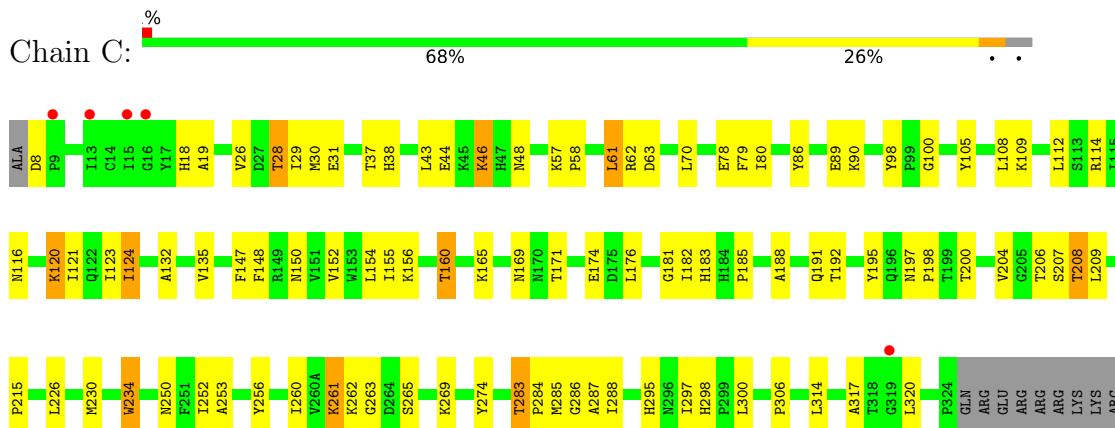
3 Residue-property plots [i](#)

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.

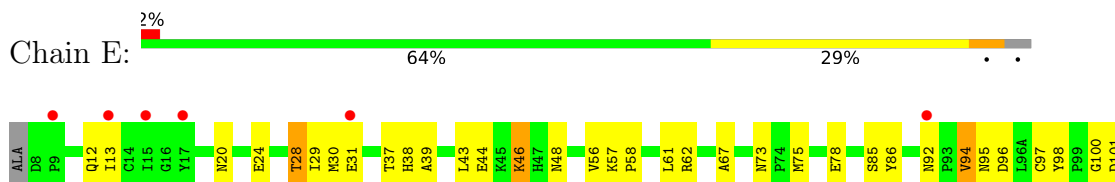
• Molecule 1: Hemagglutinin HA1 chain

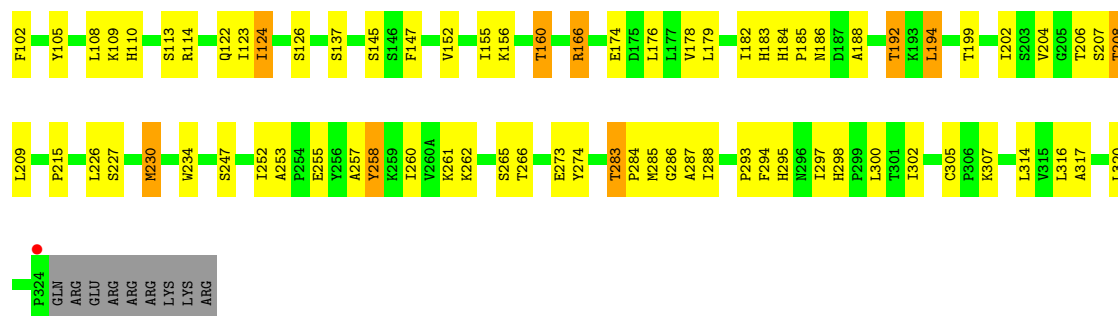


• Molecule 1: Hemagglutinin HA1 chain



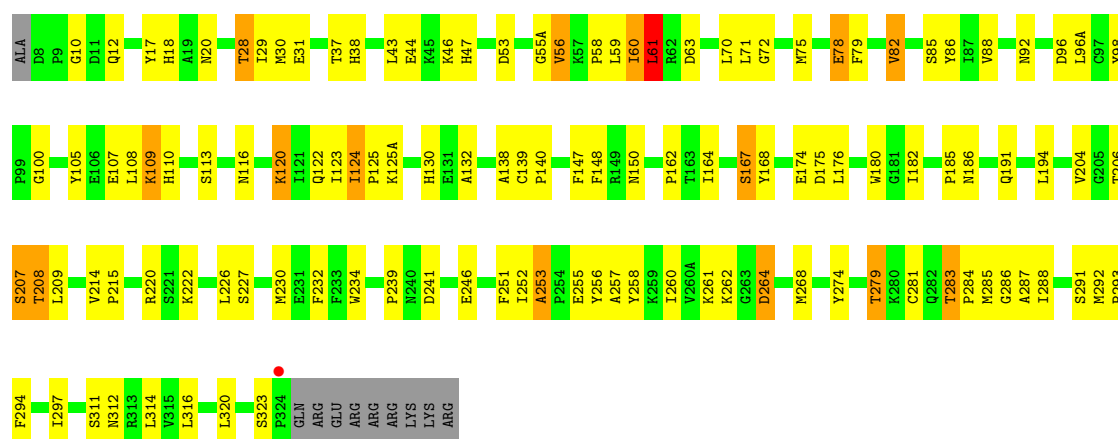
• Molecule 1: Hemagglutinin HA1 chain





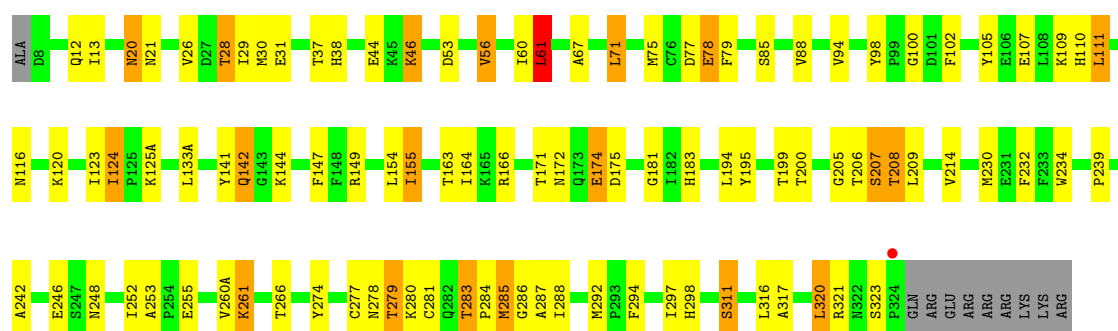
• Molecule 1: Hemagglutinin HA1 chain

Chain G: 61% 31%



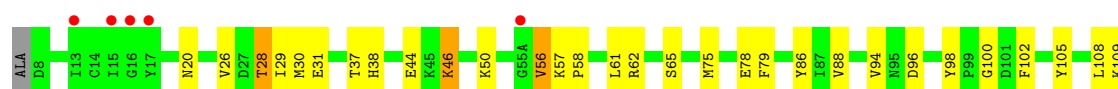
• Molecule 1: Hemagglutinin HA1 chain

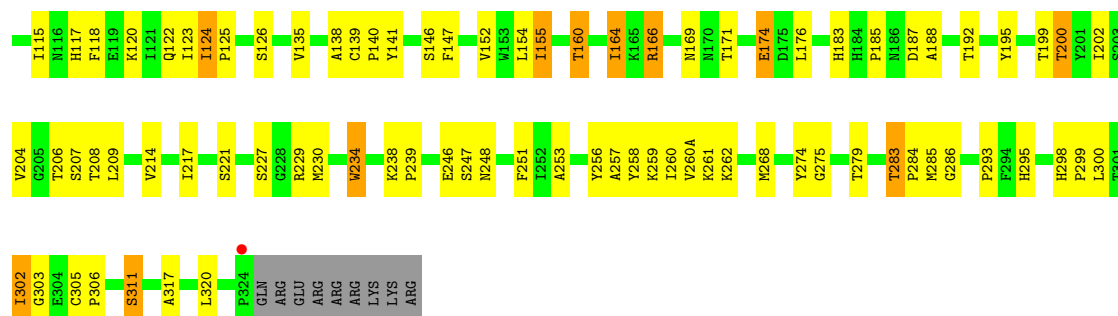
Chain I: 67% 24% 6%



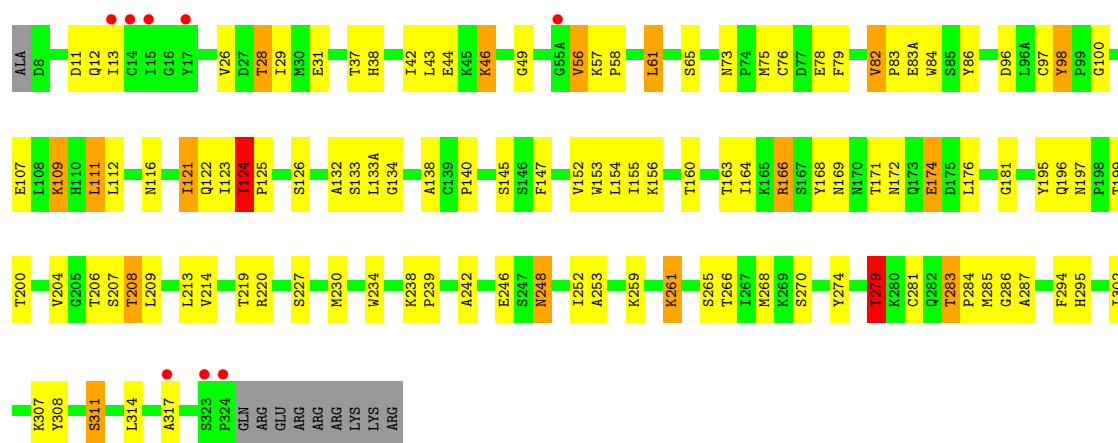
• Molecule 1: Hemagglutinin HA1 chain

Chain K: 2% 63% 29%

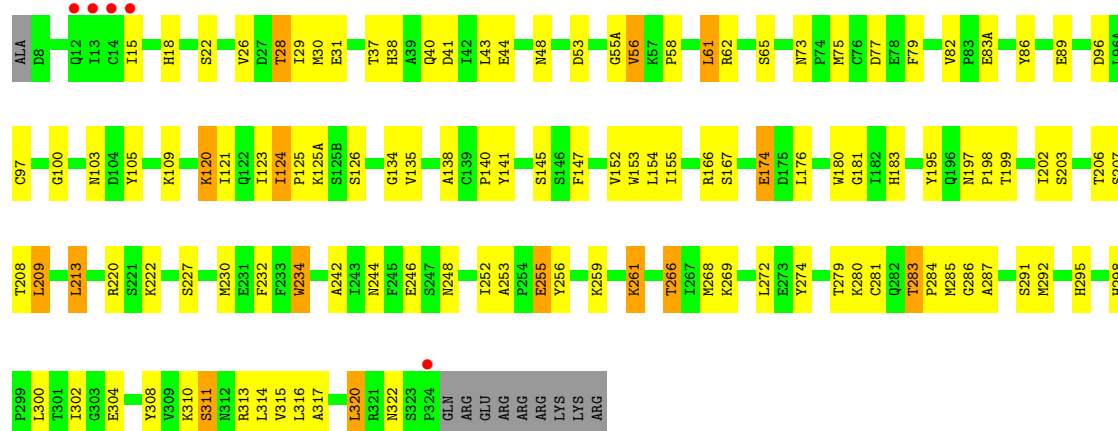




• Molecule 1: Hemagglutinin HA1 chain

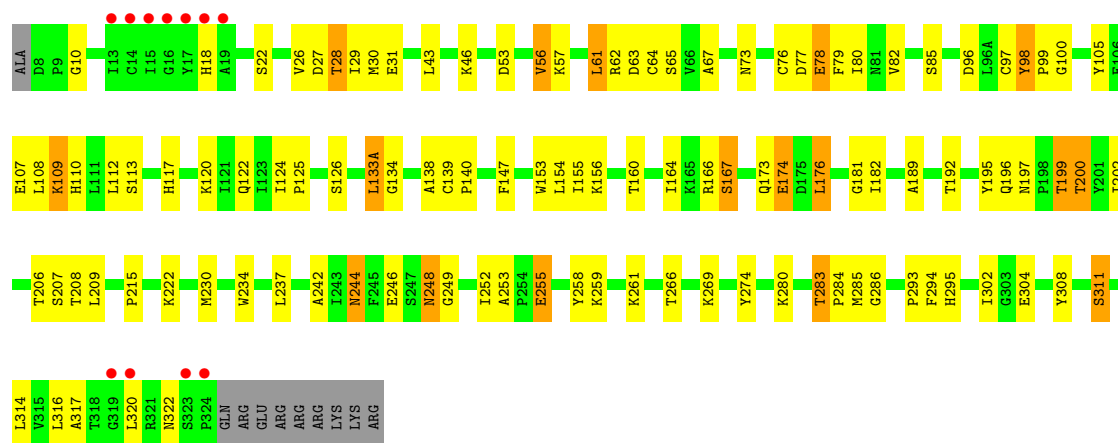


• Molecule 1: Hemagglutinin HA1 chain

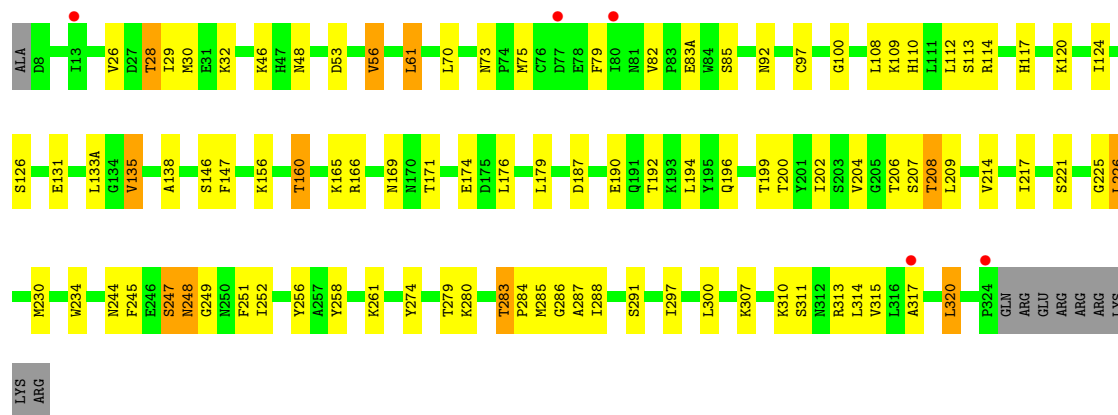


• Molecule 1: Hemagglutinin HA1 chain

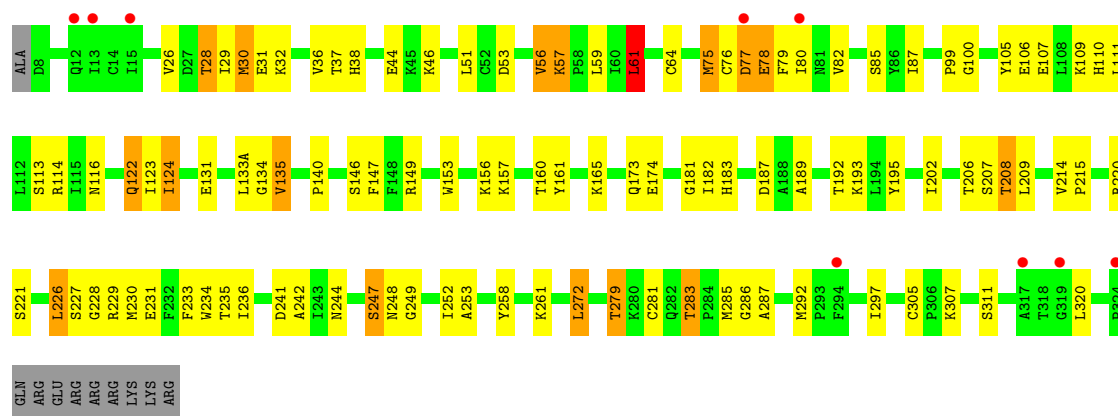




• Molecule 1: Hemagglutinin HA1 chain

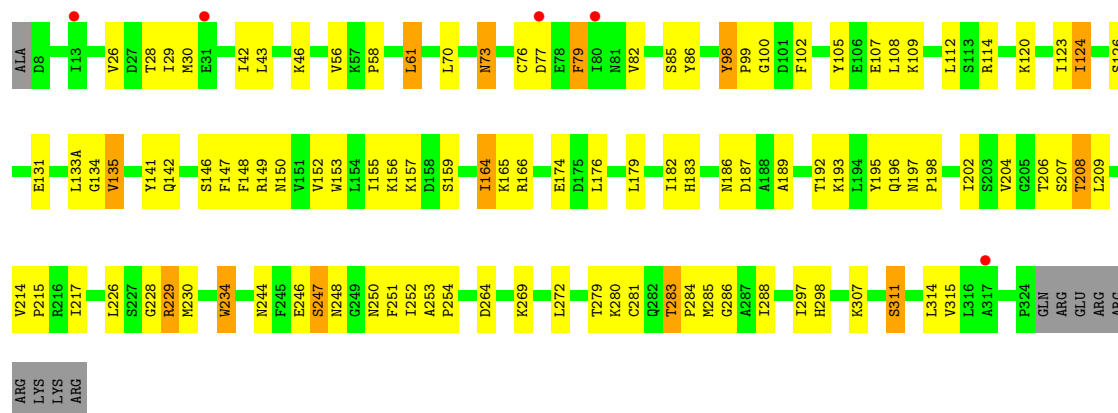


• Molecule 1: Hemagglutinin HA1 chain

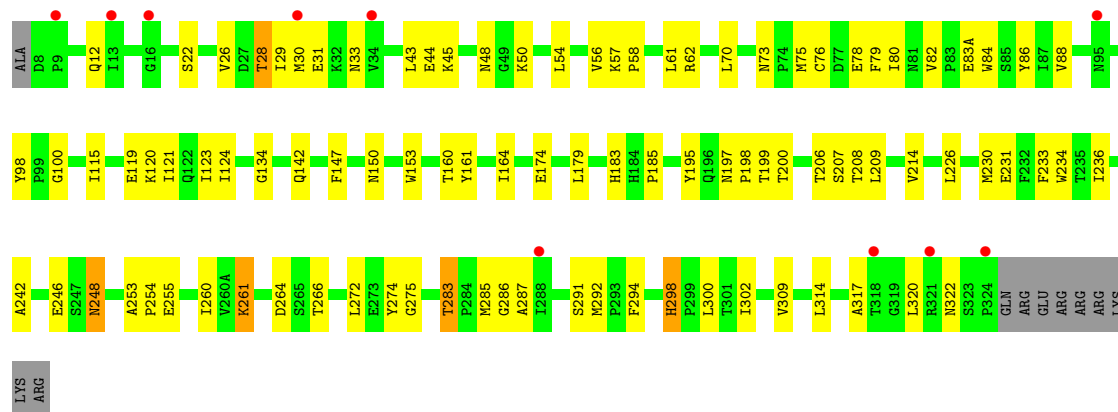


• Molecule 1: Hemagglutinin HA1 chain

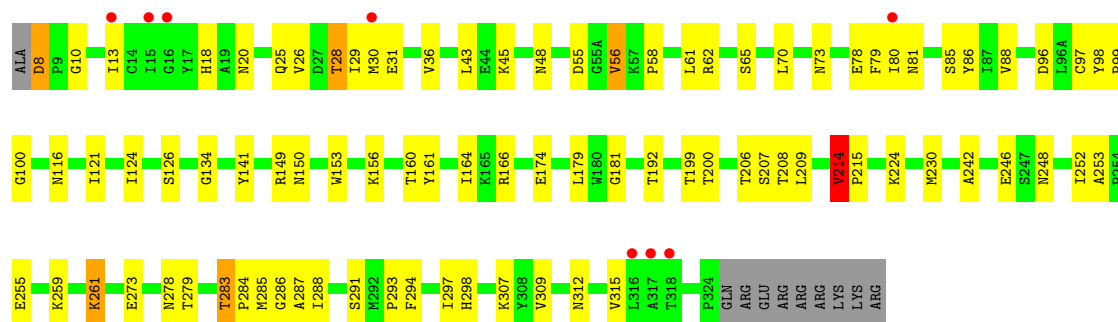




• Molecule 1: Hemagglutinin HA1 chain

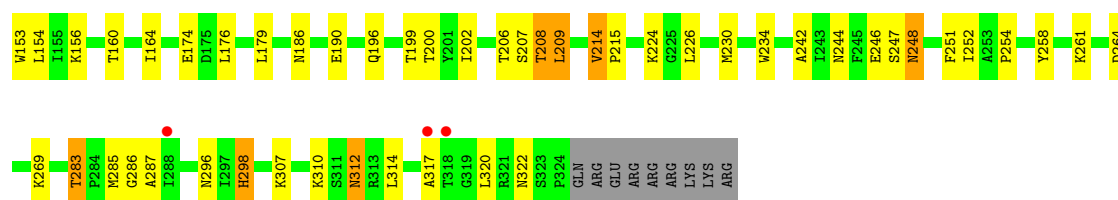


• Molecule 1: Hemagglutinin HA1 chain

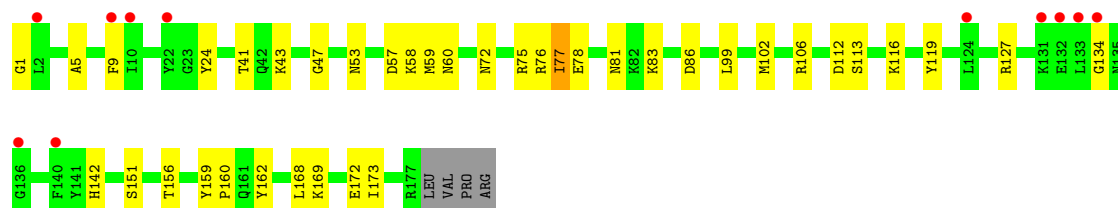
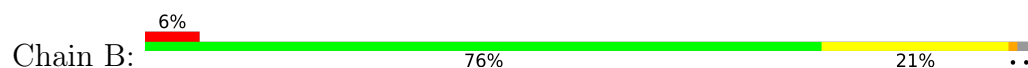


• Molecule 1: Hemagglutinin HA1 chain

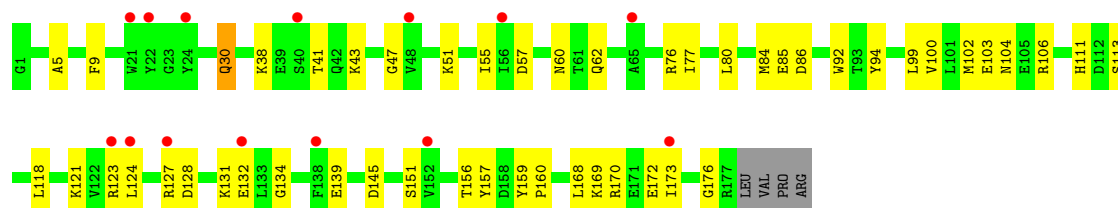




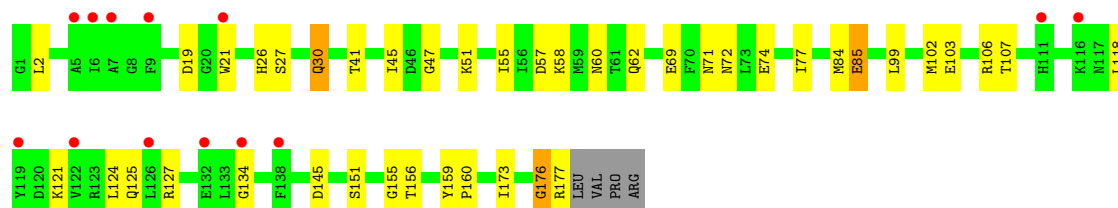
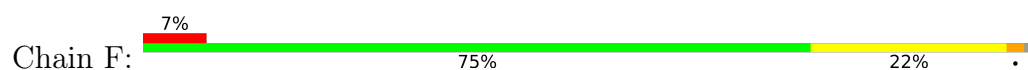
• Molecule 2: Hemagglutinin HA2 chain



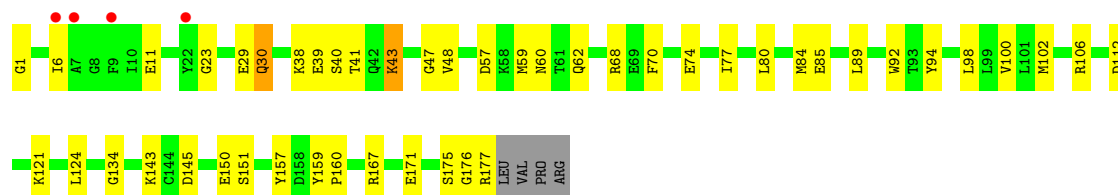
• Molecule 2: Hemagglutinin HA2 chain



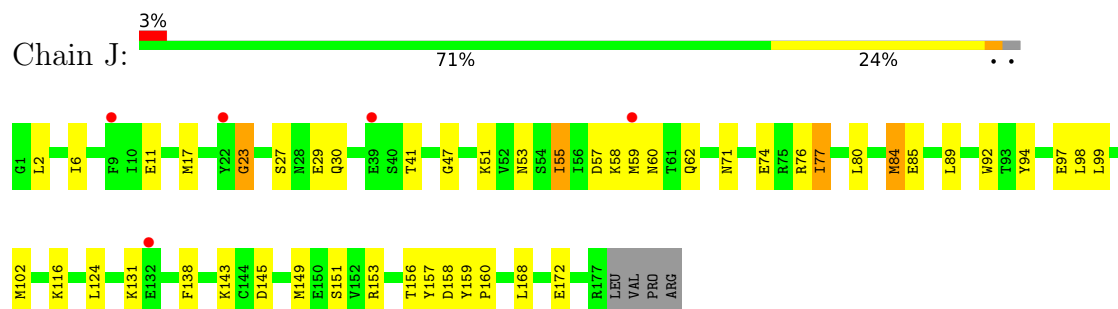
• Molecule 2: Hemagglutinin HA2 chain



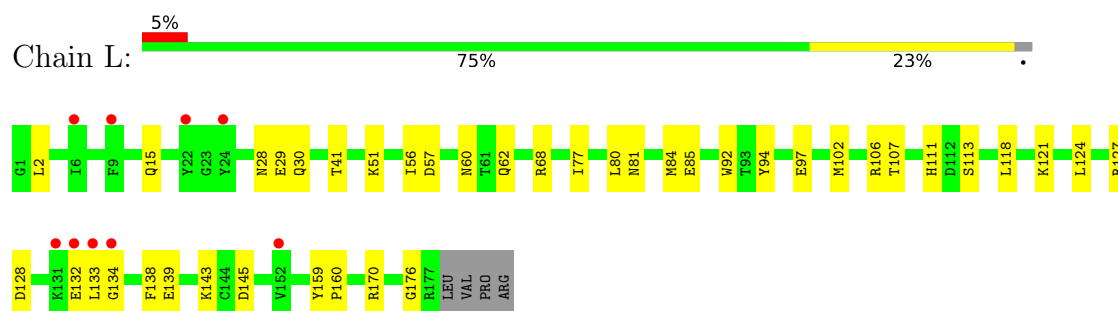
• Molecule 2: Hemagglutinin HA2 chain



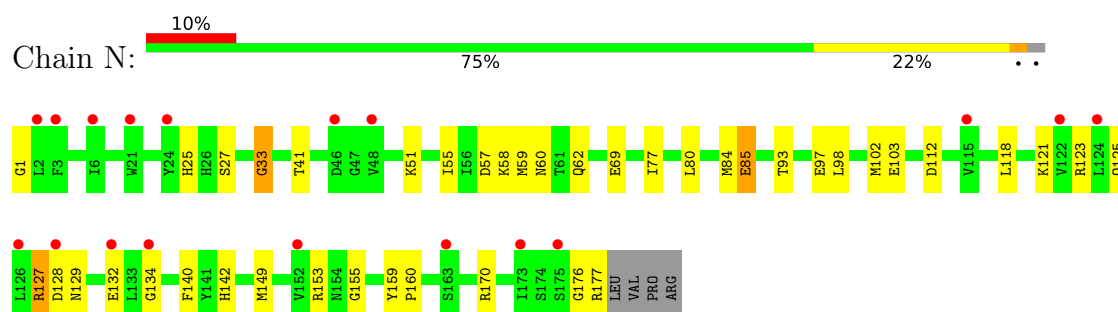
- Molecule 2: Hemagglutinin HA2 chain



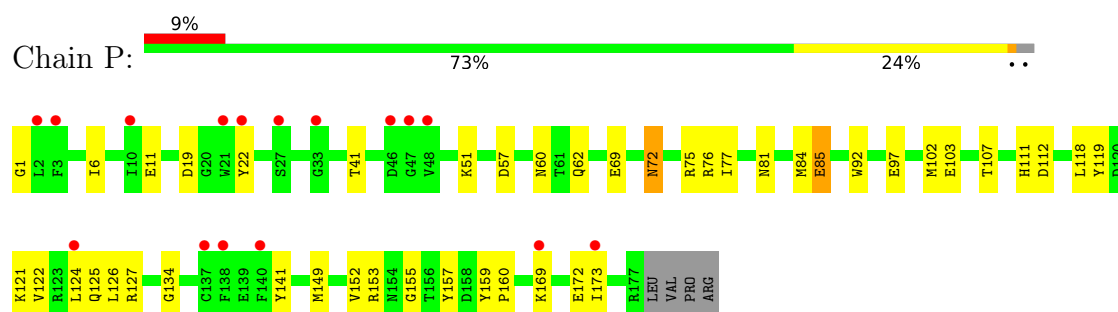
- Molecule 2: Hemagglutinin HA2 chain



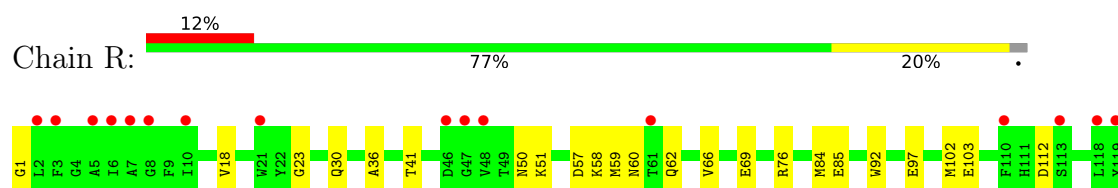
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain

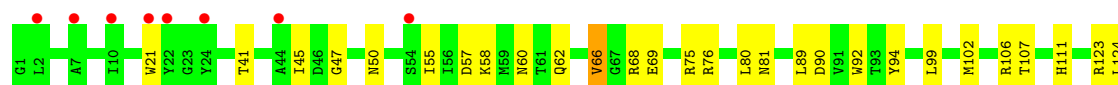
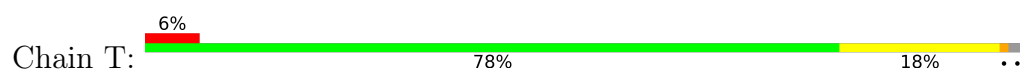


- Molecule 2: Hemagglutinin HA2 chain

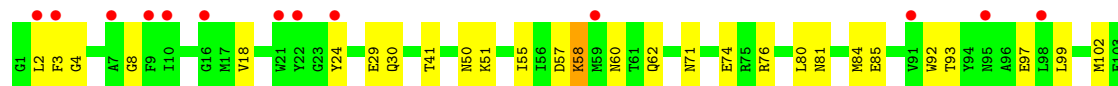
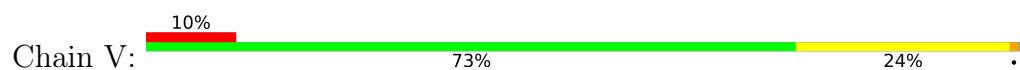




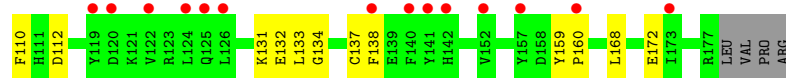
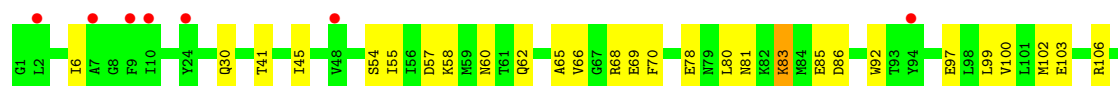
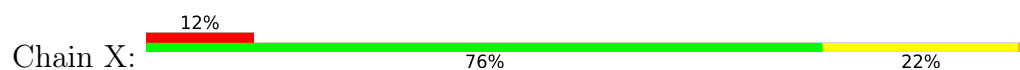
• Molecule 2: Hemagglutinin HA2 chain



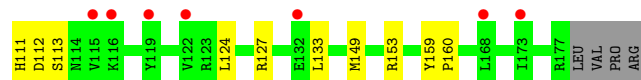
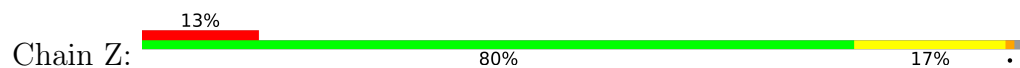
• Molecule 2: Hemagglutinin HA2 chain



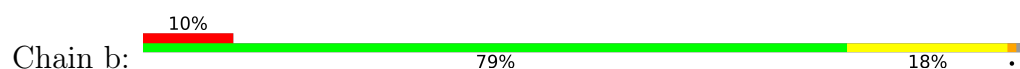
• Molecule 2: Hemagglutinin HA2 chain

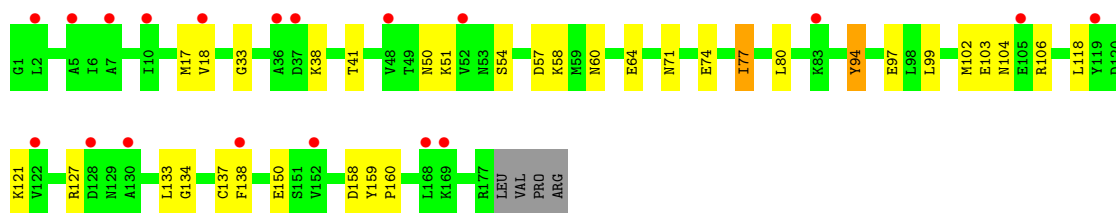


• Molecule 2: Hemagglutinin HA2 chain

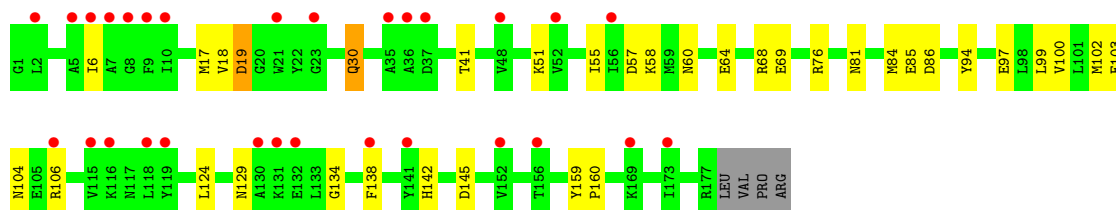
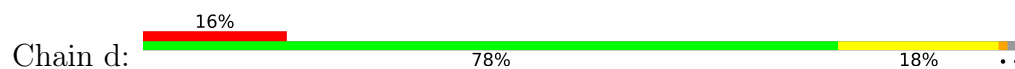


• Molecule 2: Hemagglutinin HA2 chain





• Molecule 2: Hemagglutinin HA2 chain



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



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



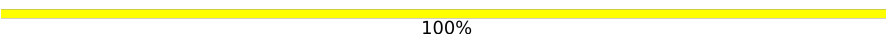
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

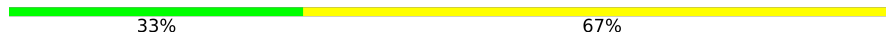


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  33% 67%

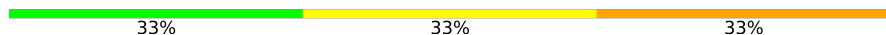
MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  67% 33%

MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:  33% 33% 33%

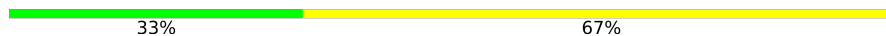
MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  67% 33%

MAG1
MAG2
BMA3

- Molecule 3: 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%

MAG1
MAG2
BMA3

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

Chain f:  100%

NAG1
NAG2

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

Chain i:  100%

NAG1
NAG2

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

Chain k:  100%

NAG1
NAG2

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

Chain m:  100%

NAG1
NAG2

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

Chain p:  50% 50%

NAG1
NAG2

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

Chain r:  100%

NAG1
NAG2

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

Chain t:  100%

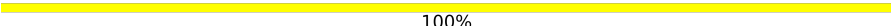
NAG1
NAG2

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

Chain u:  50% 50%

MAG1
MAG2

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

Chain v:  100%

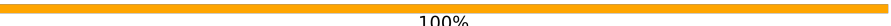
MAG1
MAG2

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

Chain x:  50% 50%

MAG1
MAG2

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

Chain z:  100%

MAG1
MAG2

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

Chain 0:  50% 50%

MAG1
MAG2

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

Chain 1:  50% 50%

MAG1
MAG2

- Molecule 5: 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 s:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.92Å 118.11Å 273.80Å 91.50° 90.18° 119.87°	Depositor
Resolution (Å)	45.28 – 3.16 45.28 – 3.16	Depositor EDS
% Data completeness (in resolution range)	91.1 (45.28-3.16) 91.1 (45.28-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.262 0.219 , 0.266	Depositor DCC
R_{free} test set	9996 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h+k,-h,l 0.004 for -k,h+k,l 0.057 for k,-h-k,l 0.057 for -h-k,h,l 0.024 for h,-h-k,-l 0.011 for -h-k,k,-l 0.000 for -h,-k,l 0.004 for k,h,-l 0.001 for -k,-h,-l 0.000 for -h,h+k,-l 0.000 for h+k,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	60964	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.86% 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: MAN, BMA, 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	0.91	1/2639 (0.0%)	1.28	17/3584 (0.5%)
1	C	0.80	0/2639	1.18	10/3584 (0.3%)
1	E	0.78	0/2639	1.20	19/3584 (0.5%)
1	G	0.94	0/2639	1.32	19/3584 (0.5%)
1	I	0.94	2/2639 (0.1%)	1.30	23/3584 (0.6%)
1	K	0.80	0/2639	1.16	17/3584 (0.5%)
1	M	0.89	0/2639	1.27	18/3584 (0.5%)
1	O	0.85	0/2639	1.20	16/3584 (0.4%)
1	Q	0.88	1/2639 (0.0%)	1.26	21/3584 (0.6%)
1	S	0.73	0/2639	1.14	13/3584 (0.4%)
1	U	0.73	0/2639	1.17	21/3584 (0.6%)
1	W	0.77	0/2639	1.17	21/3584 (0.6%)
1	Y	0.56	0/2639	1.04	12/3584 (0.3%)
1	a	0.57	0/2639	1.06	19/3584 (0.5%)
1	c	0.57	0/2639	1.03	8/3584 (0.2%)
2	B	0.56	0/1460	0.94	1/1961 (0.1%)
2	D	0.52	0/1460	0.89	2/1961 (0.1%)
2	F	0.51	0/1460	0.91	1/1961 (0.1%)
2	H	0.60	0/1460	0.99	2/1961 (0.1%)
2	J	0.58	0/1460	0.96	2/1961 (0.1%)
2	L	0.52	0/1460	0.89	1/1961 (0.1%)
2	N	0.56	0/1460	0.95	2/1961 (0.1%)
2	P	0.54	0/1460	0.92	3/1961 (0.2%)
2	R	0.56	0/1460	0.95	1/1961 (0.1%)
2	T	0.46	0/1460	0.91	1/1961 (0.1%)
2	V	0.48	0/1460	0.91	2/1961 (0.1%)
2	X	0.46	0/1460	0.87	0/1961
2	Z	0.44	0/1460	0.89	3/1961 (0.2%)
2	b	0.44	0/1460	0.89	3/1961 (0.2%)
2	d	0.43	0/1460	0.85	1/1961 (0.1%)
All	All	0.70	4/61485 (0.0%)	1.10	279/83175 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	248	ASN	CA-C	6.96	1.62	1.52
1	I	242	ALA	CA-C	6.46	1.60	1.52
1	A	243	ILE	CA-CB	-5.67	1.47	1.54
1	I	171	THR	C-O	-5.61	1.16	1.24

The worst 5 of 279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	253	ALA	CA-C-N	-10.98	108.99	120.85
1	G	253	ALA	C-N-CA	-10.98	108.99	120.85
1	I	253	ALA	CA-C-N	-10.18	109.86	120.85
1	I	253	ALA	C-N-CA	-10.18	109.86	120.85
1	E	253	ALA	CA-C-N	-9.48	111.02	120.31

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	2573	0	2521	73	0
1	C	2573	0	2522	73	0
1	E	2573	0	2521	72	0
1	G	2573	0	2521	80	0
1	I	2573	0	2521	68	0
1	K	2573	0	2521	83	0
1	M	2573	0	2521	79	0
1	O	2573	0	2520	79	0
1	Q	2573	0	2521	72	0
1	S	2573	0	2521	65	0
1	U	2573	0	2521	69	0
1	W	2573	0	2521	73	0
1	Y	2573	0	2521	53	0
1	a	2573	0	2522	50	0
1	c	2573	0	2521	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1433	0	1340	36	0
2	D	1433	0	1340	32	0
2	F	1433	0	1340	30	0
2	H	1433	0	1340	29	0
2	J	1433	0	1340	39	0
2	L	1433	0	1340	25	0
2	N	1433	0	1340	28	0
2	P	1433	0	1340	28	0
2	R	1433	0	1340	22	0
2	T	1433	0	1340	34	0
2	V	1433	0	1340	38	0
2	X	1433	0	1340	37	0
2	Z	1433	0	1340	22	0
2	b	1433	0	1340	25	0
2	d	1433	0	1340	27	0
3	e	39	0	34	1	0
3	g	39	0	34	0	0
3	h	39	0	34	0	0
3	j	39	0	34	1	0
3	l	39	0	34	0	0
3	n	39	0	34	0	0
3	o	39	0	34	1	0
3	q	39	0	34	2	0
3	w	39	0	34	2	0
3	y	39	0	34	0	0
4	0	28	0	25	1	0
4	1	28	0	25	2	0
4	f	28	0	25	2	0
4	i	28	0	25	0	0
4	k	28	0	25	0	0
4	m	28	0	25	1	0
4	p	28	0	25	0	0
4	r	28	0	25	1	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	v	28	0	25	0	0
4	x	28	0	25	0	0
4	z	28	0	25	1	0
5	s	50	0	43	5	0
6	K	14	0	13	0	0
6	O	14	0	13	0	0
6	Y	14	0	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	c	28	0	26	2	0
All	All	60964	0	58689	1310	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 11.

The worst 5 of 1310 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:K:192:THR:HG21	1:S:192:THR:HG21	1.28	1.14
5:s:3:BMA:H2	5:s:4:MAN:H5	1.11	1.09
1:I:283:THR:HG22	1:I:285:MET:H	1.24	1.03
1:O:283:THR:HG22	1:O:285:MET:H	1.27	0.98
1:A:283:THR:HG22	1:A:285:MET:H	1.27	0.98

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	323/334 (97%)	295 (91%)	28 (9%)	0	100	100
1	C	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	E	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	G	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	I	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	K	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	M	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	O	323/334 (97%)	299 (93%)	24 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	S	323/334 (97%)	302 (94%)	20 (6%)	1 (0%)	36	64
1	U	323/334 (97%)	298 (92%)	23 (7%)	2 (1%)	21	52
1	W	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Y	323/334 (97%)	297 (92%)	25 (8%)	1 (0%)	36	64
1	a	323/334 (97%)	297 (92%)	26 (8%)	0	100	100
1	c	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	36	64
2	B	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	D	175/181 (97%)	162 (93%)	12 (7%)	1 (1%)	21	52
2	F	175/181 (97%)	163 (93%)	11 (6%)	1 (1%)	21	52
2	H	175/181 (97%)	166 (95%)	9 (5%)	0	100	100
2	J	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	L	175/181 (97%)	160 (91%)	14 (8%)	1 (1%)	21	52
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	167 (95%)	8 (5%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	b	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	6943 (93%)	519 (7%)	8 (0%)	48	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	Y	248	ASN
1	S	248	ASN
1	U	78	GLU
1	c	248	ASN

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	292/300 (97%)	268 (92%)	24 (8%)	10	34
1	C	292/300 (97%)	281 (96%)	11 (4%)	29	58
1	E	292/300 (97%)	274 (94%)	18 (6%)	16	44
1	G	292/300 (97%)	274 (94%)	18 (6%)	16	44
1	I	292/300 (97%)	270 (92%)	22 (8%)	12	38
1	K	292/300 (97%)	280 (96%)	12 (4%)	27	56
1	M	292/300 (97%)	269 (92%)	23 (8%)	11	36
1	O	292/300 (97%)	274 (94%)	18 (6%)	16	44
1	Q	292/300 (97%)	270 (92%)	22 (8%)	12	38
1	S	292/300 (97%)	276 (94%)	16 (6%)	19	47
1	U	292/300 (97%)	274 (94%)	18 (6%)	16	44
1	W	292/300 (97%)	281 (96%)	11 (4%)	29	58
1	Y	292/300 (97%)	277 (95%)	15 (5%)	21	50
1	a	292/300 (97%)	278 (95%)	14 (5%)	23	52
1	c	292/300 (97%)	279 (96%)	13 (4%)	24	53
2	B	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	D	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	F	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	H	151/155 (97%)	143 (95%)	8 (5%)	20	49
2	J	151/155 (97%)	146 (97%)	5 (3%)	33	60
2	L	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	N	151/155 (97%)	146 (97%)	5 (3%)	33	60
2	P	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	R	151/155 (97%)	147 (97%)	4 (3%)	40	64
2	T	151/155 (97%)	148 (98%)	3 (2%)	48	68
2	V	151/155 (97%)	145 (96%)	6 (4%)	28	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	151/155 (97%)	145 (96%)	6 (4%)	28	56
2	Z	151/155 (97%)	146 (97%)	5 (3%)	33	60
2	b	151/155 (97%)	146 (97%)	5 (3%)	33	60
2	d	151/155 (97%)	146 (97%)	5 (3%)	33	60
All	All	6645/6825 (97%)	6318 (95%)	327 (5%)	22	51

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	174	GLU
2	N	85	GLU
1	a	283	THR
2	D	41	THR
2	V	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	30	GLN
2	d	42	GLN
2	R	161	GLN
2	X	50	ASN
1	M	197	ASN

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 ⓘ

60 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
4	NAG	0	1	4,1	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	0	2	4	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	1	1	4,1	14,14,15	0.45	0	17,19,21	1.22	2 (11%)
4	NAG	1	2	4	14,14,15	0.42	0	17,19,21	0.45	0
3	NAG	e	1	1,3	14,14,15	1.41	3 (21%)	17,19,21	1.20	1 (5%)
3	NAG	e	2	3	14,14,15	0.49	0	17,19,21	0.57	0
3	BMA	e	3	3	11,11,12	1.91	3 (27%)	15,15,17	1.71	4 (26%)
4	NAG	f	1	4,1	14,14,15	1.00	1 (7%)	17,19,21	1.25	2 (11%)
4	NAG	f	2	4	14,14,15	1.82	2 (14%)	17,19,21	1.19	1 (5%)
3	NAG	g	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.66	0
3	NAG	g	2	3	14,14,15	0.64	0	17,19,21	0.85	0
3	BMA	g	3	3	11,11,12	1.78	2 (18%)	15,15,17	2.47	5 (33%)
3	NAG	h	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.45	1 (5%)
3	NAG	h	2	3	14,14,15	0.98	1 (7%)	17,19,21	1.39	3 (17%)
3	BMA	h	3	3	11,11,12	2.44	7 (63%)	15,15,17	1.43	3 (20%)
4	NAG	i	1	4,1	14,14,15	1.18	1 (7%)	17,19,21	1.31	3 (17%)
4	NAG	i	2	4	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
3	NAG	j	1	1,3	14,14,15	1.71	2 (14%)	17,19,21	1.30	2 (11%)
3	NAG	j	2	3	14,14,15	1.22	1 (7%)	17,19,21	1.16	2 (11%)
3	BMA	j	3	3	11,11,12	2.24	5 (45%)	15,15,17	1.54	3 (20%)
4	NAG	k	1	4,1	14,14,15	1.24	1 (7%)	17,19,21	1.38	2 (11%)
4	NAG	k	2	4	14,14,15	1.81	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	l	1	1,3	14,14,15	1.27	2 (14%)	17,19,21	1.42	2 (11%)
3	NAG	l	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.61	0
3	BMA	l	3	3	11,11,12	1.94	3 (27%)	15,15,17	1.45	3 (20%)
4	NAG	m	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	m	2	4	14,14,15	1.55	2 (14%)	17,19,21	1.02	1 (5%)
3	NAG	n	1	1,3	14,14,15	0.54	0	17,19,21	0.73	0
3	NAG	n	2	3	14,14,15	0.92	1 (7%)	17,19,21	1.22	2 (11%)
3	BMA	n	3	3	11,11,12	1.96	4 (36%)	15,15,17	1.61	3 (20%)
3	NAG	o	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	o	2	3	14,14,15	0.84	1 (7%)	17,19,21	0.85	0
3	BMA	o	3	3	11,11,12	1.87	4 (36%)	15,15,17	1.94	5 (33%)
4	NAG	p	1	4,1	14,14,15	0.73	0	17,19,21	0.76	0
4	NAG	p	2	4	14,14,15	1.46	1 (7%)	17,19,21	1.35	3 (17%)
3	NAG	q	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	0.71	0
3	NAG	q	2	3	14,14,15	0.32	0	17,19,21	0.42	0
3	BMA	q	3	3	11,11,12	1.51	2 (18%)	15,15,17	2.13	3 (20%)
4	NAG	r	1	4,1	14,14,15	0.84	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	r	2	4	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
5	NAG	s	1	5,1	14,14,15	0.57	0	17,19,21	1.71	5 (29%)
5	NAG	s	2	5	14,14,15	0.45	0	17,19,21	1.03	0
5	BMA	s	3	5	11,11,12	0.70	0	15,15,17	1.78	4 (26%)
5	MAN	s	4	5	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
4	NAG	t	1	4,1	14,14,15	1.24	1 (7%)	17,19,21	1.27	2 (11%)
4	NAG	t	2	4	14,14,15	1.03	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	u	1	4,1	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	u	2	4	14,14,15	0.90	1 (7%)	17,19,21	0.89	0
4	NAG	v	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	0.97	2 (11%)
4	NAG	v	2	4	14,14,15	1.26	3 (21%)	17,19,21	1.07	1 (5%)
3	NAG	w	1	1,3	14,14,15	0.31	0	17,19,21	0.59	0
3	NAG	w	2	3	14,14,15	1.89	1 (7%)	17,19,21	1.35	2 (11%)
3	BMA	w	3	3	11,11,12	1.37	2 (18%)	15,15,17	1.32	3 (20%)
4	NAG	x	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	1.26	2 (11%)
4	NAG	x	2	4	14,14,15	0.40	0	17,19,21	0.62	0
3	NAG	y	1	1,3	14,14,15	0.64	0	17,19,21	0.98	1 (5%)
3	NAG	y	2	3	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
3	BMA	y	3	3	11,11,12	0.56	0	15,15,17	0.69	0
4	NAG	z	1	4,1	14,14,15	1.40	1 (7%)	17,19,21	1.30	3 (17%)
4	NAG	z	2	4	14,14,15	0.95	1 (7%)	17,19,21	0.86	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	0	1	4,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	0	2	4	-	2/6/23/26	0/1/1/1
4	NAG	1	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	2/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	BMA	e	3	3	-	2/2/19/22	0/1/1/1
4	NAG	f	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	1/6/23/26	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	1/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
4	NAG	i	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
3	NAG	j	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
4	NAG	k	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	0/6/23/26	0/1/1/1
3	NAG	l	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	BMA	l	3	3	-	2/2/19/22	0/1/1/1
4	NAG	m	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
3	NAG	n	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	BMA	n	3	3	-	0/2/19/22	0/1/1/1
3	NAG	o	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	o	2	3	-	1/6/23/26	0/1/1/1
3	BMA	o	3	3	-	2/2/19/22	0/1/1/1
4	NAG	p	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	p	2	4	-	0/6/23/26	0/1/1/1
3	NAG	q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	q	3	3	-	1/2/19/22	0/1/1/1
4	NAG	r	1	4,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	w	2	NAG	O5-C1	-6.85	1.32	1.43
3	j	1	NAG	O5-C1	-5.77	1.34	1.43
4	p	2	NAG	O5-C1	-4.82	1.35	1.43
4	z	1	NAG	O5-C1	-4.80	1.35	1.43
4	k	2	NAG	C1-C2	4.79	1.58	1.52

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	3	BMA	C1-O5-C5	6.01	120.24	112.19
3	q	3	BMA	C1-O5-C5	5.36	119.37	112.19
3	h	1	NAG	C1-O5-C5	5.07	118.98	112.19
4	f	2	NAG	C1-O5-C5	4.53	118.26	112.19
4	k	1	NAG	C3-C4-C5	4.17	117.79	110.23

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	w	2	NAG	O5-C5-C6-O6
4	u	2	NAG	O5-C5-C6-O6
3	y	3	BMA	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6

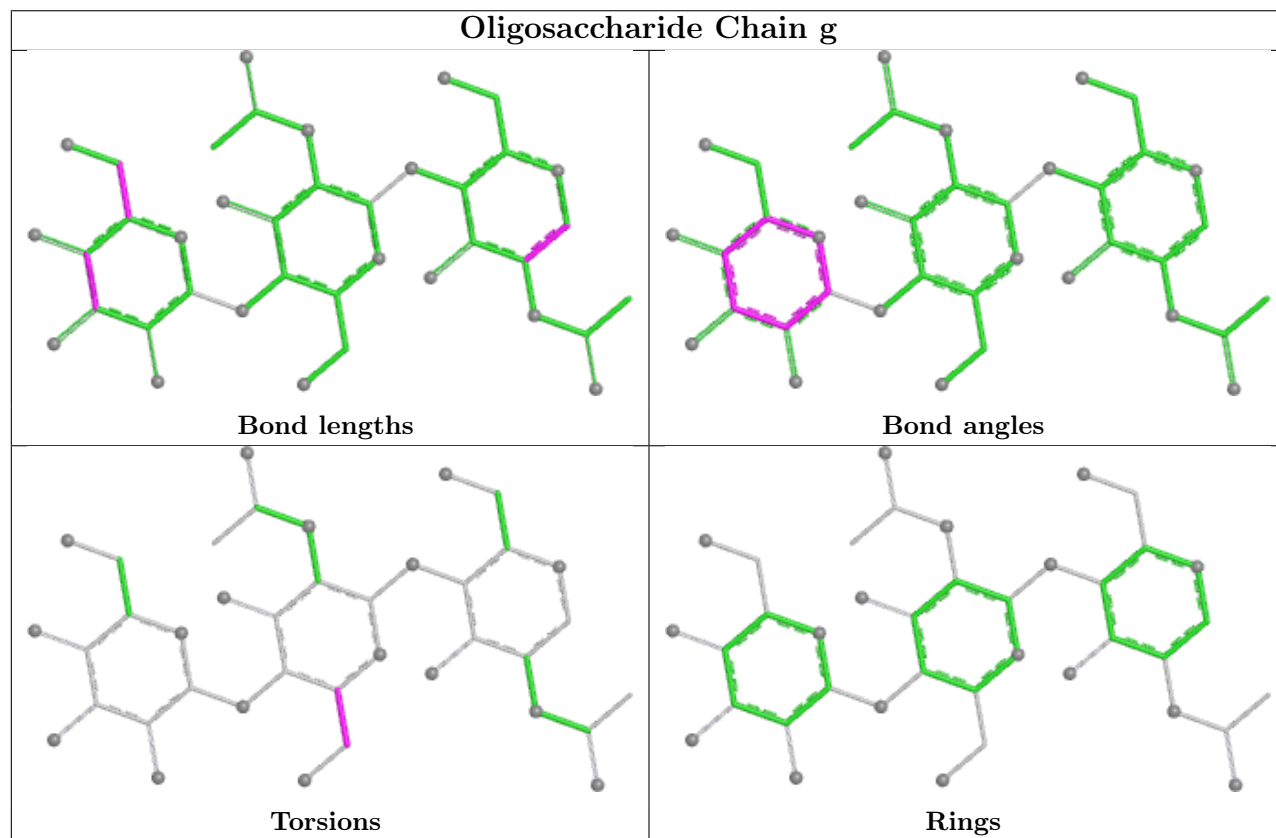
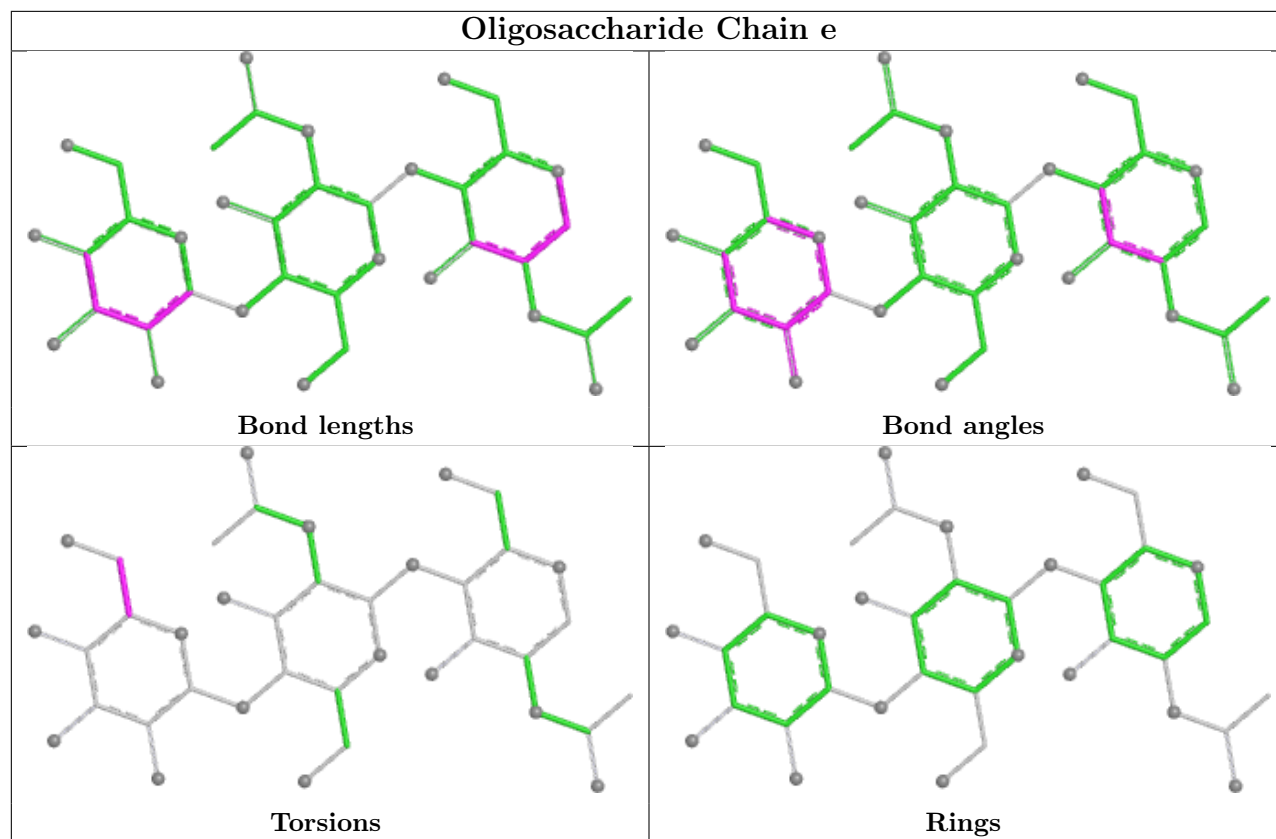
All (1) ring outliers are listed below:

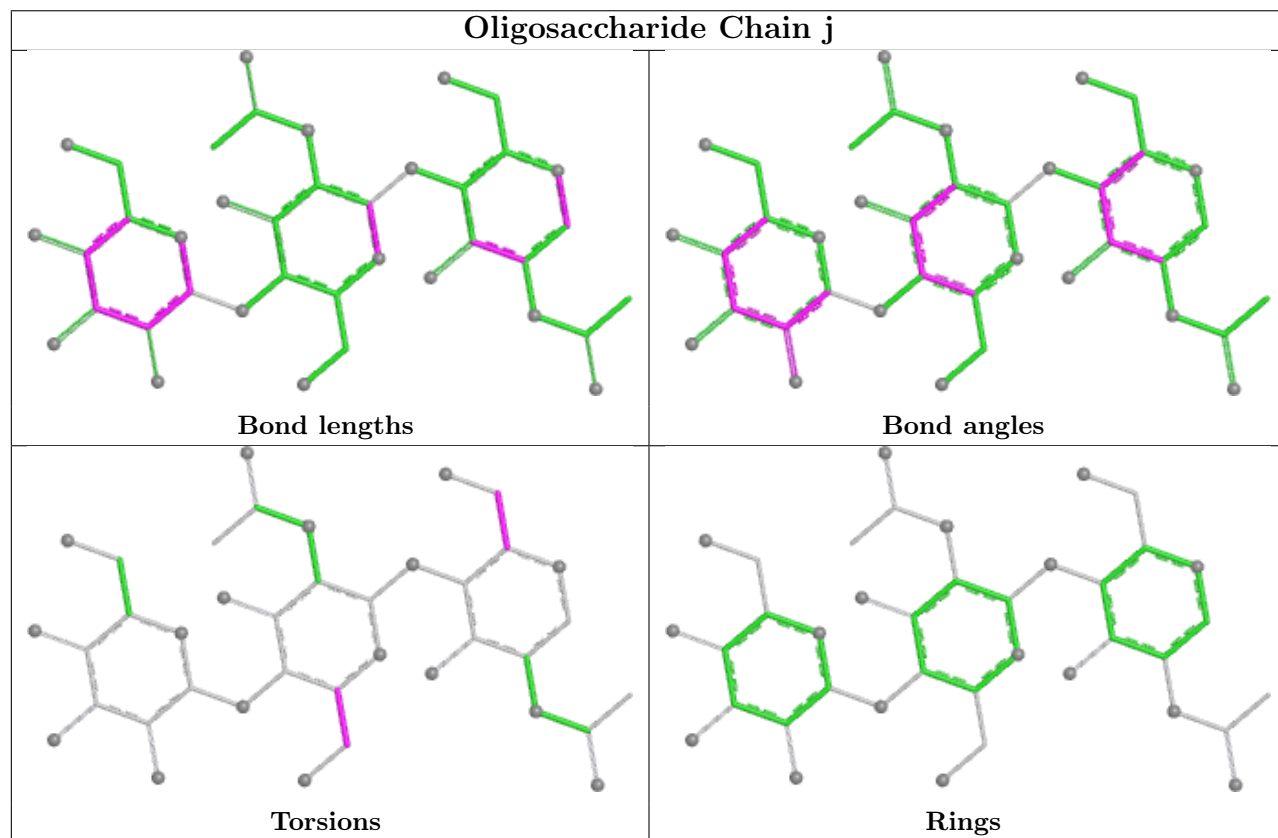
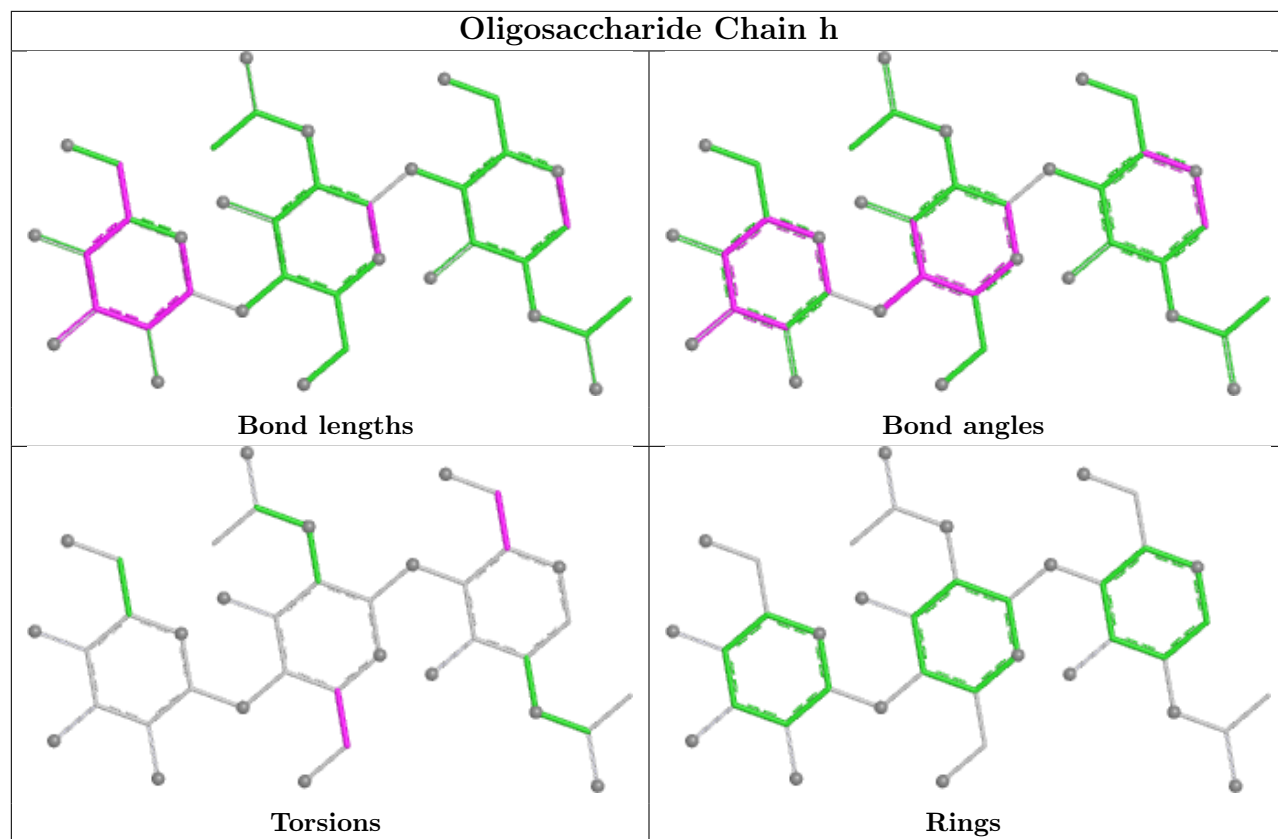
Mol	Chain	Res	Type	Atoms
3	w	3	BMA	C1-C2-C3-C4-C5-O5

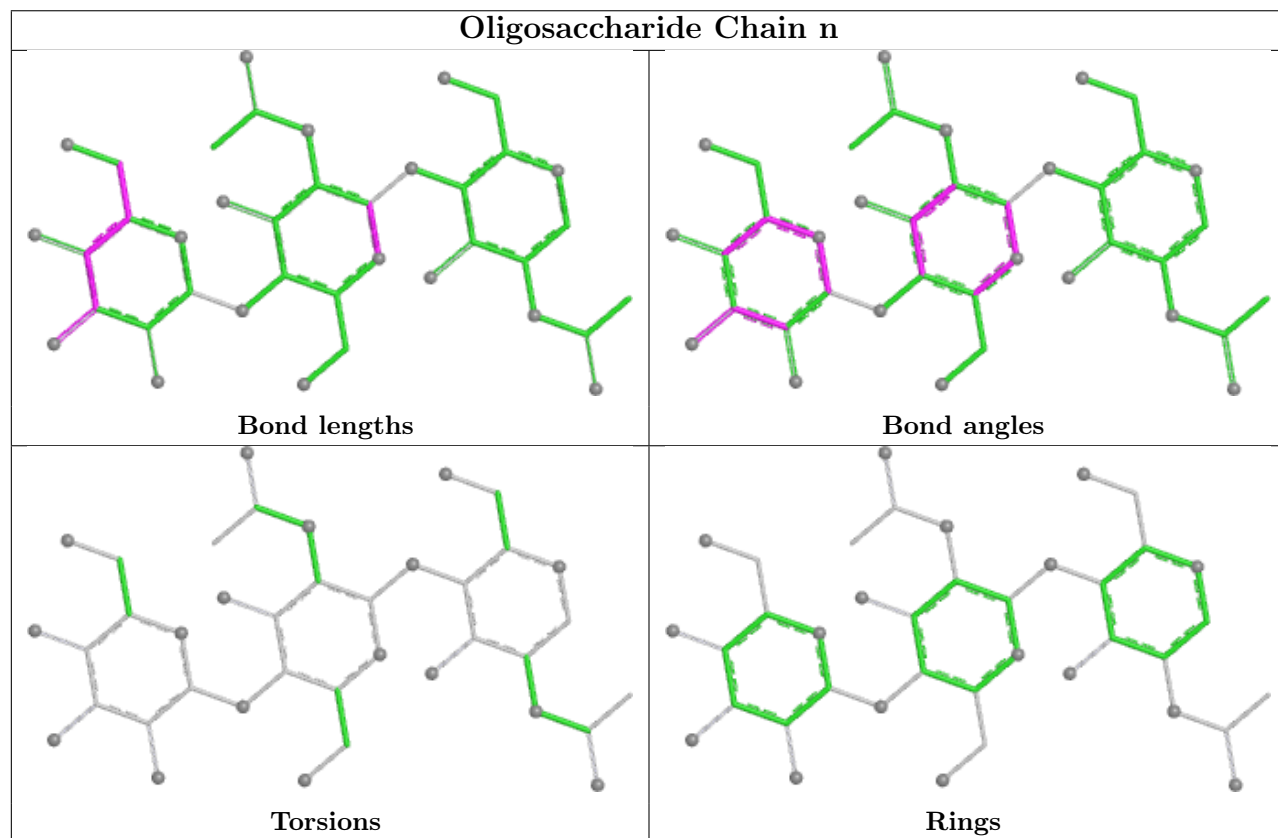
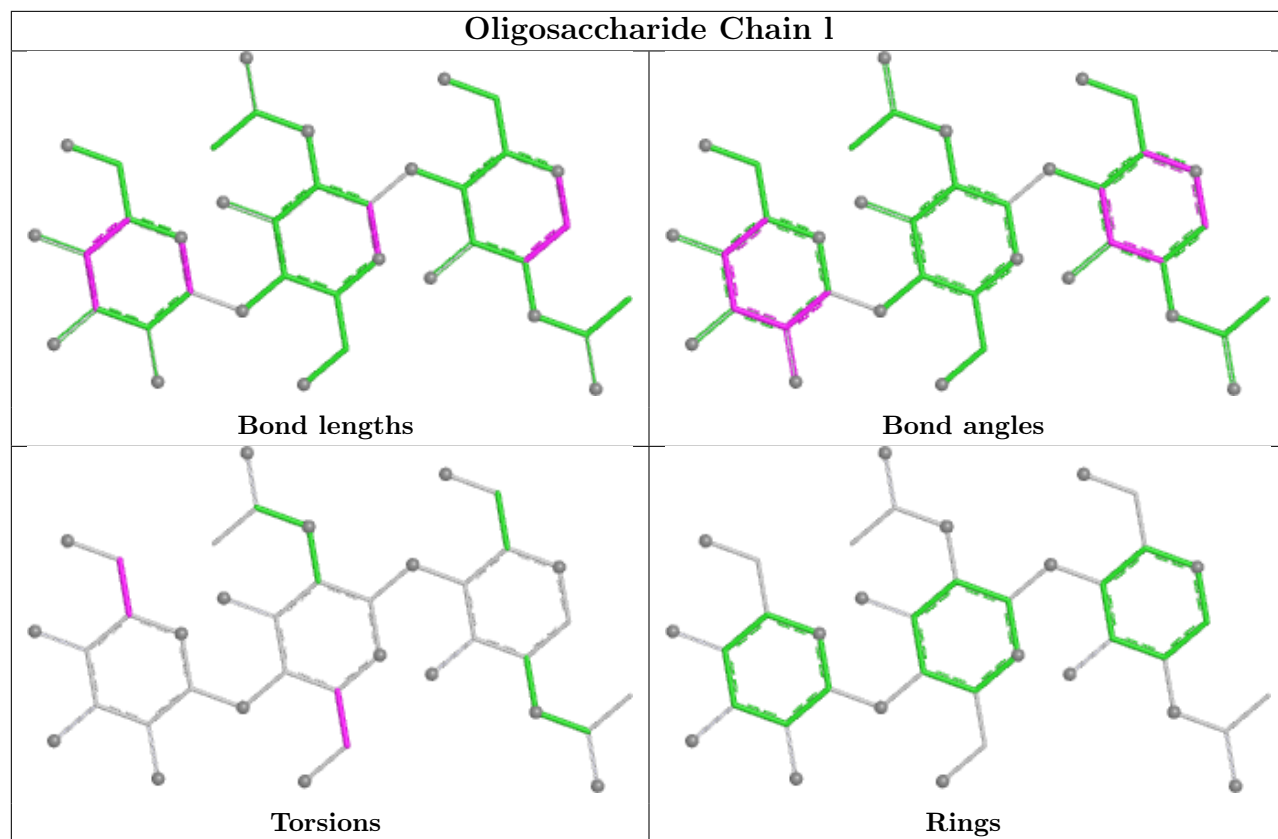
19 monomers are involved in 20 short contacts:

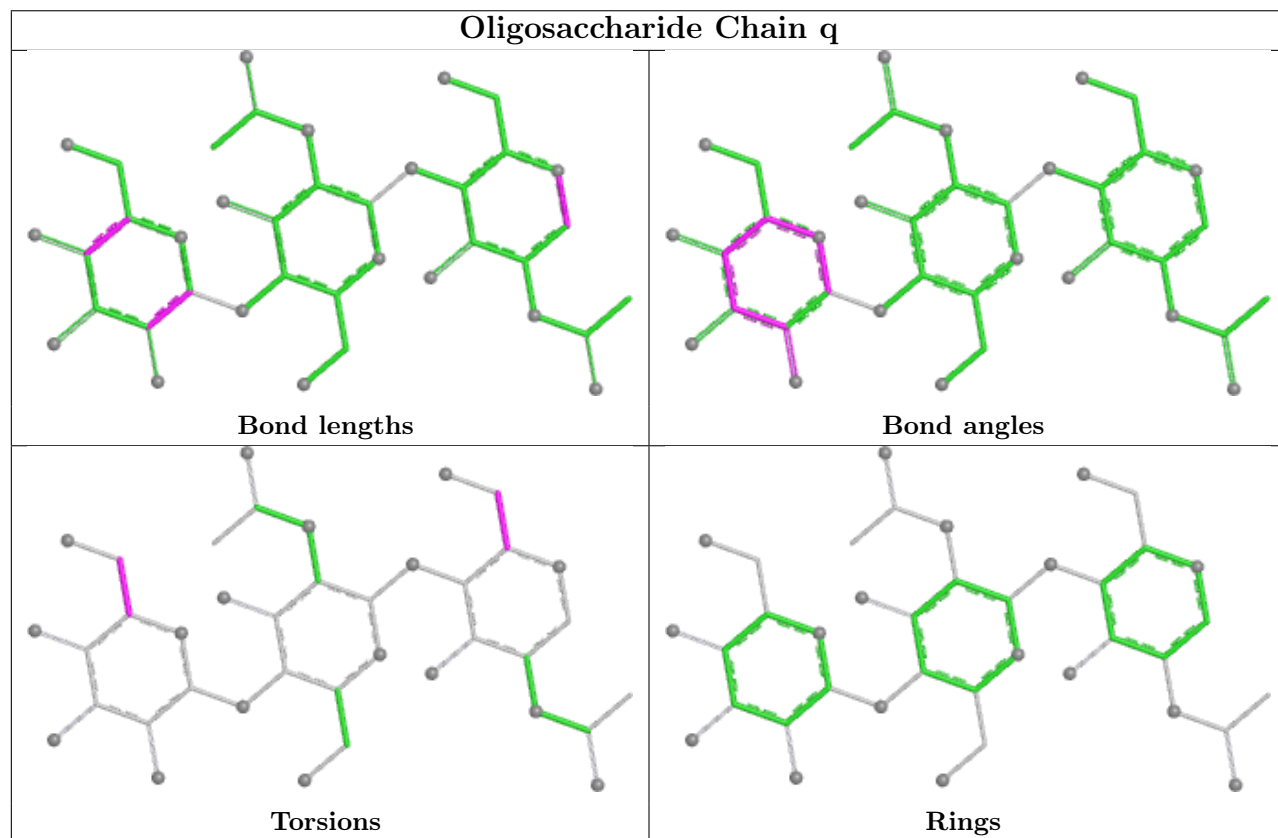
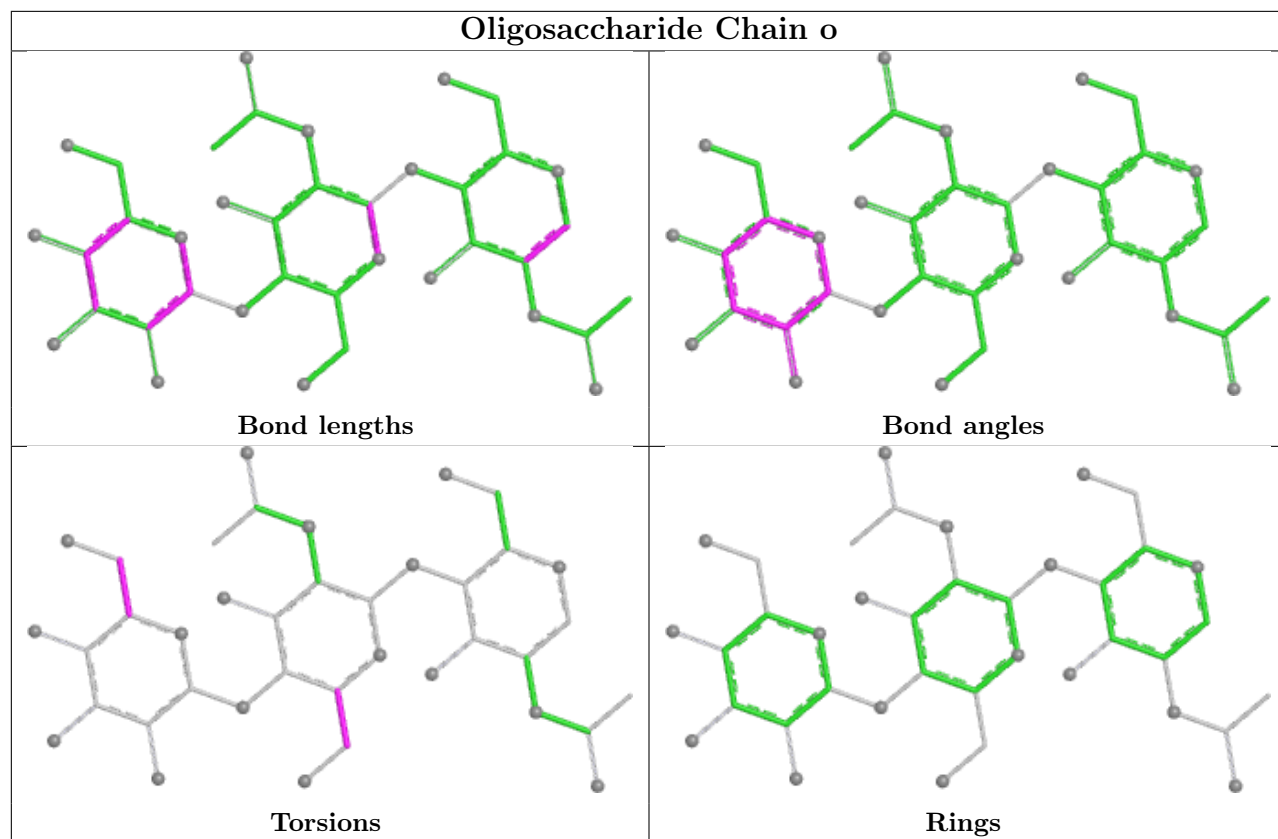
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	0	1	NAG	1	0
3	w	1	NAG	2	0
4	f	1	NAG	2	0
4	z	1	NAG	1	0
5	s	4	MAN	4	0
3	o	1	NAG	1	0
3	w	2	NAG	1	0
5	s	1	NAG	1	0
4	z	2	NAG	1	0
4	m	2	NAG	1	0
4	r	2	NAG	1	0
3	q	1	NAG	2	0
5	s	3	BMA	4	0
3	e	1	NAG	1	0
4	r	1	NAG	1	0
4	f	2	NAG	2	0
4	l	1	NAG	2	0
3	j	1	NAG	1	0
4	m	1	NAG	1	0

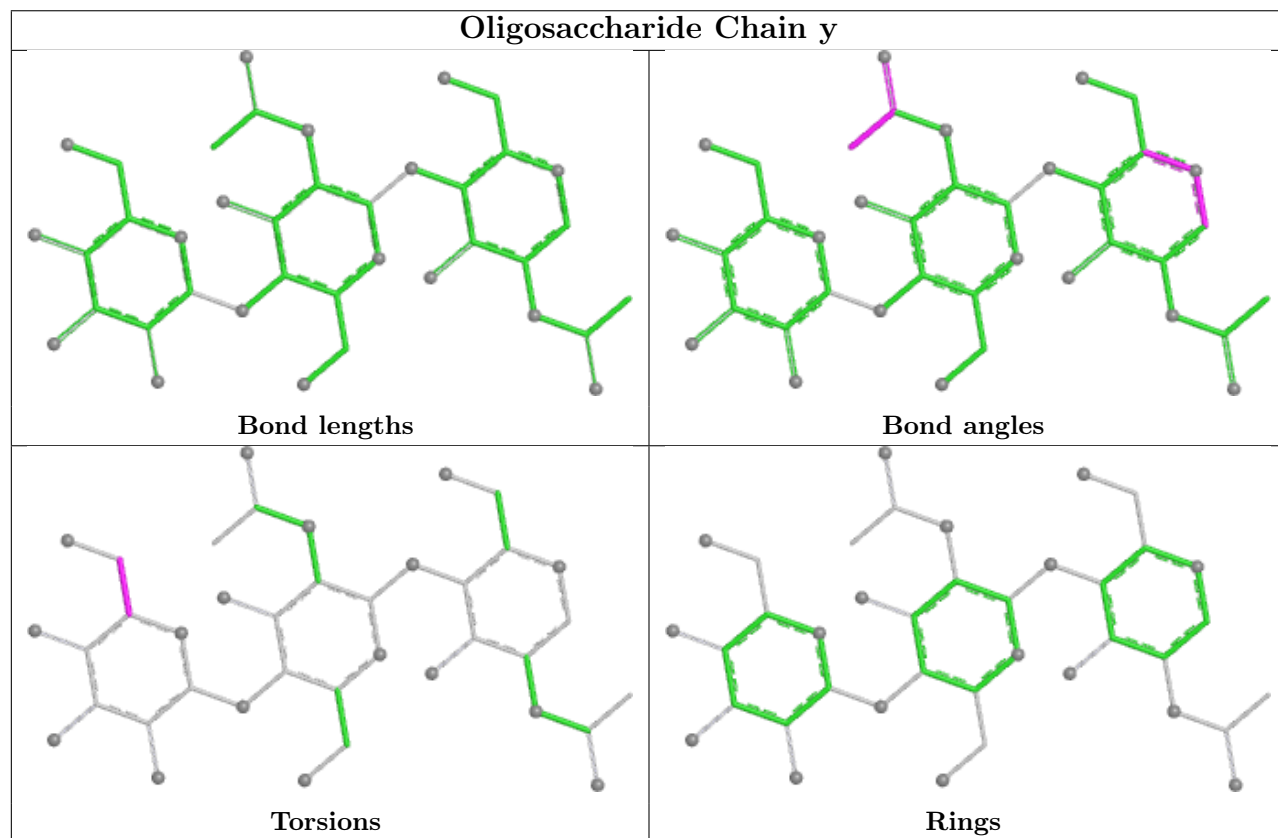
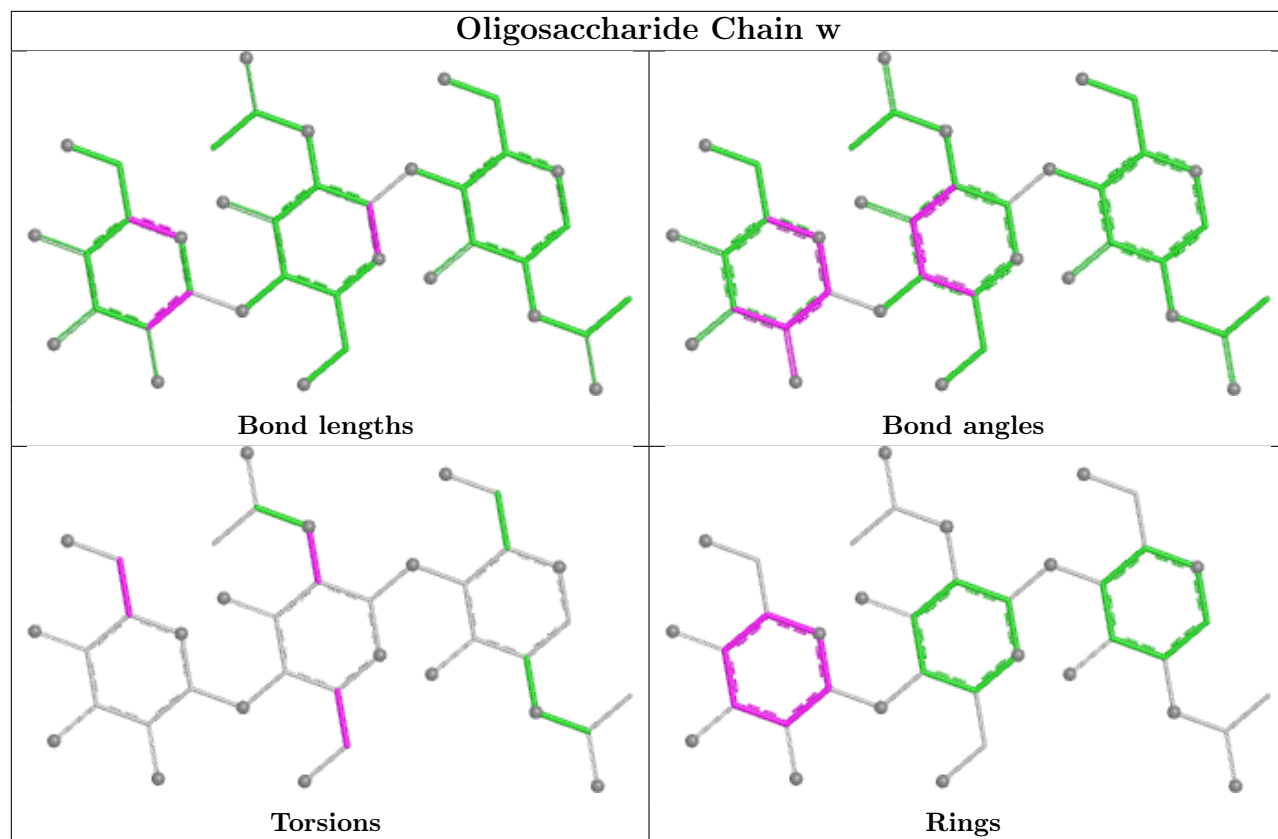
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

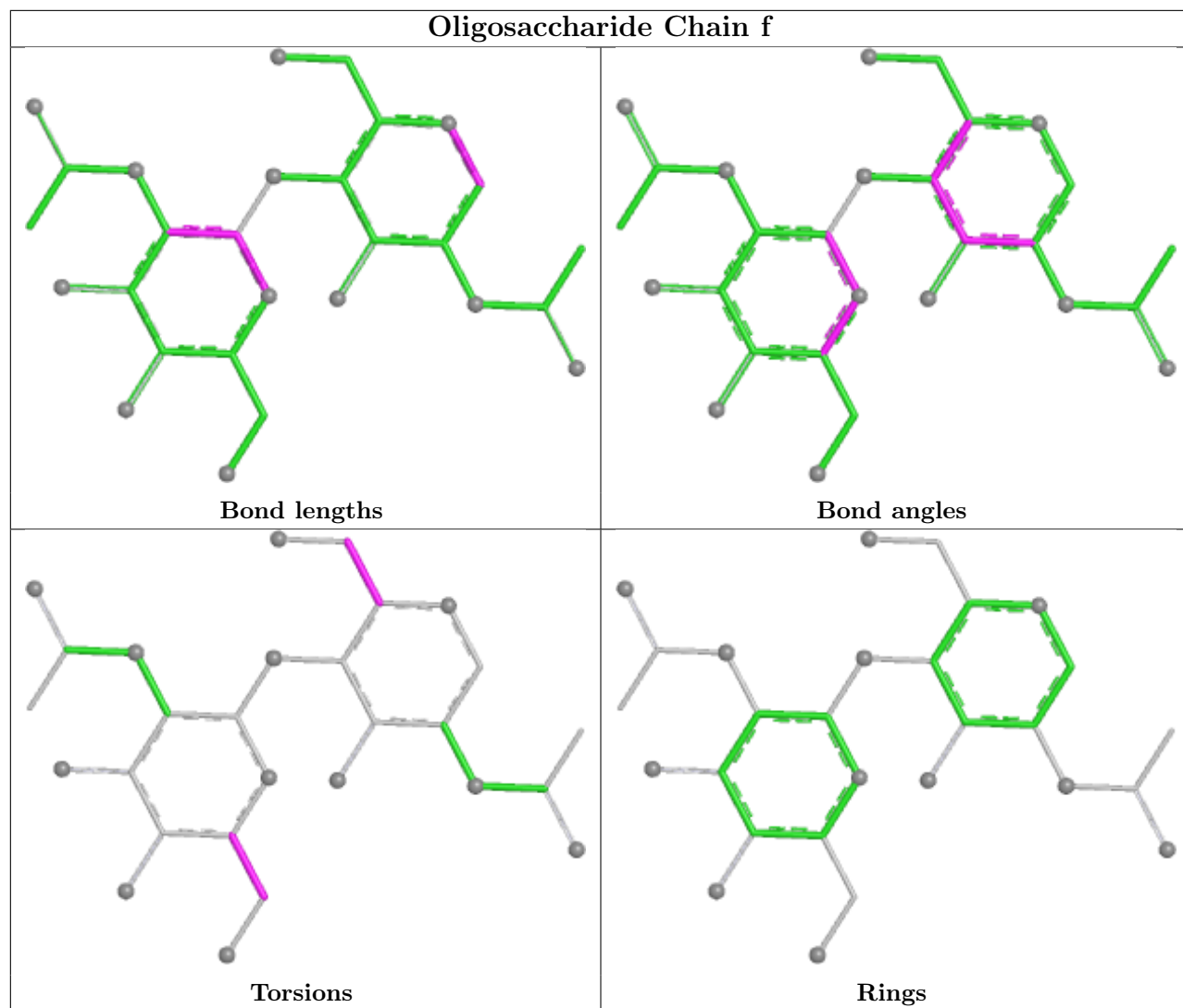


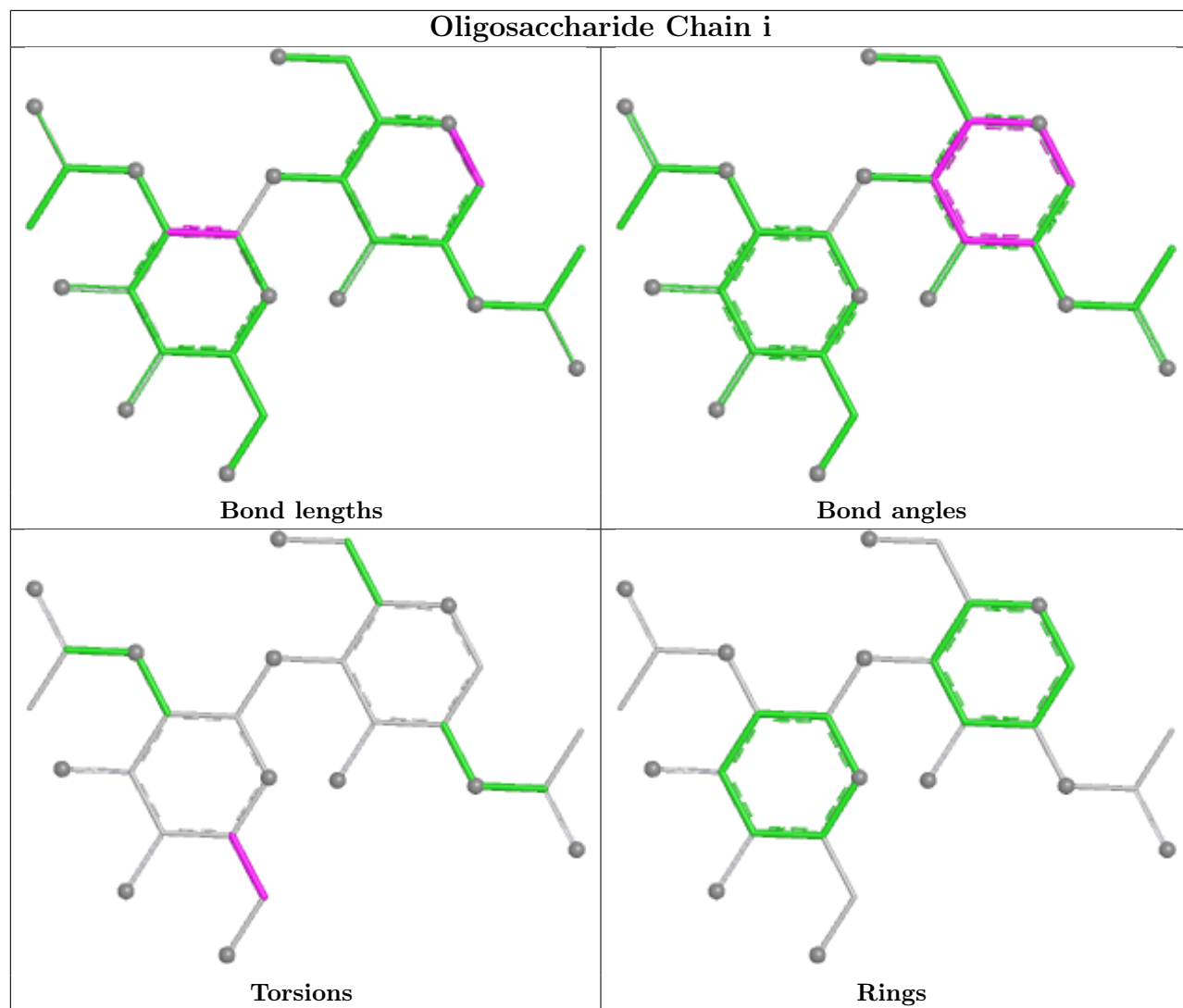


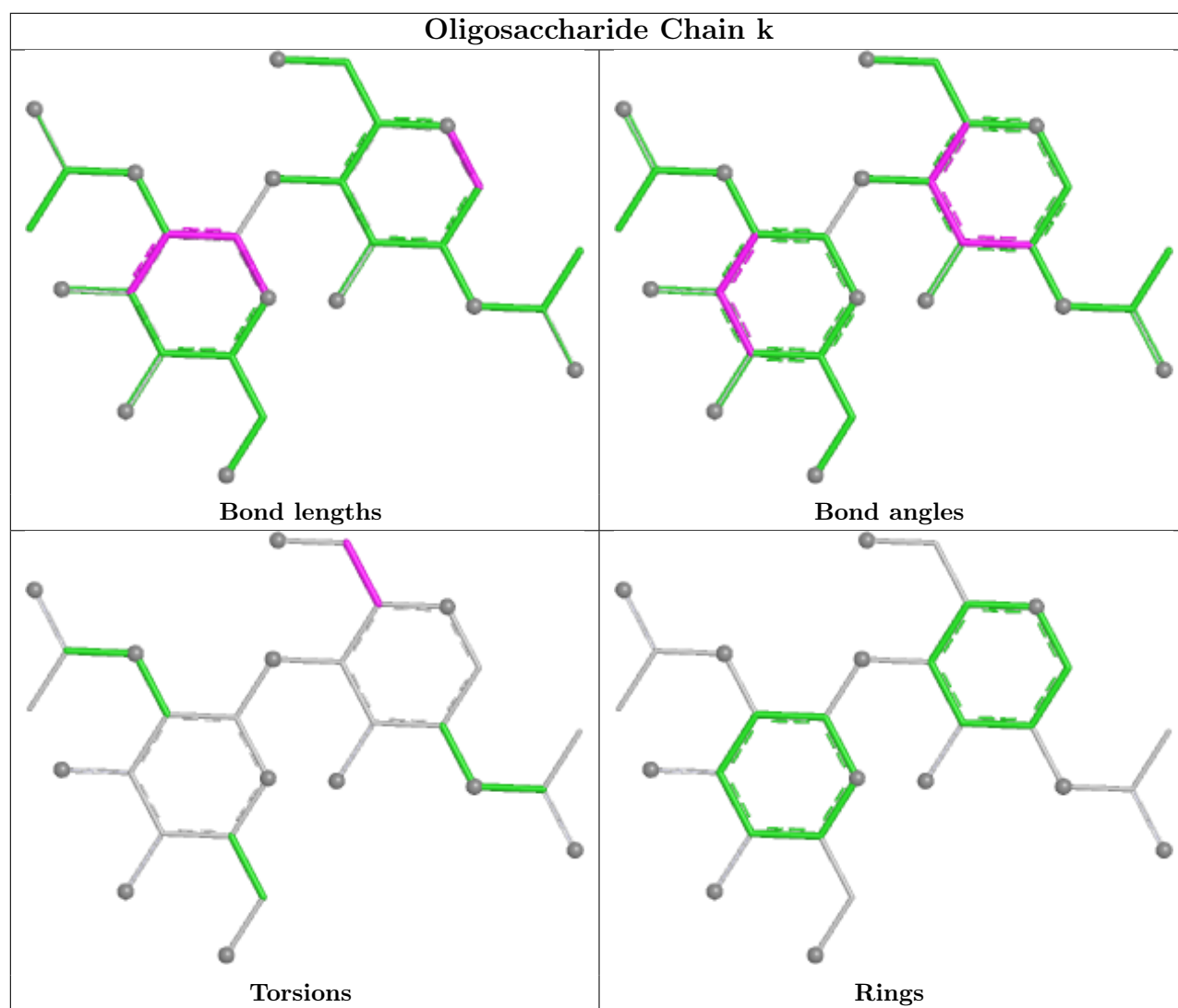


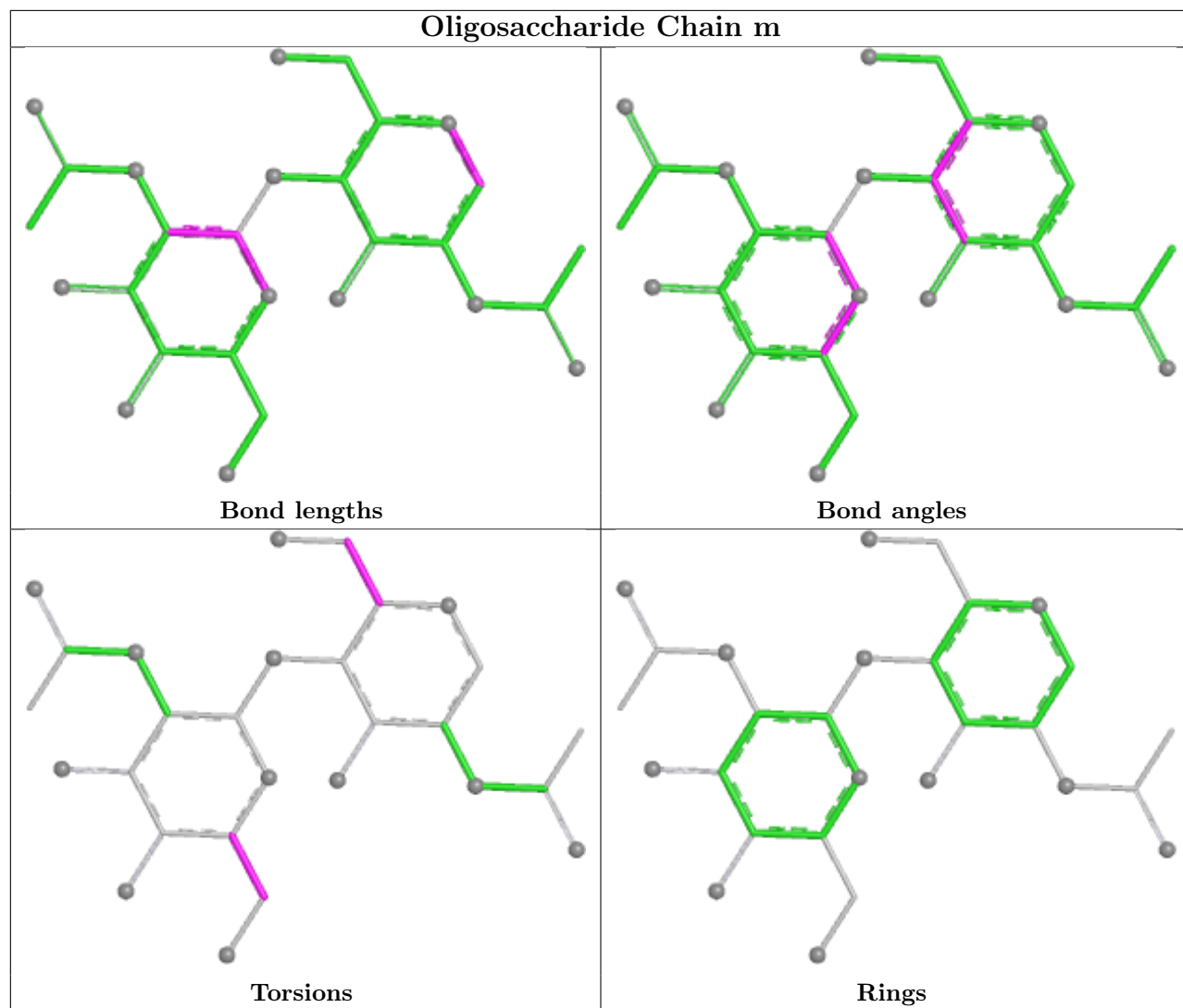


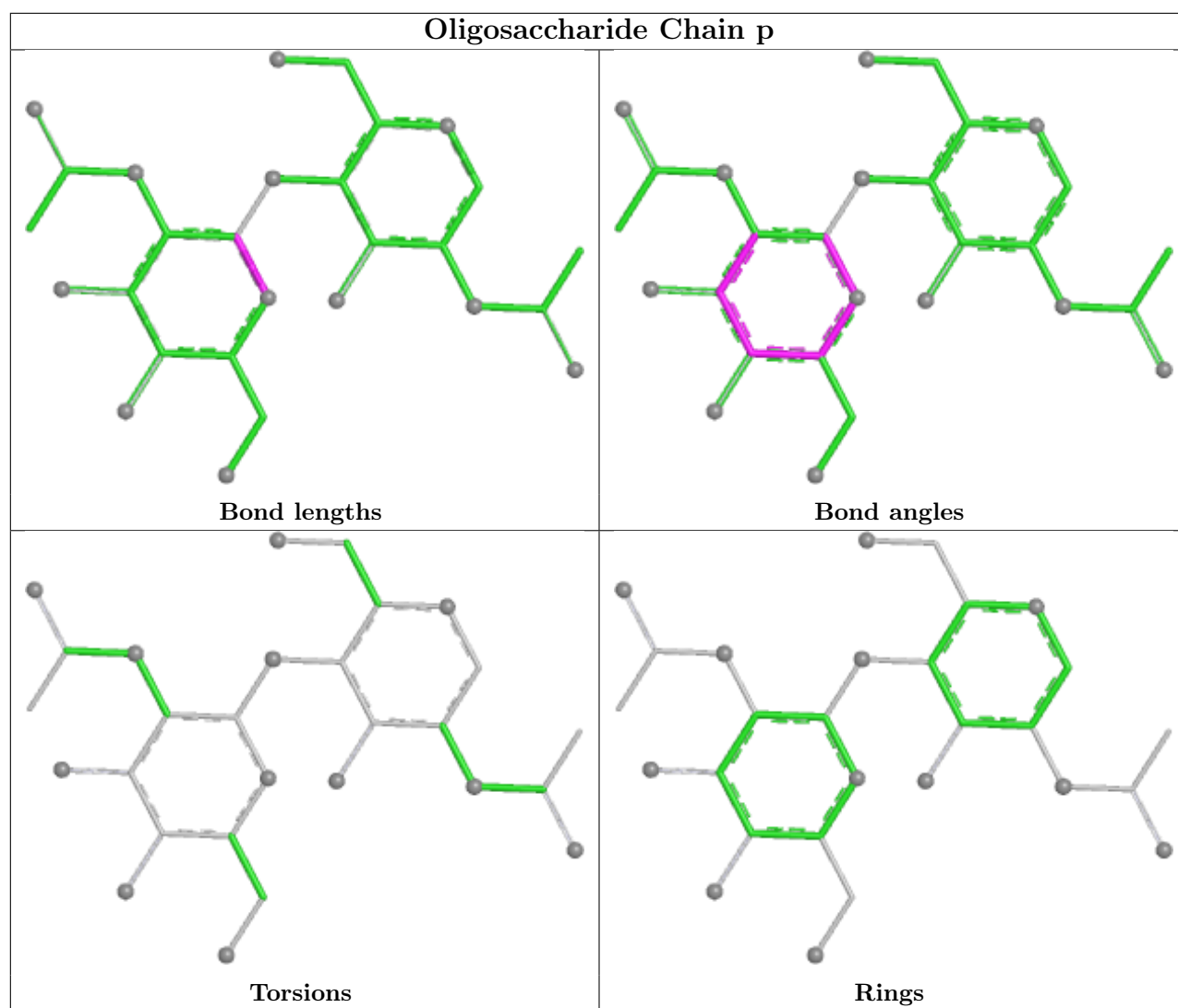


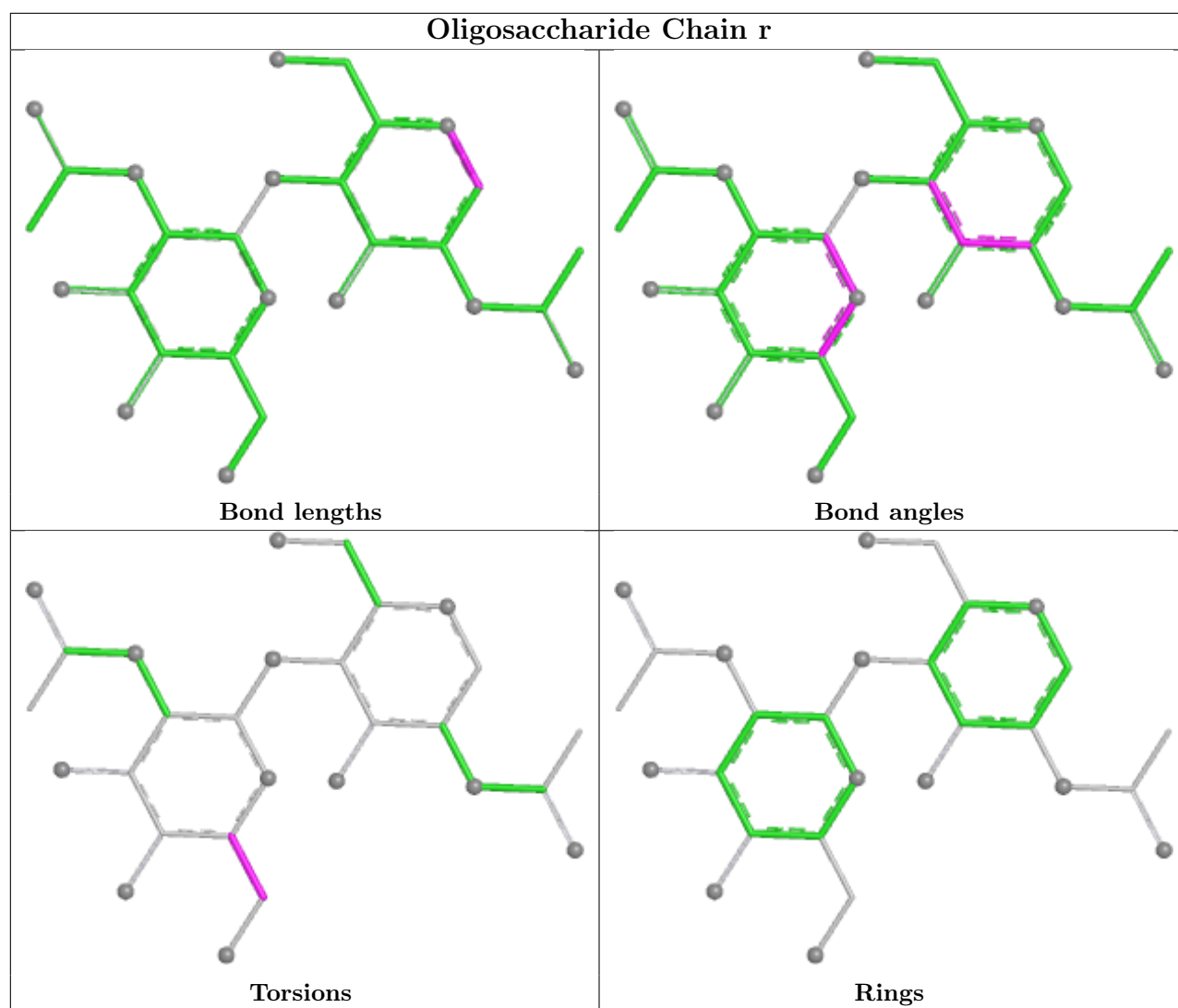


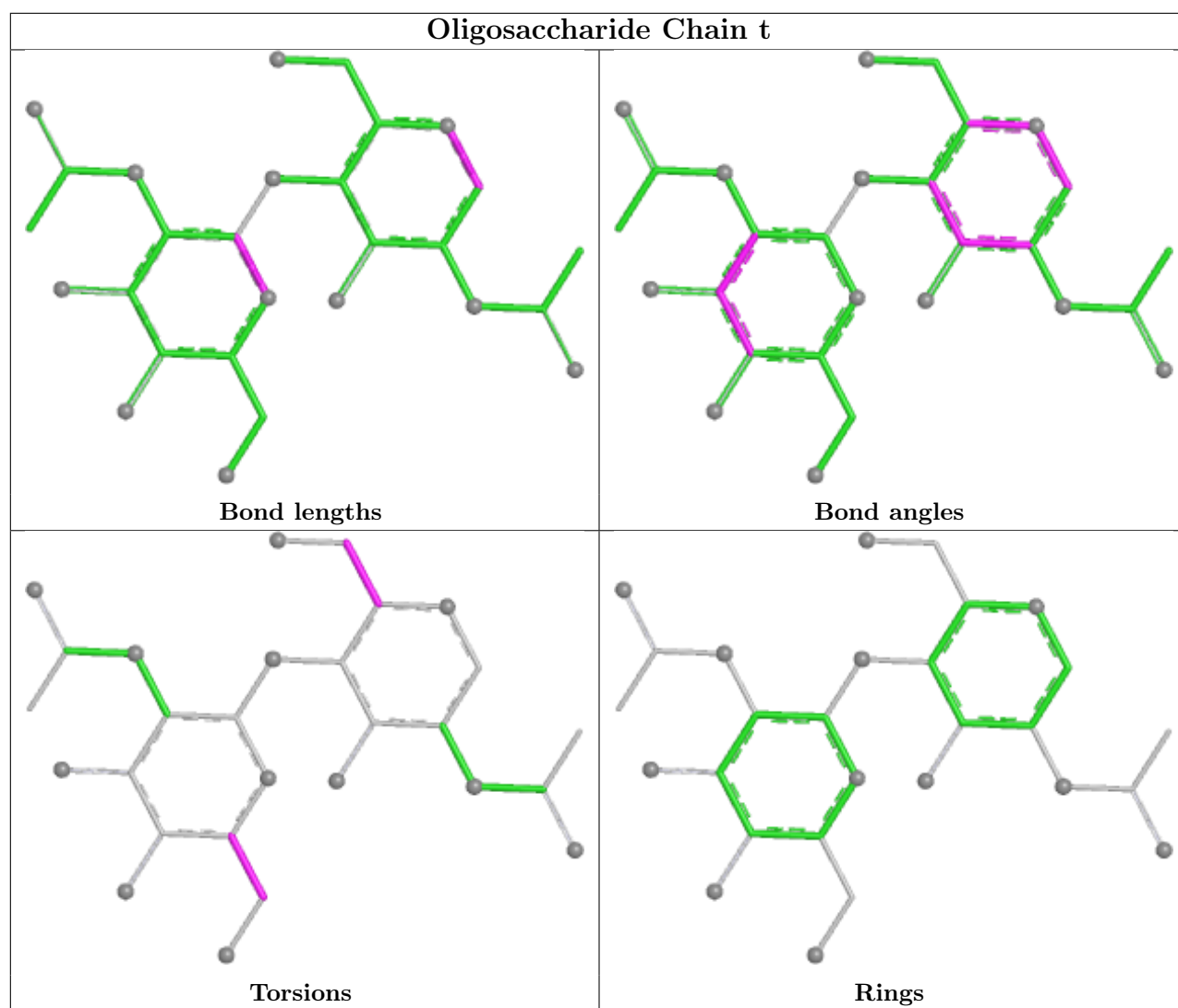


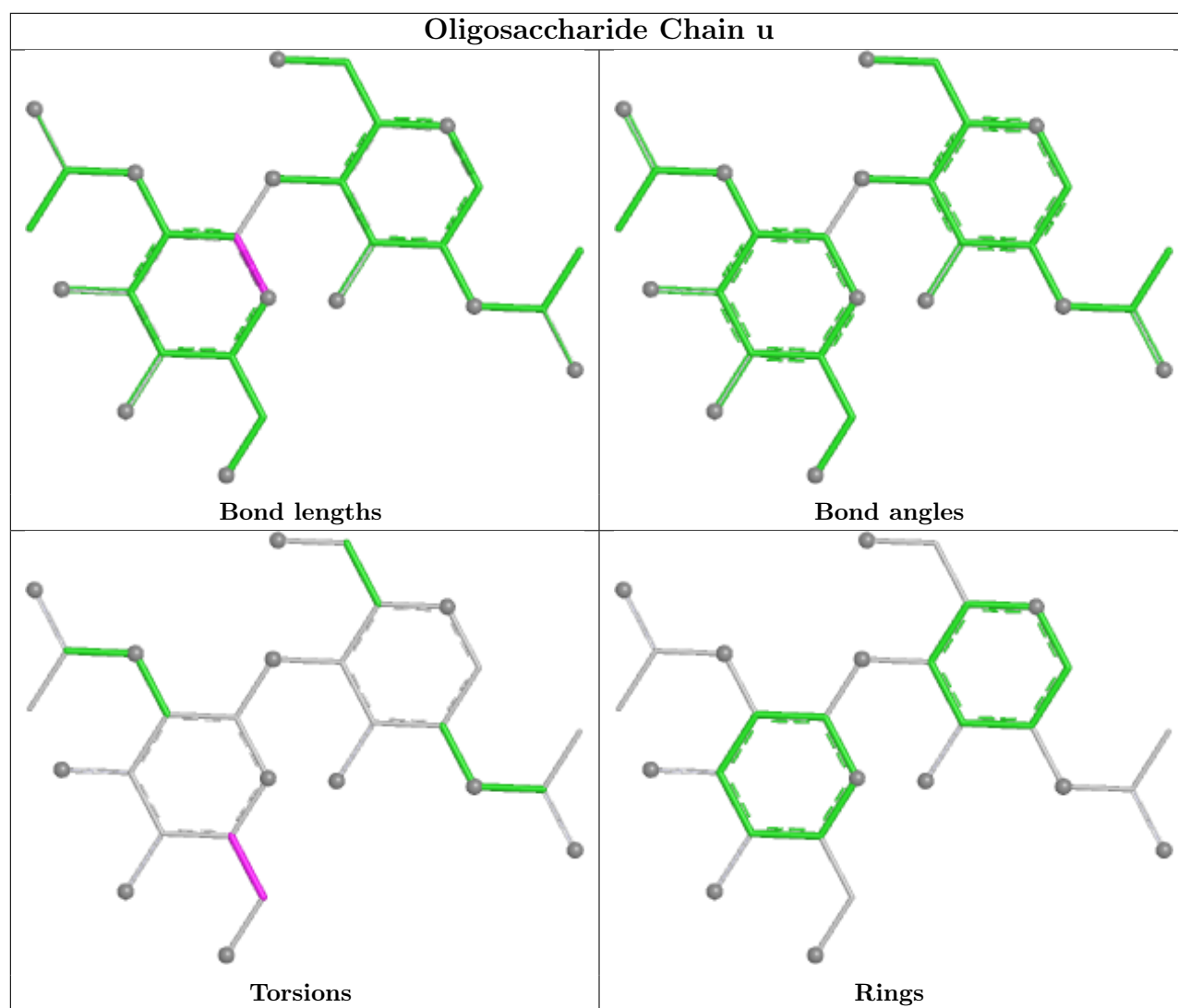


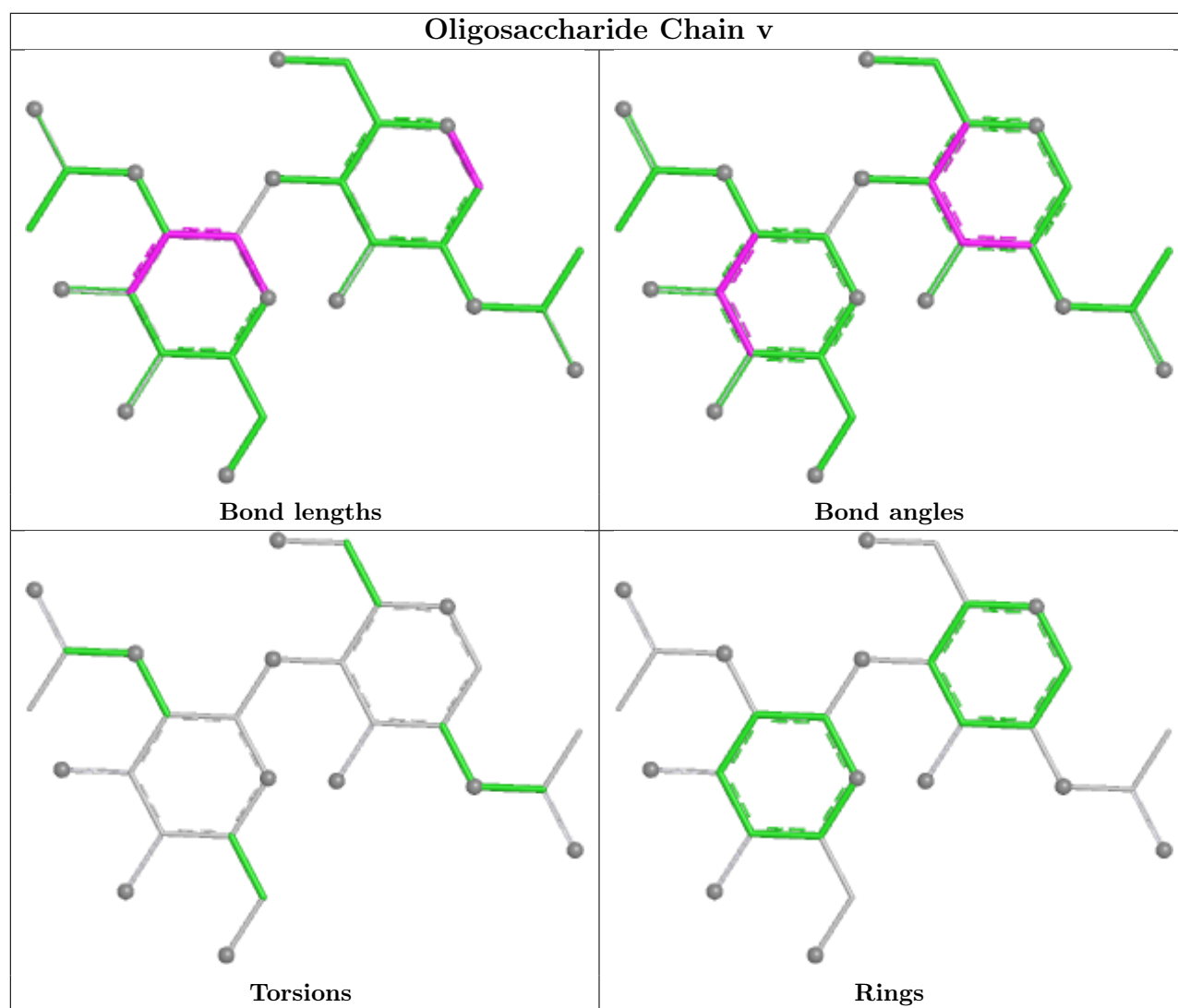


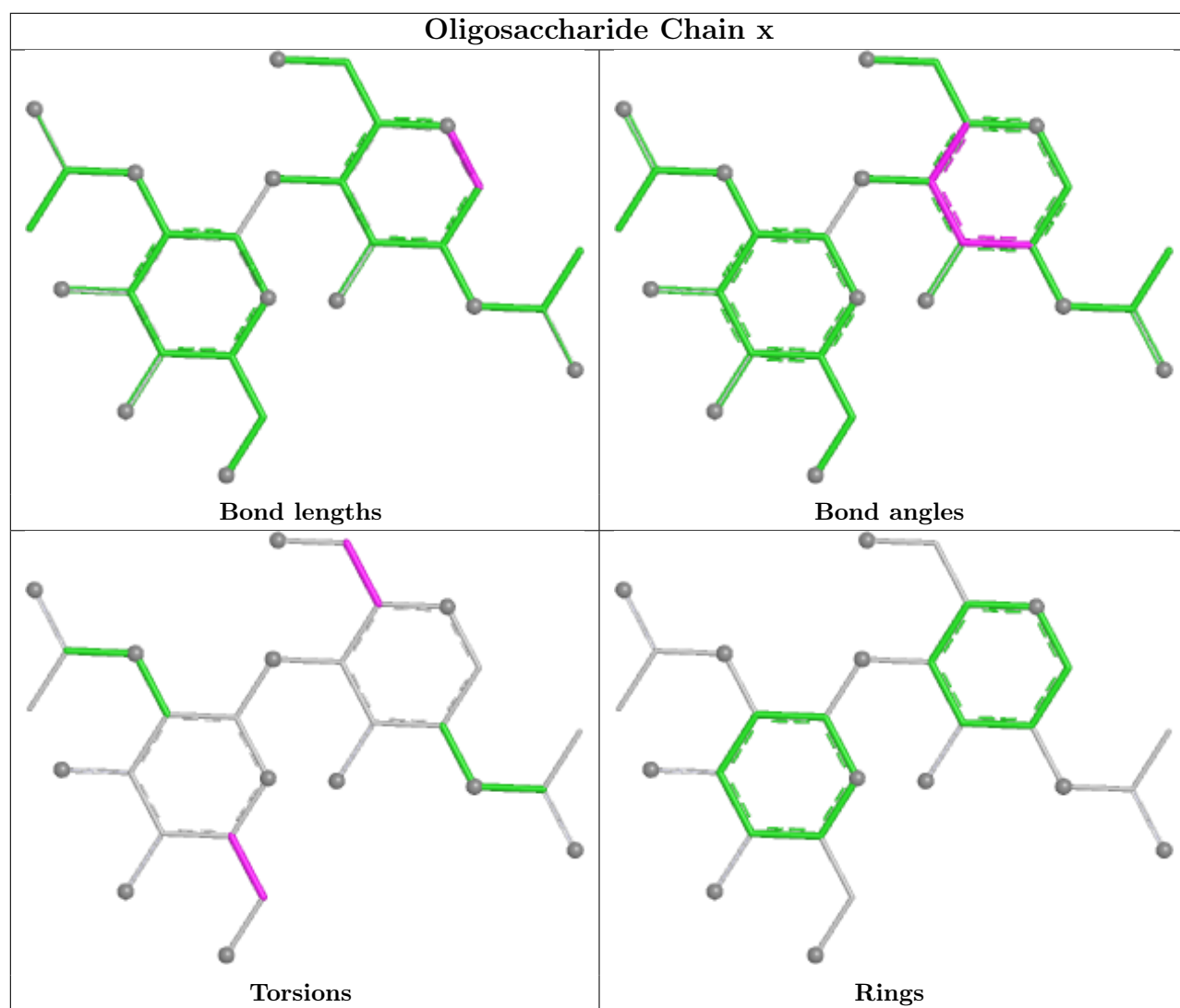


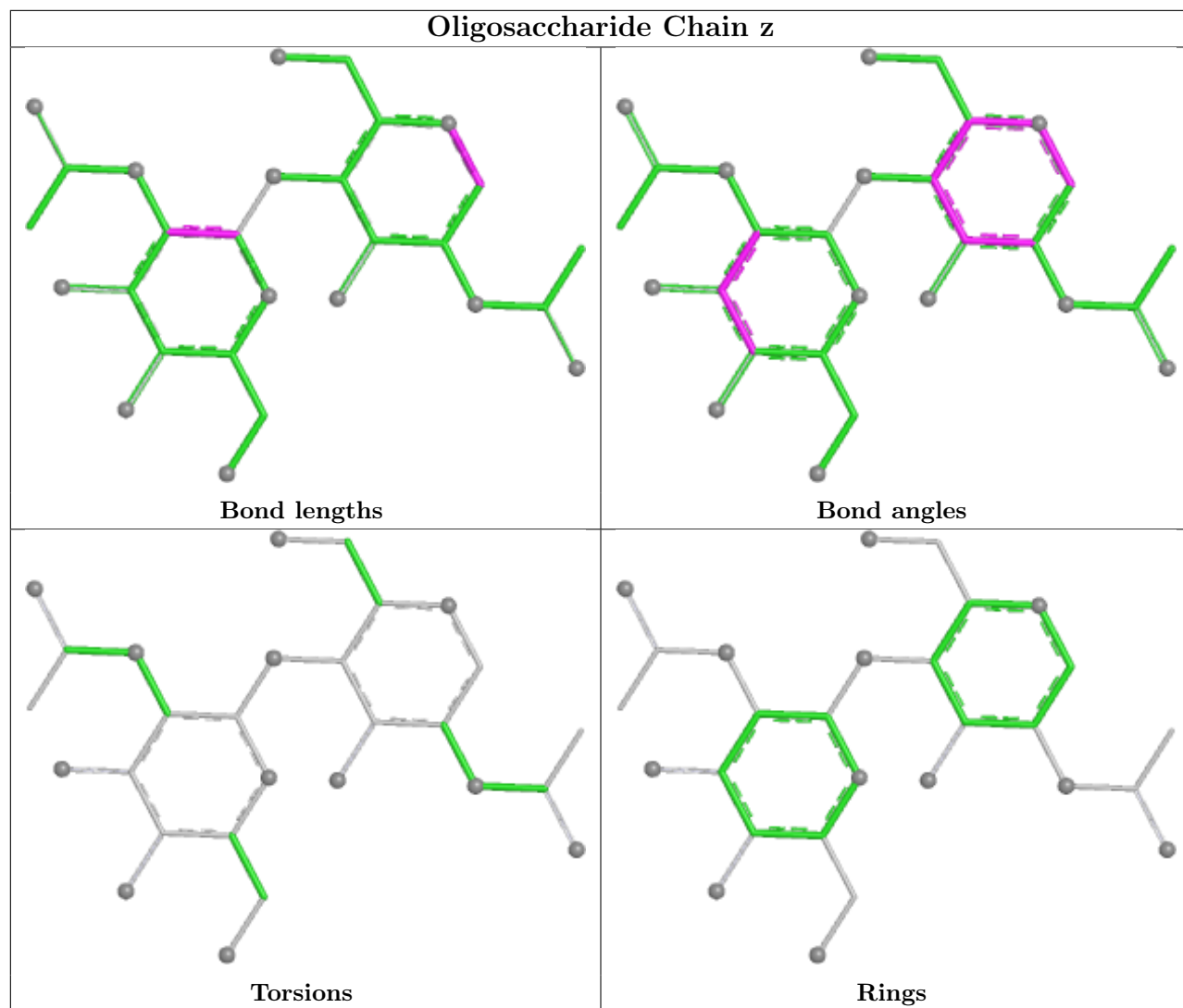


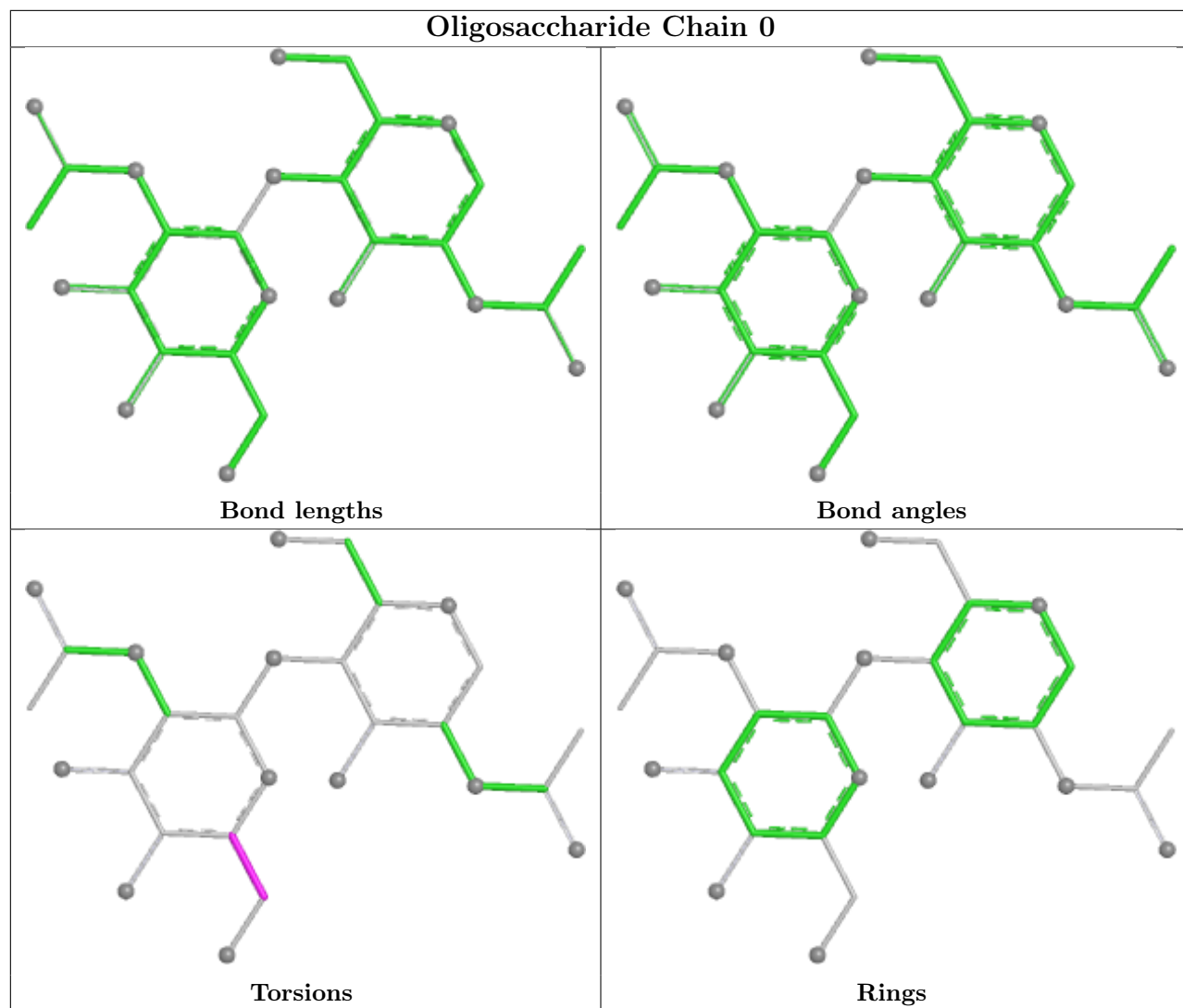


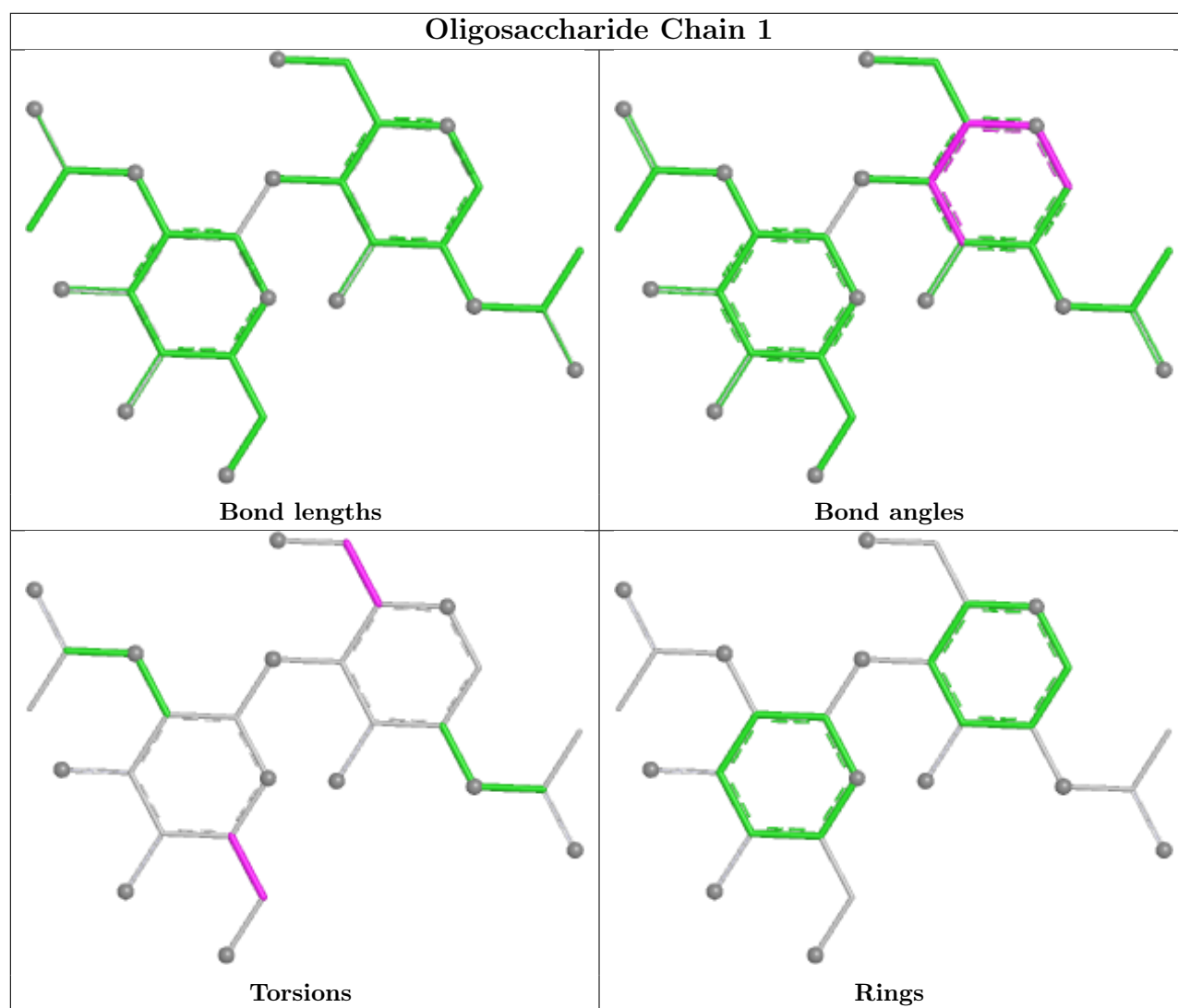


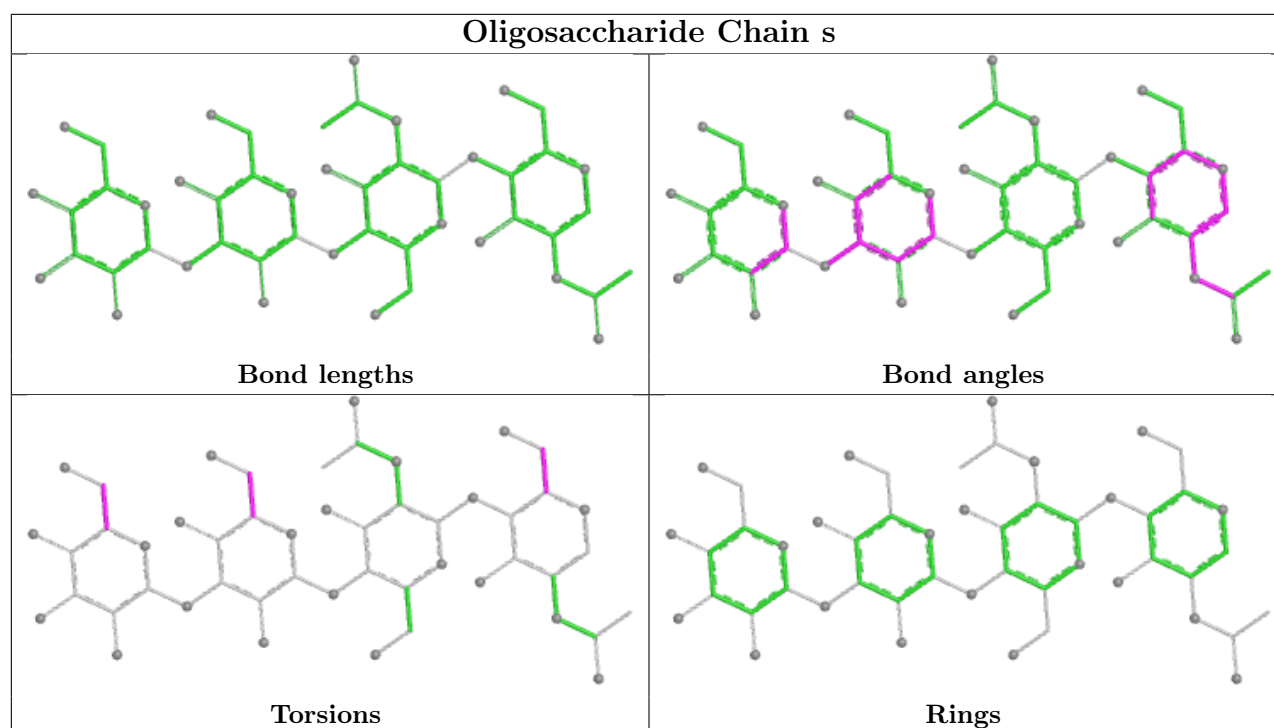












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
6	NAG	c	2001	1	14,14,15	0.56	0	17,19,21	0.50	0
6	NAG	Y	2003	1	14,14,15	0.59	0	17,19,21	0.46	0
6	NAG	c	2002	1	14,14,15	1.15	2 (14%)	17,19,21	1.19	2 (11%)
6	NAG	O	2006	1	14,14,15	1.18	2 (14%)	17,19,21	1.05	2 (11%)
6	NAG	K	2004	1	14,14,15	0.71	1 (7%)	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	c	2001	1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2003	1	-	2/6/23/26	0/1/1/1
6	NAG	c	2002	1	-	2/6/23/26	0/1/1/1
6	NAG	O	2006	1	-	0/6/23/26	0/1/1/1
6	NAG	K	2004	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	c	2002	NAG	O5-C1	-3.35	1.38	1.43
6	O	2006	NAG	O5-C1	-2.96	1.38	1.43
6	O	2006	NAG	C1-C2	2.88	1.56	1.52
6	c	2002	NAG	C1-C2	2.25	1.55	1.52
6	K	2004	NAG	C1-C2	2.15	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	c	2002	NAG	C4-C3-C2	3.36	115.95	111.02
6	O	2006	NAG	C4-C3-C2	2.75	115.04	111.02
6	O	2006	NAG	C3-C4-C5	2.16	114.15	110.23
6	c	2002	NAG	C1-O5-C5	-2.01	109.49	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	c	2002	NAG	O5-C5-C6-O6
6	Y	2003	NAG	O5-C5-C6-O6
6	Y	2003	NAG	C4-C5-C6-O6
6	c	2002	NAG	C4-C5-C6-O6
6	K	2004	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	c	2001	NAG	2	0
6	Y	2003	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	324/334 (97%)	-0.18	3 (0%) 81 64	22, 45, 100, 176	1 (0%)
1	C	324/334 (97%)	0.01	5 (1%) 72 52	30, 56, 142, 199	1 (0%)
1	E	324/334 (97%)	0.03	7 (2%) 62 41	30, 56, 144, 203	1 (0%)
1	G	324/334 (97%)	-0.24	1 (0%) 90 81	19, 46, 98, 183	1 (0%)
1	I	324/334 (97%)	-0.23	1 (0%) 90 81	24, 44, 96, 186	1 (0%)
1	K	324/334 (97%)	0.04	6 (1%) 66 45	33, 57, 143, 218	1 (0%)
1	M	324/334 (97%)	-0.06	8 (2%) 58 37	26, 50, 152, 220	1 (0%)
1	O	324/334 (97%)	-0.13	5 (1%) 72 52	25, 50, 139, 226	1 (0%)
1	Q	324/334 (97%)	-0.07	11 (3%) 48 28	25, 49, 148, 212	1 (0%)
1	S	324/334 (97%)	0.07	5 (1%) 72 52	35, 64, 158, 195	1 (0%)
1	U	324/334 (97%)	0.04	9 (2%) 55 34	31, 64, 156, 214	1 (0%)
1	W	324/334 (97%)	0.06	5 (1%) 72 52	35, 64, 147, 211	1 (0%)
1	Y	324/334 (97%)	0.29	10 (3%) 51 31	55, 91, 189, 248	1 (0%)
1	a	324/334 (97%)	0.27	8 (2%) 58 37	55, 87, 184, 263	1 (0%)
1	c	324/334 (97%)	0.27	7 (2%) 62 41	59, 90, 185, 253	1 (0%)
2	B	177/181 (97%)	0.54	11 (6%) 26 15	26, 113, 153, 173	0
2	D	177/181 (97%)	0.73	14 (7%) 18 10	41, 155, 195, 210	0
2	F	177/181 (97%)	0.72	13 (7%) 21 12	42, 154, 196, 206	0
2	H	177/181 (97%)	0.42	4 (2%) 61 40	23, 113, 154, 174	0
2	J	177/181 (97%)	0.44	5 (2%) 55 34	27, 113, 153, 166	0
2	L	177/181 (97%)	0.67	9 (5%) 33 19	42, 148, 195, 206	0
2	N	177/181 (97%)	0.79	18 (10%) 12 7	38, 158, 213, 231	0
2	P	177/181 (97%)	0.80	16 (9%) 15 9	38, 163, 213, 231	0
2	R	177/181 (97%)	0.79	21 (11%) 9 5	34, 163, 210, 222	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	177/181 (97%)	0.73	11 (6%) 26 15	45, 153, 201, 209	0
2	V	177/181 (97%)	0.76	18 (10%) 12 7	49, 153, 213, 228	0
2	X	177/181 (97%)	0.84	21 (11%) 9 5	50, 155, 204, 220	0
2	Z	177/181 (97%)	0.95	24 (13%) 7 4	74, 191, 237, 256	0
2	b	177/181 (97%)	0.99	19 (10%) 11 6	73, 187, 239, 254	0
2	d	177/181 (97%)	1.09	29 (16%) 4 2	78, 194, 247, 269	0
All	All	7515/7725 (97%)	0.27	324 (4%) 40 23	19, 79, 201, 269	15 (0%)

The worst 5 of 324 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	16	GLY	5.8
2	X	7	ALA	5.1
2	D	22	TYR	5.0
2	d	9	PHE	4.8
1	E	15	ILE	4.5

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

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

6.3 Carbohydrates ⓘ

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
3	NAG	e	1	14/15	-	-	61,66,70,73	0
3	NAG	e	2	14/15	-	-	52,75,87,93	0
3	BMA	e	3	11/12	-	-	65,90,98,98	0
3	NAG	g	1	14/15	-	-	56,75,85,89	0
3	NAG	g	2	14/15	-	-	69,81,86,90	0
3	BMA	g	3	11/12	-	-	35,55,68,70	0
3	NAG	h	1	14/15	-	-	54,72,97,102	0
3	NAG	h	2	14/15	-	-	79,102,115,117	0
3	BMA	h	3	11/12	-	-	43,57,80,88	0

Continued on next page...

Continued from previous page...

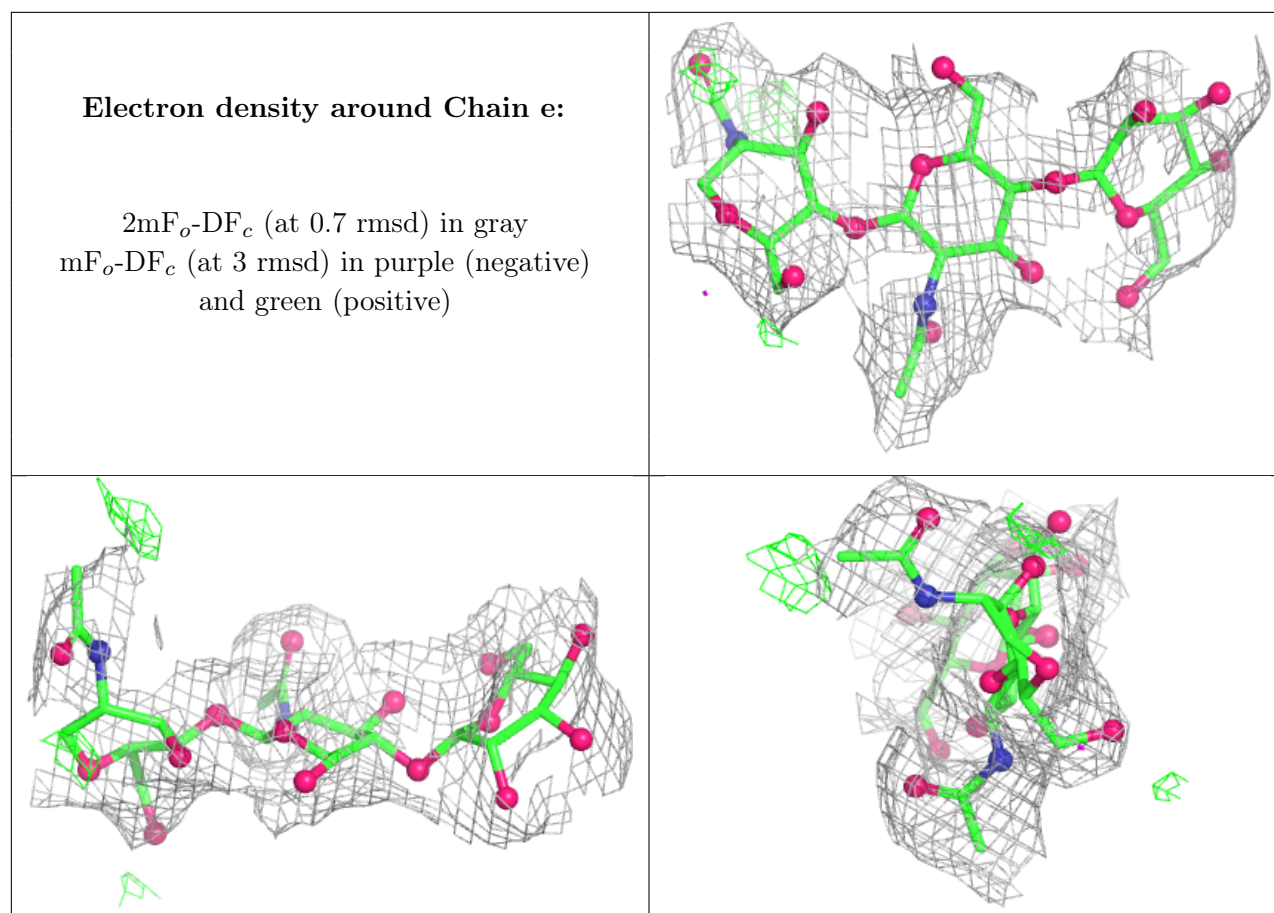
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	j	1	14/15	-	-	54,63,66,66	0
3	NAG	j	2	14/15	-	-	53,70,85,96	0
3	BMA	j	3	11/12	-	-	80,97,103,107	0
3	NAG	l	1	14/15	-	-	50,59,64,64	0
3	NAG	l	2	14/15	-	-	65,75,86,89	0
3	BMA	l	3	11/12	-	-	83,95,103,110	0
3	NAG	n	1	14/15	-	-	59,73,92,93	0
3	NAG	n	2	14/15	-	-	61,76,88,94	0
3	BMA	n	3	11/12	-	-	32,49,59,61	0
3	NAG	o	1	14/15	-	-	42,57,74,81	0
3	NAG	o	2	14/15	-	-	64,91,98,106	0
3	BMA	o	3	11/12	-	-	102,115,128,131	0
3	NAG	q	1	14/15	-	-	39,57,67,74	0
3	NAG	q	2	14/15	-	-	61,90,101,113	0
3	BMA	q	3	11/12	-	-	102,115,125,130	0
3	NAG	w	1	14/15	-	-	54,66,81,92	0
3	NAG	w	2	14/15	-	-	95,102,117,127	0
3	BMA	w	3	11/12	-	-	114,122,125,127	0
3	NAG	y	1	14/15	-	-	64,71,80,92	0
3	NAG	y	2	14/15	-	-	77,96,107,119	0
3	BMA	y	3	11/12	-	-	113,124,130,135	0
4	NAG	f	1	14/15	-	-	104,114,123,124	0
4	NAG	f	2	14/15	-	-	119,129,135,136	0
4	NAG	i	1	14/15	-	-	126,134,144,151	0
4	NAG	i	2	14/15	-	-	129,148,157,159	0
4	NAG	k	1	14/15	-	-	87,103,110,112	0
4	NAG	k	2	14/15	-	-	106,115,120,122	0
4	NAG	m	1	14/15	-	-	94,108,117,122	0
4	NAG	m	2	14/15	-	-	109,125,128,129	0
4	NAG	p	1	14/15	-	-	128,145,151,160	0
4	NAG	p	2	14/15	-	-	137,162,176,177	0
4	NAG	r	1	14/15	-	-	142,148,151,153	0
4	NAG	r	2	14/15	-	-	138,149,152,152	0
4	NAG	t	1	14/15	-	-	122,138,141,145	0
4	NAG	t	2	14/15	-	-	124,153,157,160	0
4	NAG	u	1	14/15	-	-	50,69,87,102	0
4	NAG	u	2	14/15	-	-	96,108,125,129	0
4	NAG	v	1	14/15	-	-	133,146,152,153	0
4	NAG	v	2	14/15	-	-	116,143,150,154	0
4	NAG	x	1	14/15	-	-	141,148,158,159	0
4	NAG	x	2	14/15	-	-	156,166,172,172	0
4	NAG	z	1	14/15	-	-	145,151,158,159	0

Continued on next page...

Continued from previous page...

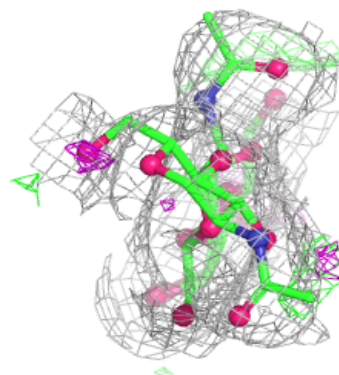
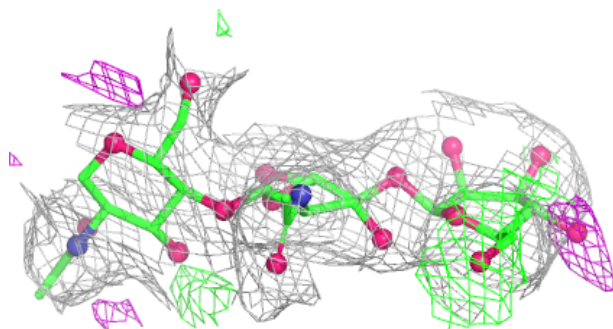
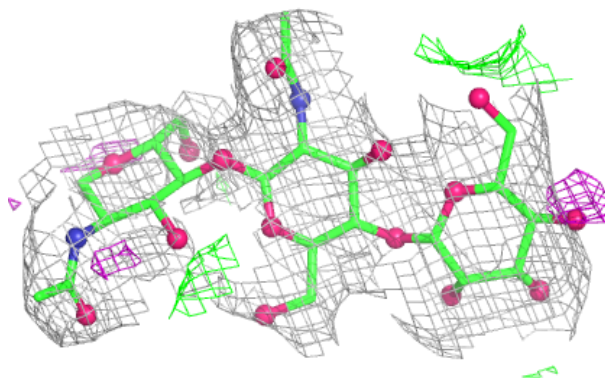
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	z	2	14/15	-	-	139,152,158,160	0
4	NAG	0	1	14/15	-	-	95,100,108,119	0
4	NAG	0	2	14/15	-	-	115,131,144,145	0
4	NAG	1	1	14/15	-	-	86,95,107,111	0
4	NAG	1	2	14/15	-	-	96,118,126,129	0
5	NAG	s	1	14/15	-	-	68,80,90,103	0
5	NAG	s	2	14/15	-	-	94,99,105,115	0
5	BMA	s	3	11/12	-	-	116,120,126,127	0
5	MAN	s	4	11/12	-	-	111,129,131,135	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.

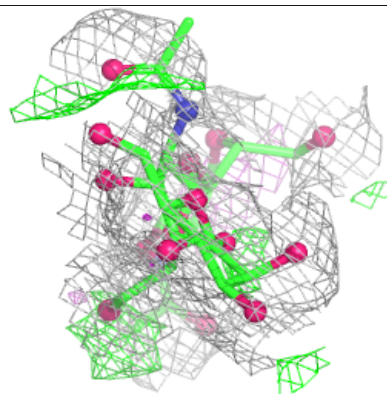
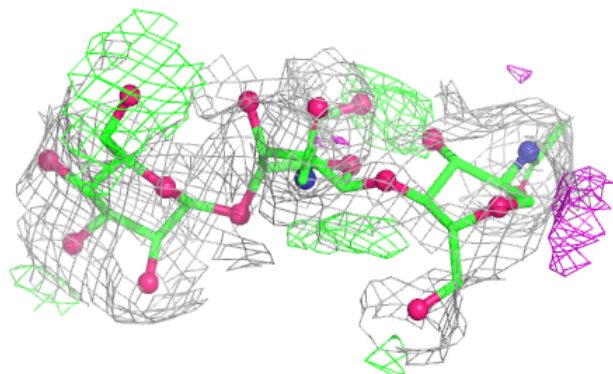
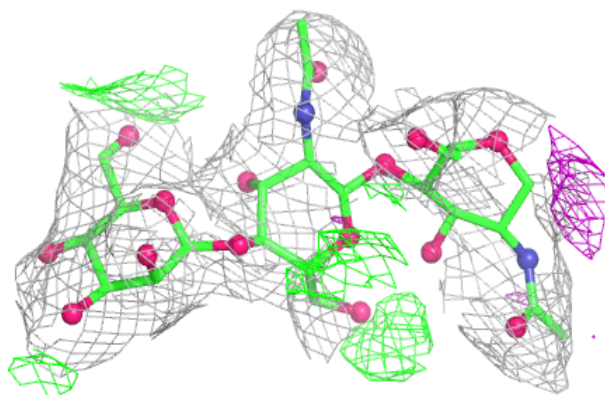


Electron density around Chain g:

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

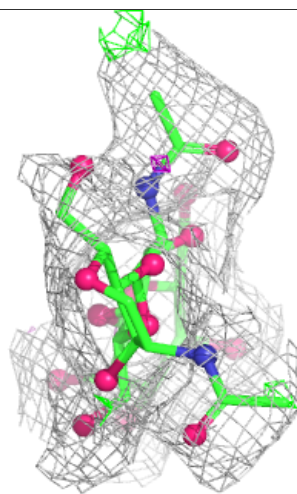
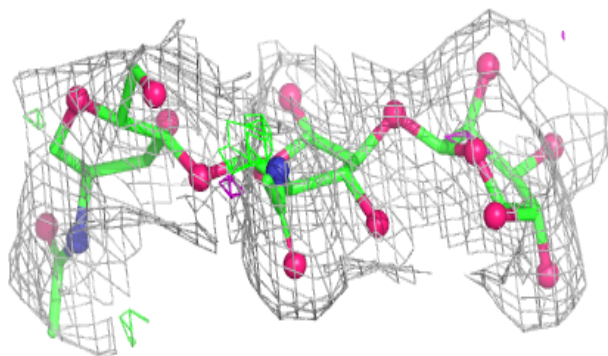
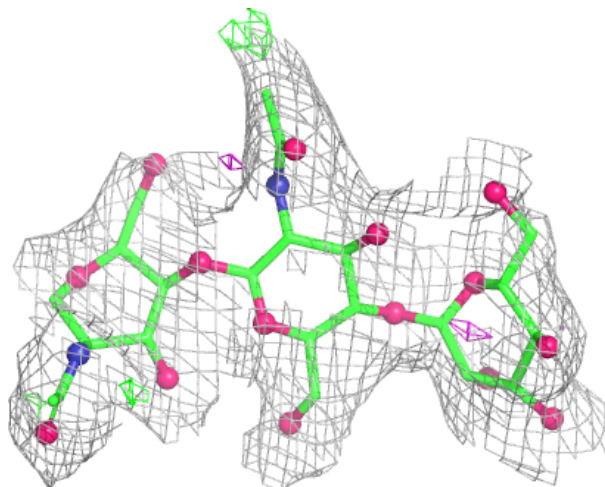
**Electron density around Chain h:**

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



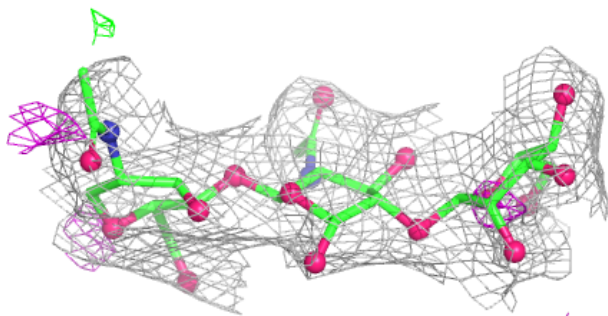
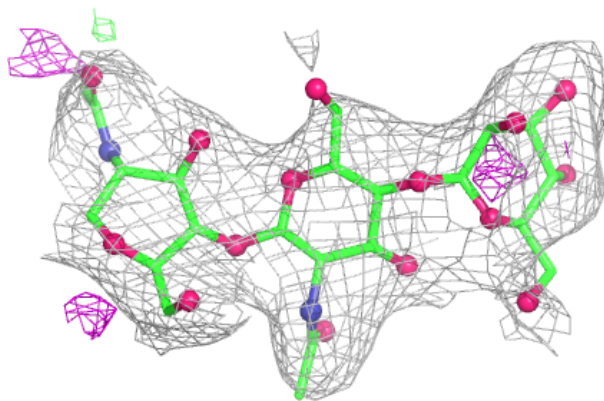
Electron density around Chain j:

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

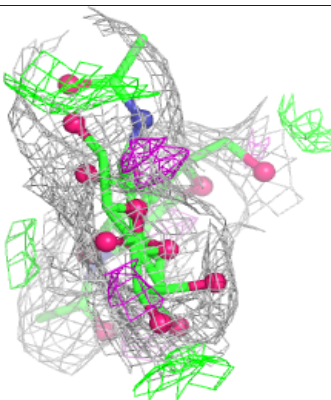
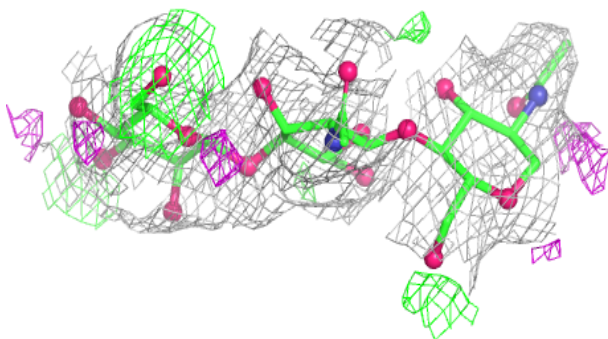
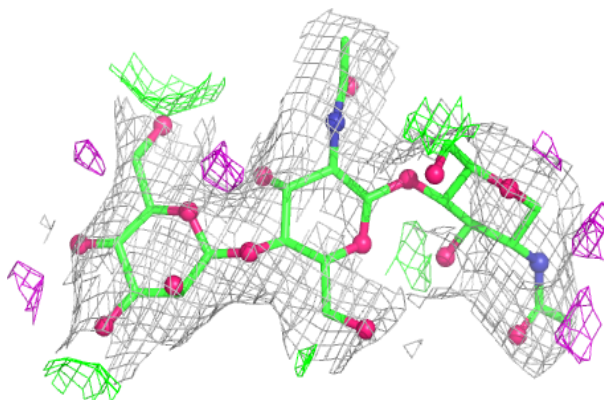


Electron density around Chain l:

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

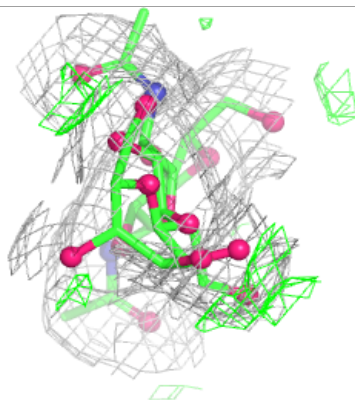
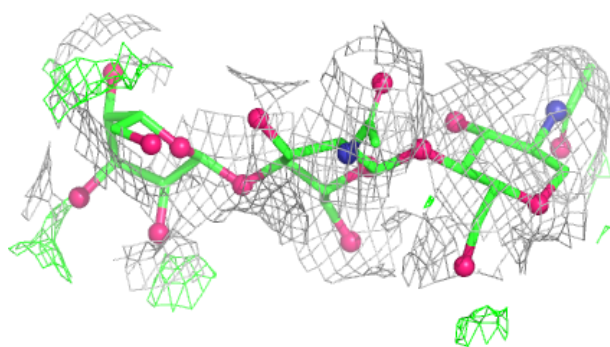
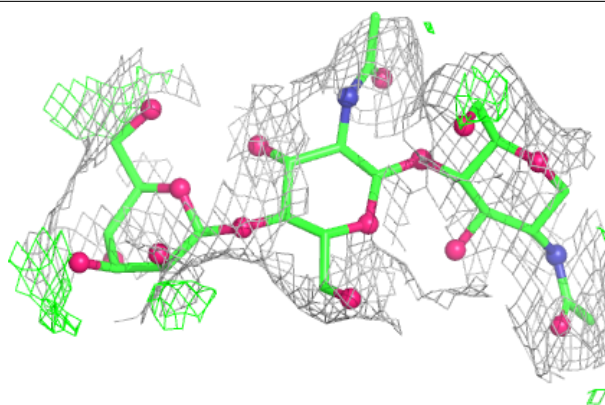
**Electron density around Chain n:**

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

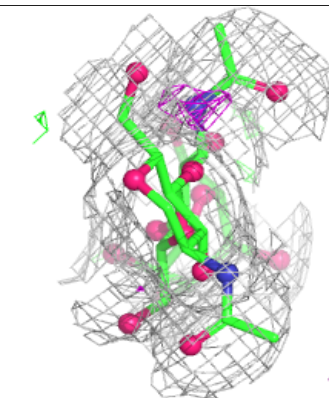
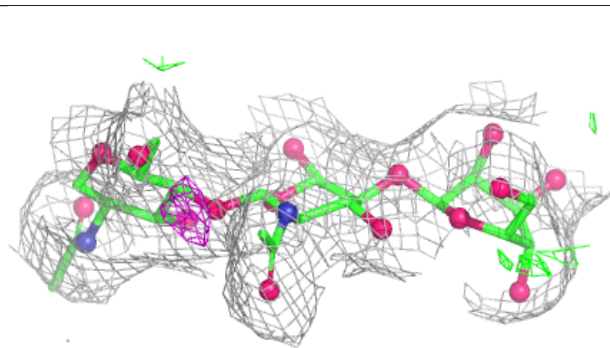
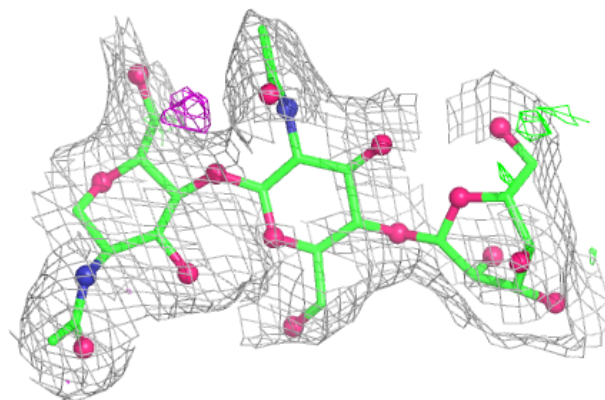


Electron density around Chain o:

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

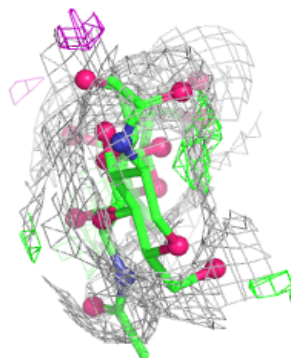
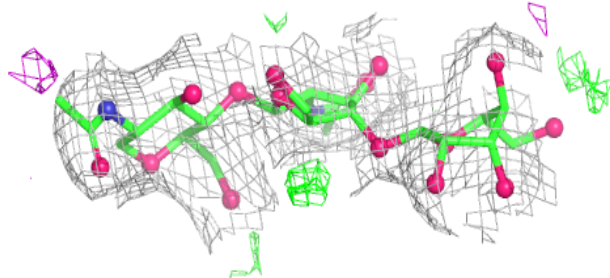
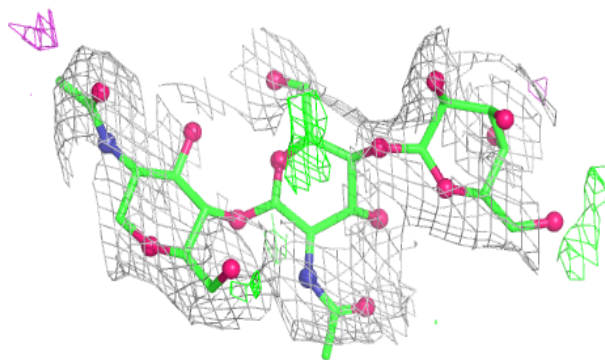
**Electron density around Chain q:**

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

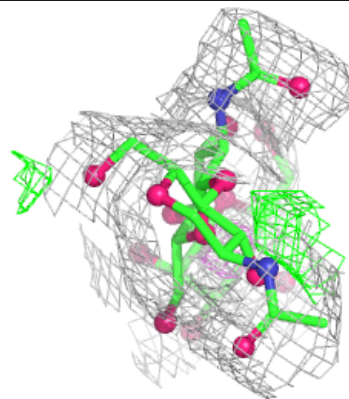
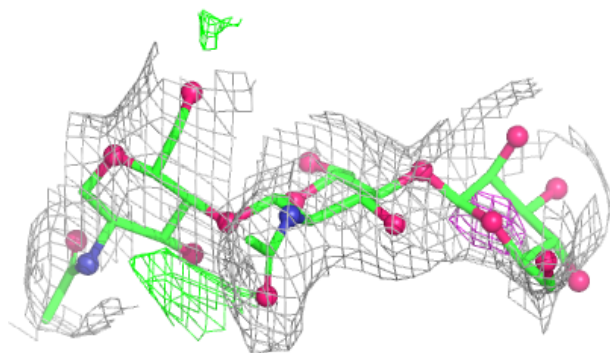
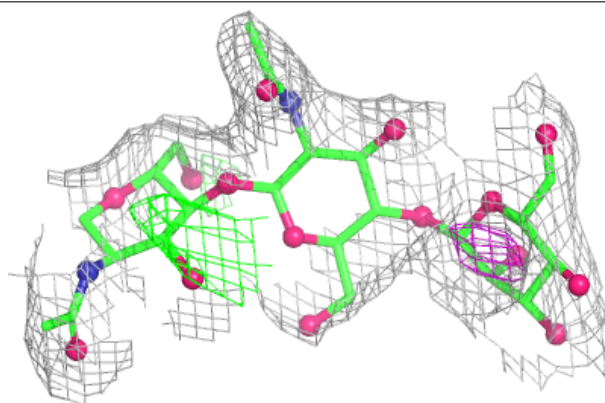


Electron density around Chain w:

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

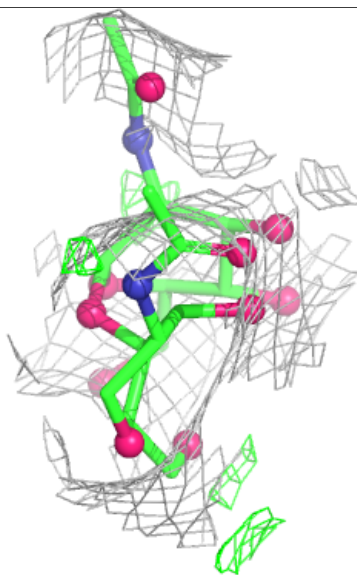
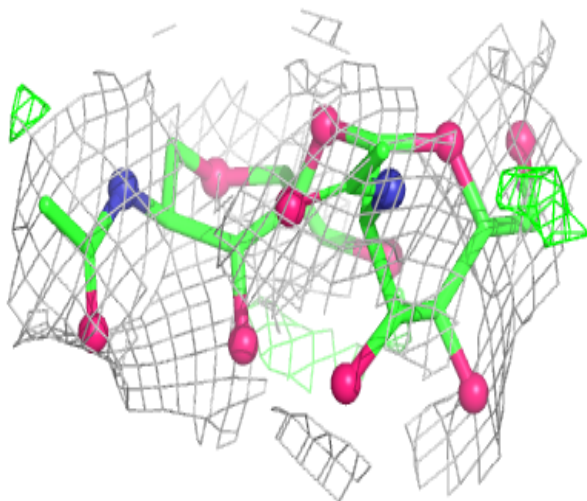
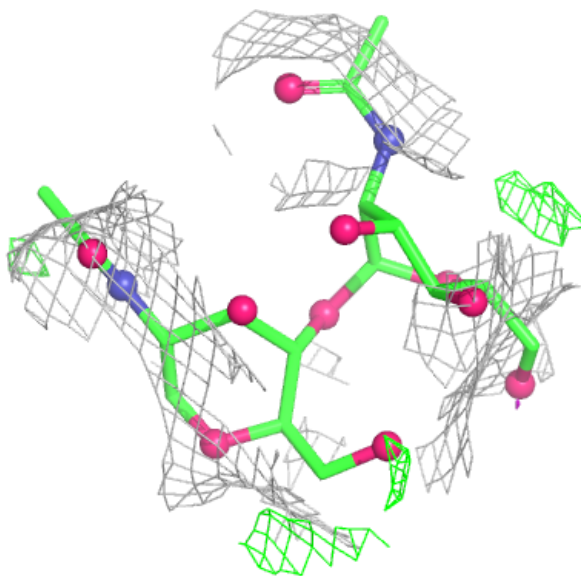
**Electron density around Chain y:**

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



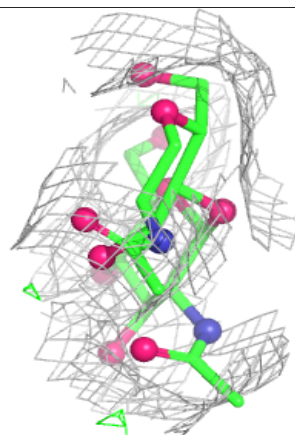
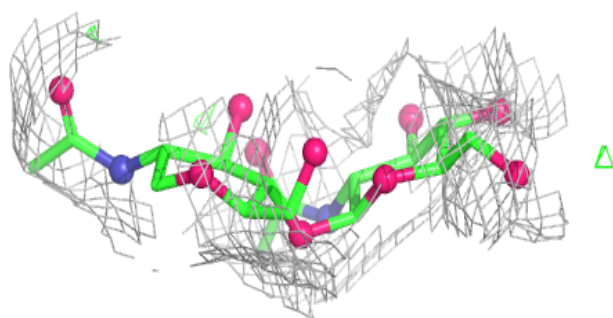
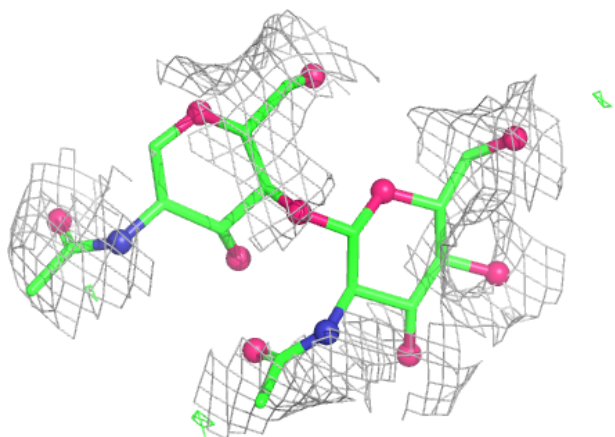
Electron density around Chain f:

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



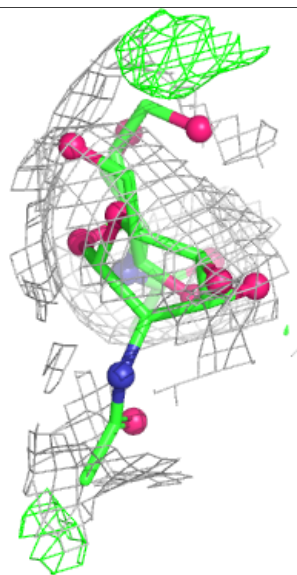
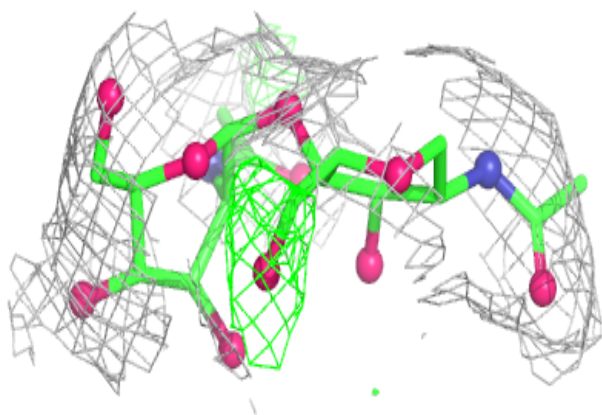
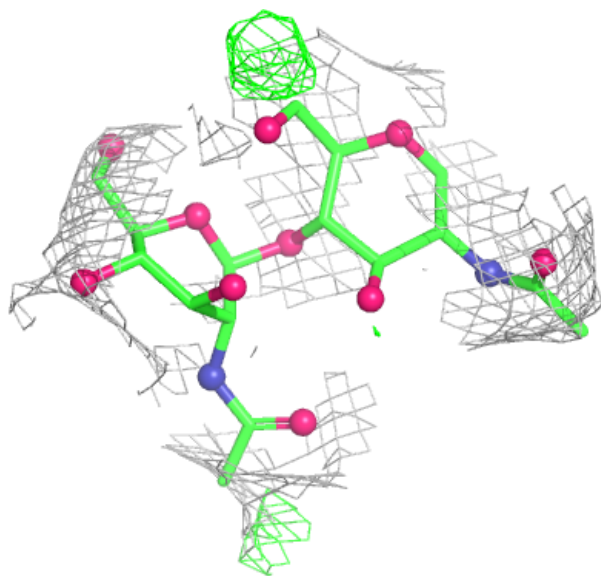
Electron density around Chain i:

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



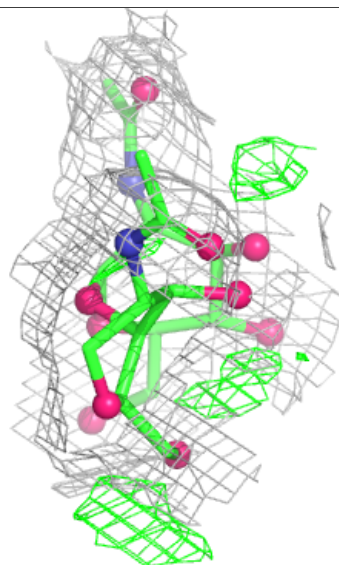
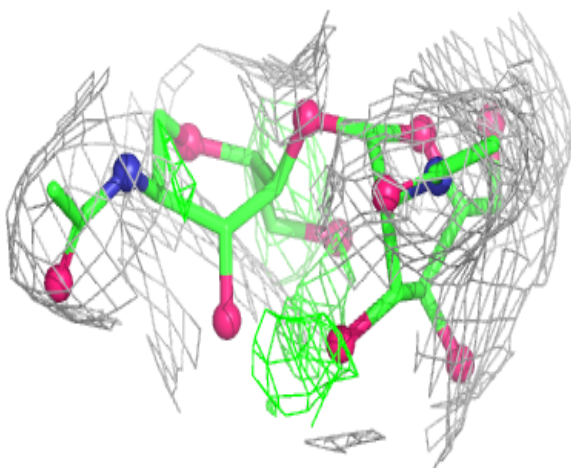
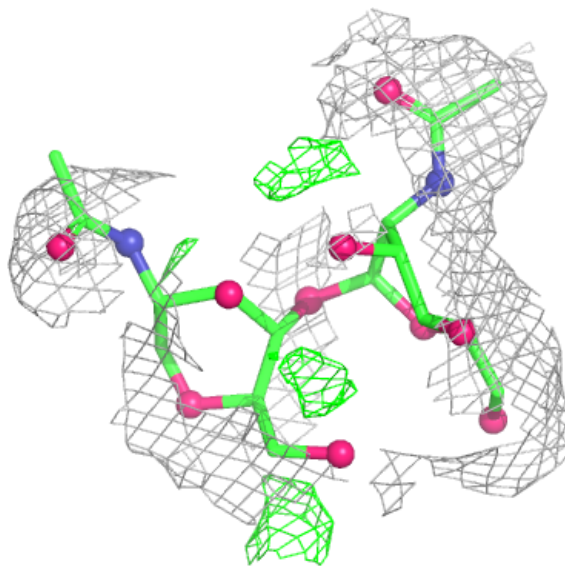
Electron density around Chain k:

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



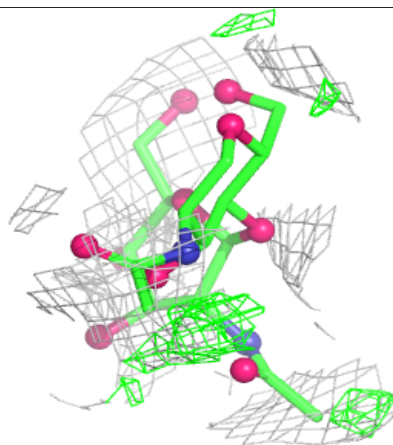
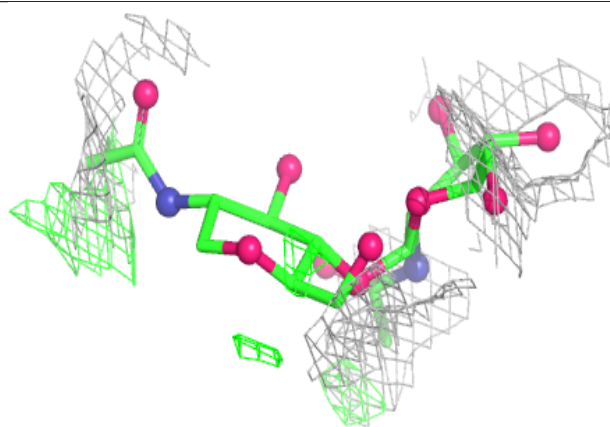
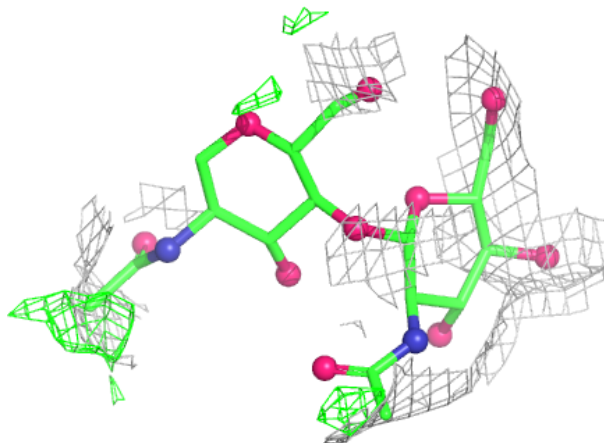
Electron density around Chain m:

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



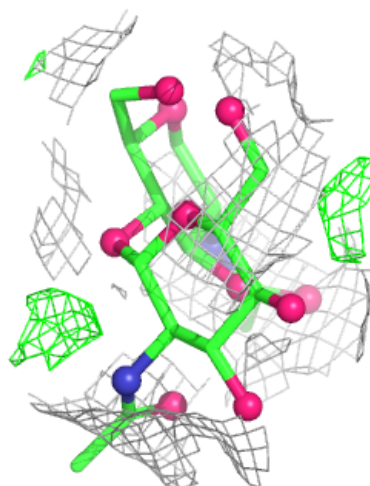
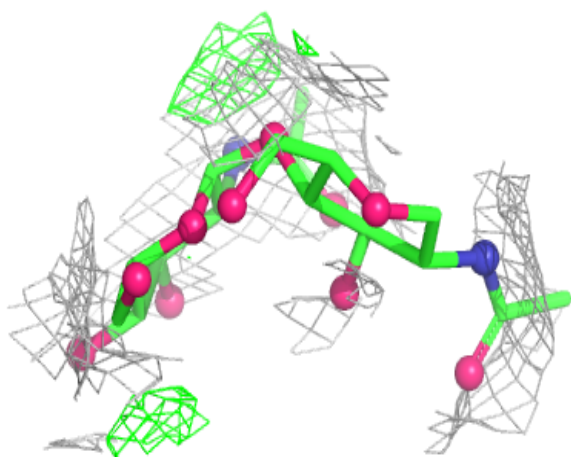
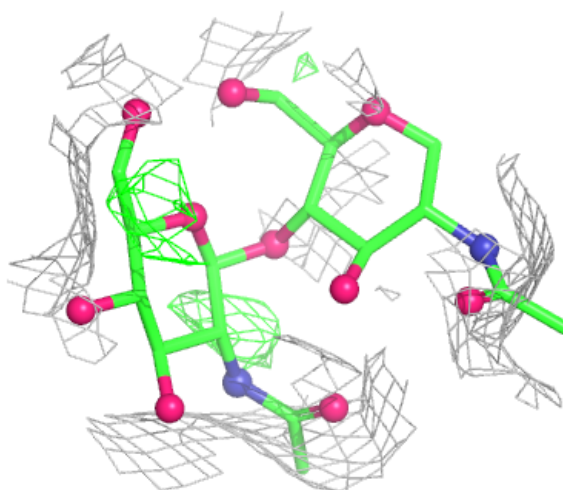
Electron density around Chain p:

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



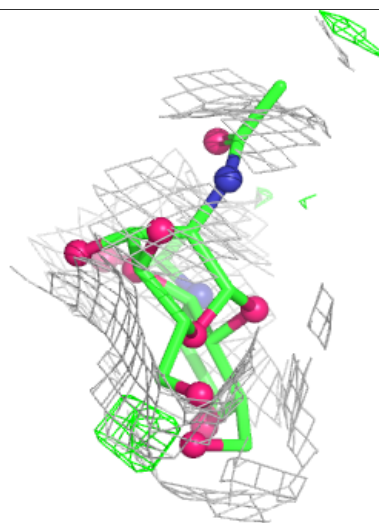
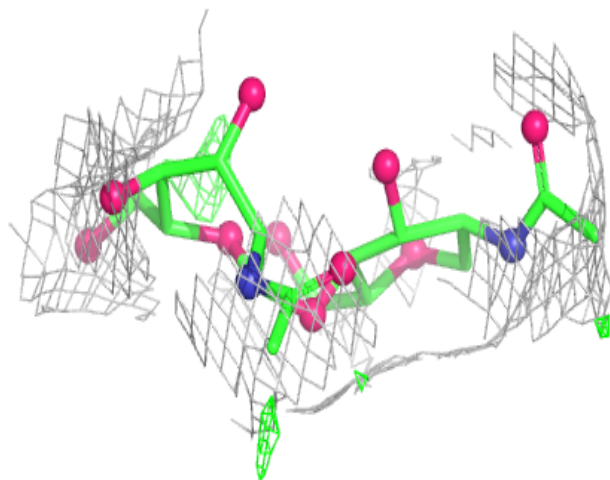
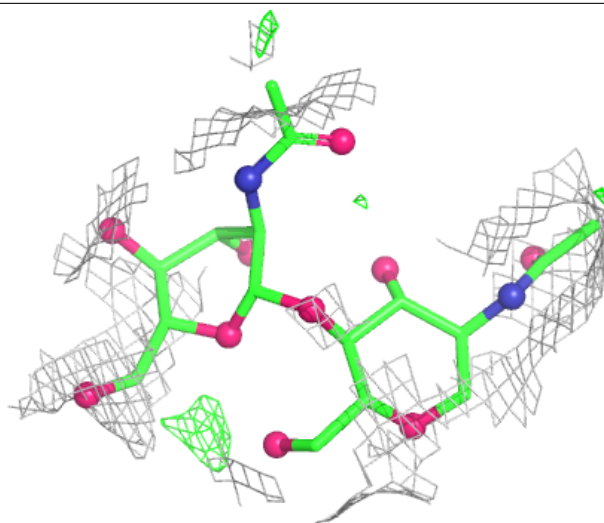
Electron density around Chain r:

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



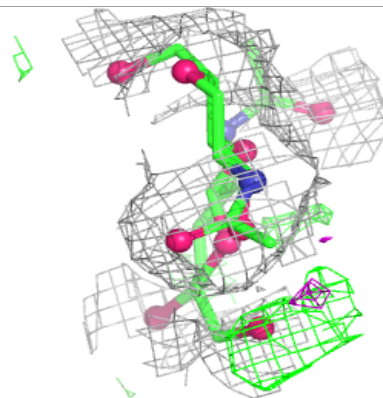
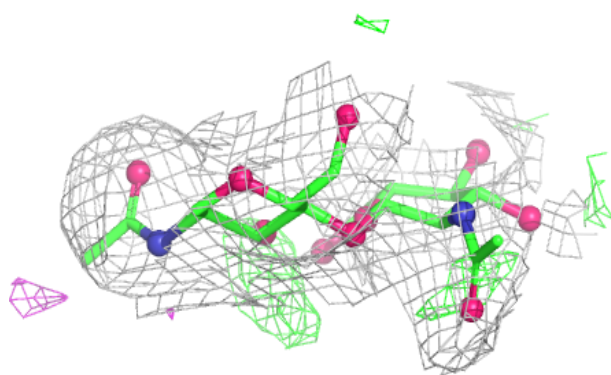
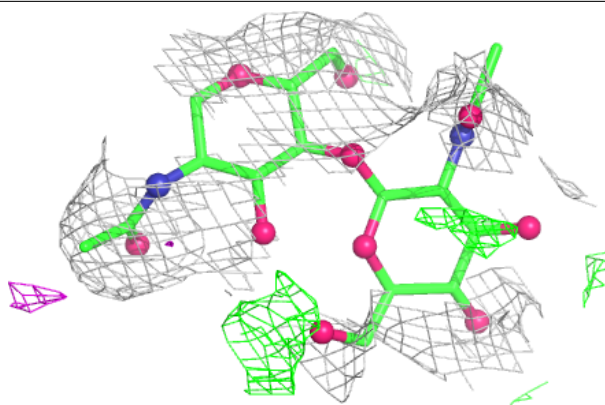
Electron density around Chain t:

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



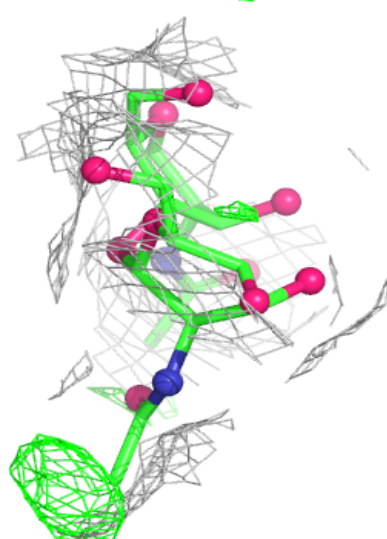
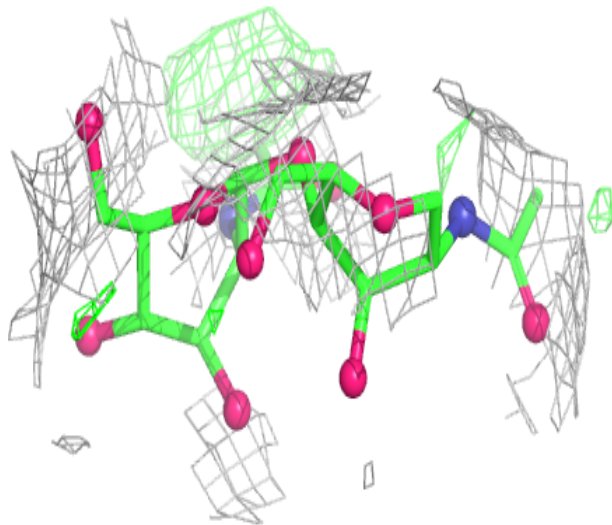
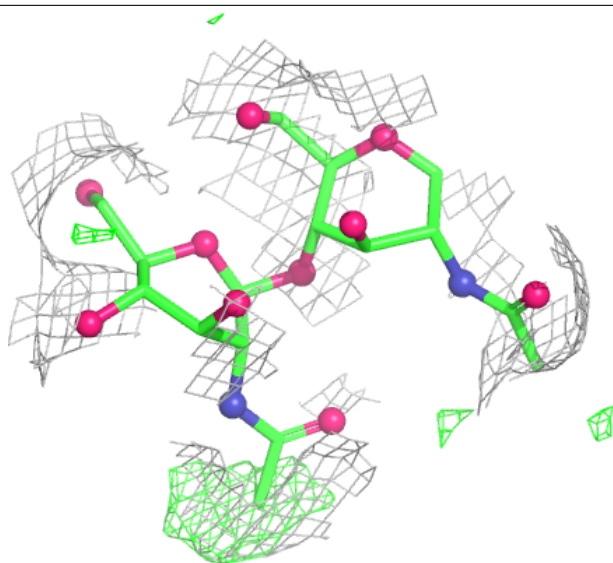
Electron density around Chain u:

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



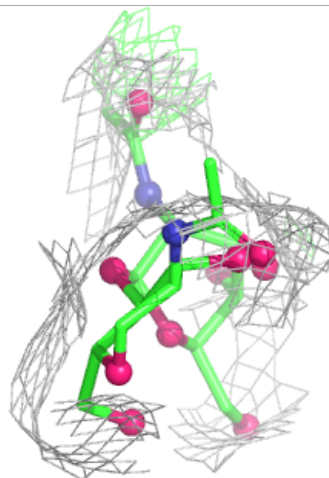
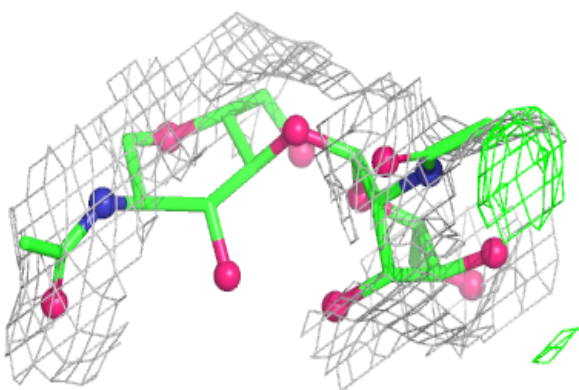
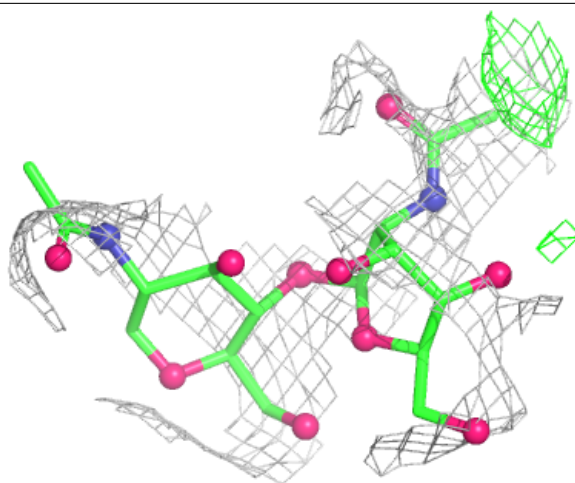
Electron density around Chain v:

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



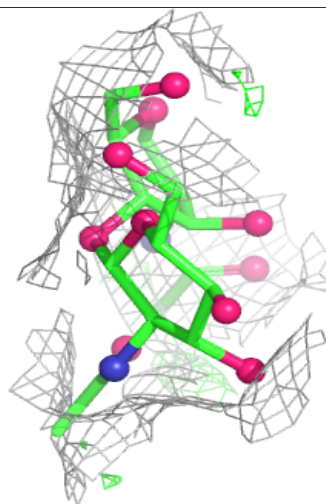
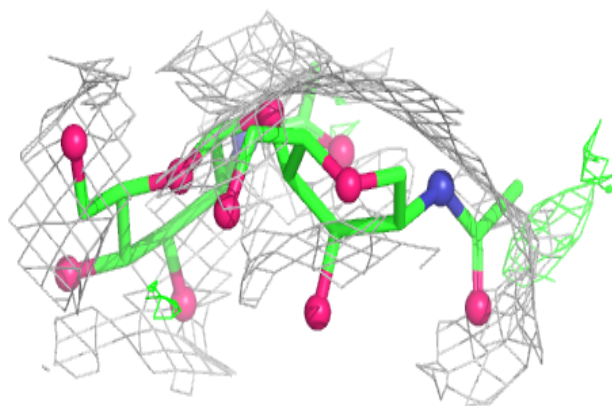
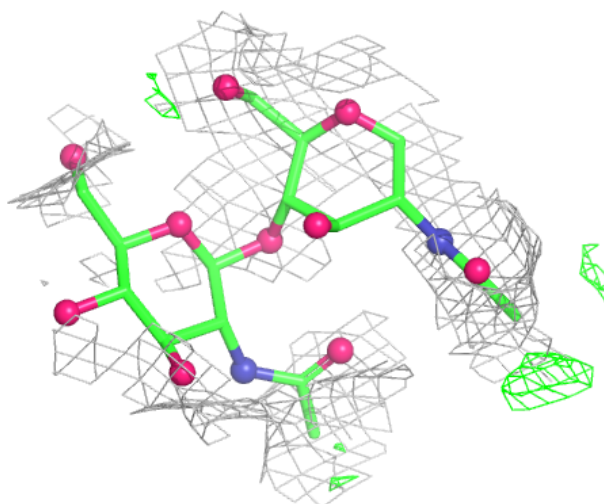
Electron density around Chain x:

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



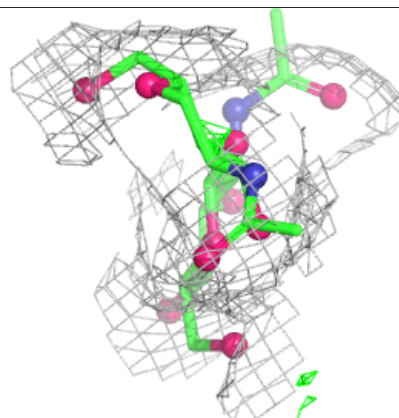
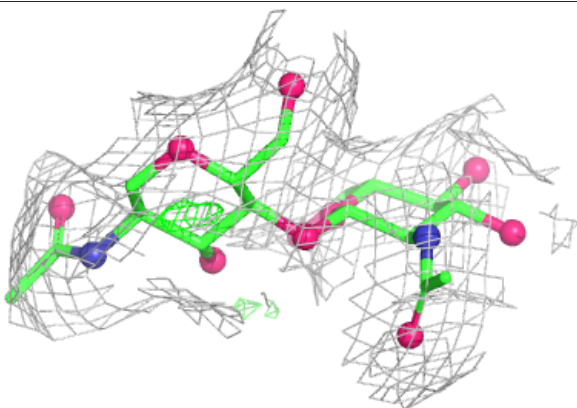
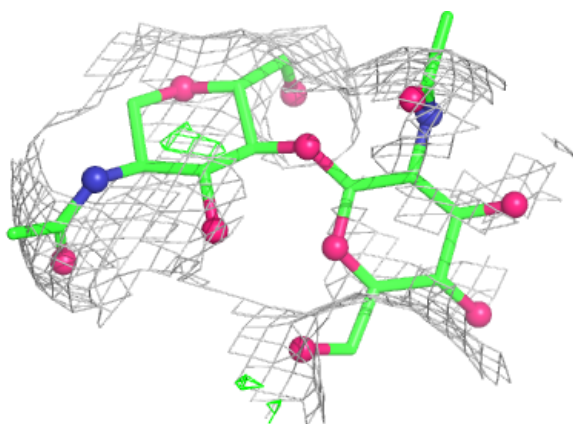
Electron density around Chain z:

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



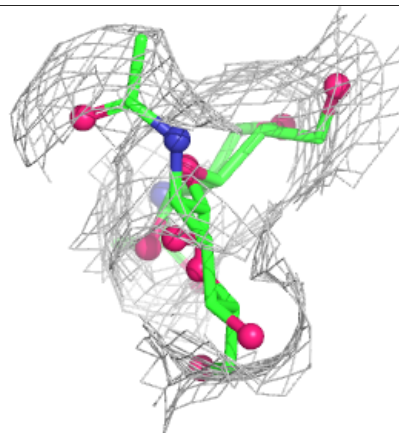
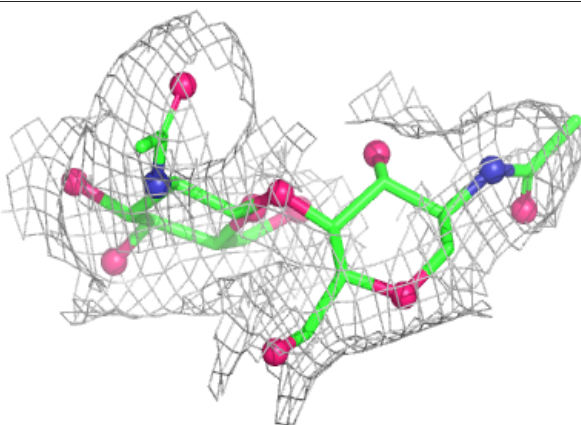
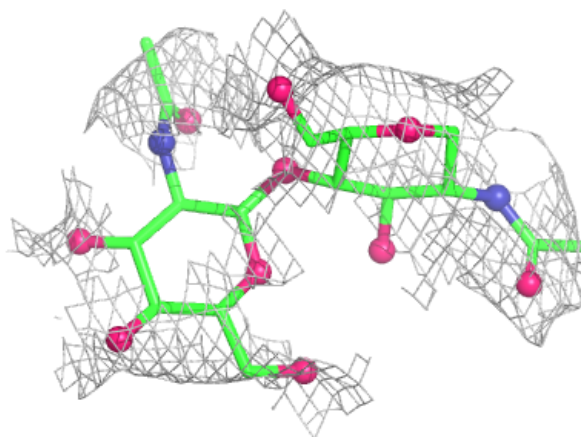
Electron density around Chain 0:

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

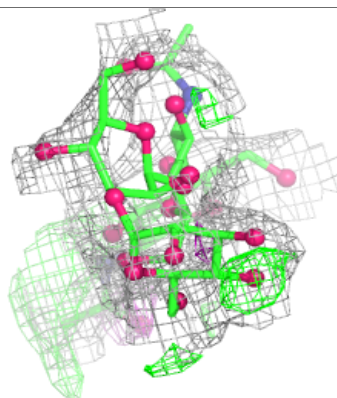
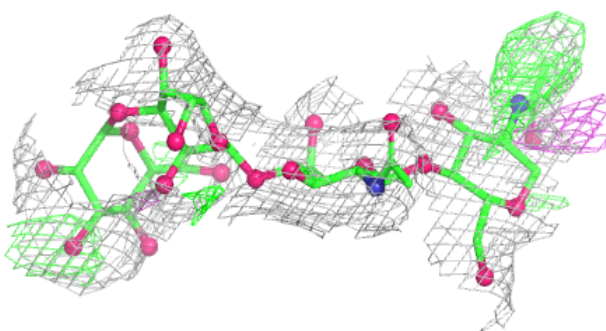
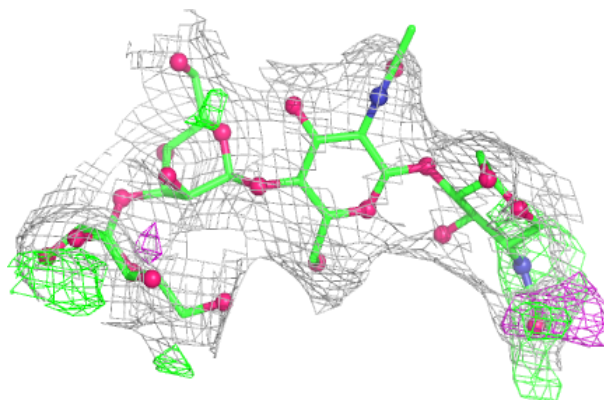


Electron density around Chain 1:

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

**Electron density around Chain s:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
6	NAG	c	2002	14/15	0.63	0.15	143,162,169,170	0
6	NAG	Y	2003	14/15	0.64	0.14	149,160,166,170	0
6	NAG	K	2004	14/15	0.69	0.12	127,140,146,149	0
6	NAG	O	2006	14/15	0.76	0.10	87,95,100,102	0
6	NAG	c	2001	14/15	0.78	0.11	94,106,117,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.