wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 02:28 PM EDT

PDB ID	:	4N5Y
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 (i) 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 (i)) were used in the production of this report:

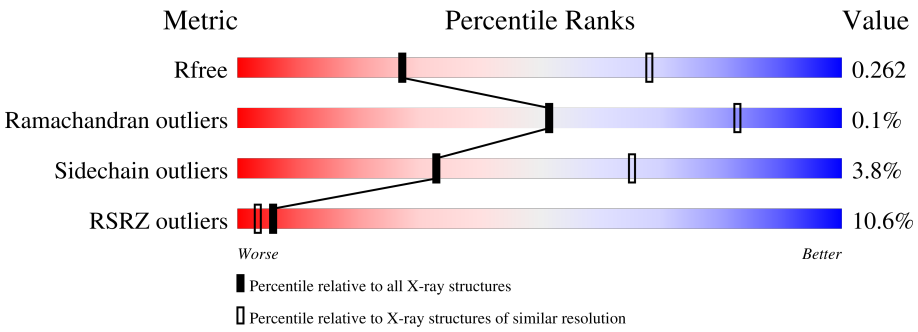
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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}	130704	1665 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 <=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	.% 90% 7% •
1	C	334	3% 93% • •
1	E	334	4% 93% • •
1	G	334	2% 92% 5% •
1	I	334	.% 90% 7% •
1	K	334	4% 94% • •
1	M	334	3% 91% 6% •

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Mol	Chain	Length	Quality of chain
1	O	334	4% 91% 5%
1	Q	334	7% 90% 7%
1	S	334	3% 93%
1	U	334	6% 92% 5%
1	W	334	4% 95%
1	Y	334	7% 93%
1	a	334	6% 93%
1	c	334	6% 93%
2	B	181	4% 94%
2	D	181	15% 96%
2	F	181	24% 96%
2	H	181	4% 96%
2	J	181	2% 96%
2	L	181	19% 97%
2	N	181	25% 97%
2	P	181	29% 97%
2	R	181	25% 97%
2	T	181	25% 97%
2	V	181	22% 96%
2	X	181	20% 96%
2	Z	181	40% 96%
2	b	181	32% 96%
2	d	181	38% 95%
3	e	3	33% 67%
3	g	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	h	3	100%
3	j	3	100%
3	l	3	100%
3	n	3	33% 67%
3	o	3	100%
3	q	3	33% 67%
3	w	3	33% 67%
3	y	3	33% 67%
4	0	2	100%
4	1	2	50% 50%
4	f	2	100%
4	i	2	50% 50%
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%

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
3	BMA	y	3	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	324	2573	1628	442	488	15	0	1	0
1	C	324	2573	1628	442	488	15	0	1	0
1	E	324	2573	1628	442	488	15	0	1	0
1	G	324	2573	1628	442	488	15	0	1	0
1	I	324	2573	1628	442	488	15	0	1	0
1	K	324	2573	1628	442	488	15	0	1	0
1	M	324	2573	1628	442	488	15	0	1	0
1	O	324	2573	1628	442	488	15	0	1	0
1	Q	324	2573	1628	442	488	15	0	1	0
1	S	324	2573	1628	442	488	15	0	1	0
1	U	324	2573	1628	442	488	15	0	1	0
1	W	324	2573	1628	442	488	15	0	1	0
1	Y	324	2573	1628	442	488	15	0	1	0
1	a	324	2573	1628	442	488	15	0	1	0
1	c	324	2573	1628	442	488	15	0	1	0

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

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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

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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
			Total	C	N	O	S			
2	B	177	1433	889	251	285	8	0	0	0
2	D	177	1433	889	251	285	8	0	0	0
2	F	177	1433	889	251	285	8	0	0	0
2	H	177	1433	889	251	285	8	0	0	0
2	J	177	1433	889	251	285	8	0	0	0
2	L	177	1433	889	251	285	8	0	0	0
2	N	177	1433	889	251	285	8	0	0	0
2	P	177	1433	889	251	285	8	0	0	0
2	R	177	1433	889	251	285	8	0	0	0

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

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

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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

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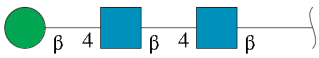
Chain	Residue	Modelled	Actual	Comment	Reference
T	181	ARG	-	expression tag	UNP Q6DQ33
V	175	SER	-	expression tag	UNP Q6DQ33
V	176	GLY	-	expression tag	UNP Q6DQ33
V	177	ARG	-	expression tag	UNP Q6DQ33
V	178	LEU	-	expression tag	UNP Q6DQ33
V	179	VAL	-	expression tag	UNP Q6DQ33
V	180	PRO	-	expression tag	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
			Total	C	N	O			
3	e	3	39	22	2	15	0	0	0
3	g	3	39	22	2	15	0	0	0
3	h	3	39	22	2	15	0	0	0
3	j	3	39	22	2	15	0	0	0
3	l	3	39	22	2	15	0	0	0
3	n	3	39	22	2	15	0	0	0
3	o	3	39	22	2	15	0	0	0
3	q	3	39	22	2	15	0	0	0
3	w	3	39	22	2	15	0	0	0
3	y	3	39	22	2	15	0	0	0

- 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
			Total	C	N	O			
4	f	2	28	16	2	10	0	0	0
4	i	2	28	16	2	10	0	0	0
4	k	2	28	16	2	10	0	0	0
4	m	2	28	16	2	10	0	0	0
4	p	2	28	16	2	10	0	0	0

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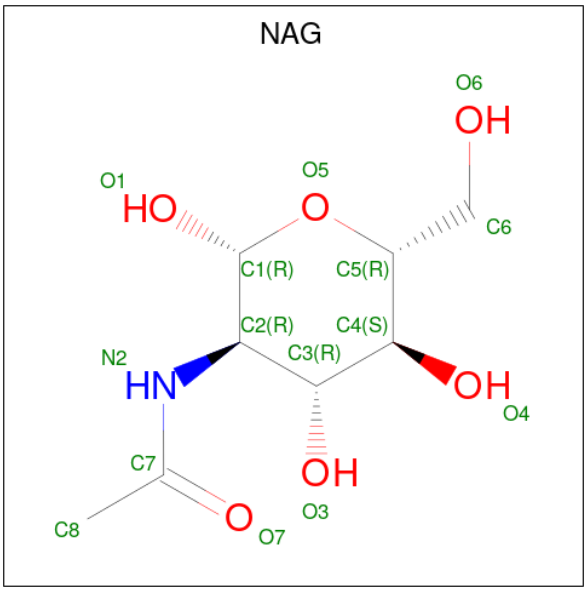
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	r	2	28	16	2	10	0	0	0
4	t	2	28	16	2	10	0	0	0
4	u	2	28	16	2	10	0	0	0
4	v	2	28	16	2	10	0	0	0
4	x	2	28	16	2	10	0	0	0
4	z	2	28	16	2	10	0	0	0
4	0	2	28	16	2	10	0	0	0
4	1	2	28	16	2	10	0	0	0

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



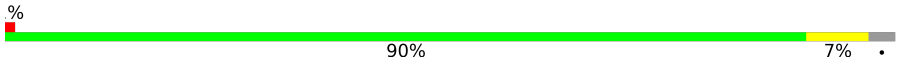
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	K	1	14	8	1	5	0	0
			Total	C	N	O		
6	O	1	14	8	1	5	0	0
			Total	C	N	O		
6	Y	1	14	8	1	5	0	0
			Total	C	N	O		
6	c	1	14	8	1	5	0	0
			Total	C	N	O		
6	c	1	14	8	1	5	0	0

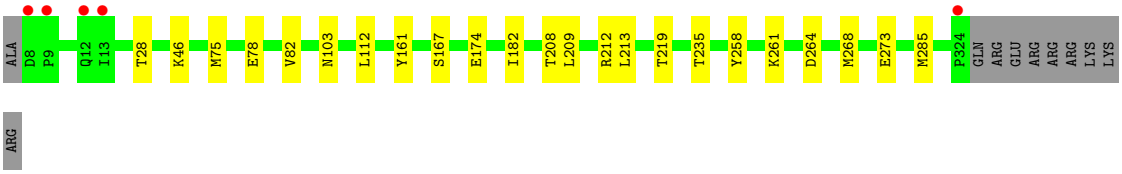
3 Residue-property plots (i)

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: Hemagglutinin HA1 chain

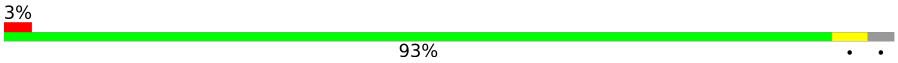
Chain A:

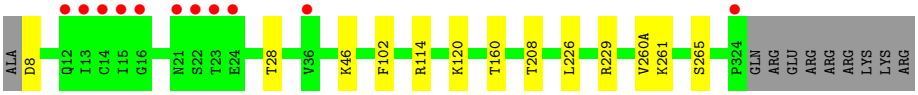




• Molecule 1: Hemagglutinin HA1 chain

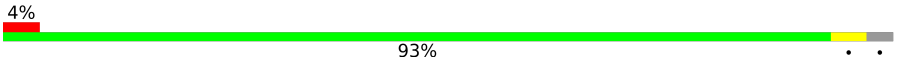
Chain C:

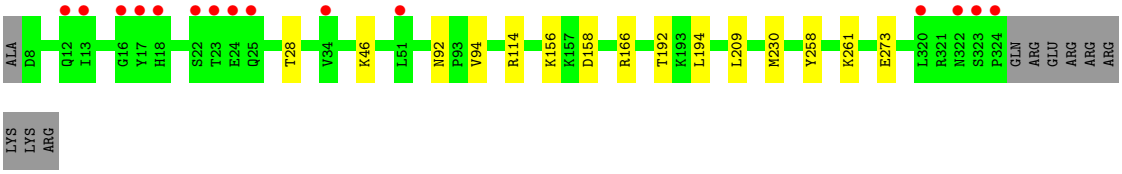




• Molecule 1: Hemagglutinin HA1 chain

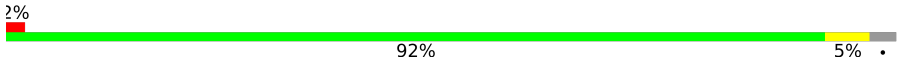
Chain E:

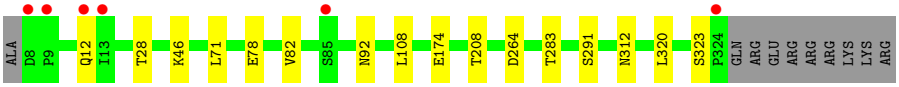




• Molecule 1: Hemagglutinin HA1 chain

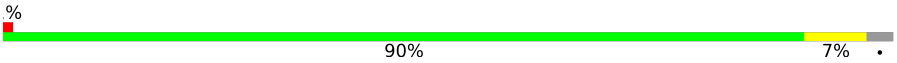
Chain G:

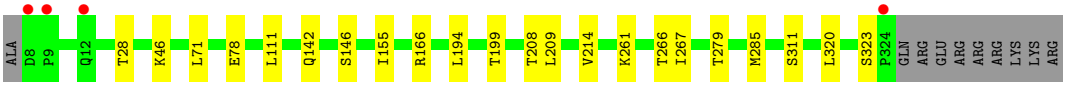




• Molecule 1: Hemagglutinin HA1 chain

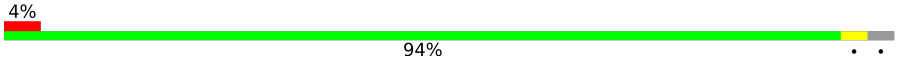
Chain I:





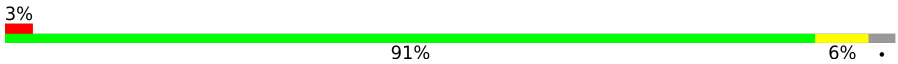
• Molecule 1: Hemagglutinin HA1 chain

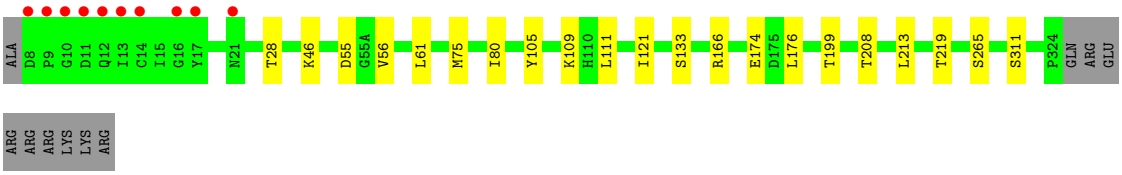
Chain K:



• Molecule 1: Hemagglutinin HA1 chain

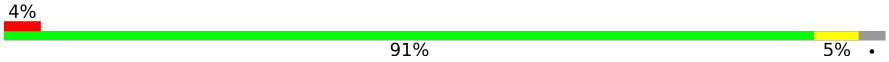
Chain M:





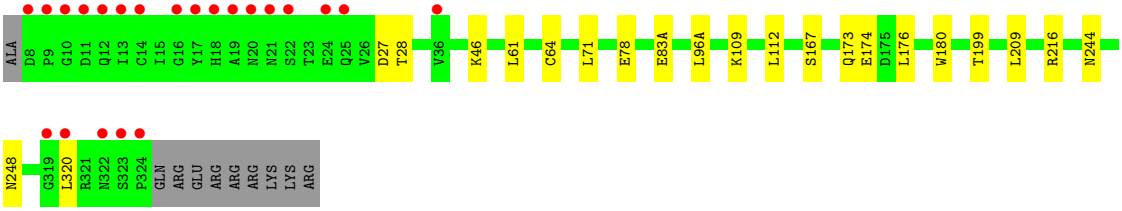
• Molecule 1: Hemagglutinin HA1 chain

Chain O:



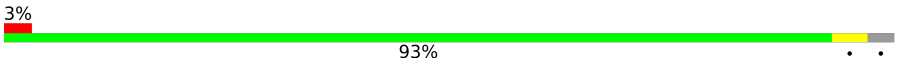
• Molecule 1: Hemagglutinin HA1 chain

Chain Q:



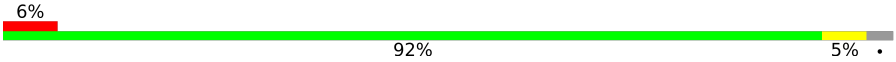
• Molecule 1: Hemagglutinin HA1 chain

Chain S:



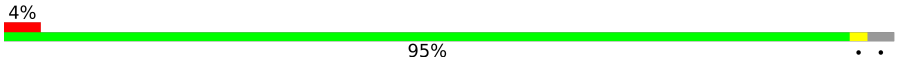
• Molecule 1: Hemagglutinin HA1 chain

Chain U:



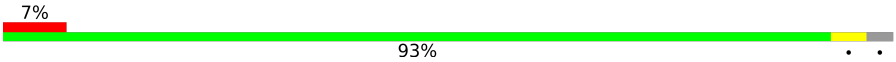
• Molecule 1: Hemagglutinin HA1 chain

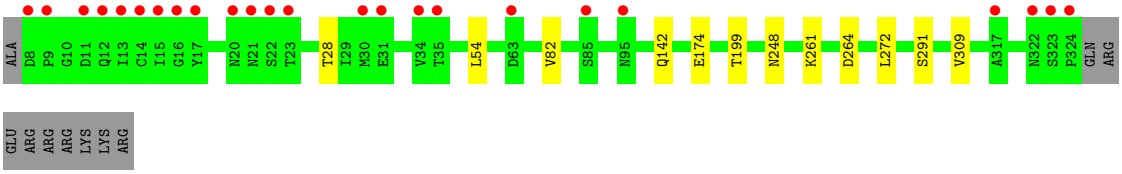
Chain W:



• Molecule 1: Hemagglutinin HA1 chain

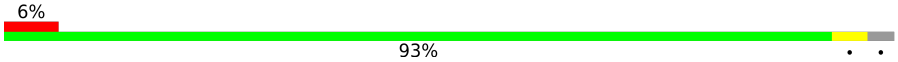
Chain Y:

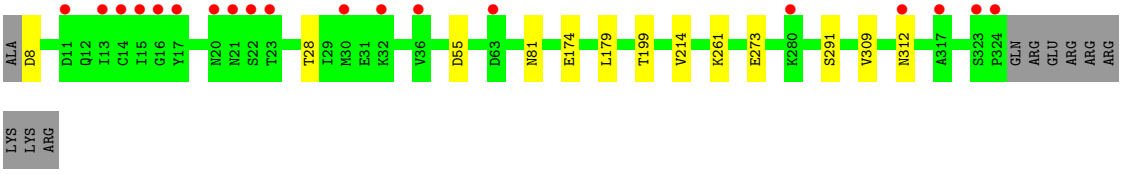




• Molecule 1: Hemagglutinin HA1 chain

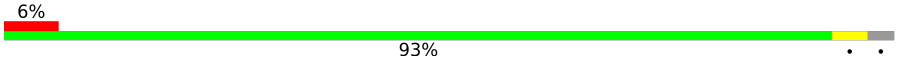
Chain a:

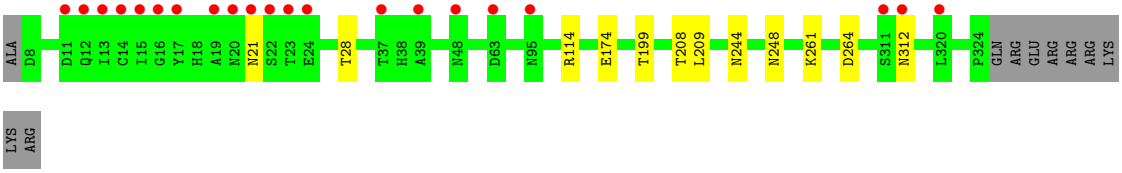




• Molecule 1: Hemagglutinin HA1 chain

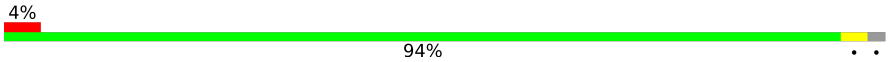
Chain c:





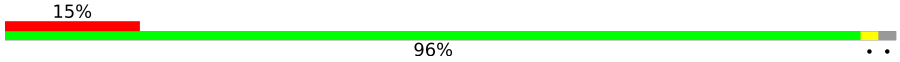
• Molecule 2: Hemagglutinin HA2 chain

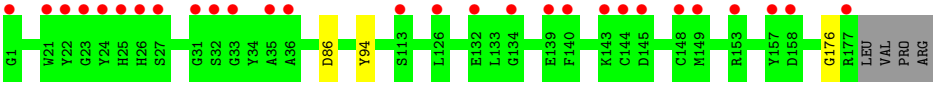
Chain B:



• Molecule 2: Hemagglutinin HA2 chain

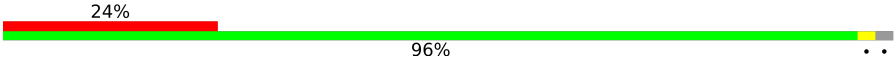
Chain D:

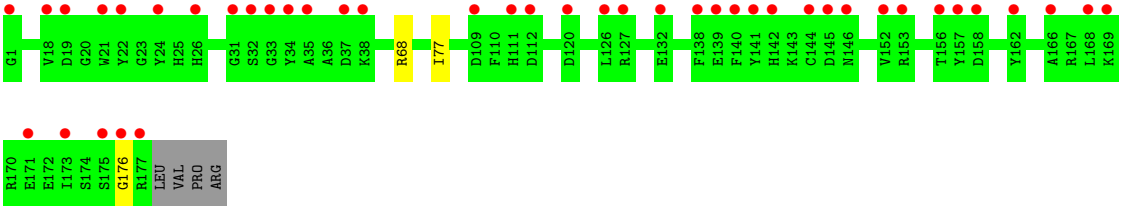




• Molecule 2: Hemagglutinin HA2 chain

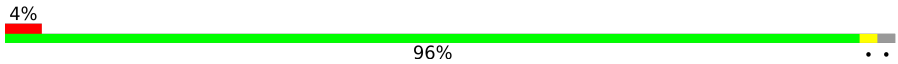
Chain F:

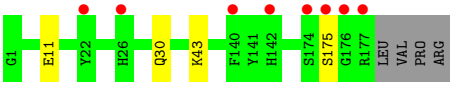




• Molecule 2: Hemagglutinin HA2 chain

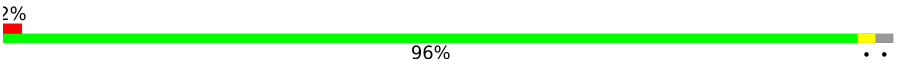
Chain H:





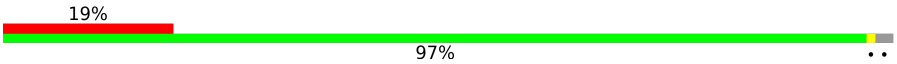
• Molecule 2: Hemagglutinin HA2 chain

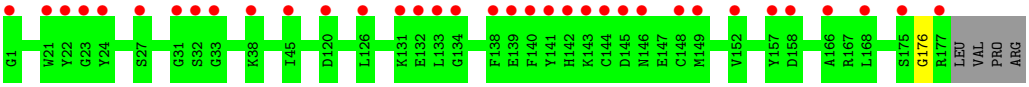
Chain J:



• Molecule 2: Hemagglutinin HA2 chain

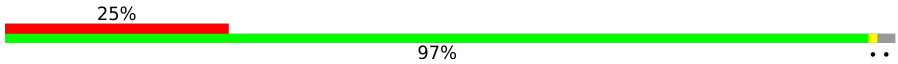
Chain L:

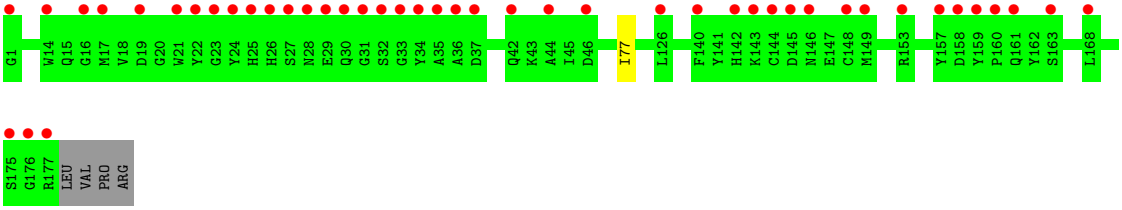




• Molecule 2: Hemagglutinin HA2 chain

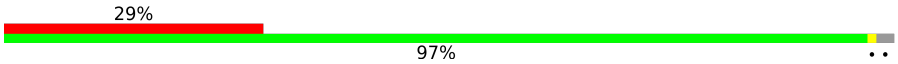
Chain N:

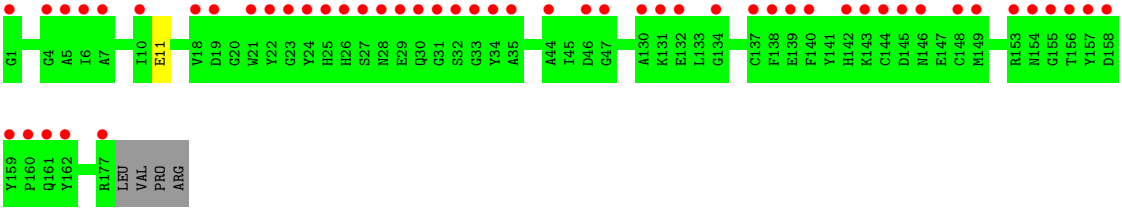




• Molecule 2: Hemagglutinin HA2 chain

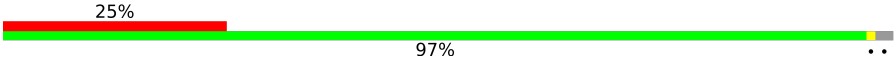
Chain P:

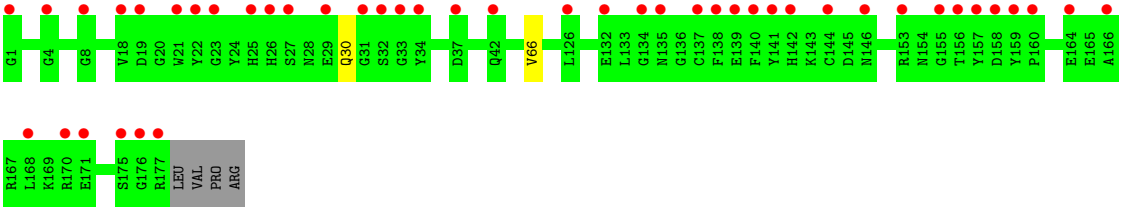




• Molecule 2: Hemagglutinin HA2 chain

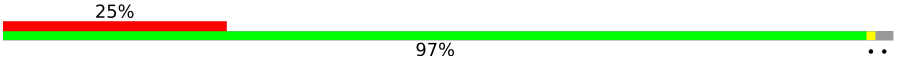
Chain R:

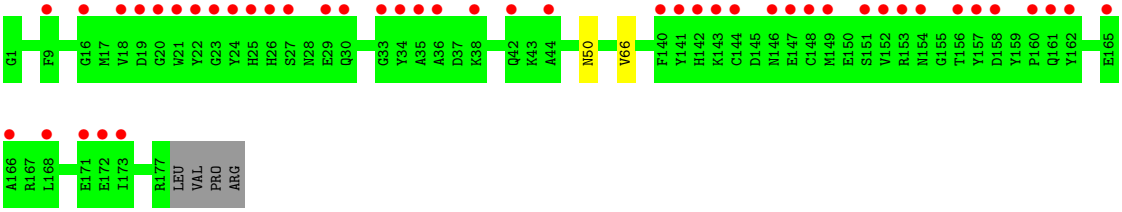




• Molecule 2: Hemagglutinin HA2 chain

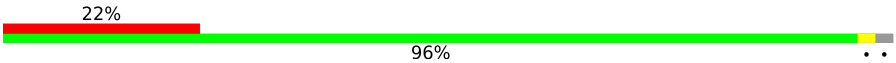
Chain T:

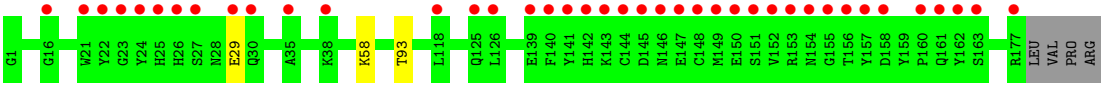




• Molecule 2: Hemagglutinin HA2 chain

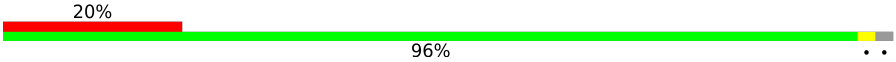
Chain V:

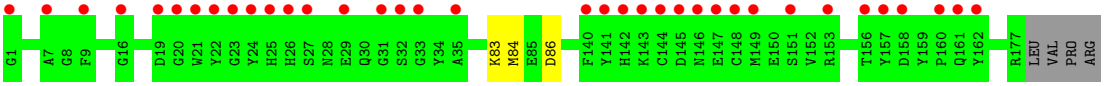




• Molecule 2: Hemagglutinin HA2 chain

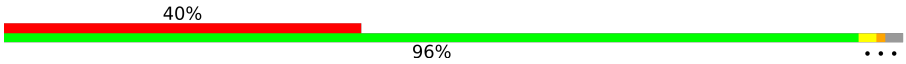
Chain X:

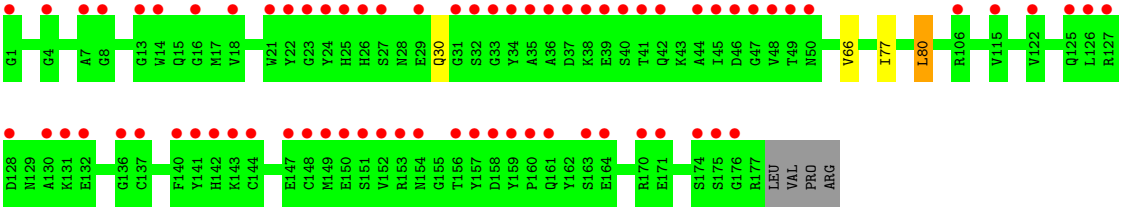




• Molecule 2: Hemagglutinin HA2 chain

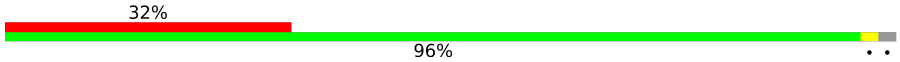
Chain Z:

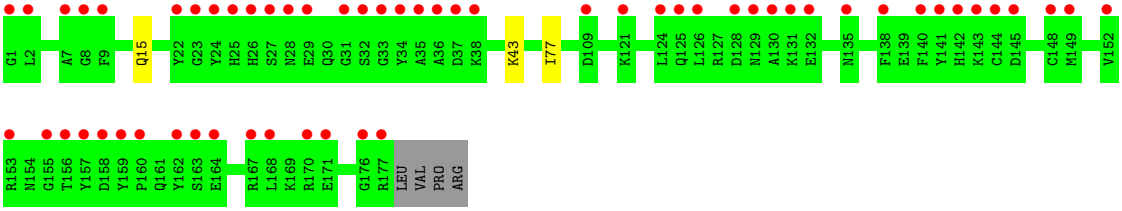




• Molecule 2: Hemagglutinin HA2 chain

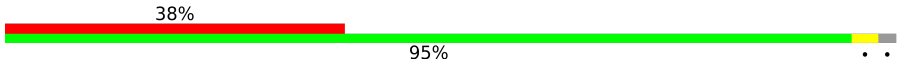
Chain b:

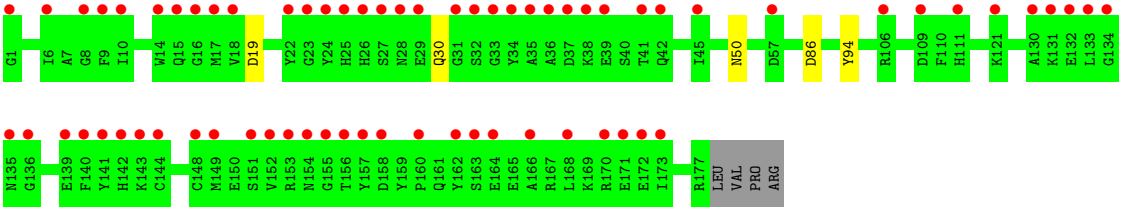




• Molecule 2: Hemagglutinin HA2 chain

Chain d:





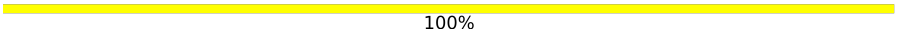
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

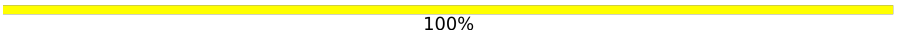
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

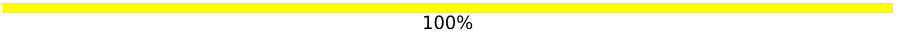
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 

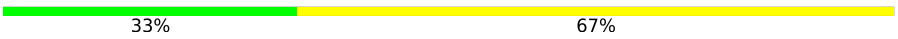
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 

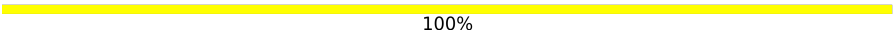
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 

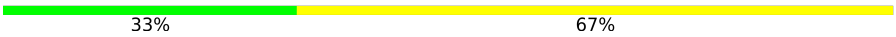
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 

• 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: 

• 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: 

• 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: 33% 67%

NAG1 NAG2 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%

NAG1 NAG2 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: 50% 50%

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%

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

Chain r: 100%

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

Chain t: 100%

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

Chain u: 50% 50%

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

Chain v: 100%

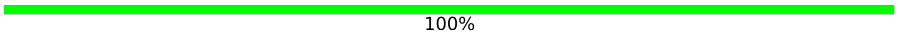
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x: 50% 50%

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

Chain z: 100%

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

Chain 0: 

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

Chain 1:

• 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:

4 Data and refinement statistics (i)

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) 91.2 (45.28-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.262 0.213 , 0.262	Depositor DCC
R_{free} test set	9993 reflections (5.00%)	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)	0.27 , 67.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, NAG, BMA

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	0.71	0/2639	0.93	4/3584 (0.1%)
1	C	0.62	0/2639	0.82	2/3584 (0.1%)
1	E	0.61	0/2639	0.81	2/3584 (0.1%)
1	G	0.73	0/2639	0.91	1/3584 (0.0%)
1	I	0.72	0/2639	0.91	2/3584 (0.1%)
1	K	0.62	0/2639	0.81	1/3584 (0.0%)
1	M	0.70	0/2639	0.88	3/3584 (0.1%)
1	O	0.68	0/2639	0.87	7/3584 (0.2%)
1	Q	0.69	1/2639 (0.0%)	0.86	4/3584 (0.1%)
1	S	0.55	0/2639	0.77	0/3584
1	U	0.58	1/2639 (0.0%)	0.76	0/3584
1	W	0.59	0/2639	0.77	1/3584 (0.0%)
1	Y	0.43	0/2639	0.67	0/3584
1	a	0.44	0/2639	0.66	0/3584
1	c	0.43	0/2639	0.67	0/3584
2	B	0.47	0/1460	0.67	1/1961 (0.1%)
2	D	0.40	0/1460	0.58	0/1961
2	F	0.40	0/1460	0.59	1/1961 (0.1%)
2	H	0.50	0/1460	0.68	0/1961
2	J	0.50	0/1460	0.68	0/1961
2	L	0.43	0/1460	0.57	0/1961
2	N	0.44	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.45	0/1460	0.63	0/1961
2	T	0.37	0/1460	0.59	0/1961
2	V	0.38	0/1460	0.56	0/1961
2	X	0.37	0/1460	0.58	0/1961
2	Z	0.32	0/1460	0.56	1/1961 (0.1%)
2	b	0.33	0/1460	0.55	0/1961
2	d	0.33	0/1460	0.53	0/1961
All	All	0.55	2/61485 (0.0%)	0.74	30/83175 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	135	VAL	CB-CG2	-5.77	1.40	1.52
1	Q	180	TRP	CB-CG	5.20	1.59	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	M	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	E	209	LEU	CA-CB-CG	7.10	131.62	115.30
1	A	212	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	Z	80	LEU	CA-CB-CG	6.29	129.76	115.30

There are no chirality outliers.

There are no planarity outliers.

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	O	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Q	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	S	323/334 (97%)	302 (94%)	20 (6%)	1 (0%)	41	73
1	U	323/334 (97%)	298 (92%)	23 (7%)	2 (1%)	25	62
1	W	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Y	323/334 (97%)	297 (92%)	25 (8%)	1 (0%)	41	73
1	a	323/334 (97%)	297 (92%)	26 (8%)	0	100	100
1	c	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	41	73
2	B	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	D	175/181 (97%)	162 (93%)	12 (7%)	1 (1%)	25	62
2	F	175/181 (97%)	163 (93%)	11 (6%)	1 (1%)	25	62
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%)	25	62
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%)	51	83

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 (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	292/300 (97%)	273 (94%)	19 (6%)	17	48
1	C	292/300 (97%)	281 (96%)	11 (4%)	33	65
1	E	292/300 (97%)	279 (96%)	13 (4%)	27	61
1	G	292/300 (97%)	277 (95%)	15 (5%)	24	56
1	I	292/300 (97%)	272 (93%)	20 (7%)	16	46
1	K	292/300 (97%)	282 (97%)	10 (3%)	37	68
1	M	292/300 (97%)	274 (94%)	18 (6%)	18	50
1	O	292/300 (97%)	277 (95%)	15 (5%)	24	56
1	Q	292/300 (97%)	275 (94%)	17 (6%)	20	52
1	S	292/300 (97%)	278 (95%)	14 (5%)	25	59
1	U	292/300 (97%)	277 (95%)	15 (5%)	24	56
1	W	292/300 (97%)	285 (98%)	7 (2%)	49	76
1	Y	292/300 (97%)	281 (96%)	11 (4%)	33	65
1	a	292/300 (97%)	279 (96%)	13 (4%)	27	61
1	c	292/300 (97%)	280 (96%)	12 (4%)	30	63
2	B	151/155 (97%)	146 (97%)	5 (3%)	38	69
2	D	151/155 (97%)	149 (99%)	2 (1%)	69	86
2	F	151/155 (97%)	150 (99%)	1 (1%)	84	93
2	H	151/155 (97%)	147 (97%)	4 (3%)	46	74
2	J	151/155 (97%)	147 (97%)	4 (3%)	46	74
2	L	151/155 (97%)	151 (100%)	0	100	100
2	N	151/155 (97%)	150 (99%)	1 (1%)	84	93
2	P	151/155 (97%)	150 (99%)	1 (1%)	84	93
2	R	151/155 (97%)	149 (99%)	2 (1%)	69	86
2	T	151/155 (97%)	149 (99%)	2 (1%)	69	86
2	V	151/155 (97%)	148 (98%)	3 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	151/155 (97%)	148 (98%)	3 (2%)	55	79
2	Z	151/155 (97%)	147 (97%)	4 (3%)	46	74
2	b	151/155 (97%)	148 (98%)	3 (2%)	55	79
2	d	151/155 (97%)	146 (97%)	5 (3%)	38	69
All	All	6645/6825 (97%)	6395 (96%)	250 (4%)	33	65

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	209	LEU
2	H	175	SER
1	S	199	THR
2	H	30	GLN
2	X	84	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	30	GLN
2	T	25	HIS
2	L	42	GLN
2	T	81	ASN
1	M	196	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.38	0	17,19,21	0.48	0
4	NAG	0	2	4	14,14,15	0.31	0	17,19,21	0.60	0
4	NAG	1	1	4,1	14,14,15	0.46	0	17,19,21	1.21	2 (11%)
4	NAG	1	2	4	14,14,15	0.44	0	17,19,21	0.43	0
3	NAG	e	1	3,1	14,14,15	1.35	3 (21%)	17,19,21	1.19	1 (5%)
3	NAG	e	2	3	14,14,15	0.51	0	17,19,21	0.56	0
3	BMA	e	3	3	11,11,12	1.97	3 (27%)	15,15,17	1.92	5 (33%)
4	NAG	f	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	1.26	2 (11%)
4	NAG	f	2	4	14,14,15	1.79	2 (14%)	17,19,21	1.17	1 (5%)
3	NAG	g	1	3,1	14,14,15	0.60	0	17,19,21	0.64	0
3	NAG	g	2	3	14,14,15	0.65	0	17,19,21	0.85	0
3	BMA	g	3	3	11,11,12	1.80	2 (18%)	15,15,17	2.77	5 (33%)
3	NAG	h	1	3,1	14,14,15	0.83	1 (7%)	17,19,21	1.45	1 (5%)
3	NAG	h	2	3	14,14,15	1.02	1 (7%)	17,19,21	1.39	3 (17%)
3	BMA	h	3	3	11,11,12	2.50	7 (63%)	15,15,17	1.53	4 (26%)
4	NAG	i	1	4,1	14,14,15	1.23	1 (7%)	17,19,21	1.30	3 (17%)
4	NAG	i	2	4	14,14,15	0.57	0	17,19,21	0.44	0
3	NAG	j	1	3,1	14,14,15	1.78	2 (14%)	17,19,21	1.30	2 (11%)
3	NAG	j	2	3	14,14,15	1.28	1 (7%)	17,19,21	1.15	2 (11%)
3	BMA	j	3	3	11,11,12	2.30	5 (45%)	15,15,17	1.64	4 (26%)
4	NAG	k	1	4,1	14,14,15	1.30	1 (7%)	17,19,21	1.38	2 (11%)
4	NAG	k	2	4	14,14,15	1.77	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	l	1	3,1	14,14,15	1.29	1 (7%)	17,19,21	1.42	2 (11%)
3	NAG	l	2	3	14,14,15	0.73	1 (7%)	17,19,21	0.60	0
3	BMA	l	3	3	11,11,12	1.99	3 (27%)	15,15,17	1.55	3 (20%)
4	NAG	m	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	m	2	4	14,14,15	1.51	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	n	1	3,1	14,14,15	0.51	0	17,19,21	0.72	0
3	NAG	n	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.21	2 (11%)
3	BMA	n	3	3	11,11,12	2.01	4 (36%)	15,15,17	1.71	4 (26%)
3	NAG	o	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
3	NAG	o	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BMA	o	3	3	11,11,12	1.93	5 (45%)	15,15,17	2.03	6 (40%)
4	NAG	p	1	4,1	14,14,15	0.72	0	17,19,21	0.75	0
4	NAG	p	2	4	14,14,15	1.51	1 (7%)	17,19,21	1.35	3 (17%)
3	NAG	q	1	3,1	14,14,15	0.96	1 (7%)	17,19,21	0.70	0
3	NAG	q	2	3	14,14,15	0.33	0	17,19,21	0.41	0
3	BMA	q	3	3	11,11,12	1.55	2 (18%)	15,15,17	2.23	4 (26%)
4	NAG	r	1	4,1	14,14,15	0.87	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	r	2	4	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
5	NAG	s	1	1,5	14,14,15	0.57	0	17,19,21	1.69	5 (29%)
5	NAG	s	2	5	14,14,15	0.46	0	17,19,21	1.03	0
5	BMA	s	3	5	11,11,12	0.72	0	15,15,17	1.96	4 (26%)
5	MAN	s	4	5	11,11,12	0.74	0	15,15,17	1.52	1 (6%)
4	NAG	t	1	4,1	14,14,15	1.28	1 (7%)	17,19,21	1.27	3 (17%)
4	NAG	t	2	4	14,14,15	1.05	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	u	1	4,1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	u	2	4	14,14,15	0.93	1 (7%)	17,19,21	0.88	0
4	NAG	v	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	0.97	2 (11%)
4	NAG	v	2	4	14,14,15	1.24	3 (21%)	17,19,21	1.06	1 (5%)
3	NAG	w	1	3,1	14,14,15	0.31	0	17,19,21	0.58	0
3	NAG	w	2	3	14,14,15	1.98	1 (7%)	17,19,21	1.35	2 (11%)
3	BMA	w	3	3	11,11,12	1.39	2 (18%)	15,15,17	1.43	3 (20%)
4	NAG	x	1	4,1	14,14,15	1.19	1 (7%)	17,19,21	1.26	2 (11%)
4	NAG	x	2	4	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	y	1	3,1	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
3	NAG	y	2	3	14,14,15	0.59	0	17,19,21	0.92	0
3	BMA	y	3	3	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
4	NAG	z	1	4,1	14,14,15	1.46	1 (7%)	17,19,21	1.30	3 (17%)
4	NAG	z	2	4	14,14,15	0.91	1 (7%)	17,19,21	0.85	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
4	NAG	0	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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	3,1	-	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
4	NAG	r	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	s	1	1,5	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	w	2	3	-	4/6/23/26	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	3,1	-	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 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	w	2	NAG	O5-C1	-7.22	1.32	1.43
3	j	1	NAG	O5-C1	-6.08	1.34	1.43
4	p	2	NAG	O5-C1	-5.08	1.35	1.43
4	z	1	NAG	O5-C1	-5.06	1.35	1.43
4	f	2	NAG	O5-C1	4.94	1.51	1.43

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	g	3	BMA	C1-O5-C5	5.94	120.24	112.19
3	g	3	BMA	O5-C1-C2	5.74	119.63	110.77
3	q	3	BMA	C1-O5-C5	5.30	119.37	112.19
5	s	4	MAN	O5-C1-C2	5.07	118.59	110.77
3	h	1	NAG	C1-O5-C5	5.01	118.98	112.19

There are no chirality outliers.

5 of 61 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
5	s	4	MAN	O5-C5-C6-O6
3	y	3	BMA	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6

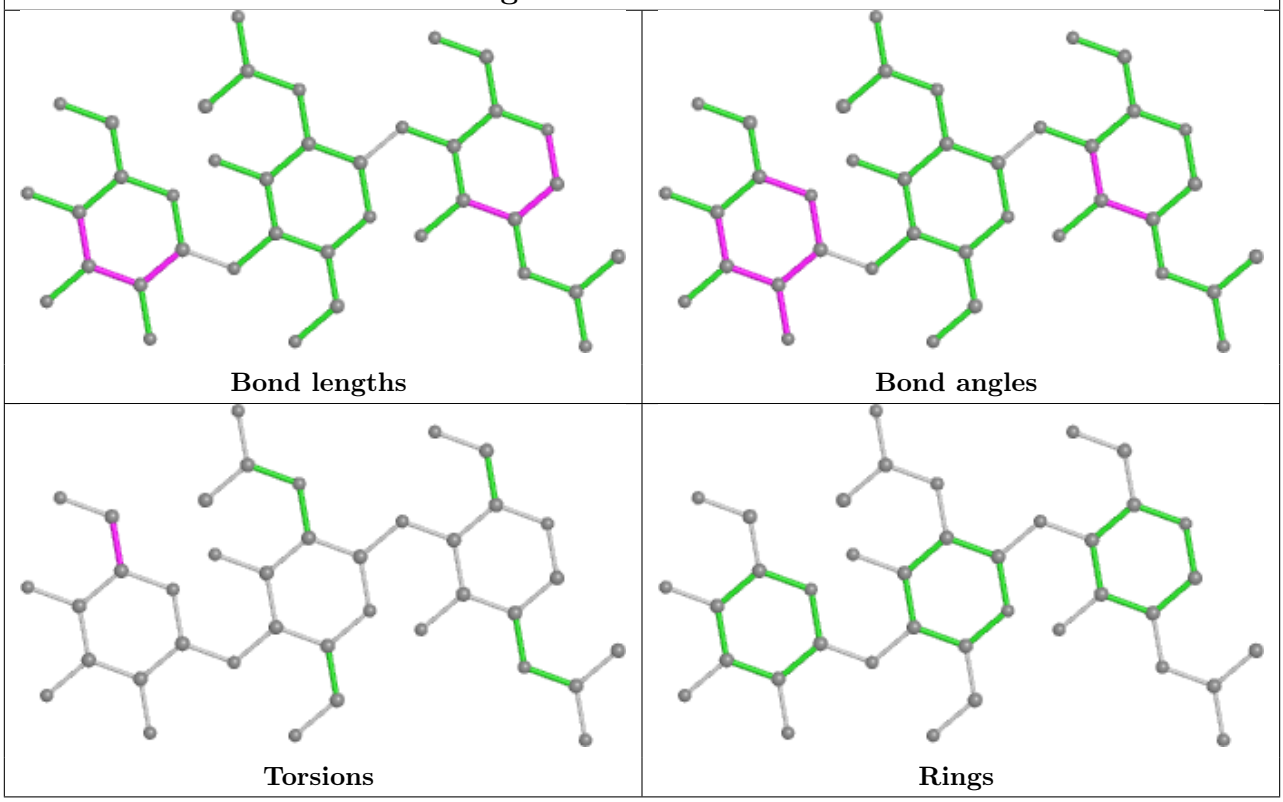
All (1) ring outliers are listed below:

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

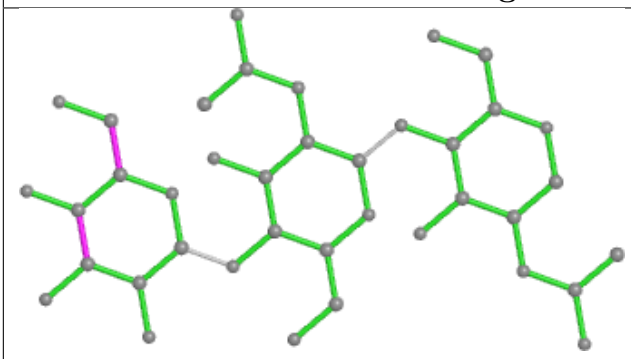
No monomer is involved in short contacts.

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

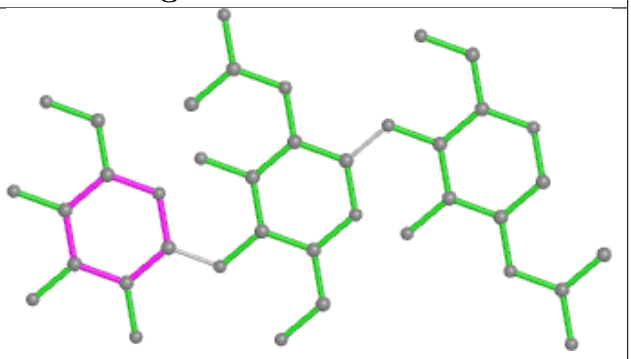
Oligosaccharide Chain e



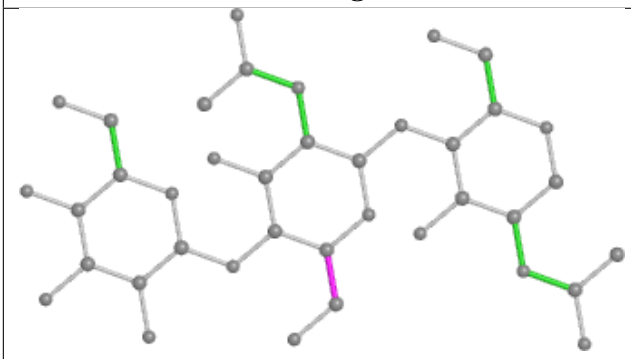
Oligosaccharide Chain g



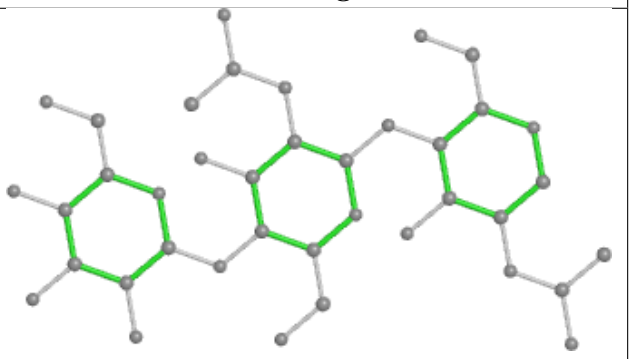
Bond lengths



Bond angles

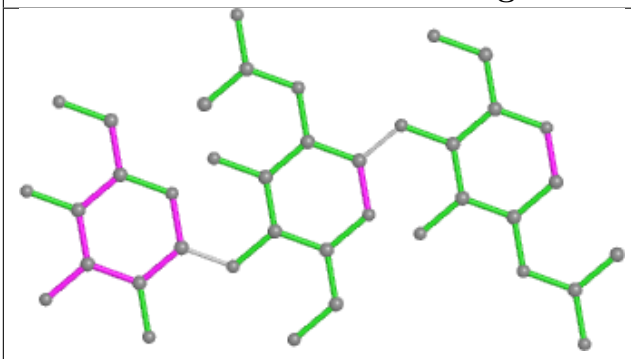


Torsions

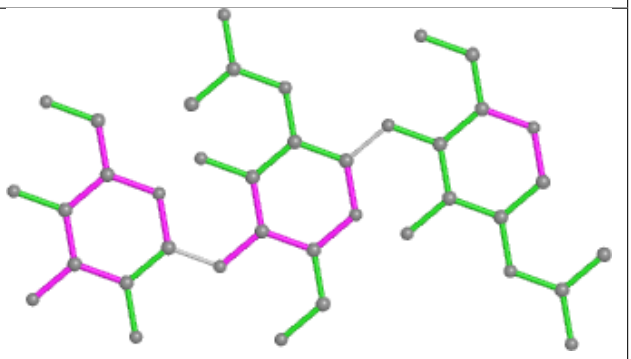


Rings

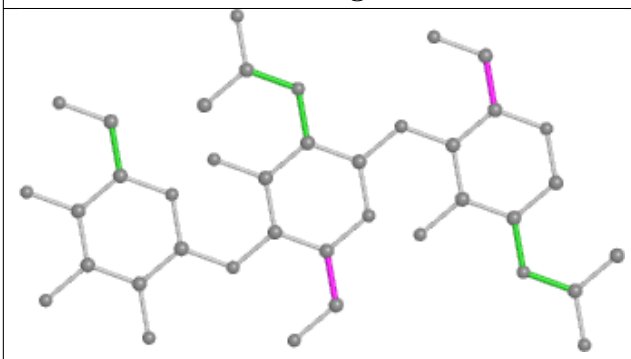
Oligosaccharide Chain h



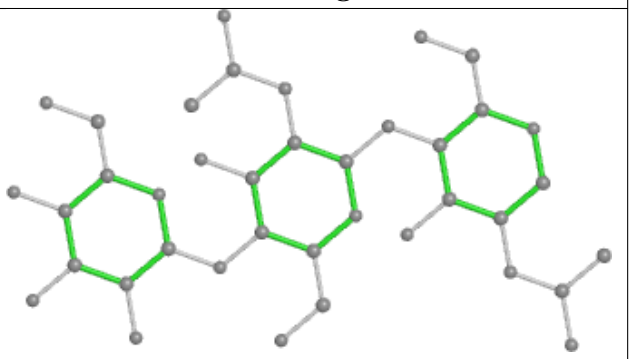
Bond lengths



Bond angles

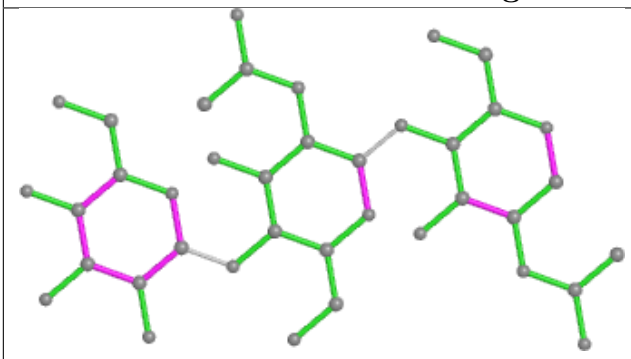


Torsions

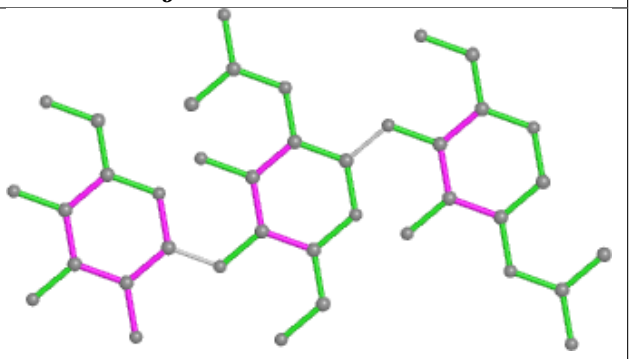


Rings

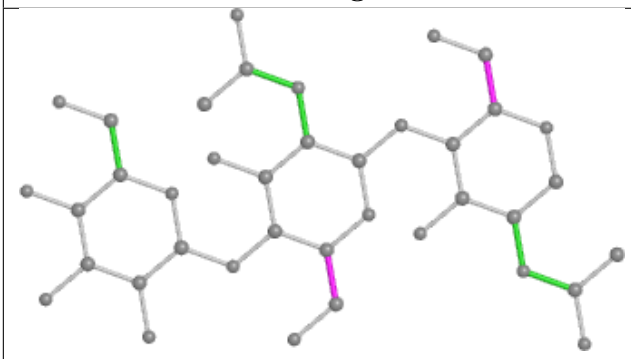
Oligosaccharide Chain j



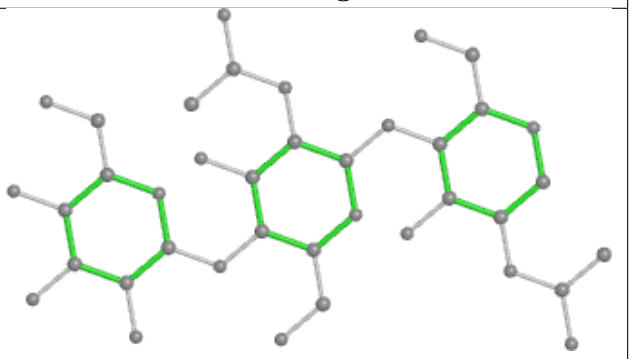
Bond lengths



Bond angles

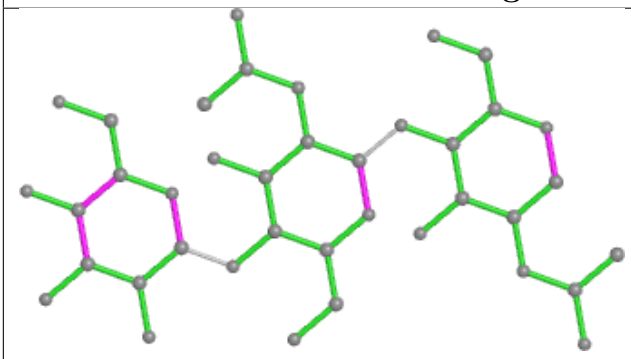


Torsions

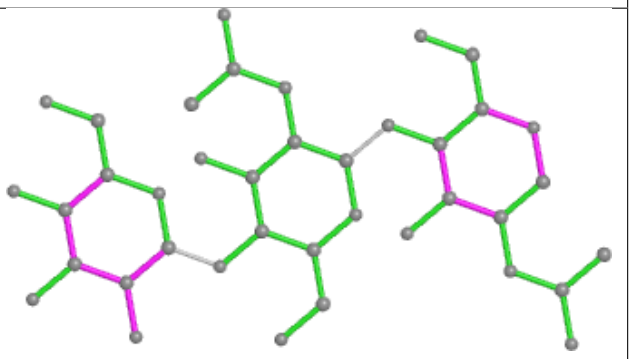


Rings

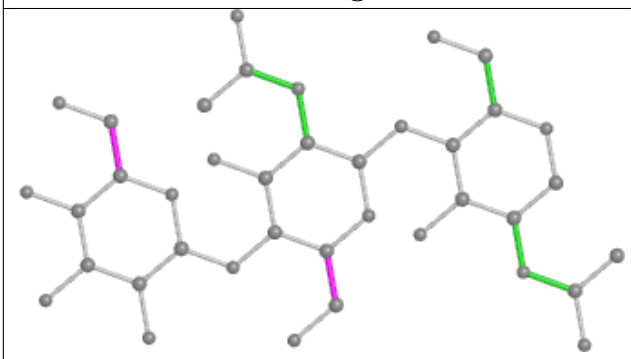
Oligosaccharide Chain l



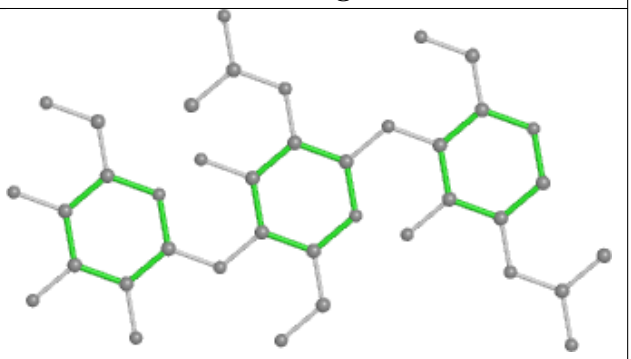
Bond lengths



Bond angles

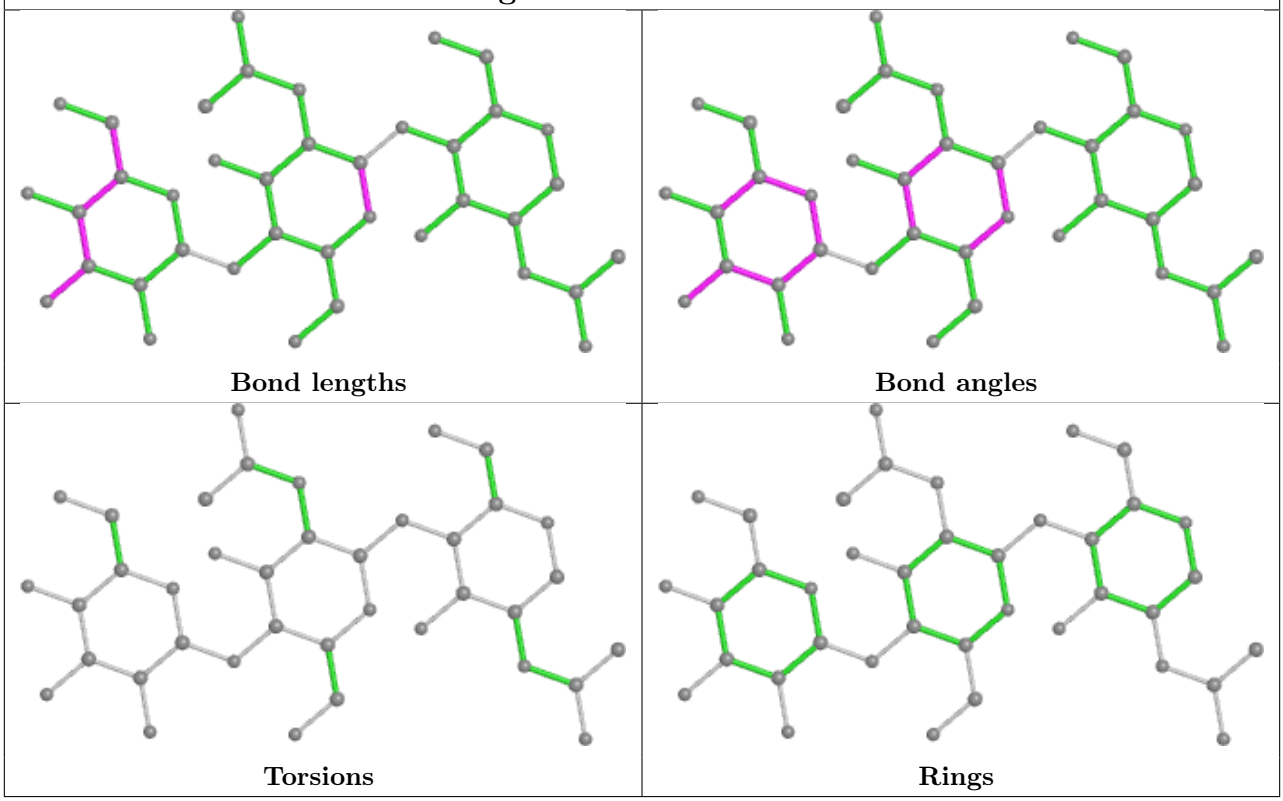


Torsions

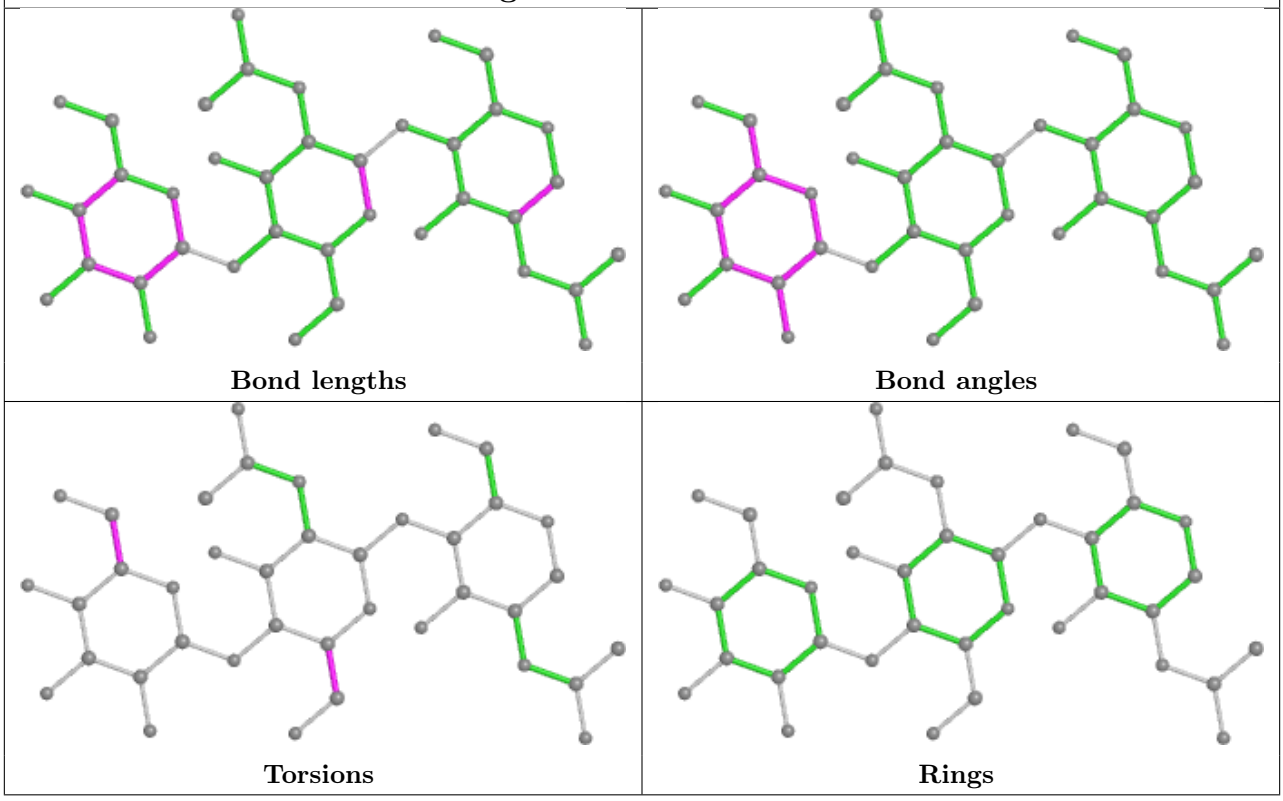


Rings

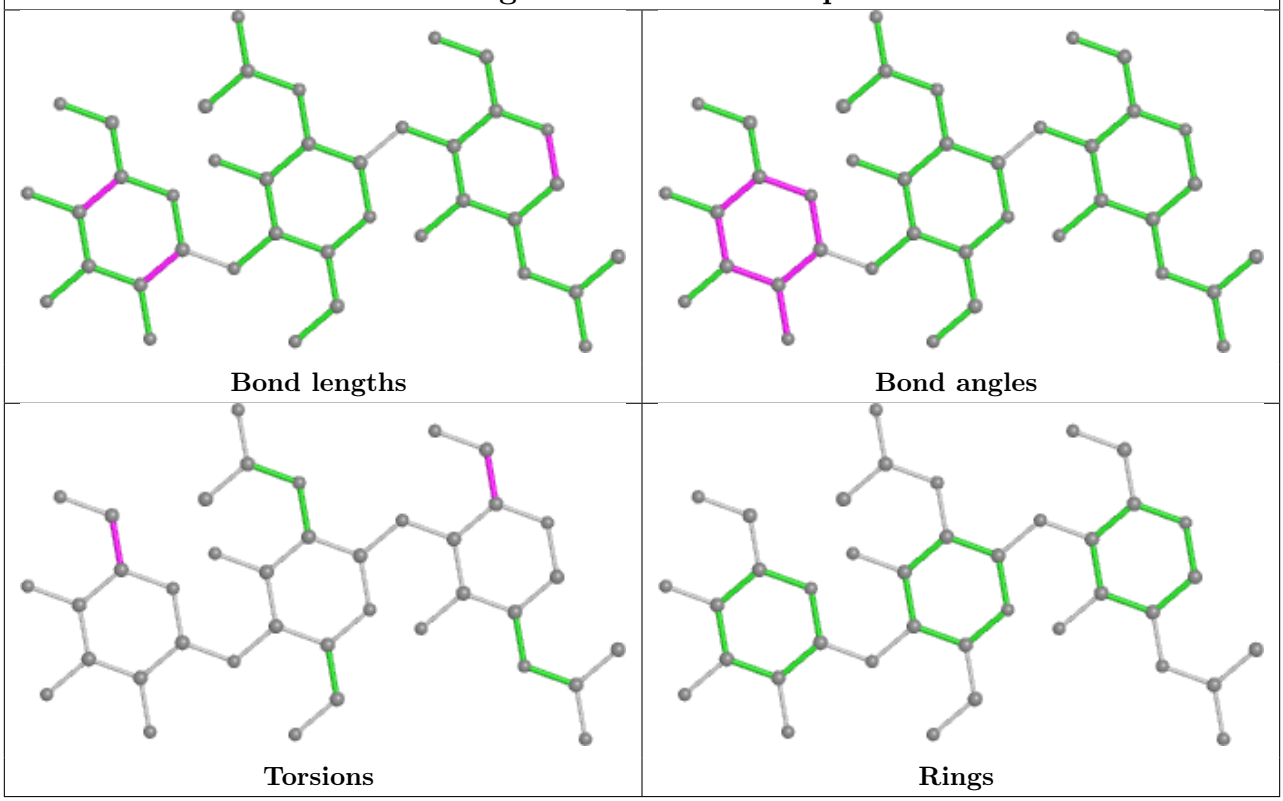
Oligosaccharide Chain n



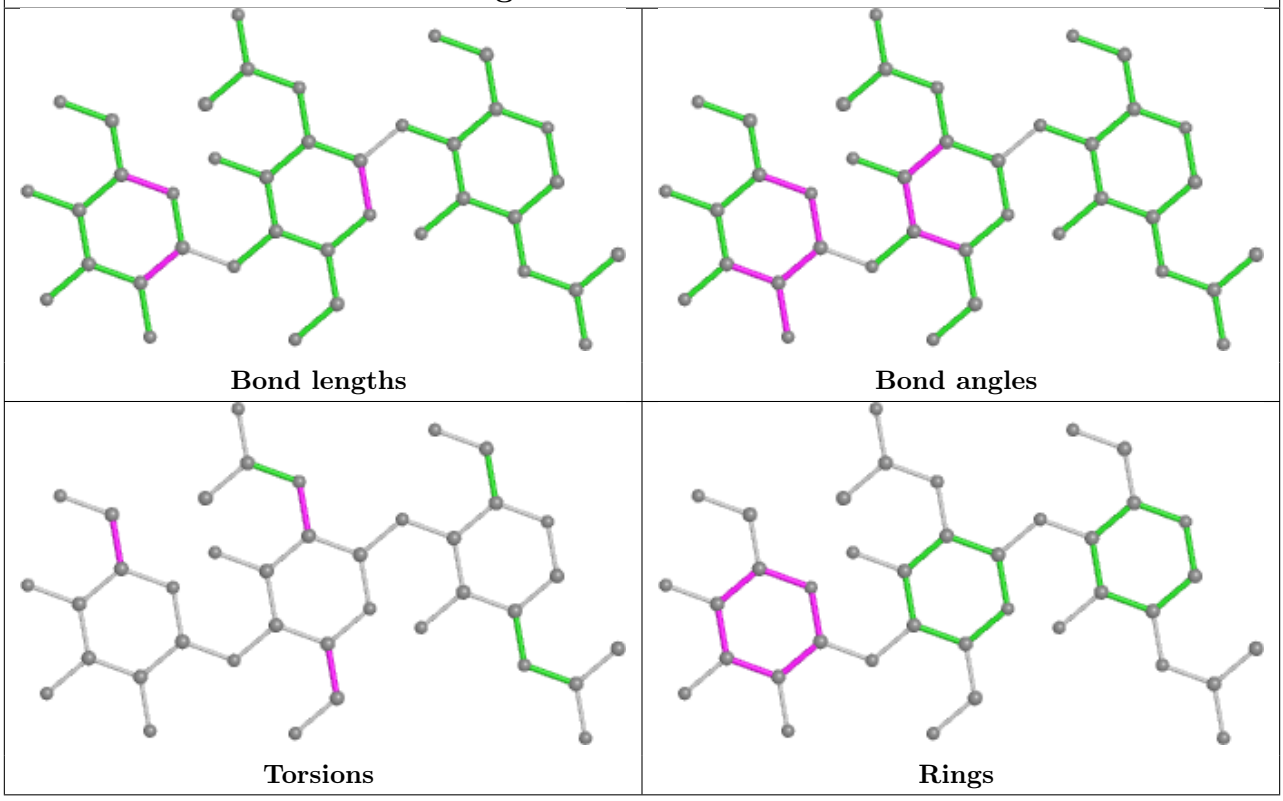
Oligosaccharide Chain o



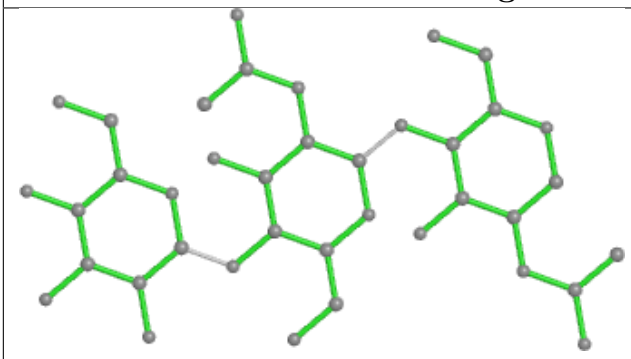
Oligosaccharide Chain q



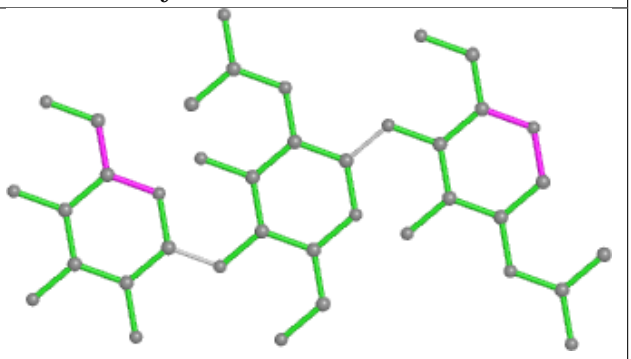
Oligosaccharide Chain w



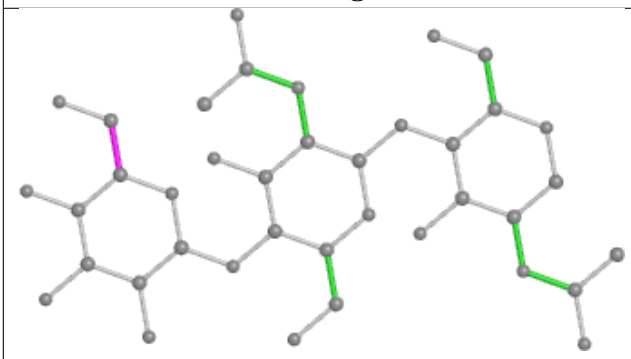
Oligosaccharide Chain y



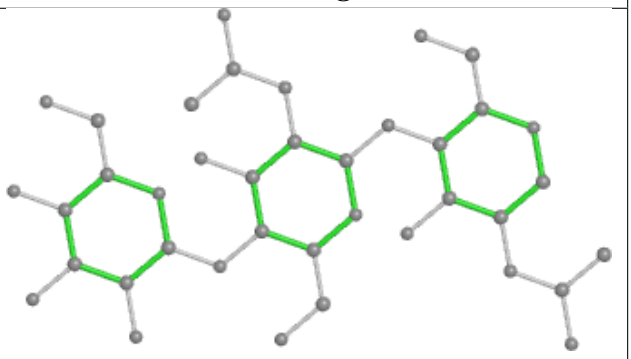
Bond lengths



Bond angles

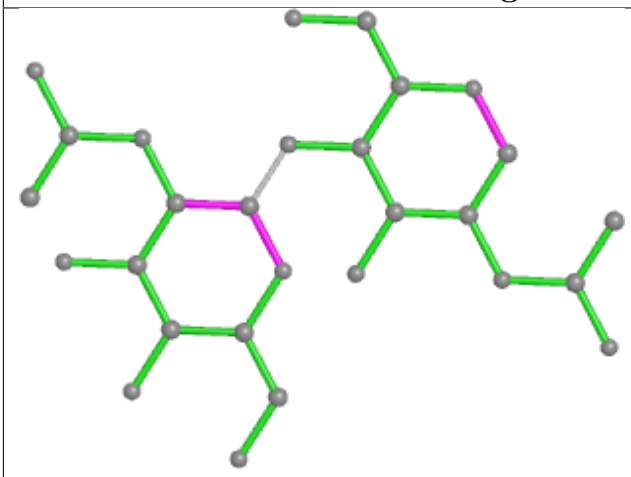


Torsions



Rings

Oligosaccharide Chain f



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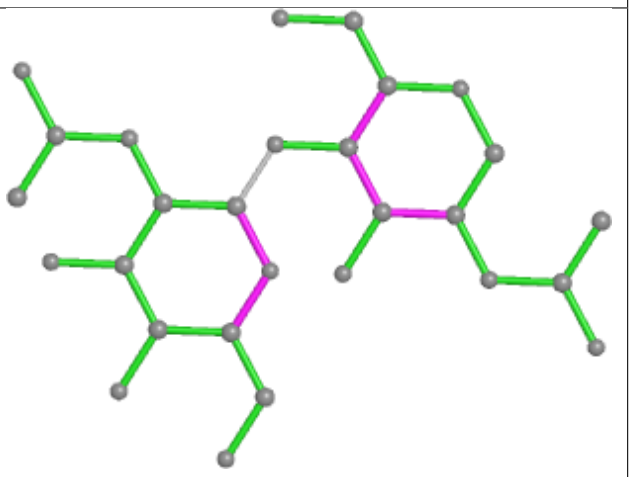

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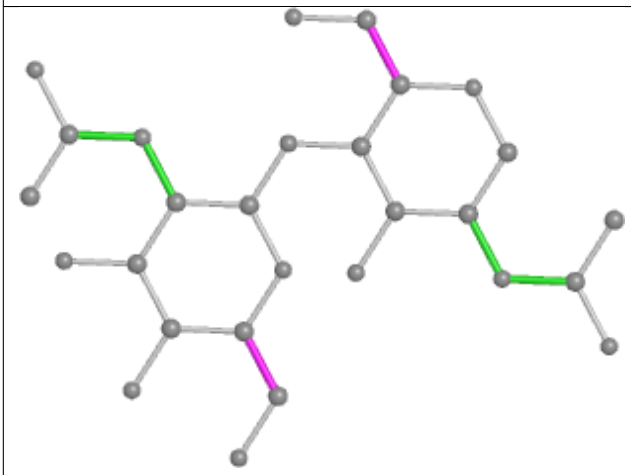

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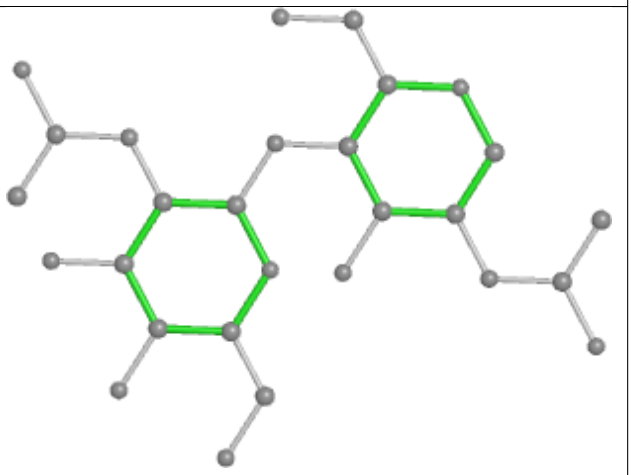
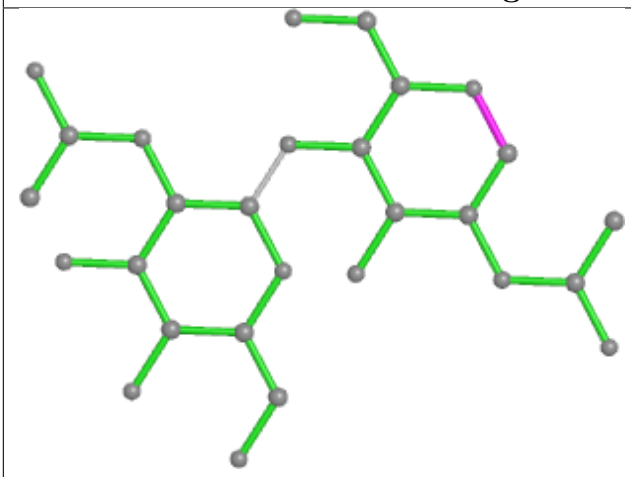


Rings

Oligosaccharide Chain i



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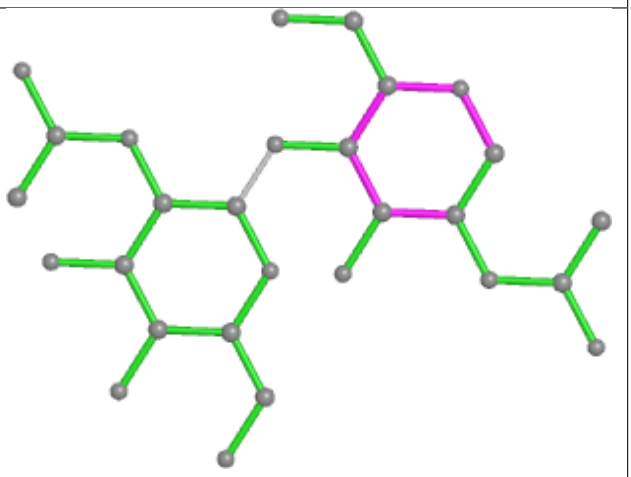
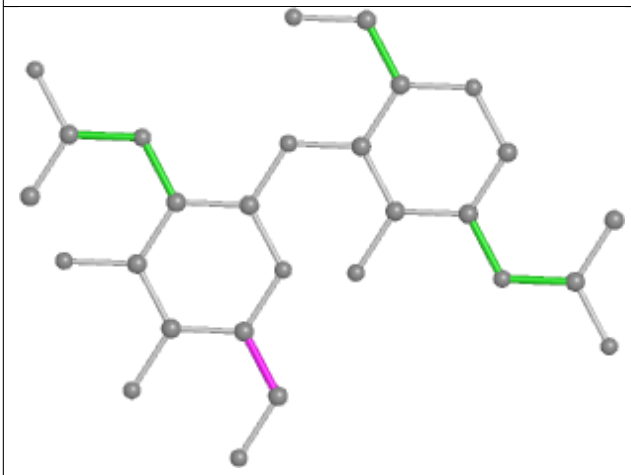


Bond angles



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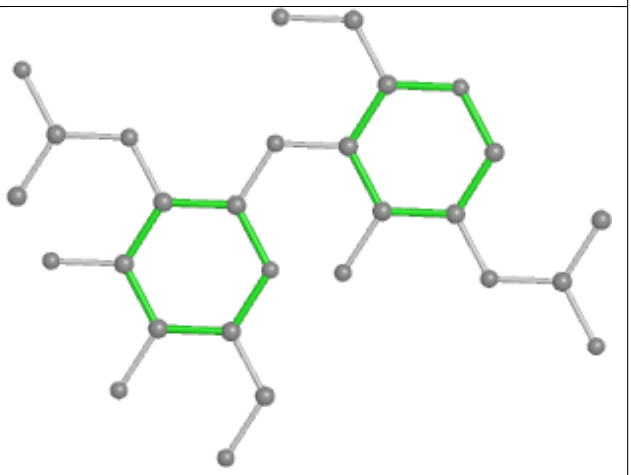
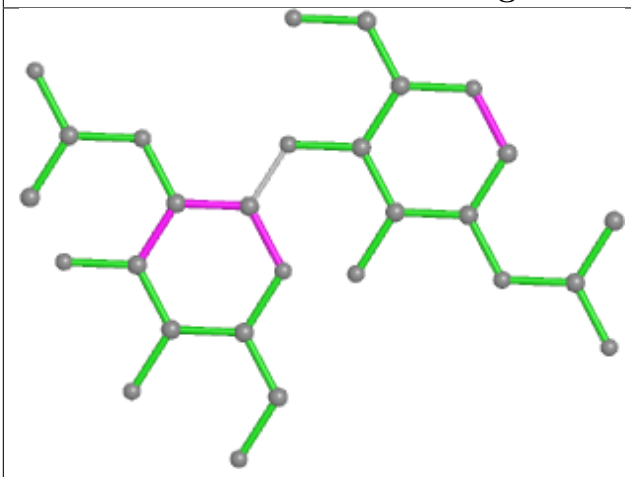


Rings

Oligosaccharide Chain k



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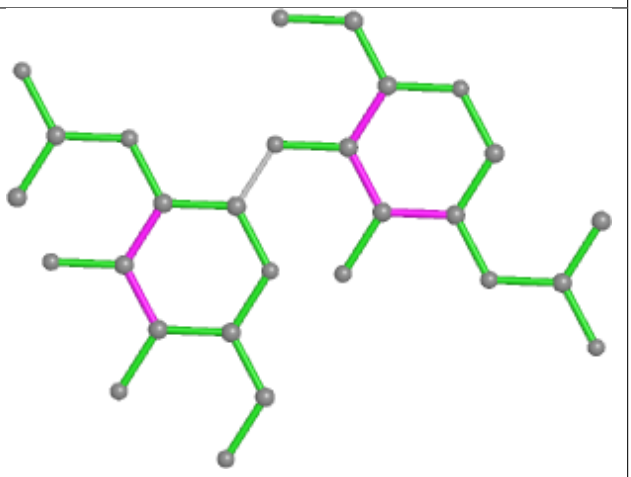

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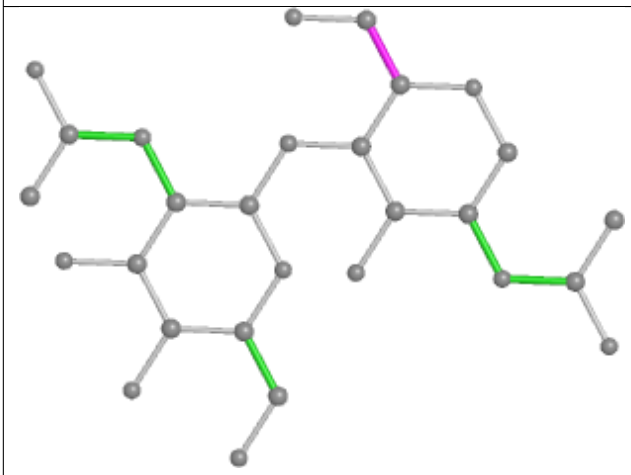

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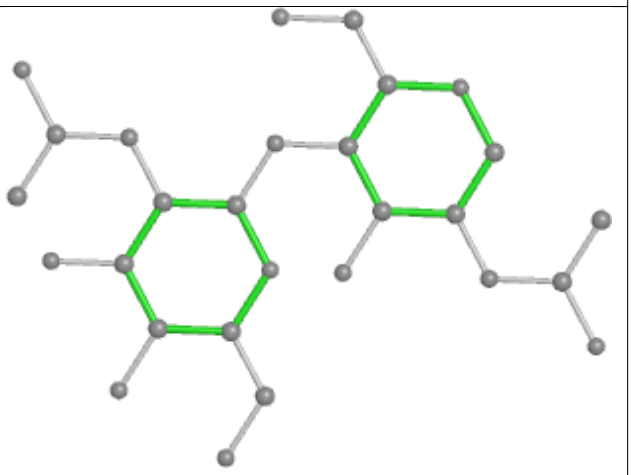
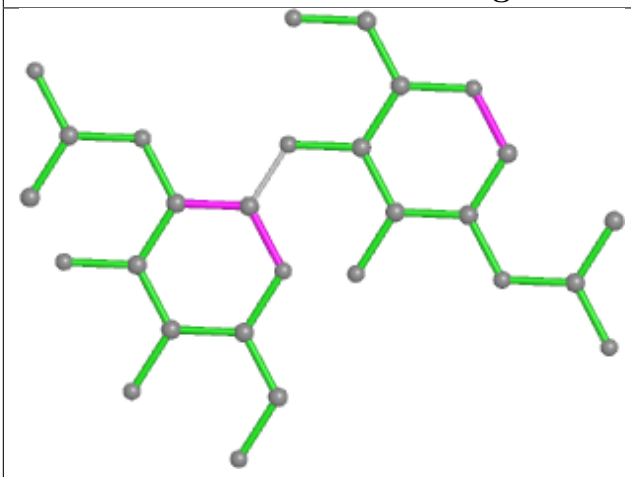


Rings

Oligosaccharide Chain m



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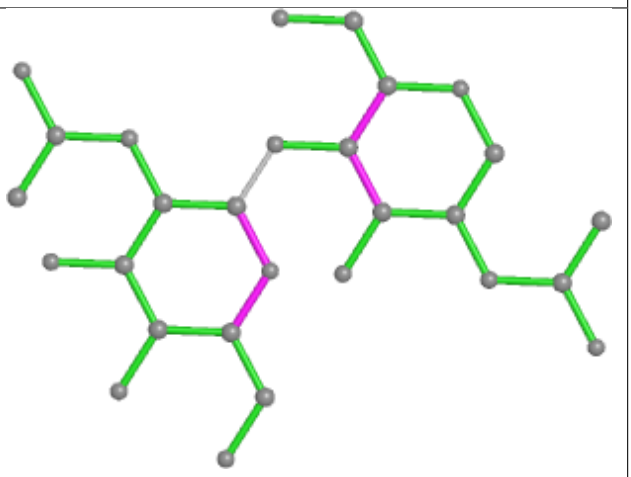
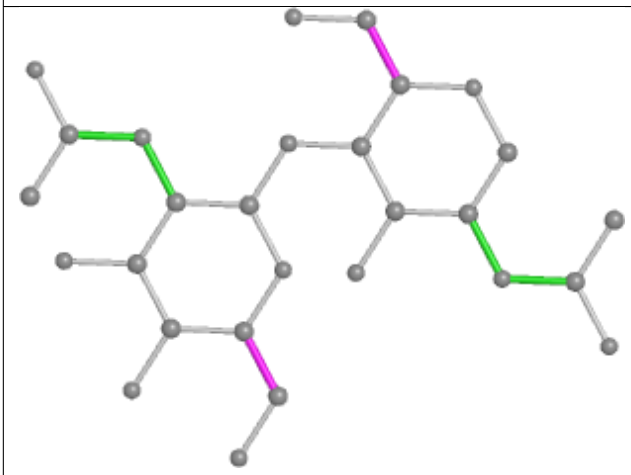


Bond angles



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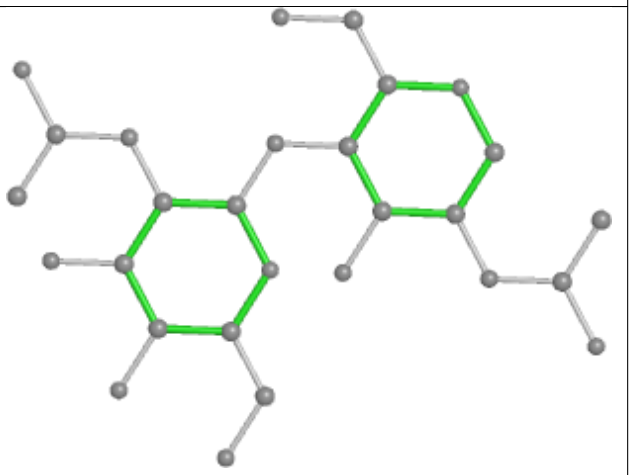
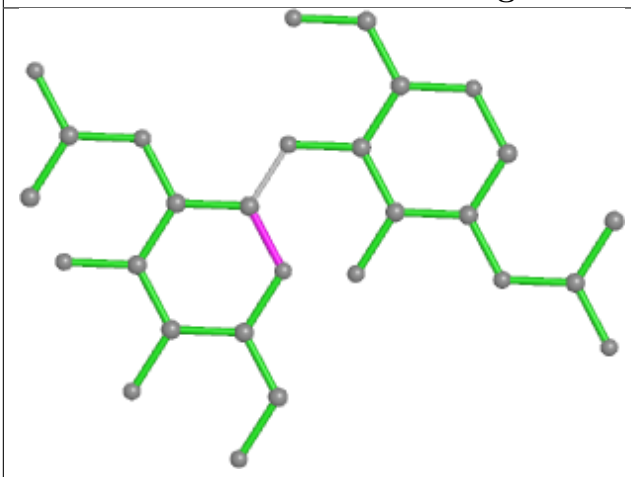


Rings

Oligosaccharide Chain p



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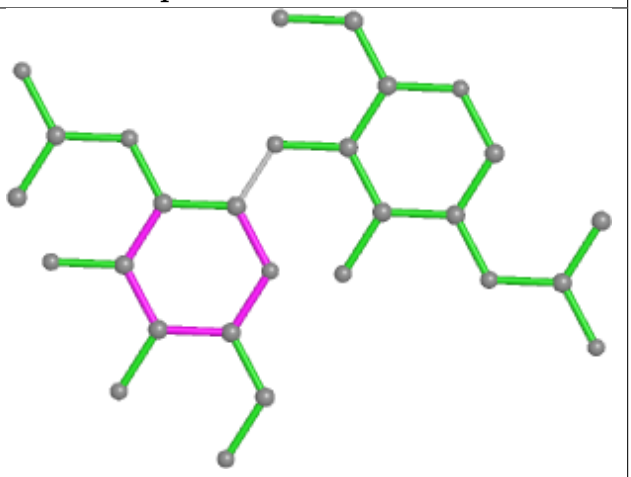
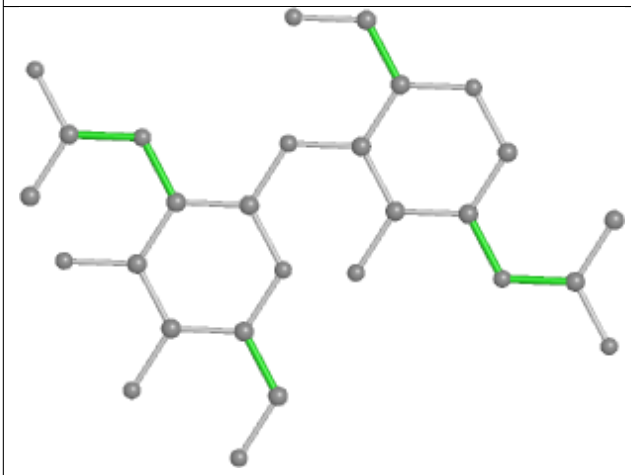


Bond angles



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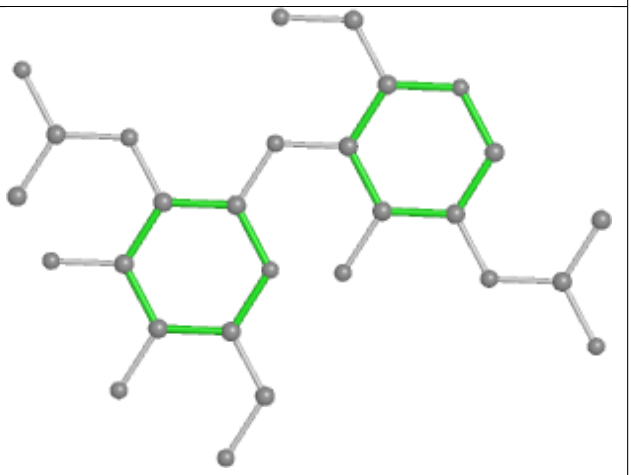
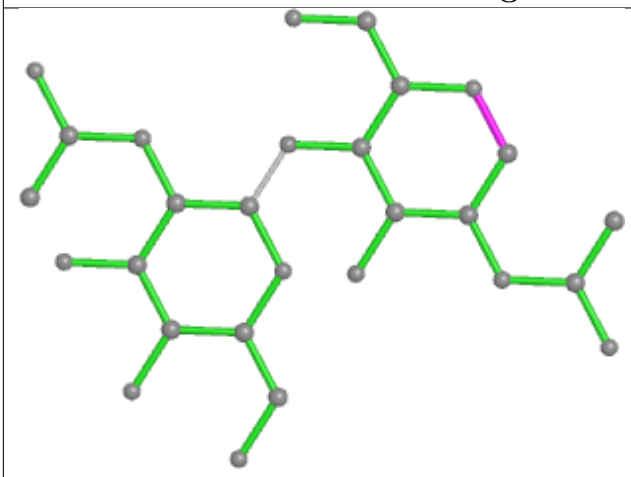


Rings

Oligosaccharide Chain r



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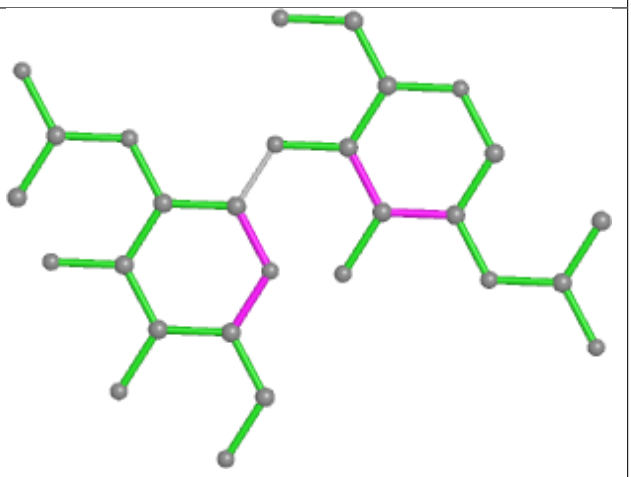

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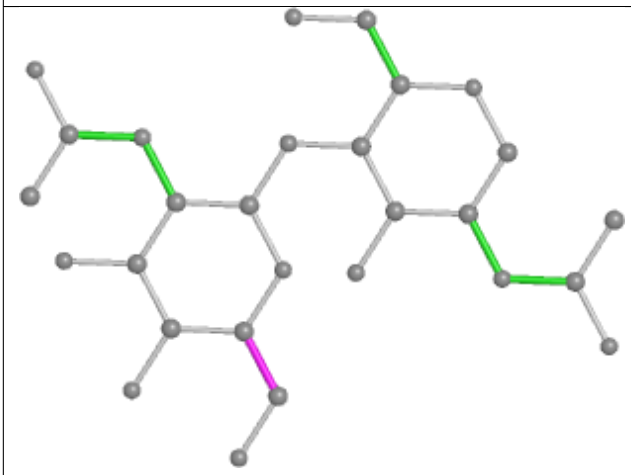

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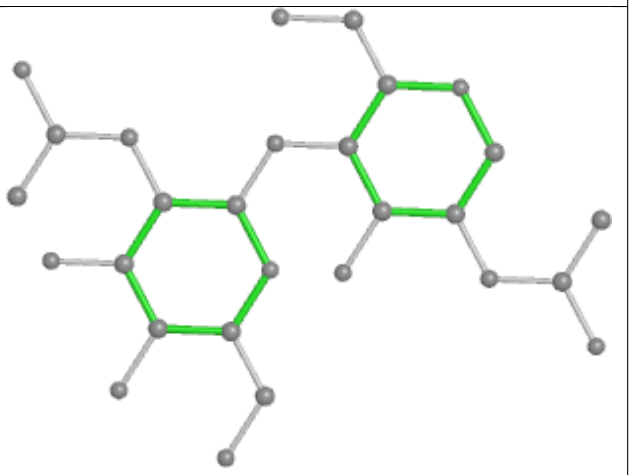
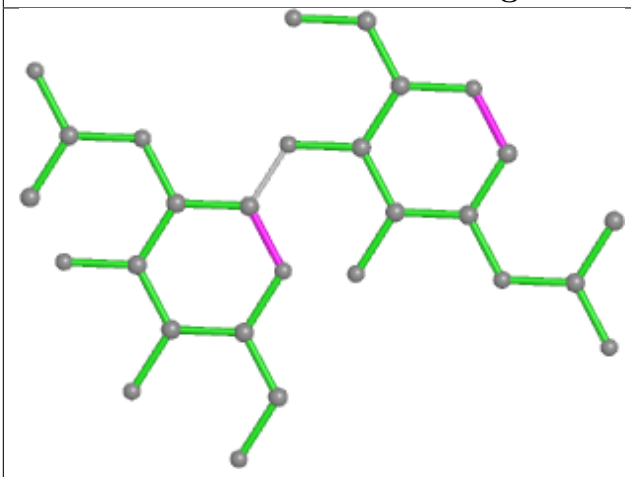


Rings

Oligosaccharide Chain t



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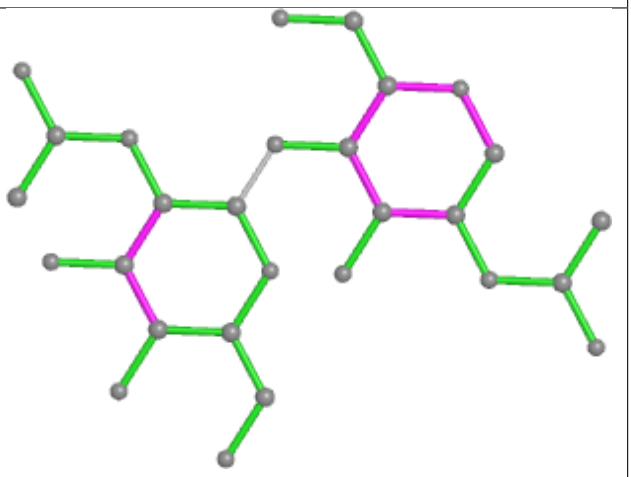

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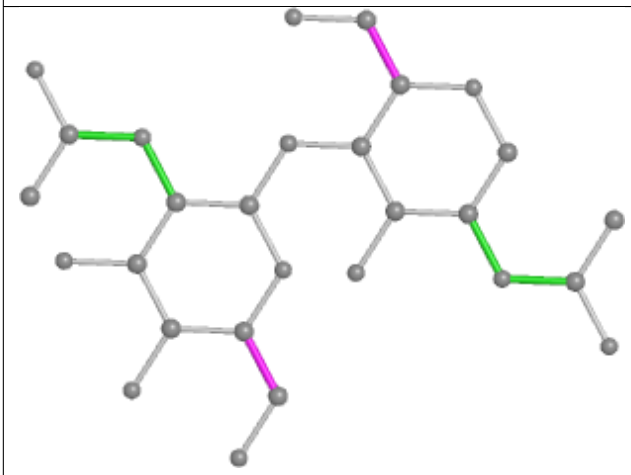

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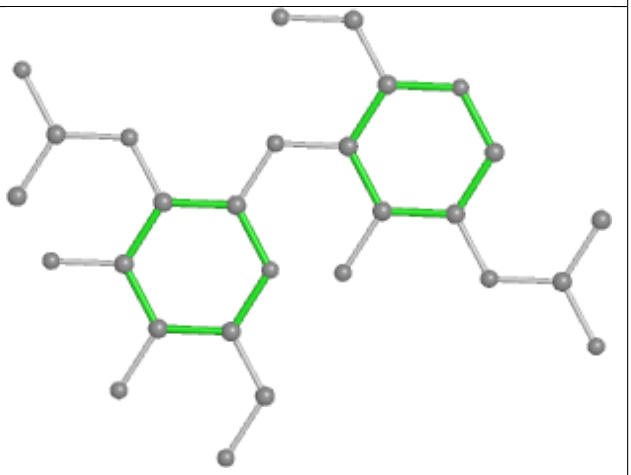
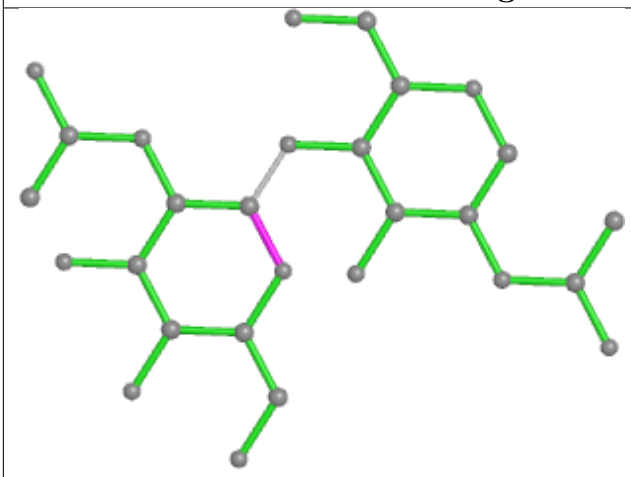


Rings

Oligosaccharide Chain u



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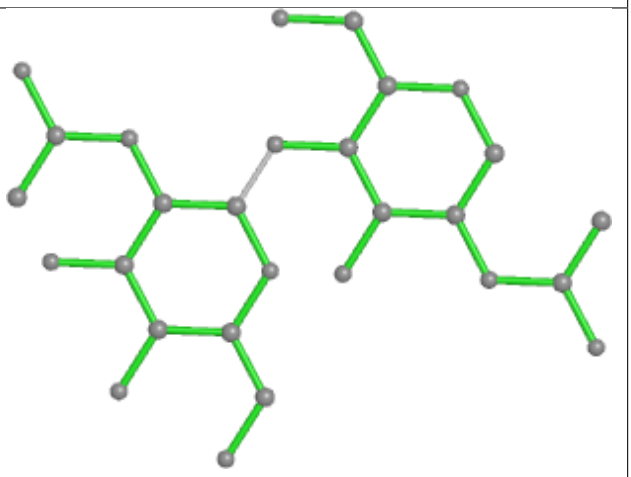
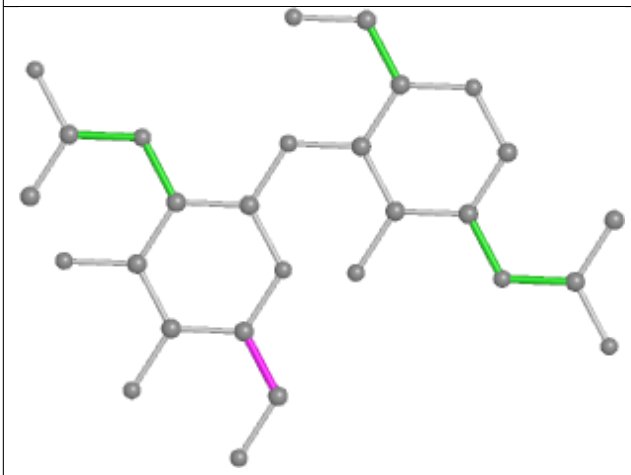


Bond angles



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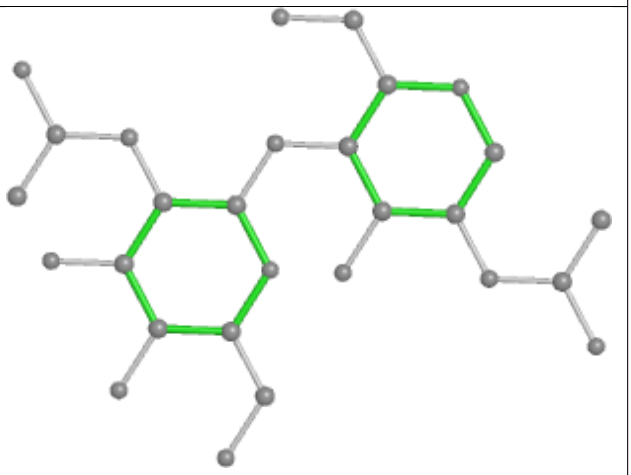

Rings

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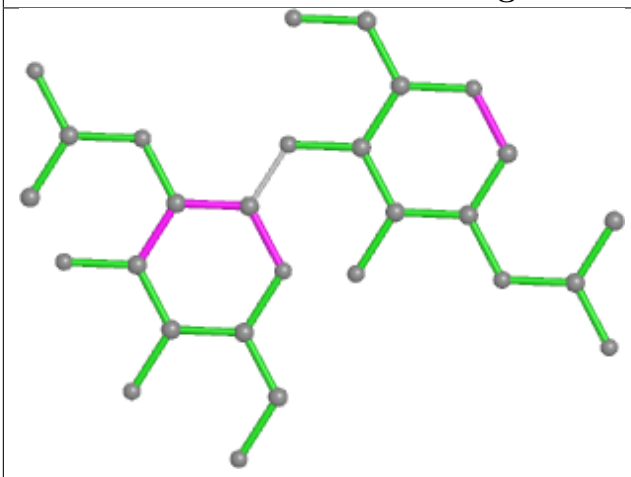

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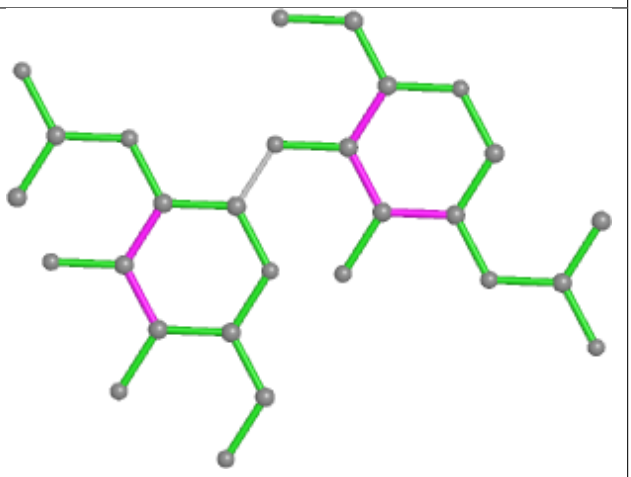

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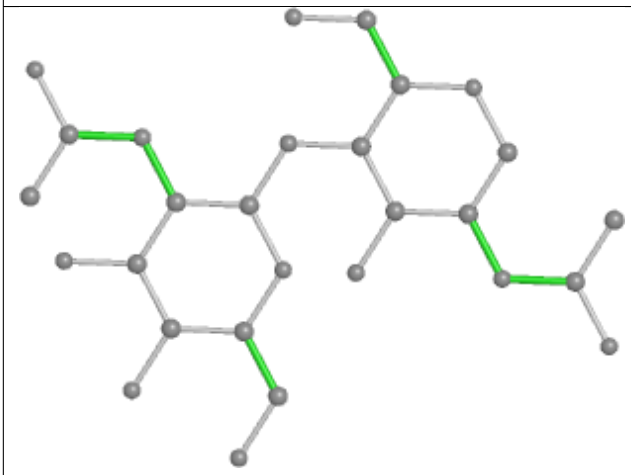

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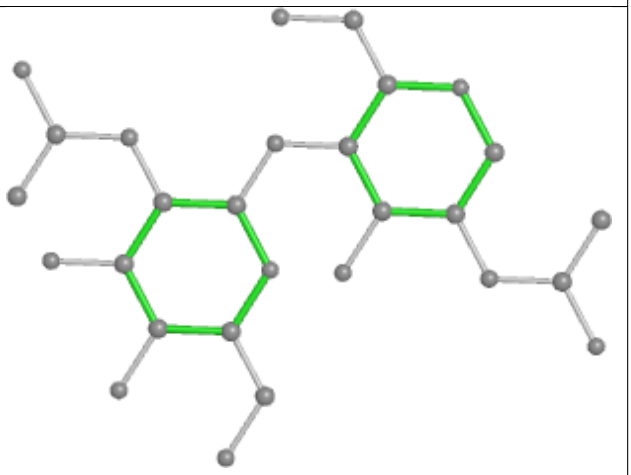

Rings

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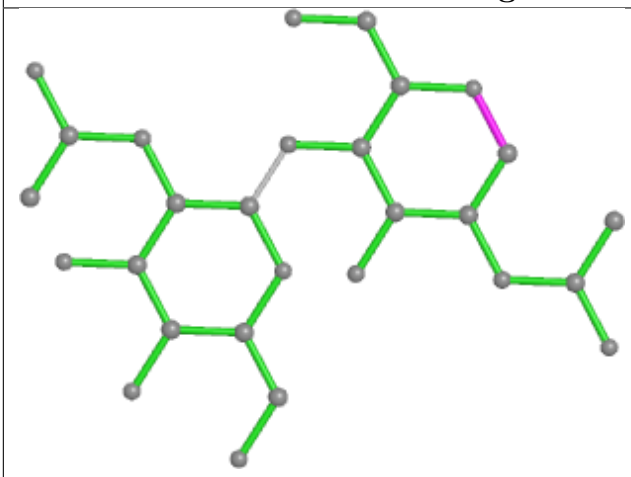

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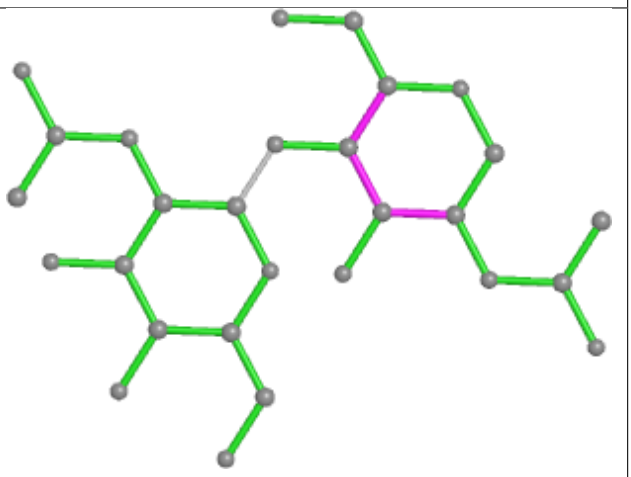

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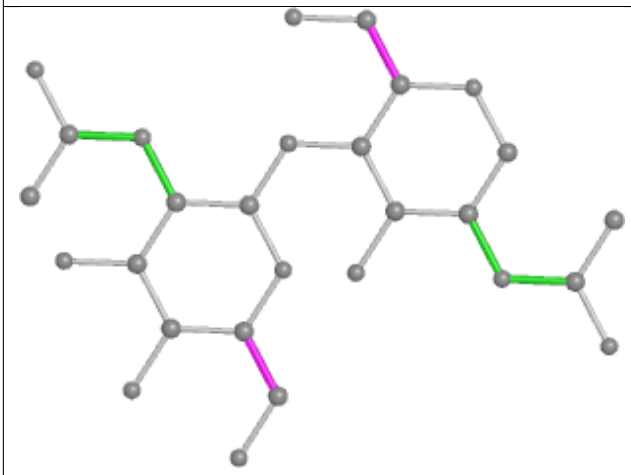

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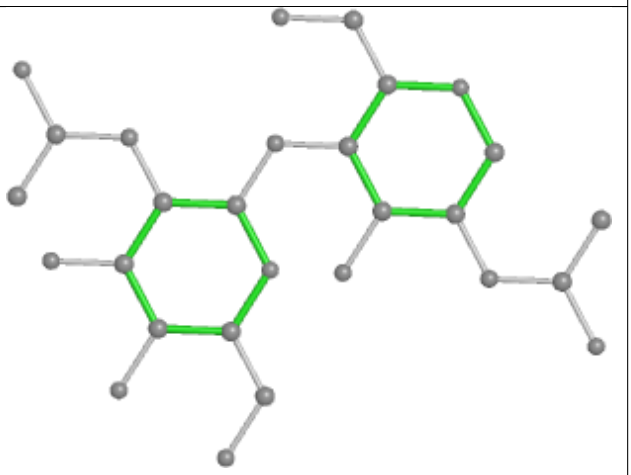
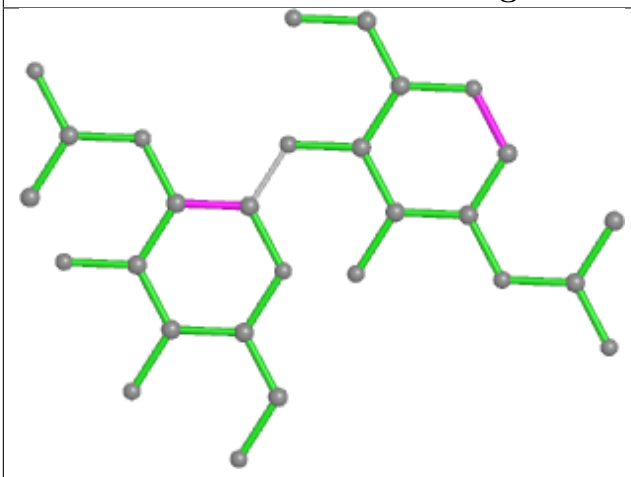


Rings

Oligosaccharide Chain z



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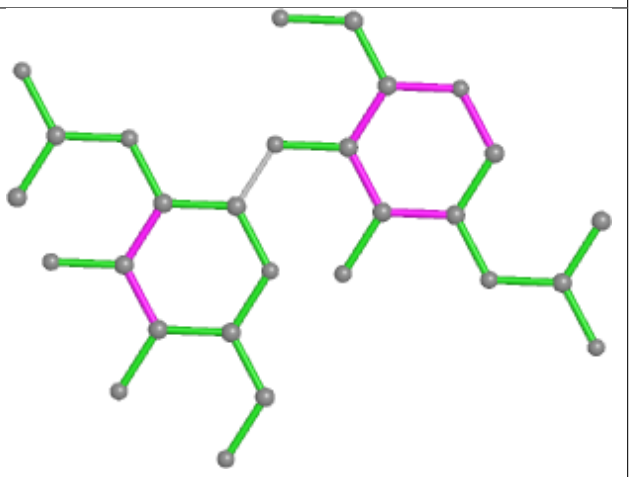
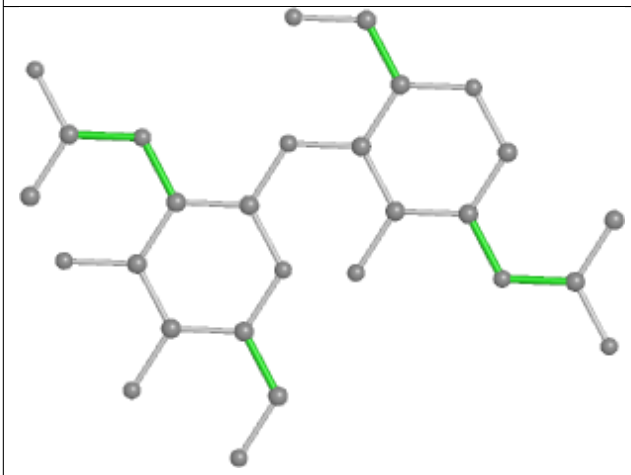


Bond angles



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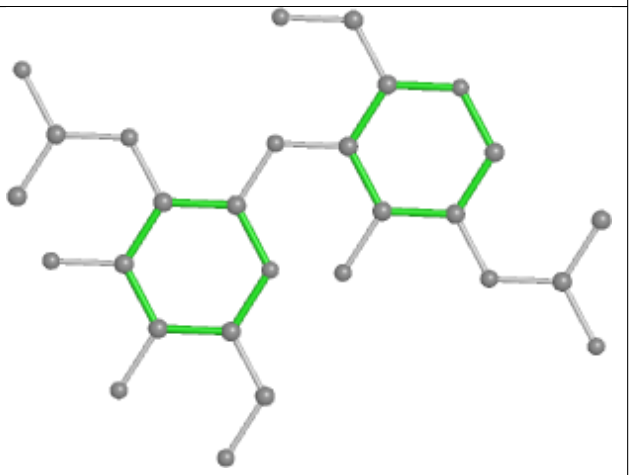
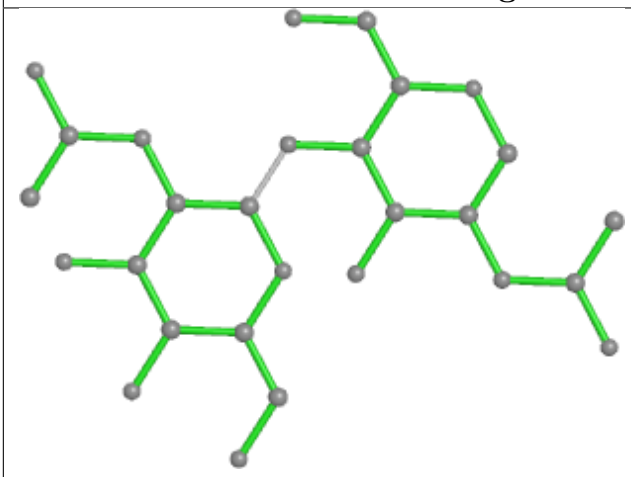


Rings

Oligosaccharide Chain 0



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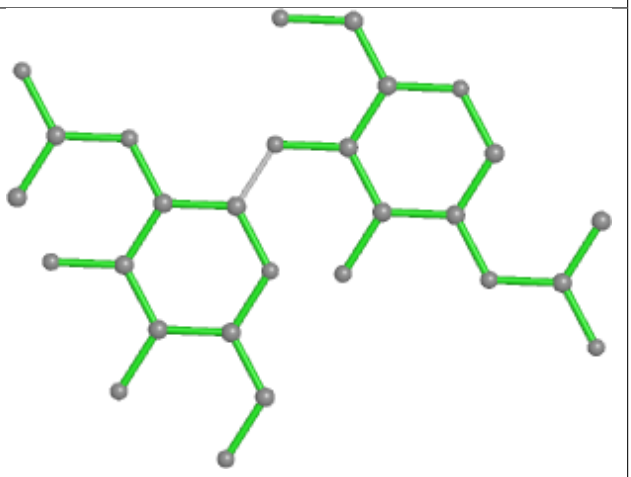
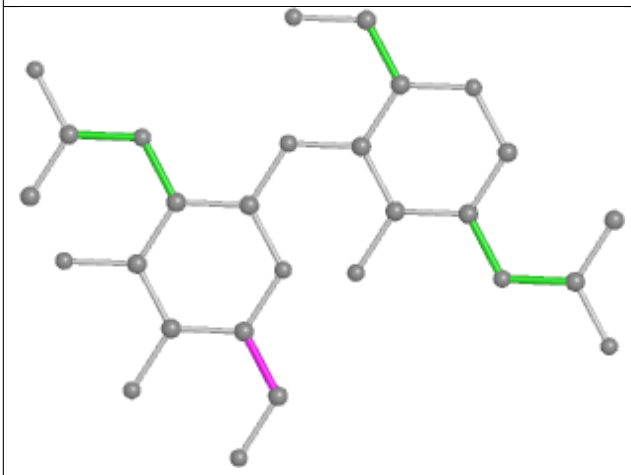


Bond angles



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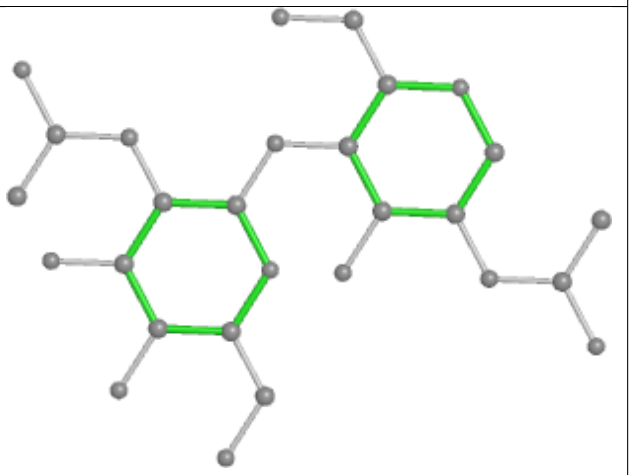
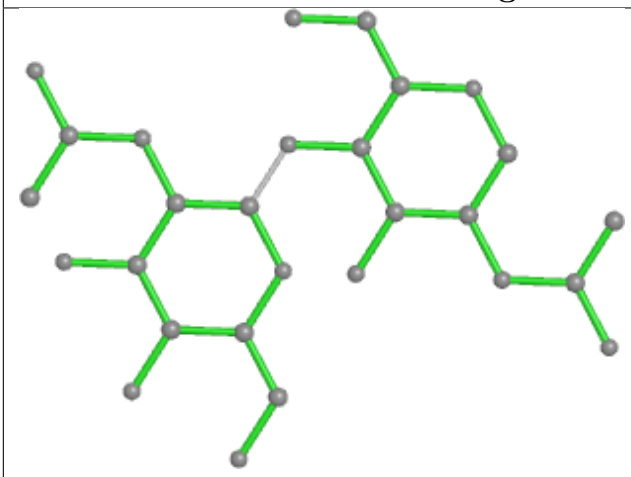


Rings

Oligosaccharide Chain 1



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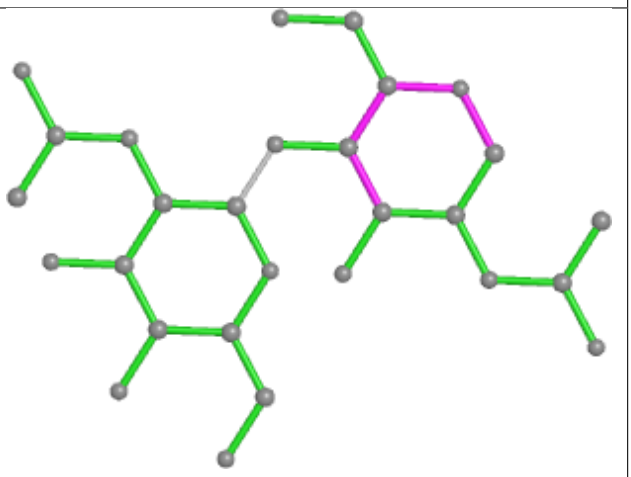

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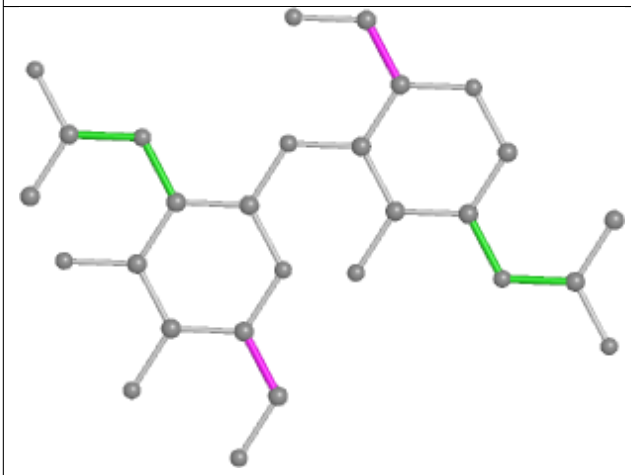
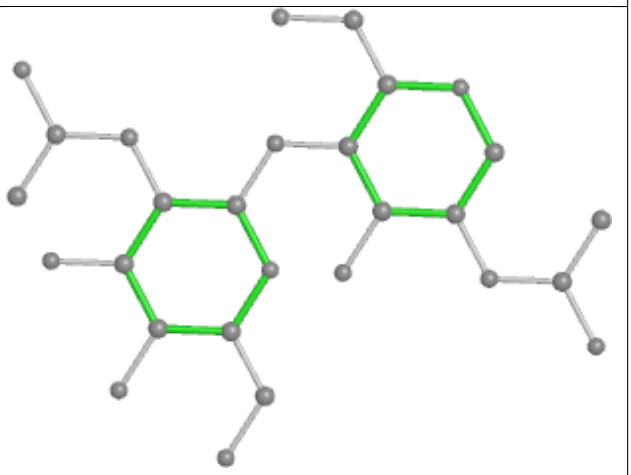
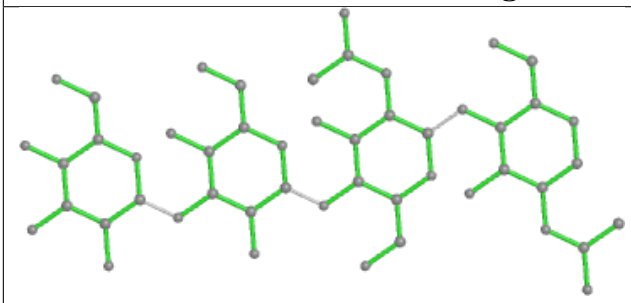


Torsions

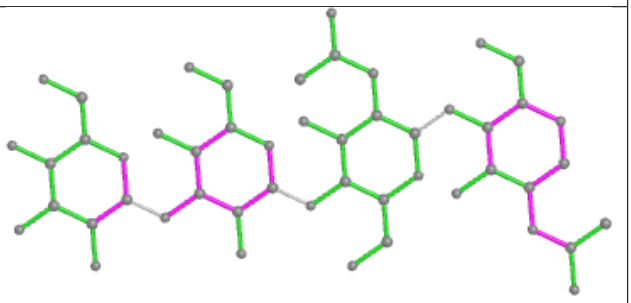


Rings

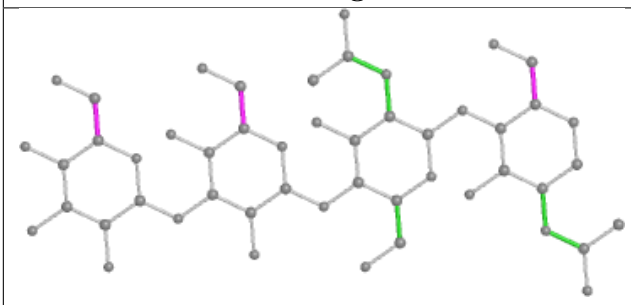
Oligosaccharide Chain s



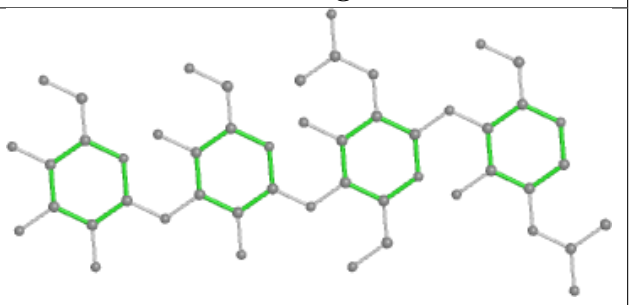
Bond lengths



Bond angles



Torsions



Rings

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	2002	1	14,14,15	1.17	2 (14%)	17,19,21	1.19	1 (5%)
6	NAG	O	2006	1	14,14,15	1.17	2 (14%)	17,19,21	1.04	2 (11%)
6	NAG	K	2004	1	14,14,15	0.69	0	17,19,21	0.53	0
6	NAG	Y	2003	1	14,14,15	0.56	0	17,19,21	0.45	0
6	NAG	c	2001	1	14,14,15	0.54	0	17,19,21	0.49	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	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
6	NAG	Y	2003	1	-	2/6/23/26	0/1/1/1
6	NAG	c	2001	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	c	2002	NAG	O5-C1	-3.53	1.38	1.43
6	O	2006	NAG	O5-C1	-3.12	1.38	1.43
6	O	2006	NAG	C1-C2	2.63	1.56	1.52
6	c	2002	NAG	C1-C2	2.06	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	c	2002	NAG	C4-C3-C2	3.36	115.95	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	2006	NAG	C4-C3-C2	2.75	115.04	111.02
6	O	2006	NAG	C3-C4-C5	2.19	114.15	110.24

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	c	2002	NAG	C4-C5-C6-O6
6	Y	2003	NAG	C4-C5-C6-O6
6	K	2004	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/334 (97%)	-0.25	5 (1%)	73	61	22, 45, 101, 176	0
1	C	324/334 (97%)	-0.09	11 (3%)	45	28	30, 56, 143, 199	0
1	E	324/334 (97%)	-0.08	15 (4%)	32	18	30, 56, 144, 203	0
1	G	324/334 (97%)	-0.26	6 (1%)	66	53	19, 46, 102, 183	0
1	I	324/334 (97%)	-0.33	4 (1%)	79	68	24, 44, 100, 186	0
1	K	324/334 (97%)	-0.02	14 (4%)	35	21	33, 57, 143, 218	0
1	M	324/334 (97%)	-0.16	10 (3%)	49	32	26, 50, 152, 220	0
1	O	324/334 (97%)	-0.10	12 (3%)	41	25	25, 50, 140, 226	0
1	Q	324/334 (97%)	-0.07	22 (6%)	17	9	25, 49, 151, 212	0
1	S	324/334 (97%)	-0.05	11 (3%)	45	28	35, 64, 158, 195	0
1	U	324/334 (97%)	-0.03	19 (5%)	22	12	31, 64, 158, 214	0
1	W	324/334 (97%)	-0.08	13 (4%)	38	23	35, 64, 148, 211	0
1	Y	324/334 (97%)	0.28	24 (7%)	14	8	55, 91, 189, 248	0
1	a	324/334 (97%)	0.27	19 (5%)	22	12	55, 87, 184, 263	0
1	c	324/334 (97%)	0.33	21 (6%)	18	10	59, 90, 185, 253	0
2	B	177/181 (97%)	0.36	8 (4%)	33	19	26, 113, 153, 173	0
2	D	177/181 (97%)	0.81	28 (15%)	2	1	41, 155, 195, 210	0
2	F	177/181 (97%)	1.11	43 (24%)	0	0	42, 154, 196, 206	0
2	H	177/181 (97%)	0.31	8 (4%)	33	19	23, 113, 154, 174	0
2	J	177/181 (97%)	0.17	3 (1%)	70	57	27, 113, 153, 166	0
2	L	177/181 (97%)	1.07	35 (19%)	1	0	42, 148, 195, 206	0
2	N	177/181 (97%)	1.22	45 (25%)	0	0	38, 158, 213, 231	0
2	P	177/181 (97%)	1.38	52 (29%)	0	0	38, 163, 213, 231	0
2	R	177/181 (97%)	1.26	45 (25%)	0	0	34, 163, 210, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	T	177/181 (97%)	1.09	46 (25%)	0	0	45, 153, 201, 209	0
2	V	177/181 (97%)	1.22	40 (22%)	0	0	49, 153, 213, 228	0
2	X	177/181 (97%)	1.06	36 (20%)	1	0	50, 155, 204, 220	0
2	Z	177/181 (97%)	2.03	73 (41%)	0	0	74, 191, 237, 256	0
2	b	177/181 (97%)	1.84	58 (32%)	0	0	73, 187, 239, 254	0
2	d	177/181 (97%)	2.07	68 (38%)	0	0	78, 194, 247, 269	0
All	All	7515/7725 (97%)	0.37	794 (10%)	6	3	19, 79, 201, 269	0

The worst 5 of 794 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	16	GLY	17.9
1	O	13	ILE	15.1
2	d	23	GLY	15.1
2	b	141	TYR	14.4
1	U	12	GLN	14.1

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
3	BMA	y	3	11/12	0.47	0.44	113,124,130,135	0
3	BMA	o	3	11/12	0.64	0.21	102,115,128,131	0
4	NAG	f	2	14/15	0.68	0.26	119,129,135,136	0
4	NAG	i	2	14/15	0.69	0.36	129,148,157,159	0
4	NAG	u	2	14/15	0.70	0.25	96,108,125,129	0
5	MAN	s	4	11/12	0.70	0.29	111,129,131,135	0
3	NAG	h	2	14/15	0.71	0.26	79,102,115,117	0
3	BMA	h	3	11/12	0.73	0.20	43,57,80,88	0
3	BMA	j	3	11/12	0.75	0.29	80,97,103,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	p	2	14/15	0.75	0.26	137,162,176,177	0
3	BMA	w	3	11/12	0.76	0.23	114,122,125,127	0
4	NAG	v	1	14/15	0.77	0.18	133,146,152,153	0
4	NAG	x	2	14/15	0.78	0.20	156,166,172,172	0
3	BMA	n	3	11/12	0.78	0.21	32,49,59,61	0
4	NAG	0	2	14/15	0.79	0.24	115,131,144,145	0
5	BMA	s	3	11/12	0.79	0.18	116,120,126,127	0
3	BMA	q	3	11/12	0.79	0.14	102,115,125,130	0
4	NAG	v	2	14/15	0.80	0.17	116,143,150,154	0
4	NAG	t	2	14/15	0.81	0.23	124,153,157,160	0
4	NAG	z	1	14/15	0.81	0.23	145,151,158,159	0
4	NAG	m	1	14/15	0.81	0.20	94,108,117,122	0
3	BMA	l	3	11/12	0.81	0.39	83,95,103,110	0
4	NAG	r	2	14/15	0.81	0.20	138,149,152,152	0
4	NAG	x	1	14/15	0.82	0.15	141,148,158,159	0
5	NAG	s	1	14/15	0.82	0.23	68,80,90,103	0
4	NAG	f	1	14/15	0.82	0.20	104,114,123,124	0
3	NAG	w	2	14/15	0.82	0.22	95,102,117,127	0
3	BMA	e	3	11/12	0.83	0.22	65,90,98,98	0
4	NAG	k	1	14/15	0.83	0.20	87,103,110,112	0
4	NAG	m	2	14/15	0.84	0.14	109,125,128,129	0
3	NAG	g	1	14/15	0.84	0.32	56,75,85,89	0
4	NAG	r	1	14/15	0.84	0.19	142,148,151,153	0
3	NAG	o	2	14/15	0.84	0.22	64,91,98,106	0
3	BMA	g	3	11/12	0.84	0.17	35,55,68,70	0
4	NAG	p	1	14/15	0.85	0.12	128,145,151,160	0
3	NAG	y	2	14/15	0.86	0.29	77,96,107,119	0
4	NAG	z	2	14/15	0.86	0.21	139,152,158,160	0
3	NAG	n	1	14/15	0.87	0.28	59,73,92,93	0
3	NAG	y	1	14/15	0.87	0.17	64,71,80,92	0
4	NAG	1	1	14/15	0.88	0.28	86,95,107,111	0
3	NAG	q	2	14/15	0.88	0.25	61,90,101,113	0
3	NAG	h	1	14/15	0.89	0.22	54,72,97,102	0
4	NAG	k	2	14/15	0.89	0.13	106,115,120,122	0
4	NAG	1	2	14/15	0.89	0.31	96,118,126,129	0
3	NAG	j	2	14/15	0.90	0.23	53,70,85,96	0
4	NAG	t	1	14/15	0.90	0.14	122,138,141,145	0
4	NAG	i	1	14/15	0.90	0.20	126,134,144,151	0
4	NAG	0	1	14/15	0.90	0.19	95,100,108,119	0
4	NAG	u	1	14/15	0.90	0.17	50,69,87,102	0
3	NAG	g	2	14/15	0.91	0.24	69,81,86,90	0
5	NAG	s	2	14/15	0.91	0.21	94,99,105,115	0

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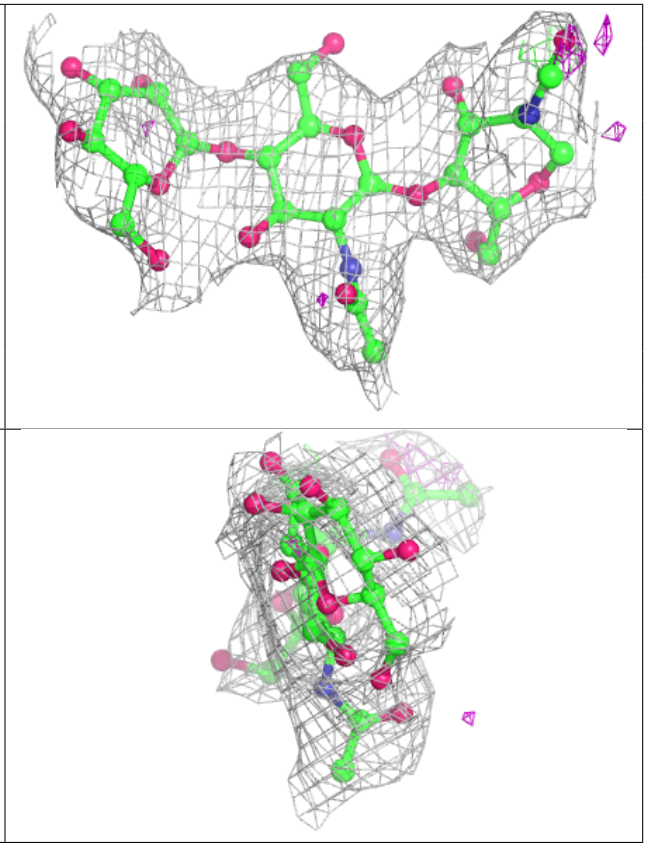
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	w	1	14/15	0.91	0.20	54,66,81,92	0
3	NAG	n	2	14/15	0.91	0.21	61,76,88,94	0
3	NAG	l	2	14/15	0.92	0.27	65,75,86,89	0
3	NAG	l	1	14/15	0.93	0.22	50,59,64,64	0
3	NAG	e	1	14/15	0.93	0.22	61,66,70,73	0
3	NAG	o	1	14/15	0.94	0.16	42,57,74,81	0
3	NAG	j	1	14/15	0.95	0.18	54,63,66,66	0
3	NAG	q	1	14/15	0.95	0.28	39,57,67,74	0
3	NAG	e	2	14/15	0.96	0.19	52,75,87,93	0

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

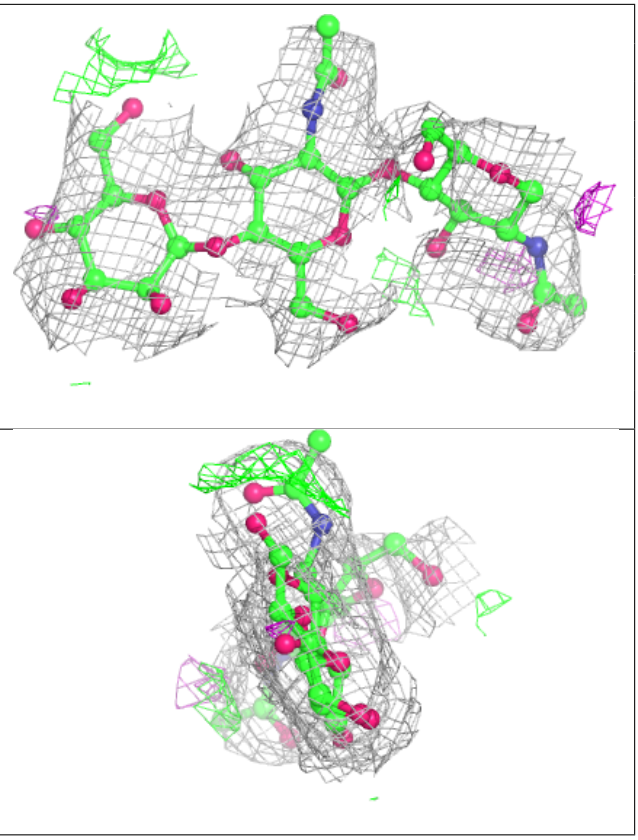
Electron density around Chain e:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



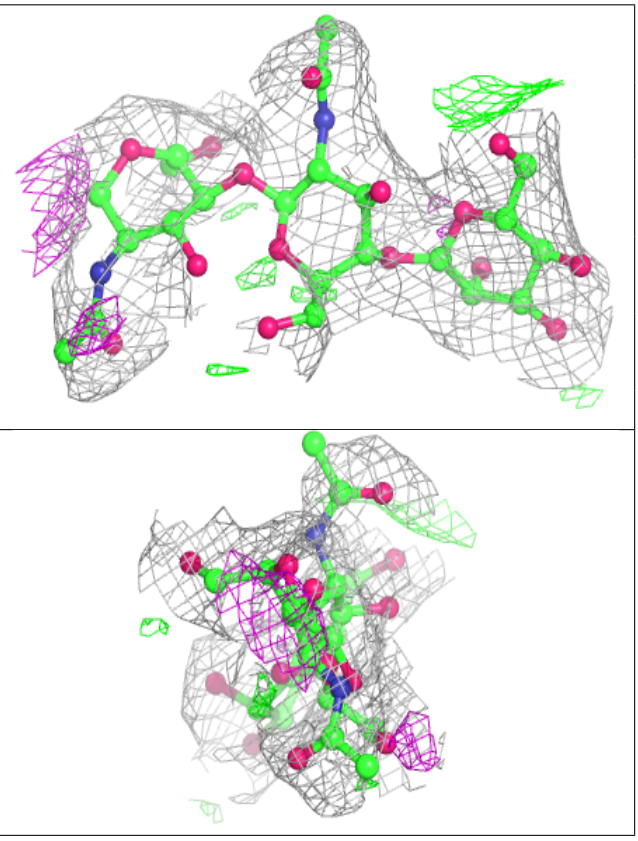
Electron density around Chain g:

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



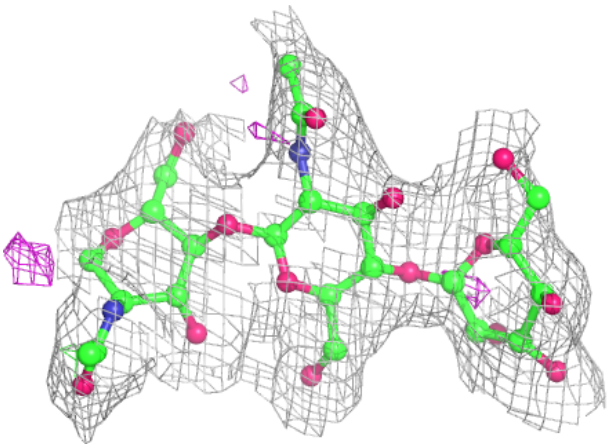
Electron density around Chain h:

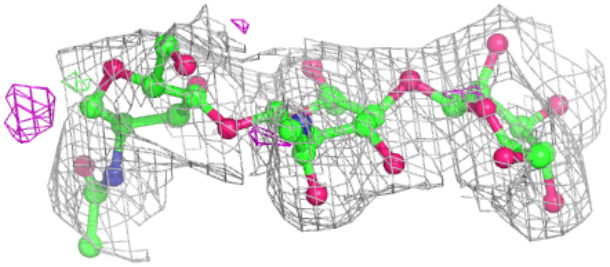
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

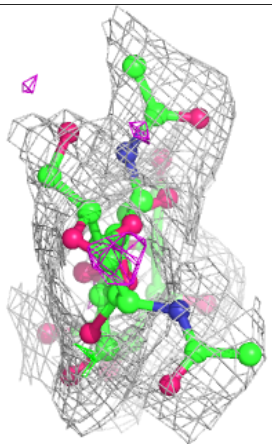


Electron density around Chain j:

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

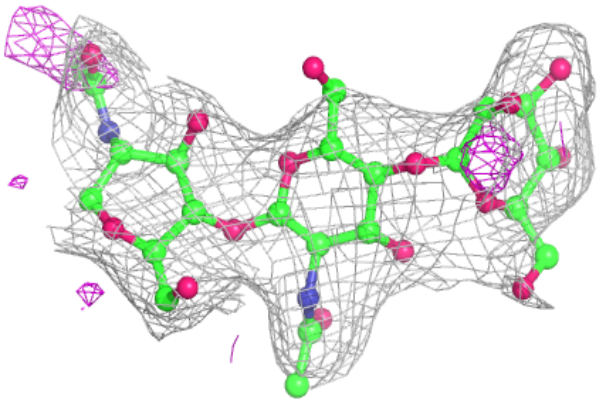


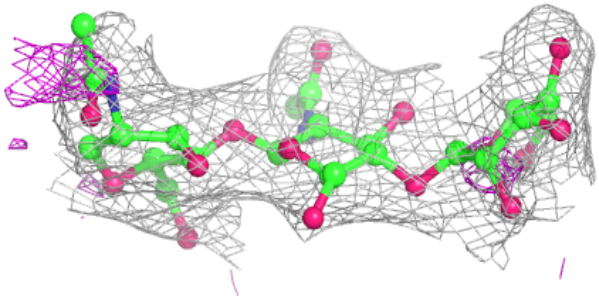


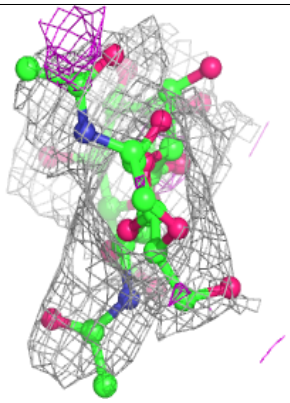


Electron density around Chain l:

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

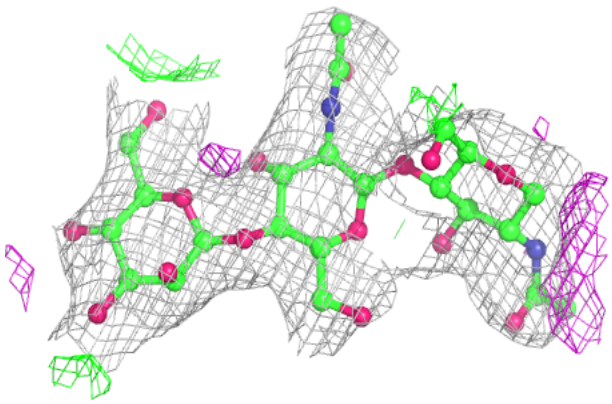


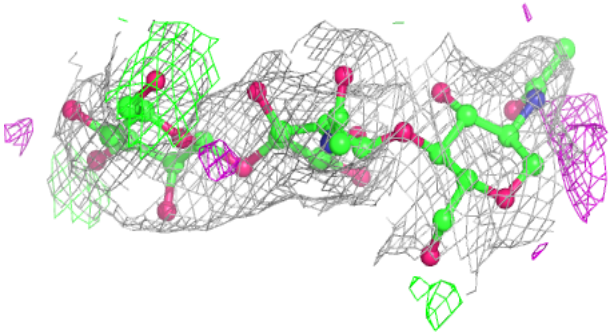


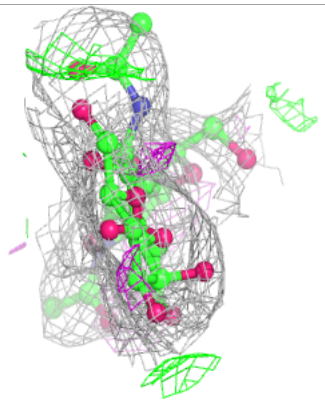


Electron density around Chain n:

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

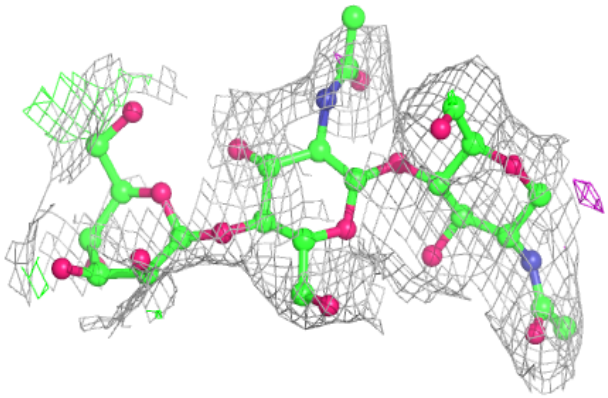


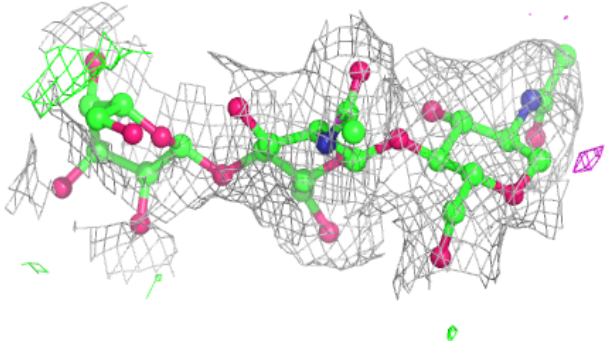


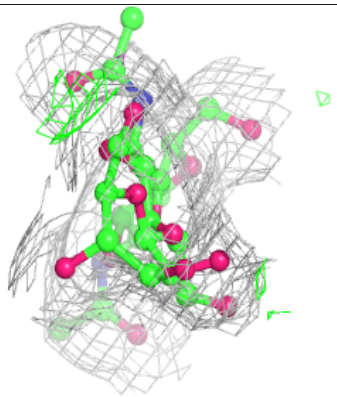


Electron density around Chain o:

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

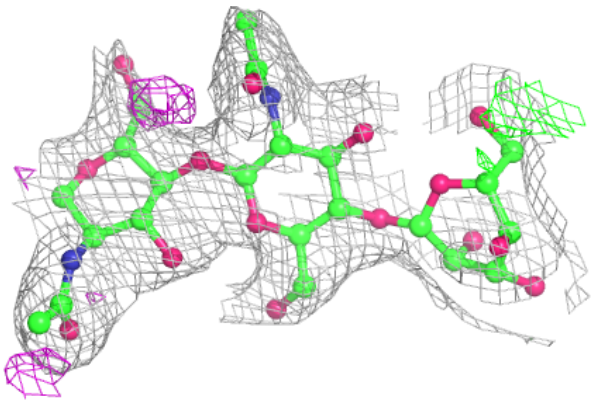


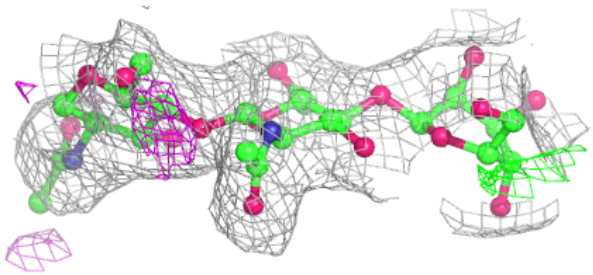


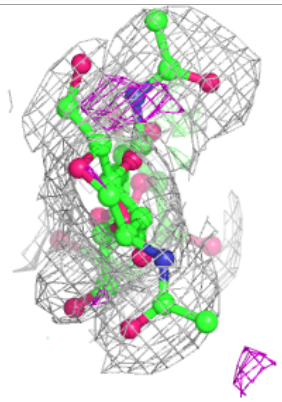


Electron density around Chain q:

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

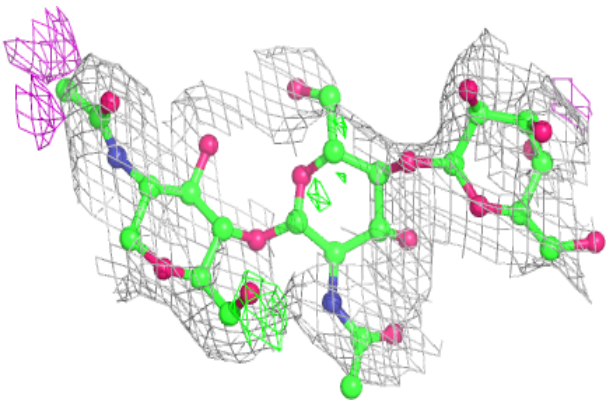


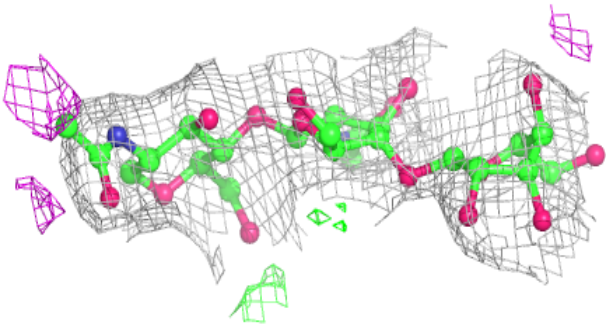


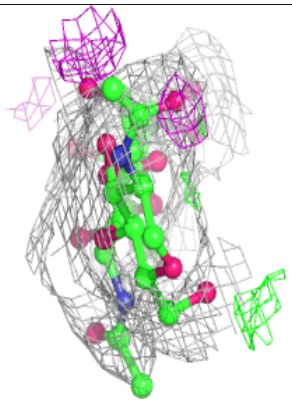


Electron density around Chain w:

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

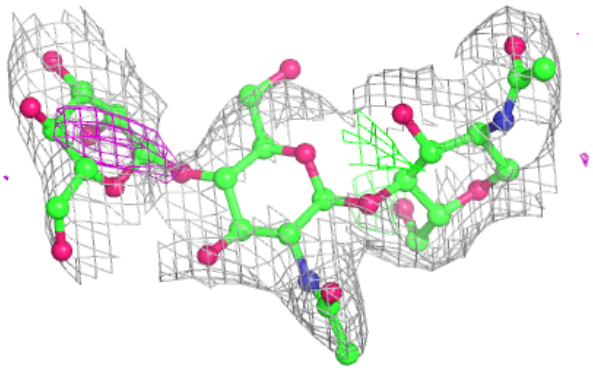


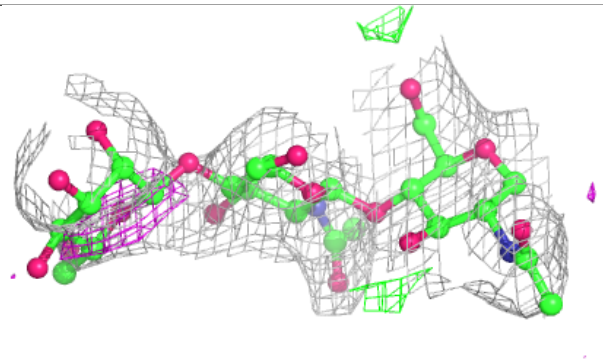


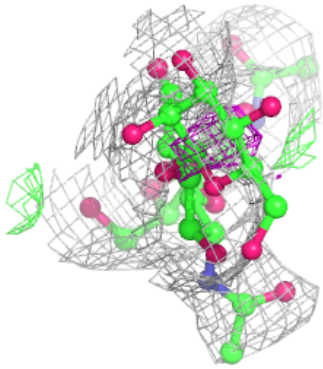


Electron density around Chain y:

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

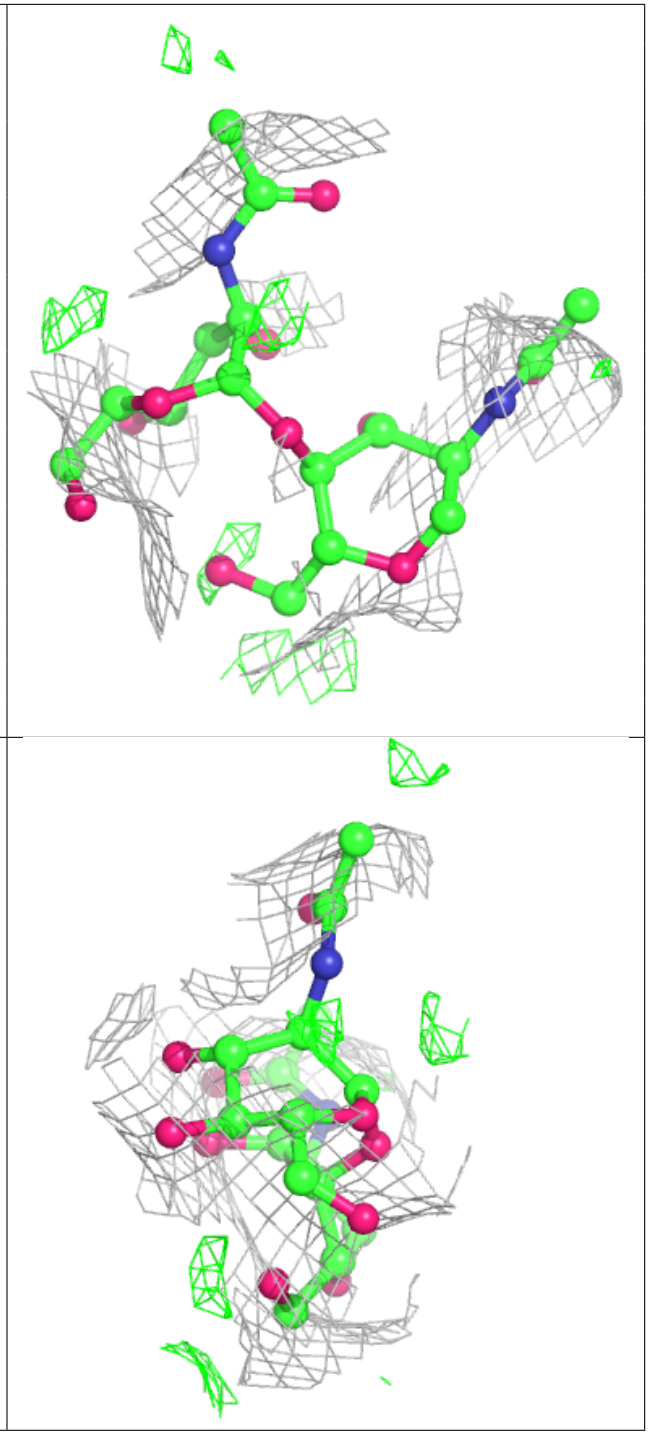






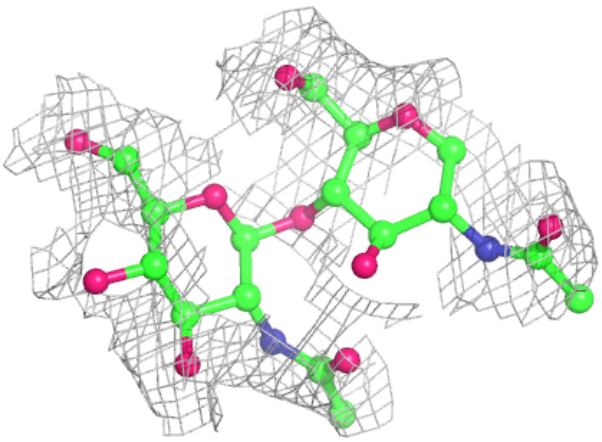
Electron density around Chain f:

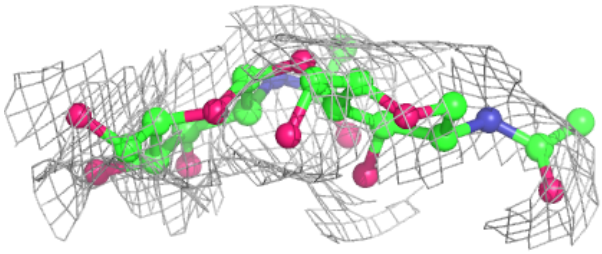
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

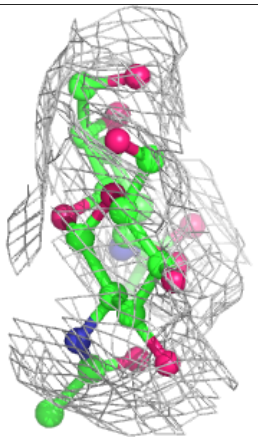


Electron density around Chain i:

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

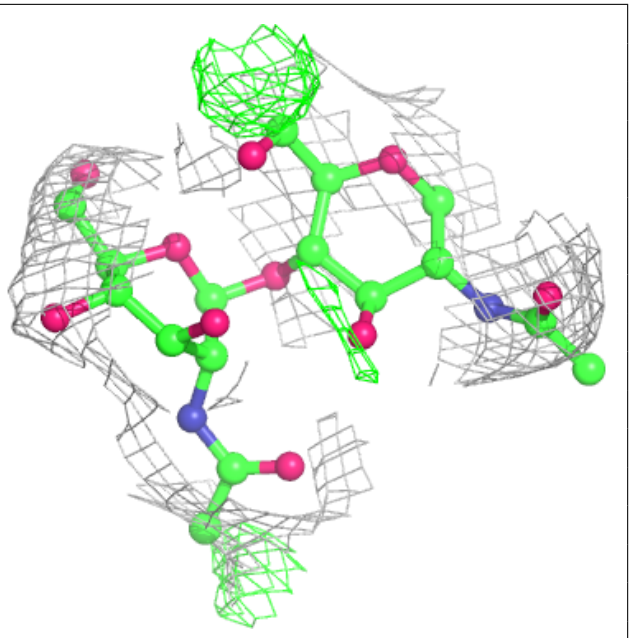


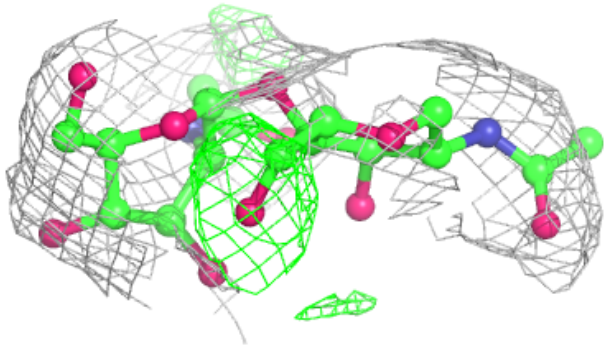


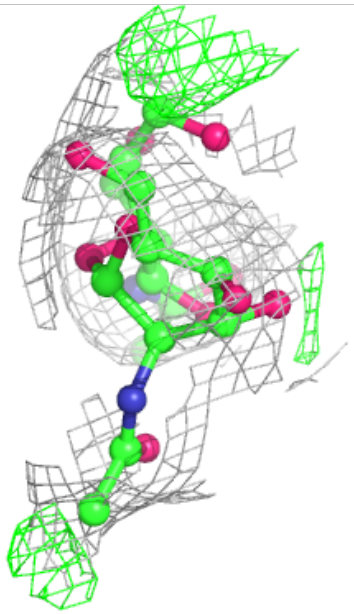


Electron density around Chain k:

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

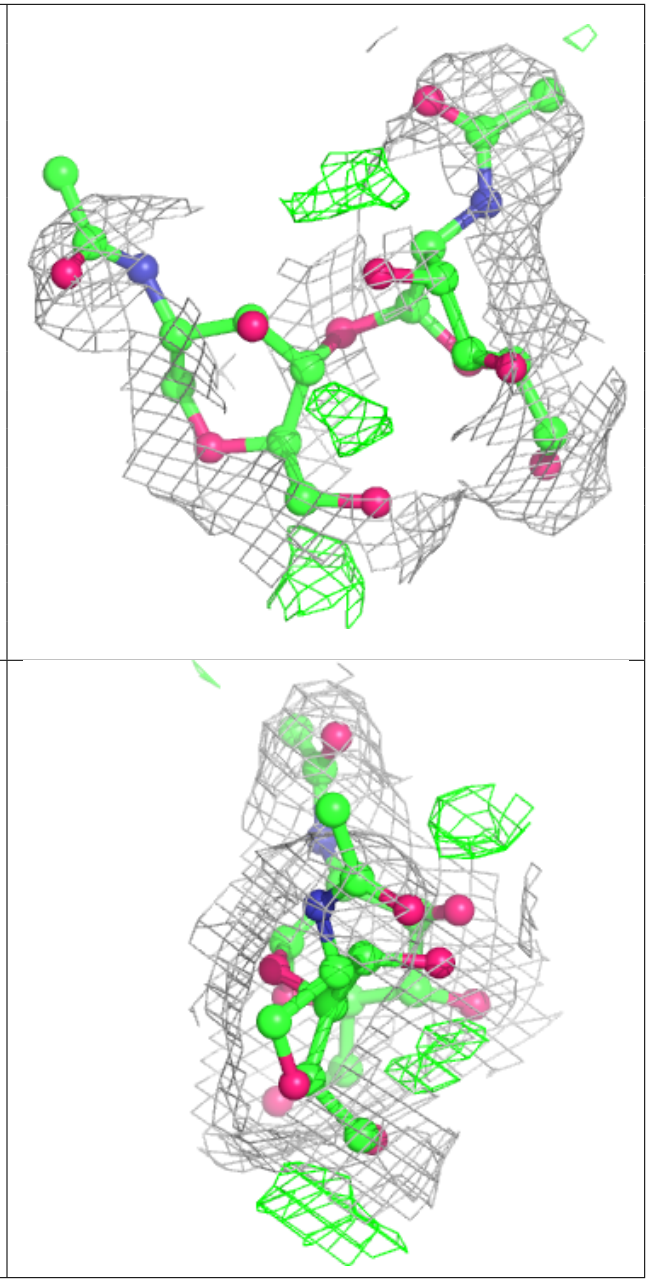






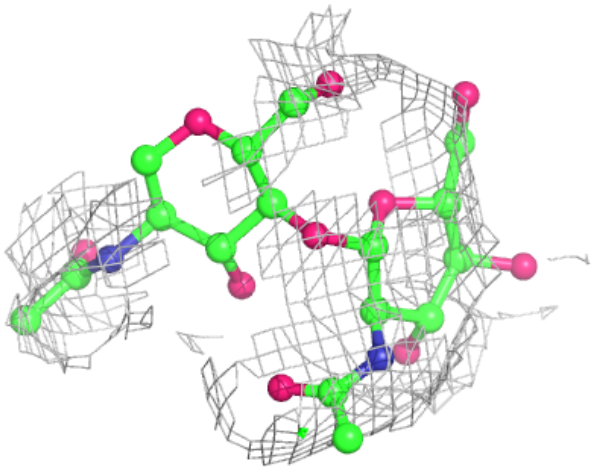
Electron density around Chain m:

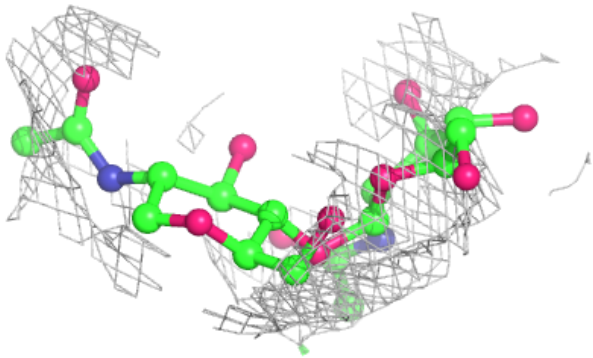
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

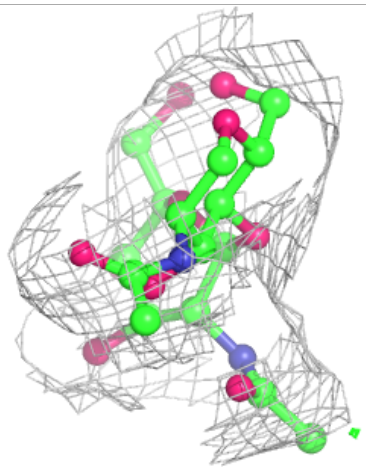


Electron density around Chain p:

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

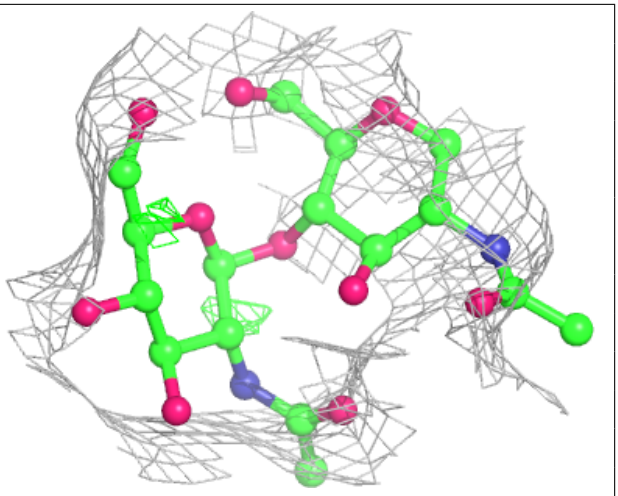


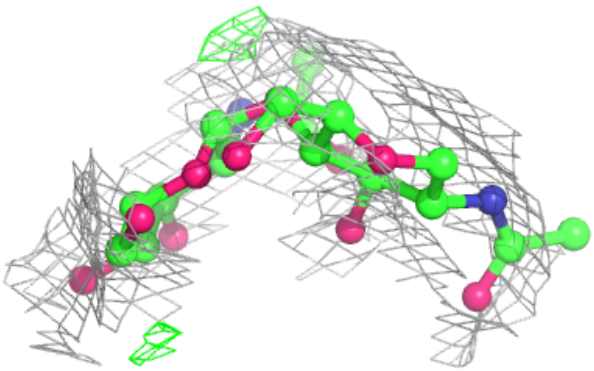


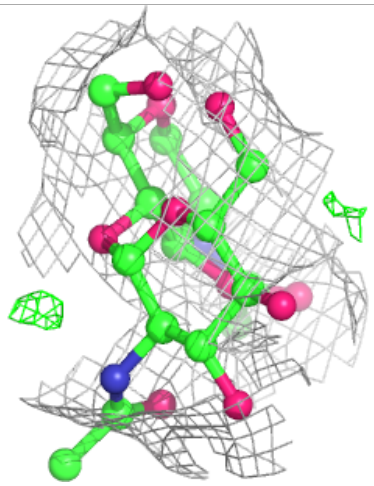


Electron density around Chain r:

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

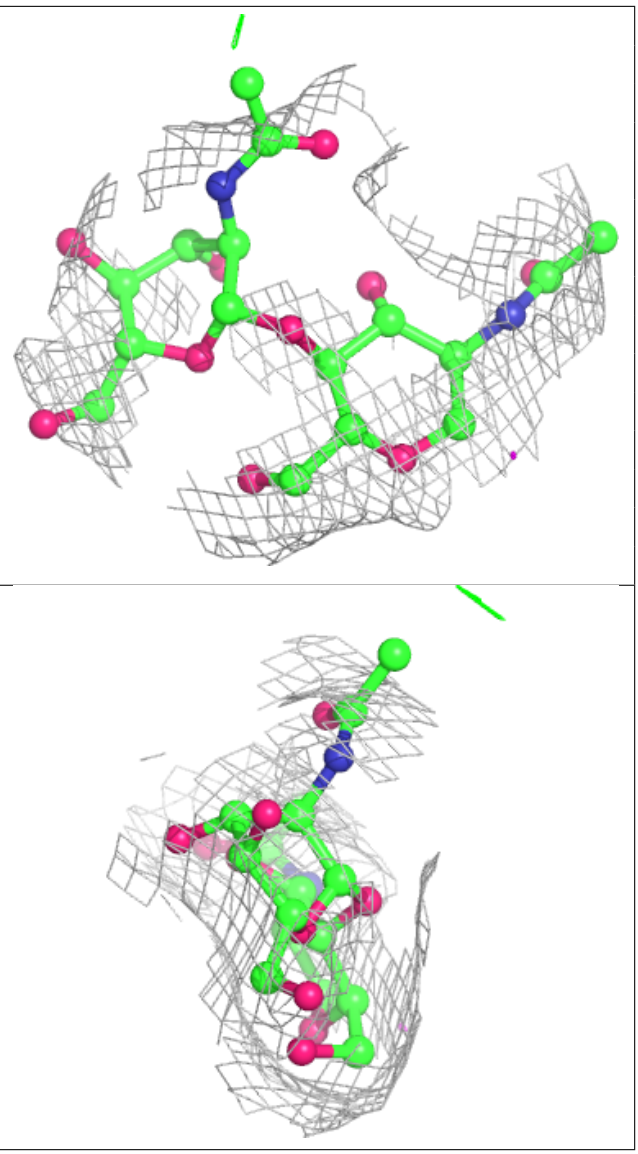






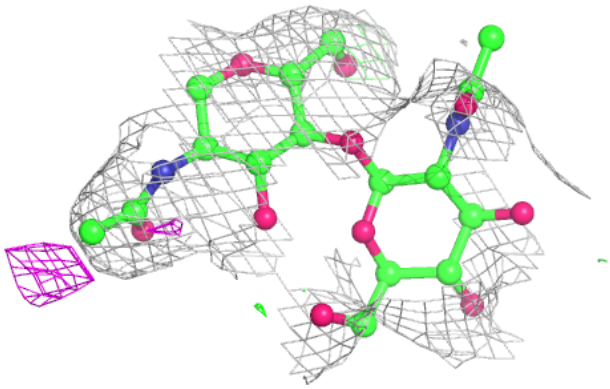
Electron density around Chain t:

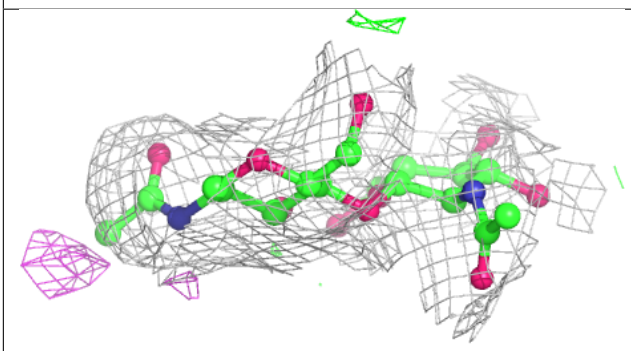
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

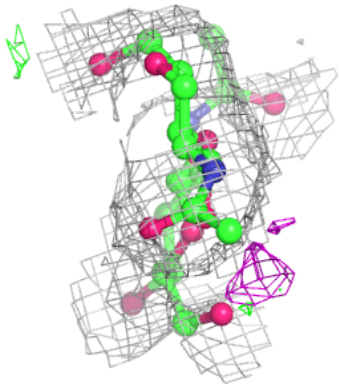


Electron density around Chain u:

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

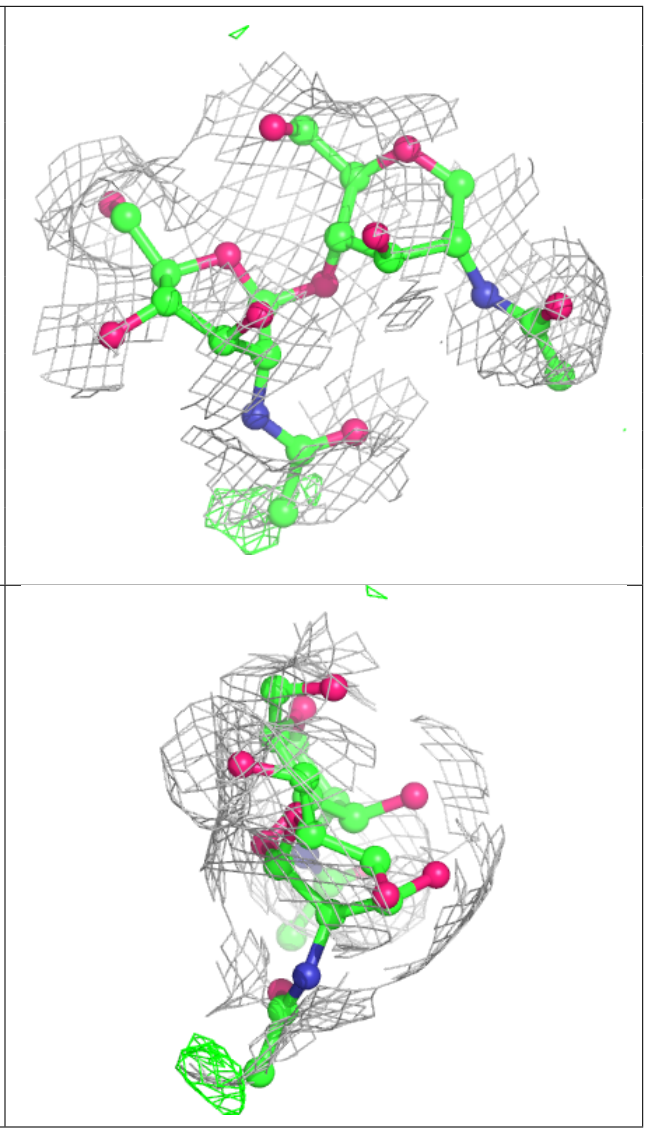






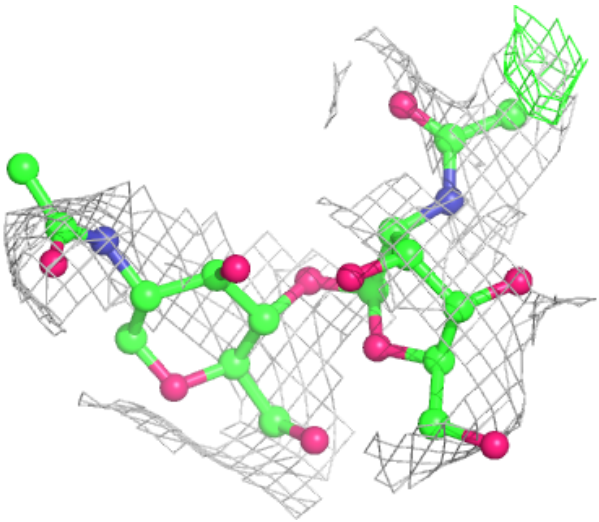
Electron density around Chain v:

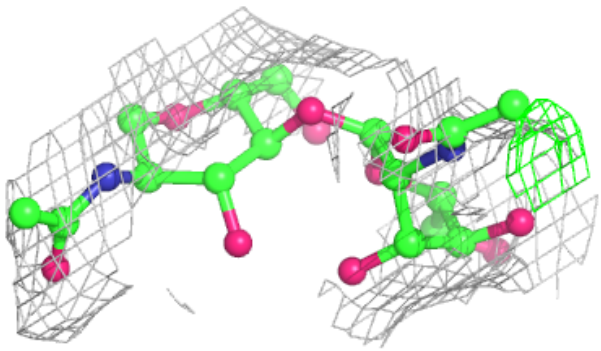
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

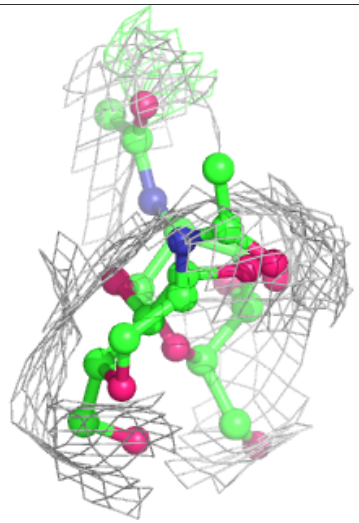


Electron density around Chain x:

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

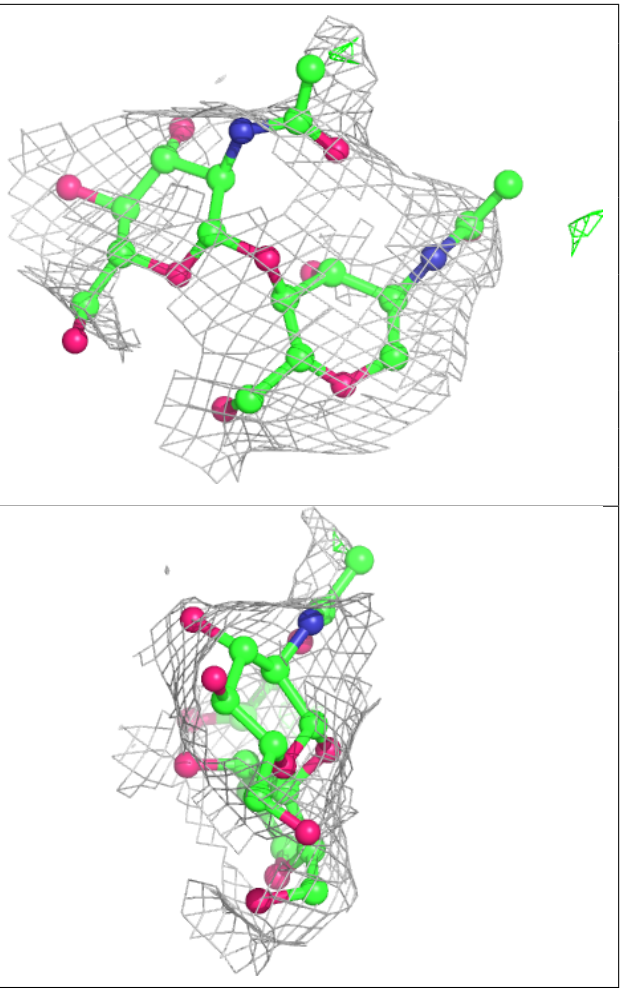






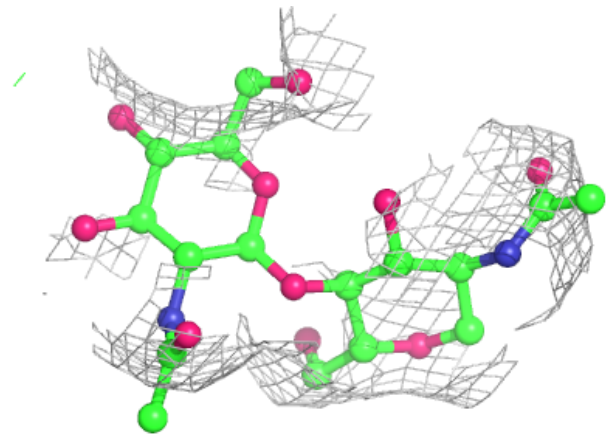
Electron density around Chain z:

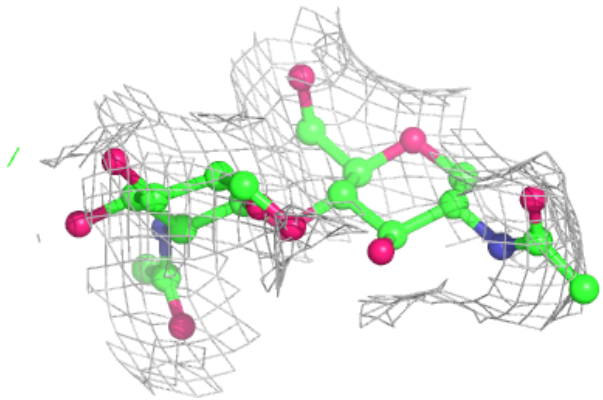
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

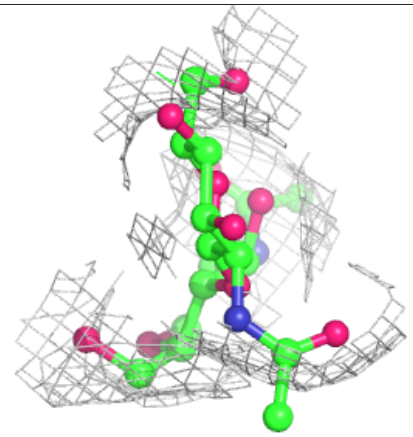


Electron density around Chain 0:

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

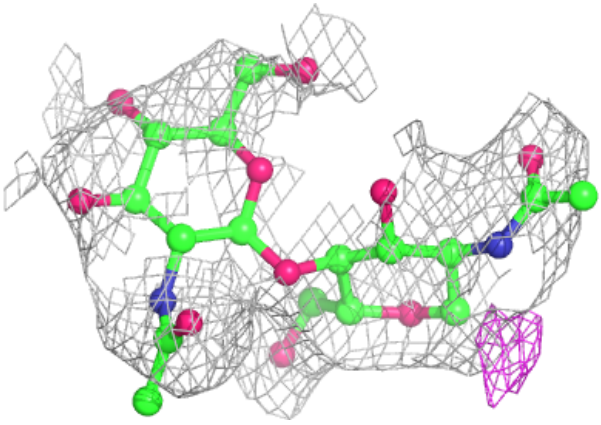


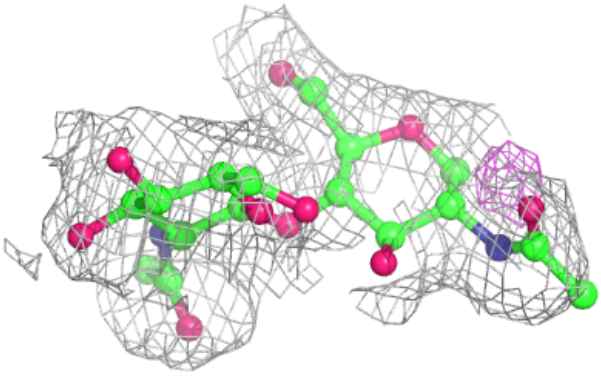




Electron density around Chain 1:

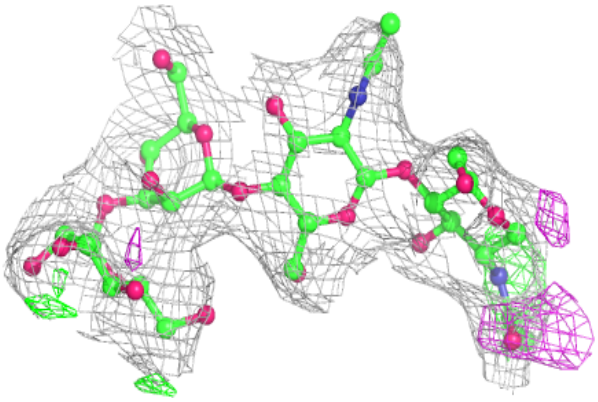
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

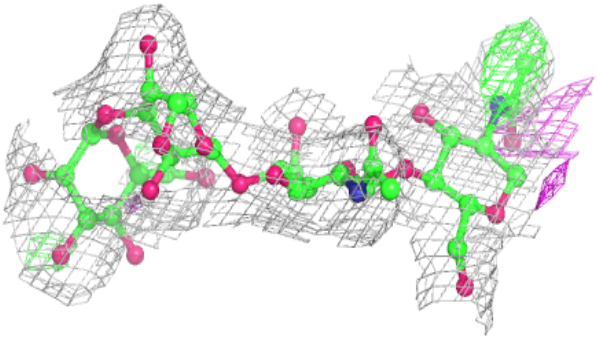


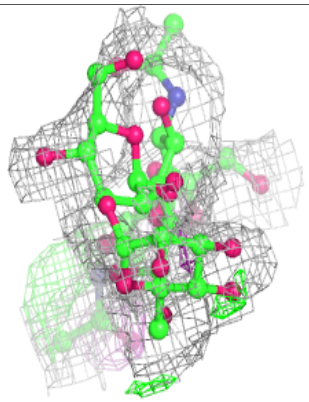


Electron density around Chain s:

$2mF_o$-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(Å^2)	Q<0.9
6	NAG	Y	2003	14/15	0.65	0.26	149,160,166,170	0
6	NAG	c	2002	14/15	0.67	0.19	143,162,169,170	0
6	NAG	c	2001	14/15	0.80	0.28	94,106,117,123	0
6	NAG	O	2006	14/15	0.87	0.23	87,95,100,102	0
6	NAG	K	2004	14/15	0.88	0.10	127,140,146,149	0

6.5 Other polymers (i)

There are no such residues in this entry.