Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

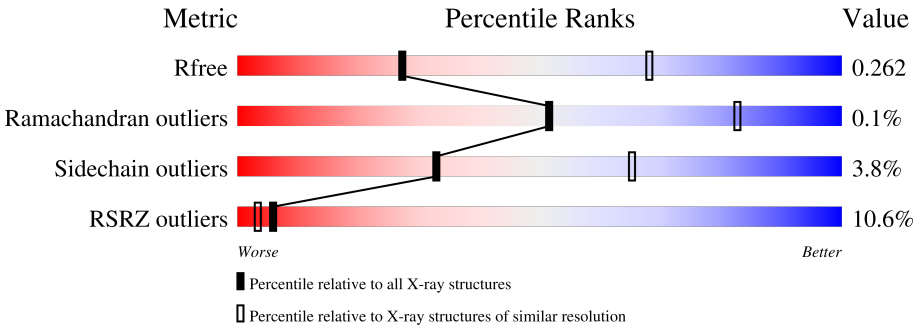
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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
1	A	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	C	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	E	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	G	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	I	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	K	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	M	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	O	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	S	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	U	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	W	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	a	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	c	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			

There are 105 discrepancies between the modelled and reference sequences:

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

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

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

There are 105 discrepancies between the modelled and reference sequences:

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

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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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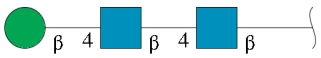
Chain	Residue	Modelled	Actual	Comment	Reference
T	181	ARG	-	expression tag	UNP Q6DQ33
V	175	SER	-	expression tag	UNP Q6DQ33
V	176	GLY	-	expression tag	UNP Q6DQ33
V	177	ARG	-	expression tag	UNP Q6DQ33
V	178	LEU	-	expression tag	UNP Q6DQ33
V	179	VAL	-	expression tag	UNP Q6DQ33
V	180	PRO	-	expression tag	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
3	e	3	Total C N O 39 22 2 15	0	0	0
3	g	3	Total C N O 39 22 2 15	0	0	0
3	h	3	Total C N O 39 22 2 15	0	0	0
3	j	3	Total C N O 39 22 2 15	0	0	0
3	l	3	Total C N O 39 22 2 15	0	0	0
3	n	3	Total C N O 39 22 2 15	0	0	0
3	o	3	Total C N O 39 22 2 15	0	0	0
3	q	3	Total C N O 39 22 2 15	0	0	0
3	w	3	Total C N O 39 22 2 15	0	0	0
3	y	3	Total C N O 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
4	f	2	Total C N O 28 16 2 10	0	0	0
4	i	2	Total C N O 28 16 2 10	0	0	0
4	k	2	Total C N O 28 16 2 10	0	0	0
4	m	2	Total C N O 28 16 2 10	0	0	0
4	p	2	Total C N O 28 16 2 10	0	0	0

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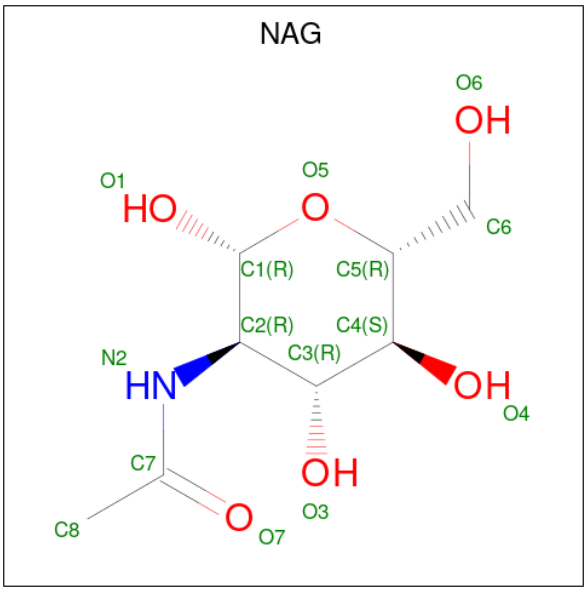
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	r	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	t	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	u	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	v	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	x	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	z	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	0	2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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	s	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



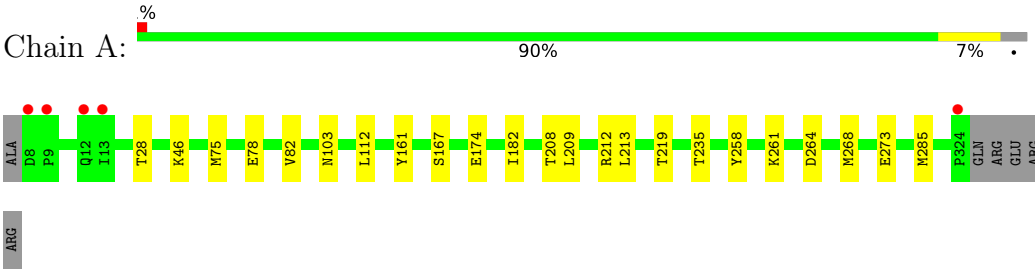
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total C N O 14 8 1 5	0	0
6	O	1	Total C N O 14 8 1 5	0	0
6	Y	1	Total C N O 14 8 1 5	0	0
6	c	1	Total C N O 14 8 1 5	0	0
6	c	1	Total C N O 14 8 1 5	0	0

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.

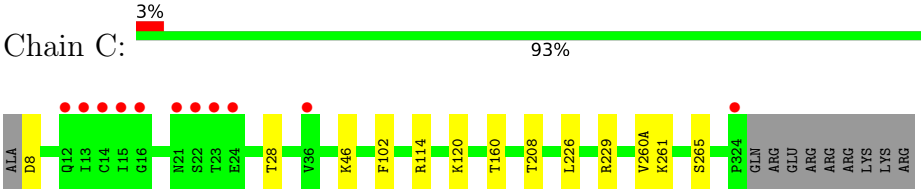
• Molecule 1: Hemagglutinin HA1 chain

Chain A:



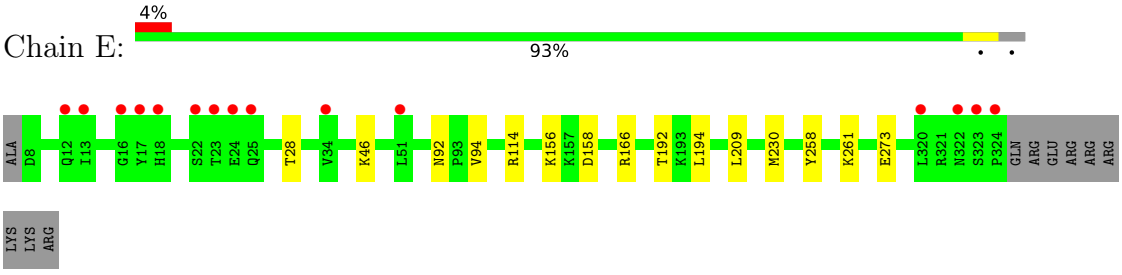
• Molecule 1: Hemagglutinin HA1 chain

Chain C:



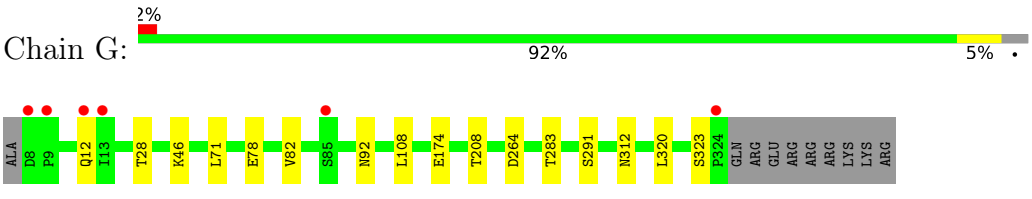
• Molecule 1: Hemagglutinin HA1 chain

Chain E:



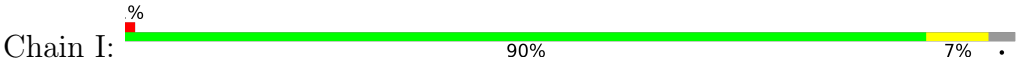
• Molecule 1: Hemagglutinin HA1 chain

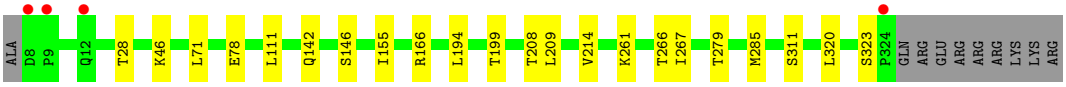
Chain G:



• Molecule 1: Hemagglutinin HA1 chain

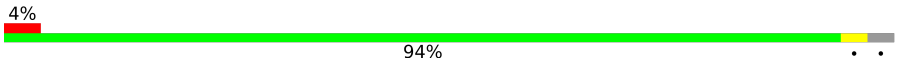
Chain I:





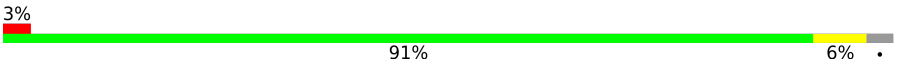
• Molecule 1: Hemagglutinin HA1 chain

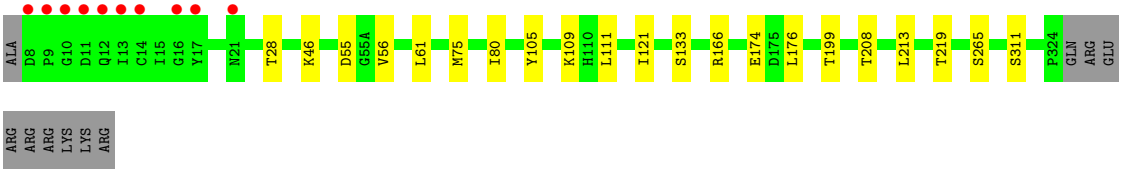
Chain K:



• Molecule 1: Hemagglutinin HA1 chain

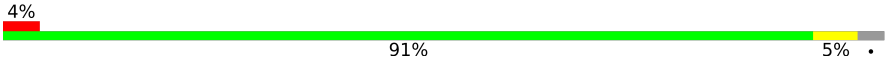
Chain M:





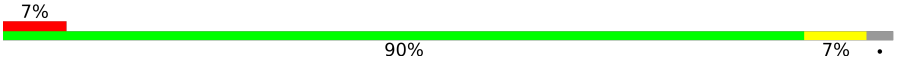
• Molecule 1: Hemagglutinin HA1 chain

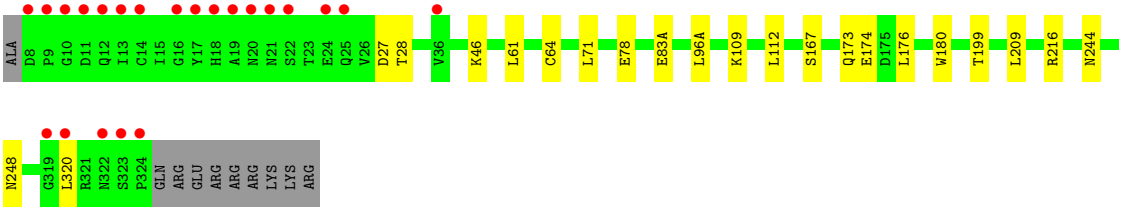
Chain O:



• Molecule 1: Hemagglutinin HA1 chain

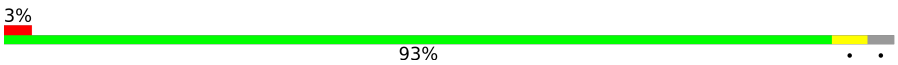
Chain Q:





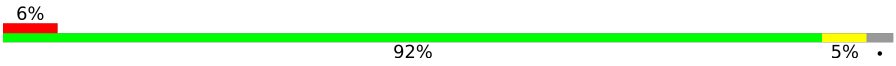
• Molecule 1: Hemagglutinin HA1 chain

Chain S:

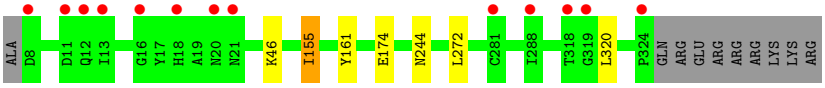


• Molecule 1: Hemagglutinin HA1 chain

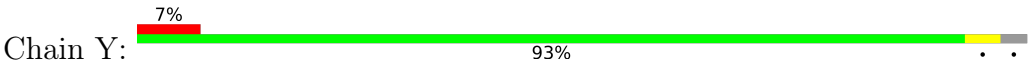
Chain U:



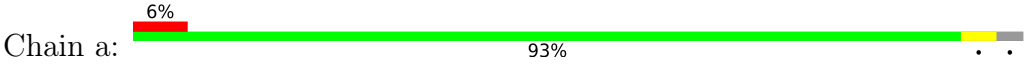
• Molecule 1: Hemagglutinin HA1 chain

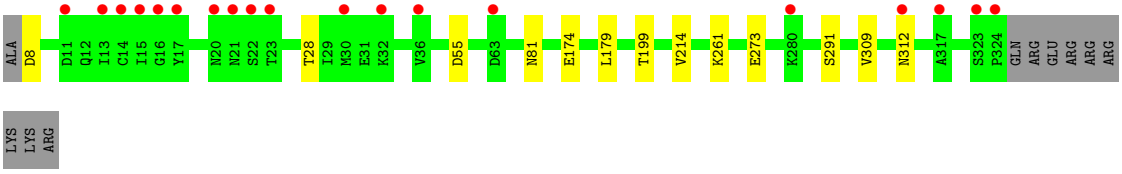


• Molecule 1: Hemagglutinin HA1 chain

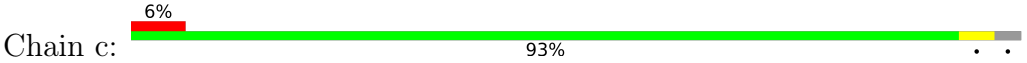


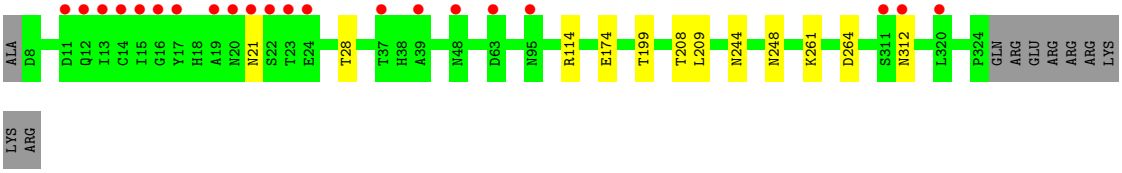
• Molecule 1: Hemagglutinin HA1 chain



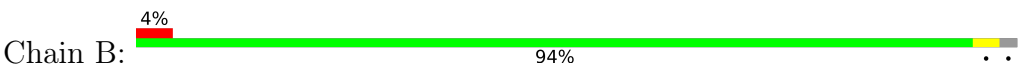


• Molecule 1: Hemagglutinin HA1 chain



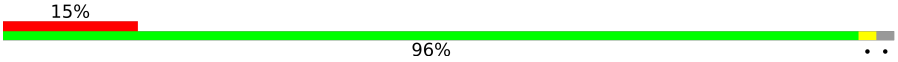


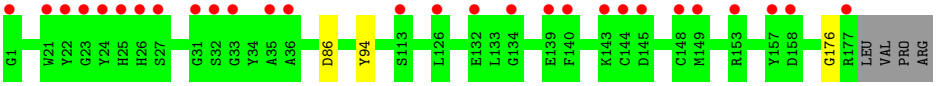
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain

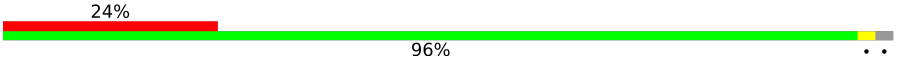
Chain D:

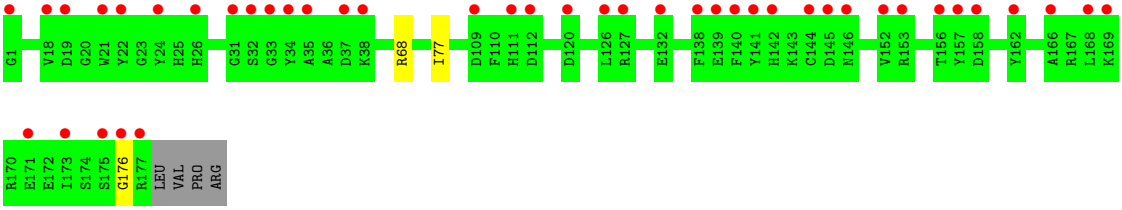




• Molecule 2: Hemagglutinin HA2 chain

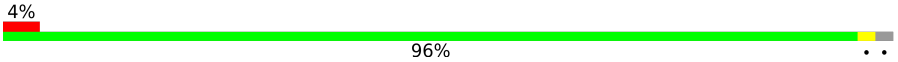
Chain F:

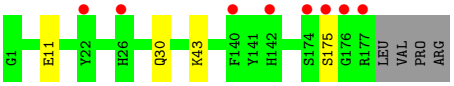




• Molecule 2: Hemagglutinin HA2 chain

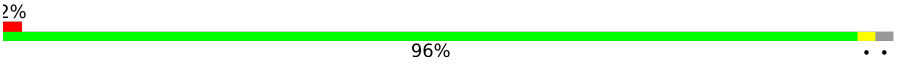
Chain H:





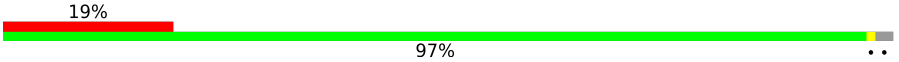
• Molecule 2: Hemagglutinin HA2 chain

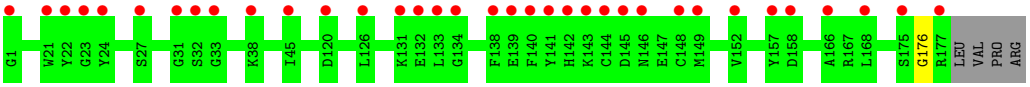
Chain J:



• Molecule 2: Hemagglutinin HA2 chain

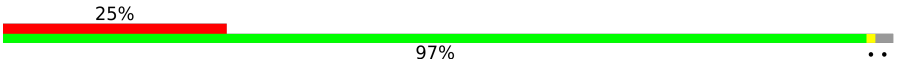
Chain L:

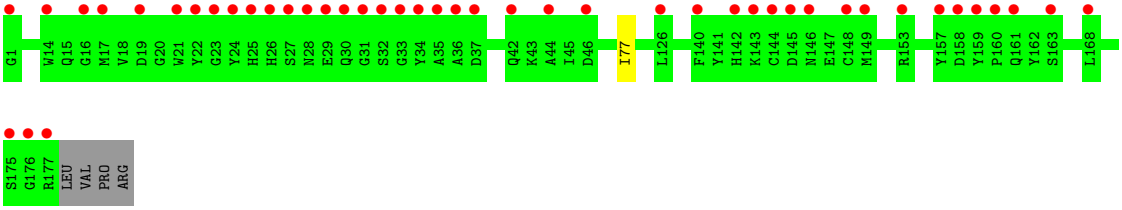




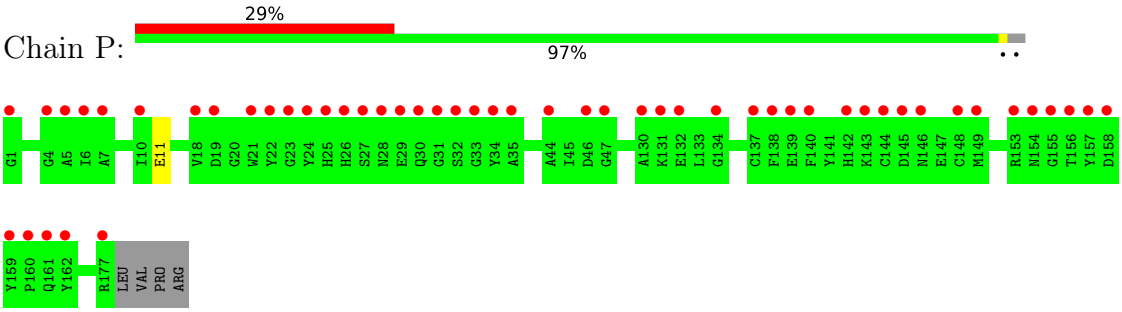
• Molecule 2: Hemagglutinin HA2 chain

Chain N:

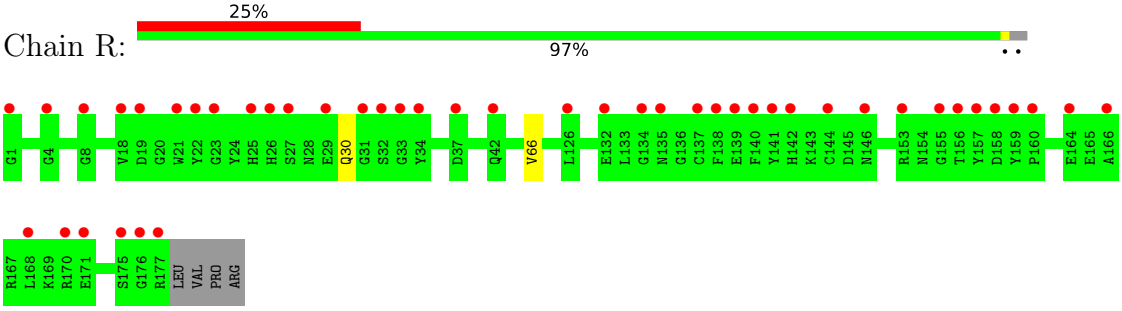




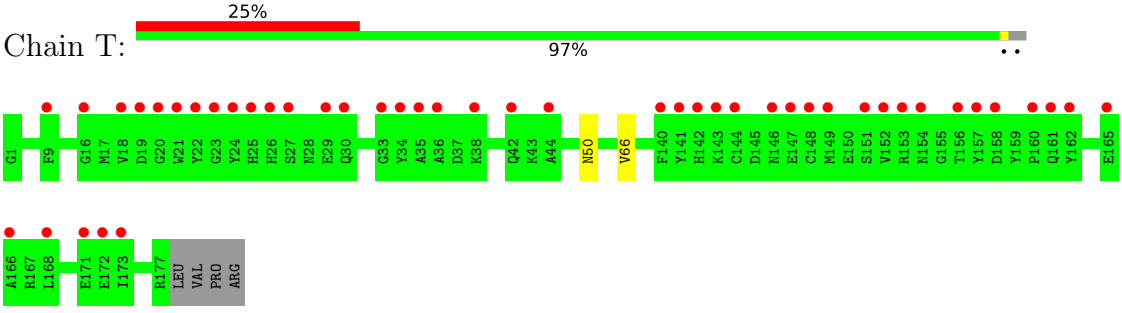
• Molecule 2: Hemagglutinin HA2 chain



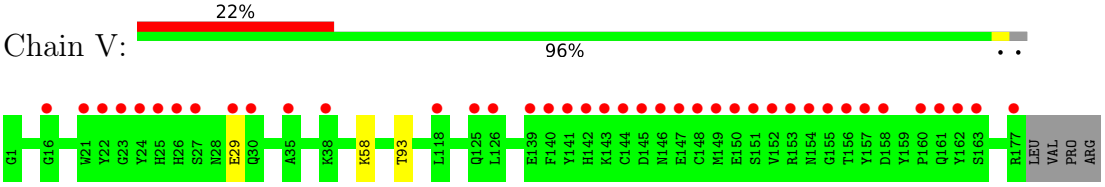
• Molecule 2: Hemagglutinin HA2 chain



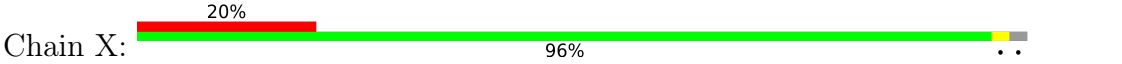
• Molecule 2: Hemagglutinin HA2 chain

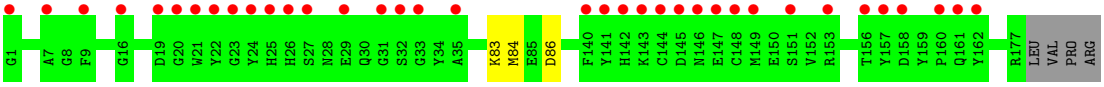


• Molecule 2: Hemagglutinin HA2 chain

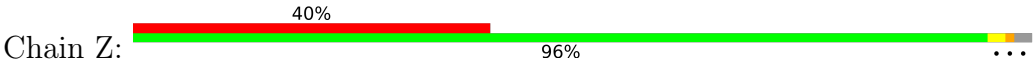


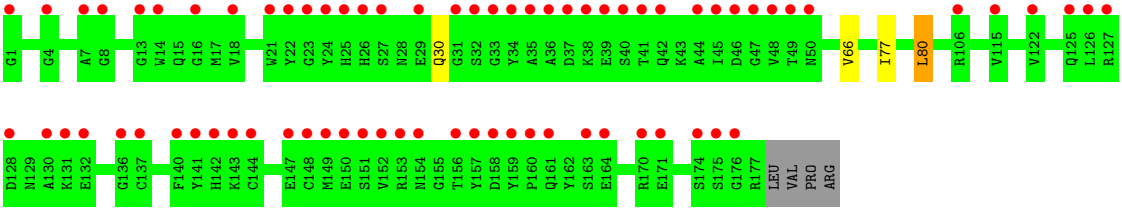
• Molecule 2: Hemagglutinin HA2 chain



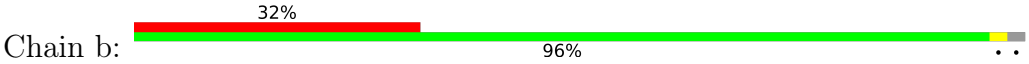


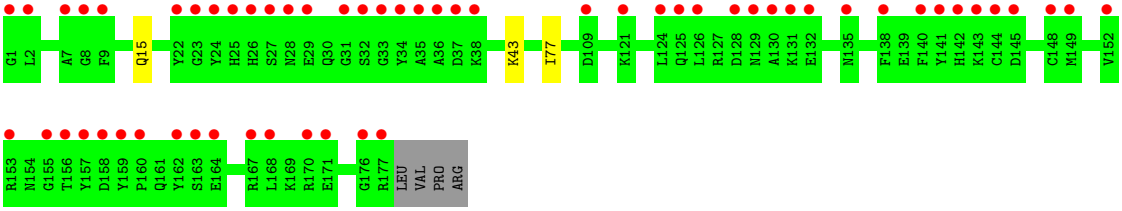
• Molecule 2: Hemagglutinin HA2 chain



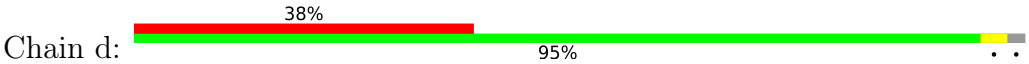


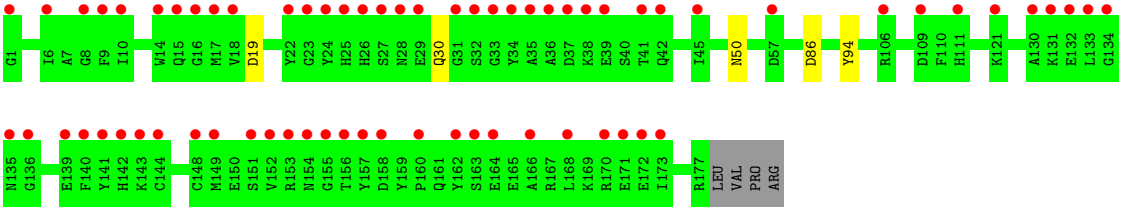
• Molecule 2: Hemagglutinin HA2 chain





• Molecule 2: Hemagglutinin HA2 chain



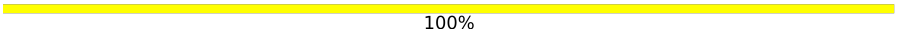


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

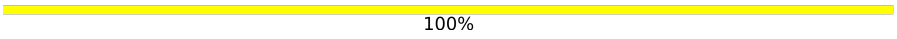
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



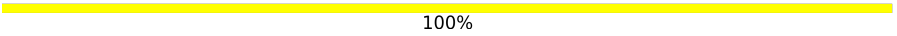
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



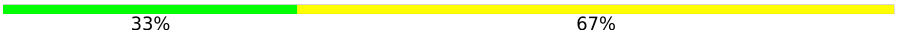
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



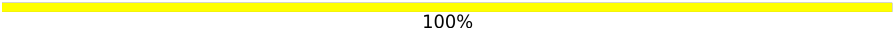
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

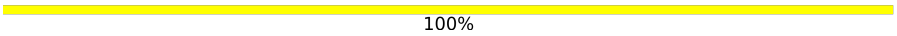
Chain w:

• 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:

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

Chain f:

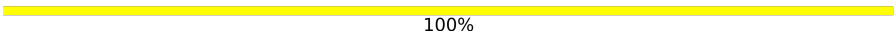


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

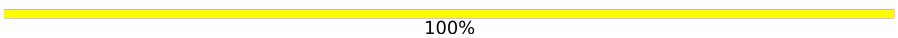
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



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

Chain m:

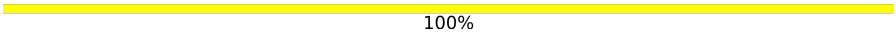


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

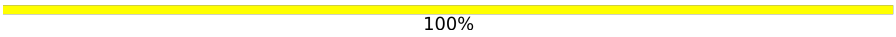
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



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

Chain t:

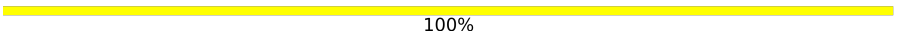


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

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

Chain v:

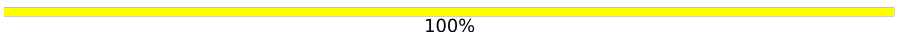


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

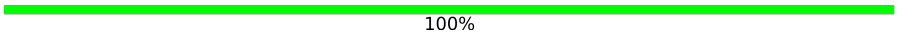
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



• 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

5.1 Standard geometry

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

All (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
1	A	213	LEU	CA-CB-CG	6.23	129.62	115.30
1	O	57	LYS	CD-CE-NZ	5.82	125.08	111.70
1	O	96(A)	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	209	LEU	CA-CB-CG	5.76	128.55	115.30
1	Q	216	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	Q	71	LEU	CA-CB-CG	5.52	128.00	115.30
1	Q	96(A)	LEU	CA-CB-CG	5.52	128.00	115.30
1	K	179	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	E	194	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	Q	209	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	226	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	O	213	LEU	CB-CG-CD2	5.31	120.03	111.00
1	O	241	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	W	155	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	G	108	LEU	CB-CG-CD2	-5.21	102.14	111.00
2	F	68	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	C	229	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	I	267	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	A	161	TYR	CA-CB-CG	5.11	123.11	113.40
1	I	209	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	O	194	LEU	CB-CG-CD2	-5.09	102.34	111.00
2	B	73	LEU	CA-CB-CG	5.09	127.00	115.30
1	O	241	ASP	CB-CG-OD1	5.07	122.86	118.30
1	M	80	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	M	105	TYR	CB-CG-CD2	-5.04	117.98	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
2	F	176	GLY
2	L	176	GLY
2	D	176	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	46	LYS

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Mol	Chain	Res	Type
1	A	75	MET
1	A	78	GLU
1	A	82	VAL
1	A	103	ASN
1	A	112	LEU
1	A	167	SER
1	A	174	GLU
1	A	182	ILE
1	A	208	THR
1	A	219	THR
1	A	235	THR
1	A	258	TYR
1	A	261	LYS
1	A	264	ASP
1	A	268	MET
1	A	273	GLU
1	A	285	MET
1	C	8	ASP
1	C	28	THR
1	C	46	LYS
1	C	102	PHE
1	C	114	ARG
1	C	120	LYS
1	C	160	THR
1	C	208	THR
1	C	260(A)	VAL
1	C	261	LYS
1	C	265	SER
1	E	28	THR
1	E	46	LYS
1	E	92	ASN
1	E	94	VAL
1	E	114	ARG
1	E	156	LYS
1	E	158	ASP
1	E	166	ARG
1	E	192	THR
1	E	230	MET
1	E	258	TYR
1	E	261	LYS
1	E	273	GLU
1	G	12	GLN

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Mol	Chain	Res	Type
1	G	28	THR
1	G	46	LYS
1	G	71	LEU
1	G	78	GLU
1	G	82	VAL
1	G	92	ASN
1	G	174	GLU
1	G	208	THR
1	G	264	ASP
1	G	283	THR
1	G	291	SER
1	G	312	ASN
1	G	320	LEU
1	G	323	SER
1	I	28	THR
1	I	46	LYS
1	I	71	LEU
1	I	78	GLU
1	I	111	LEU
1	I	142	GLN
1	I	146	SER
1	I	155	ILE
1	I	166	ARG
1	I	194	LEU
1	I	199	THR
1	I	208	THR
1	I	214	VAL
1	I	261	LYS
1	I	266	THR
1	I	279	THR
1	I	285	MET
1	I	311	SER
1	I	320	LEU
1	I	323	SER
1	K	28	THR
1	K	46	LYS
1	K	56	VAL
1	K	94	VAL
1	K	114	ARG
1	K	166	ARG
1	K	187	ASP
1	K	199	THR

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Mol	Chain	Res	Type
1	K	260(A)	VAL
1	K	261	LYS
1	M	28	THR
1	M	46	LYS
1	M	55	ASP
1	M	56	VAL
1	M	61	LEU
1	M	75	MET
1	M	109	LYS
1	M	111	LEU
1	M	121	ILE
1	M	133	SER
1	M	166	ARG
1	M	174	GLU
1	M	176	LEU
1	M	199	THR
1	M	208	THR
1	M	219	THR
1	M	265	SER
1	M	311	SER
1	O	28	THR
1	O	56	VAL
1	O	61	LEU
1	O	96(A)	LEU
1	O	120	LYS
1	O	174	GLU
1	O	176	LEU
1	O	199	THR
1	O	208	THR
1	O	209	LEU
1	O	248	ASN
1	O	291	SER
1	O	310	LYS
1	O	311	SER
1	O	320	LEU
1	Q	27	ASP
1	Q	28	THR
1	Q	46	LYS
1	Q	61	LEU
1	Q	64	CYS
1	Q	78	GLU
1	Q	83(A)	GLU

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Mol	Chain	Res	Type
1	Q	109	LYS
1	Q	112	LEU
1	Q	167	SER
1	Q	173	GLN
1	Q	174	GLU
1	Q	176	LEU
1	Q	199	THR
1	Q	244	ASN
1	Q	248	ASN
1	Q	320	LEU
1	S	28	THR
1	S	46	LYS
1	S	75	MET
1	S	114	ARG
1	S	160	THR
1	S	199	THR
1	S	226	LEU
1	S	244	ASN
1	S	260(A)	VAL
1	S	283	THR
1	S	291	SER
1	S	300	LEU
1	S	311	SER
1	S	320	LEU
1	U	28	THR
1	U	30	MET
1	U	46	LYS
1	U	75	MET
1	U	111	LEU
1	U	114	ARG
1	U	122	GLN
1	U	161	TYR
1	U	174	GLU
1	U	226	LEU
1	U	244	ASN
1	U	258	TYR
1	U	272	LEU
1	U	279	THR
1	U	300	LEU
1	W	46	LYS
1	W	155	ILE
1	W	161	TYR

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Mol	Chain	Res	Type
1	W	174	GLU
1	W	244	ASN
1	W	272	LEU
1	W	320	LEU
1	Y	28	THR
1	Y	54	LEU
1	Y	82	VAL
1	Y	142	GLN
1	Y	174	GLU
1	Y	199	THR
1	Y	261	LYS
1	Y	264	ASP
1	Y	272	LEU
1	Y	291	SER
1	Y	309	VAL
1	a	8	ASP
1	a	28	THR
1	a	55	ASP
1	a	81	ASN
1	a	174	GLU
1	a	179	LEU
1	a	199	THR
1	a	214	VAL
1	a	261	LYS
1	a	273	GLU
1	a	291	SER
1	a	309	VAL
1	a	312	ASN
1	c	21[A]	ASN
1	c	21[B]	ASN
1	c	28	THR
1	c	114	ARG
1	c	174	GLU
1	c	199	THR
1	c	208	THR
1	c	209	LEU
1	c	244	ASN
1	c	261	LYS
1	c	264	ASP
1	c	312	ASN
2	B	22	TYR
2	B	43	LYS

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Mol	Chain	Res	Type
2	B	77	ILE
2	B	84	MET
2	B	86	ASP
2	D	86	ASP
2	D	94	TYR
2	F	77	ILE
2	H	11	GLU
2	H	30	GLN
2	H	43	LYS
2	H	175	SER
2	J	11	GLU
2	J	68	ARG
2	J	77	ILE
2	J	116	LYS
2	N	77	ILE
2	P	11	GLU
2	R	30	GLN
2	R	66	VAL
2	T	50	ASN
2	T	66	VAL
2	V	29	GLU
2	V	58	LYS
2	V	93	THR
2	X	83	LYS
2	X	84	MET
2	X	86	ASP
2	Z	30	GLN
2	Z	66	VAL
2	Z	77	ILE
2	Z	80	LEU
2	b	15	GLN
2	b	43	LYS
2	b	77	ILE
2	d	19	ASP
2	d	30	GLN
2	d	50	ASN
2	d	86	ASP
2	d	94	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	C	18	HIS
1	E	25	GLN
1	E	186	ASN
1	I	38	HIS
1	K	122	GLN
1	M	196	GLN
1	Q	122	GLN
1	S	197	ASN
1	W	186	ASN
1	W	196	GLN
1	Y	110	HIS
1	Y	197	ASN
2	F	62	GLN
2	H	30	GLN
2	H	146	ASN
2	L	42	GLN
2	T	25	HIS
2	T	81	ASN
2	X	30	GLN
2	X	81	ASN
2	b	62	GLN
2	d	81	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
4	k	1	NAG	O5-C1	-4.67	1.36	1.43
3	j	2	NAG	O5-C1	-4.55	1.36	1.43
3	j	3	BMA	C4-C3	4.46	1.63	1.52
4	k	2	NAG	C1-C2	4.37	1.58	1.52
4	f	2	NAG	C1-C2	4.36	1.58	1.52
4	t	1	NAG	O5-C1	-4.35	1.36	1.43
4	k	2	NAG	O5-C1	-4.33	1.36	1.43
4	i	1	NAG	O5-C1	-4.31	1.36	1.43
4	x	1	NAG	O5-C1	-4.12	1.37	1.43
3	l	1	NAG	O5-C1	-4.00	1.37	1.43
4	m	2	NAG	C1-C2	3.95	1.58	1.52
4	m	2	NAG	O5-C1	3.87	1.49	1.43
3	e	3	BMA	C4-C3	3.76	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	3	BMA	C1-C2	3.75	1.60	1.52
3	e	1	NAG	C1-C2	3.71	1.57	1.52
4	f	1	NAG	O5-C1	-3.65	1.37	1.43
3	h	3	BMA	C2-C3	3.63	1.57	1.52
3	q	3	BMA	C4-C5	3.50	1.60	1.53
3	l	3	BMA	O5-C1	-3.47	1.38	1.43
3	h	2	NAG	O5-C1	-3.46	1.38	1.43
3	o	3	BMA	C4-C5	3.43	1.60	1.53
3	g	3	BMA	C4-C3	3.42	1.61	1.52
3	l	3	BMA	C4-C5	3.41	1.60	1.53
3	j	3	BMA	C4-C5	3.40	1.60	1.53
3	o	3	BMA	O5-C1	-3.36	1.38	1.43
3	h	3	BMA	C4-C5	3.28	1.59	1.53
3	j	3	BMA	O5-C1	-3.28	1.38	1.43
4	t	2	NAG	O5-C1	-3.26	1.38	1.43
3	l	3	BMA	C4-C3	3.23	1.60	1.52
3	h	3	BMA	C1-C2	3.23	1.59	1.52
3	q	1	NAG	O5-C1	-3.17	1.38	1.43
3	n	3	BMA	C4-C5	3.17	1.59	1.53
4	u	2	NAG	O5-C1	-3.09	1.38	1.43
3	w	3	BMA	C1-C2	3.04	1.59	1.52
3	n	3	BMA	O3-C3	3.02	1.50	1.43
3	h	1	NAG	O5-C1	3.01	1.48	1.43
4	v	2	NAG	O5-C1	-3.00	1.38	1.43
4	v	1	NAG	O5-C1	-2.97	1.39	1.43
3	h	3	BMA	C4-C3	2.82	1.59	1.52
4	v	2	NAG	C1-C2	2.79	1.56	1.52
4	r	1	NAG	O5-C1	-2.76	1.39	1.43
3	e	3	BMA	C2-C3	2.75	1.56	1.52
3	h	3	BMA	O3-C3	2.74	1.49	1.43
3	n	2	NAG	O5-C1	-2.71	1.39	1.43
4	m	1	NAG	O5-C1	-2.66	1.39	1.43
3	e	1	NAG	O5-C1	-2.63	1.39	1.43
3	g	3	BMA	C6-C5	2.62	1.60	1.51
3	l	2	NAG	O5-C1	-2.60	1.39	1.43
3	o	2	NAG	O5-C1	-2.55	1.39	1.43
3	h	3	BMA	C6-C5	2.52	1.60	1.51
3	w	3	BMA	O5-C5	2.45	1.48	1.43
3	q	3	BMA	C1-C2	2.41	1.57	1.52
4	z	2	NAG	C1-C2	2.41	1.55	1.52
3	o	3	BMA	C1-C2	2.32	1.57	1.52
3	o	3	BMA	C4-C3	2.30	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	n	3	BMA	C6-C5	2.29	1.59	1.51
3	j	3	BMA	C1-C2	2.28	1.57	1.52
4	k	2	NAG	C3-C2	2.25	1.57	1.52
3	h	3	BMA	O5-C1	2.21	1.47	1.43
3	j	3	BMA	C2-C3	2.16	1.55	1.52
3	j	1	NAG	C3-C2	2.10	1.57	1.52
3	n	3	BMA	C4-C3	2.09	1.57	1.52
4	v	2	NAG	C3-C2	2.06	1.56	1.52
3	o	3	BMA	C2-C3	2.04	1.55	1.52
3	e	1	NAG	C3-C2	2.01	1.56	1.52
3	o	1	NAG	C1-C2	2.01	1.55	1.52

All (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
4	f	2	NAG	C1-O5-C5	4.48	118.26	112.19
4	k	1	NAG	C3-C4-C5	4.23	117.79	110.24
5	s	3	BMA	C3-C4-C5	4.23	117.78	110.24
3	l	1	NAG	C4-C3-C2	4.05	116.95	111.02
3	j	1	NAG	C4-C3-C2	4.00	116.88	111.02
4	f	1	NAG	C3-C4-C5	3.89	117.17	110.24
3	e	1	NAG	C4-C3-C2	3.86	116.67	111.02
3	g	3	BMA	C1-C2-C3	3.85	114.40	109.67
3	o	3	BMA	C1-O5-C5	3.77	117.31	112.19
4	m	2	NAG	C1-O5-C5	3.70	117.21	112.19
3	h	2	NAG	C3-C4-C5	3.61	116.68	110.24
4	p	2	NAG	C4-C3-C2	3.57	116.25	111.02
3	n	3	BMA	C1-O5-C5	3.56	117.01	112.19
4	z	1	NAG	C4-C3-C2	3.56	116.23	111.02
4	v	2	NAG	C4-C3-C2	3.55	116.21	111.02
4	m	1	NAG	C3-C4-C5	3.52	116.53	110.24
5	s	3	BMA	O5-C1-C2	-3.51	105.36	110.77
3	j	3	BMA	C3-C4-C5	3.46	116.41	110.24
4	i	1	NAG	C4-C3-C2	3.46	116.09	111.02
4	1	1	NAG	C1-O5-C5	3.43	116.83	112.19
3	e	3	BMA	O5-C1-C2	3.42	116.05	110.77
3	q	3	BMA	C3-C4-C5	3.42	116.34	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	3	BMA	C3-C4-C5	3.35	116.21	110.24
3	g	3	BMA	C2-C3-C4	3.33	116.67	110.89
3	g	3	BMA	C3-C4-C5	3.31	116.15	110.24
4	t	1	NAG	C4-C3-C2	3.27	115.81	111.02
3	e	3	BMA	O2-C2-C1	3.26	115.83	109.15
5	s	3	BMA	O3-C3-C4	-3.26	102.81	110.35
4	k	2	NAG	C4-C3-C2	3.25	115.78	111.02
5	s	3	BMA	O3-C3-C2	3.25	116.21	109.99
5	s	1	NAG	C1-C2-N2	3.22	116.00	110.49
3	w	2	NAG	C4-C3-C2	3.21	115.73	111.02
3	l	1	NAG	C1-O5-C5	-3.21	107.84	112.19
4	x	1	NAG	C4-C3-C2	3.15	115.64	111.02
3	o	3	BMA	C3-C4-C5	3.10	115.77	110.24
3	o	3	BMA	C1-C2-C3	3.10	113.48	109.67
4	p	2	NAG	C1-O5-C5	-3.05	108.06	112.19
5	s	1	NAG	O5-C1-C2	-3.02	106.53	111.29
3	n	2	NAG	C4-C3-C2	2.96	115.36	111.02
3	w	2	NAG	C3-C4-C5	2.94	115.48	110.24
3	e	3	BMA	C1-O5-C5	-2.91	108.25	112.19
4	x	1	NAG	C3-C4-C5	2.89	115.39	110.24
3	l	3	BMA	O2-C2-C1	2.86	115.01	109.15
3	w	3	BMA	O2-C2-C3	-2.86	104.41	110.14
3	h	3	BMA	O3-C3-C2	2.83	115.41	109.99
3	q	3	BMA	O5-C1-C2	2.82	115.12	110.77
3	j	3	BMA	O2-C2-C1	2.80	114.88	109.15
4	z	1	NAG	C3-C4-C5	2.72	115.08	110.24
3	w	3	BMA	C1-O5-C5	2.70	115.85	112.19
3	h	2	NAG	C1-O5-C5	2.68	115.83	112.19
3	y	3	BMA	O5-C5-C6	2.68	111.40	107.20
3	j	2	NAG	C3-C4-C5	2.66	114.98	110.24
3	e	3	BMA	C2-C3-C4	2.66	115.49	110.89
4	f	1	NAG	C4-C3-C2	2.65	114.91	111.02
3	j	2	NAG	C4-C3-C2	2.57	114.79	111.02
4	k	1	NAG	C4-C3-C2	2.57	114.78	111.02
4	r	1	NAG	C4-C3-C2	2.56	114.77	111.02
3	w	3	BMA	O2-C2-C1	2.55	114.37	109.15
4	1	1	NAG	C3-C4-C5	2.52	114.74	110.24
3	j	3	BMA	C2-C3-C4	2.51	115.24	110.89
4	t	1	NAG	C1-O5-C5	-2.51	108.79	112.19
3	l	3	BMA	C2-C3-C4	2.49	115.21	110.89
3	n	3	BMA	O3-C3-C2	2.49	114.76	109.99
4	i	1	NAG	C1-O5-C5	-2.46	108.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	q	3	BMA	O2-C2-C3	-2.43	105.27	110.14
3	o	3	BMA	C2-C3-C4	2.42	115.09	110.89
3	o	3	BMA	O2-C2-C3	-2.42	105.29	110.14
3	n	2	NAG	C1-O5-C5	-2.42	108.92	112.19
4	z	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	j	1	NAG	C3-C4-C5	2.38	114.48	110.24
4	v	1	NAG	C4-C3-C2	2.36	114.48	111.02
5	s	1	NAG	C3-C4-C5	-2.34	106.06	110.24
4	z	1	NAG	C1-O5-C5	-2.34	109.02	112.19
3	n	3	BMA	O5-C1-C2	2.30	114.32	110.77
3	h	3	BMA	C3-C4-C5	2.30	114.33	110.24
4	i	1	NAG	C3-C4-C5	2.28	114.31	110.24
4	t	2	NAG	C4-C3-C2	2.26	114.33	111.02
3	n	3	BMA	O5-C5-C4	-2.24	105.37	110.83
3	h	2	NAG	O4-C4-C5	2.24	114.86	109.30
3	e	3	BMA	C1-C2-C3	2.23	112.41	109.67
3	y	1	NAG	C1-O5-C5	2.20	115.17	112.19
4	v	1	NAG	C3-C4-C5	2.18	114.12	110.24
4	p	2	NAG	C3-C4-C5	2.17	114.11	110.24
5	s	1	NAG	C1-O5-C5	2.13	115.08	112.19
3	o	3	BMA	O5-C5-C6	-2.13	103.87	107.20
5	s	1	NAG	C2-N2-C7	-2.11	119.90	122.90
3	h	3	BMA	O5-C5-C6	2.08	110.47	107.20
4	r	2	NAG	C1-O5-C5	2.03	114.94	112.19
3	j	3	BMA	O5-C1-C2	2.03	113.90	110.77
3	h	3	BMA	C1-O5-C5	2.02	114.93	112.19
4	t	1	NAG	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (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
4	i	2	NAG	O5-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
4	1	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	t	2	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
4	k	1	NAG	C4-C5-C6-O6
4	u	2	NAG	C4-C5-C6-O6
4	1	2	NAG	C4-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
5	s	1	NAG	O5-C5-C6-O6
3	y	3	BMA	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
4	1	1	NAG	C4-C5-C6-O6
4	0	2	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
3	w	2	NAG	C1-C2-N2-C7
3	w	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
3	q	1	NAG	C4-C5-C6-O6
4	t	2	NAG	C4-C5-C6-O6
5	s	4	MAN	C4-C5-C6-O6
4	1	1	NAG	O5-C5-C6-O6
5	s	1	NAG	C4-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
3	l	3	BMA	C4-C5-C6-O6
3	e	3	BMA	O5-C5-C6-O6
3	q	1	NAG	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
3	w	3	BMA	O5-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
4	x	1	NAG	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
3	q	3	BMA	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
5	s	3	BMA	C4-C5-C6-O6
4	x	1	NAG	O5-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
4	r	2	NAG	O5-C5-C6-O6
3	e	3	BMA	C4-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	x	2	NAG	O5-C5-C6-O6
3	w	2	NAG	C3-C2-N2-C7

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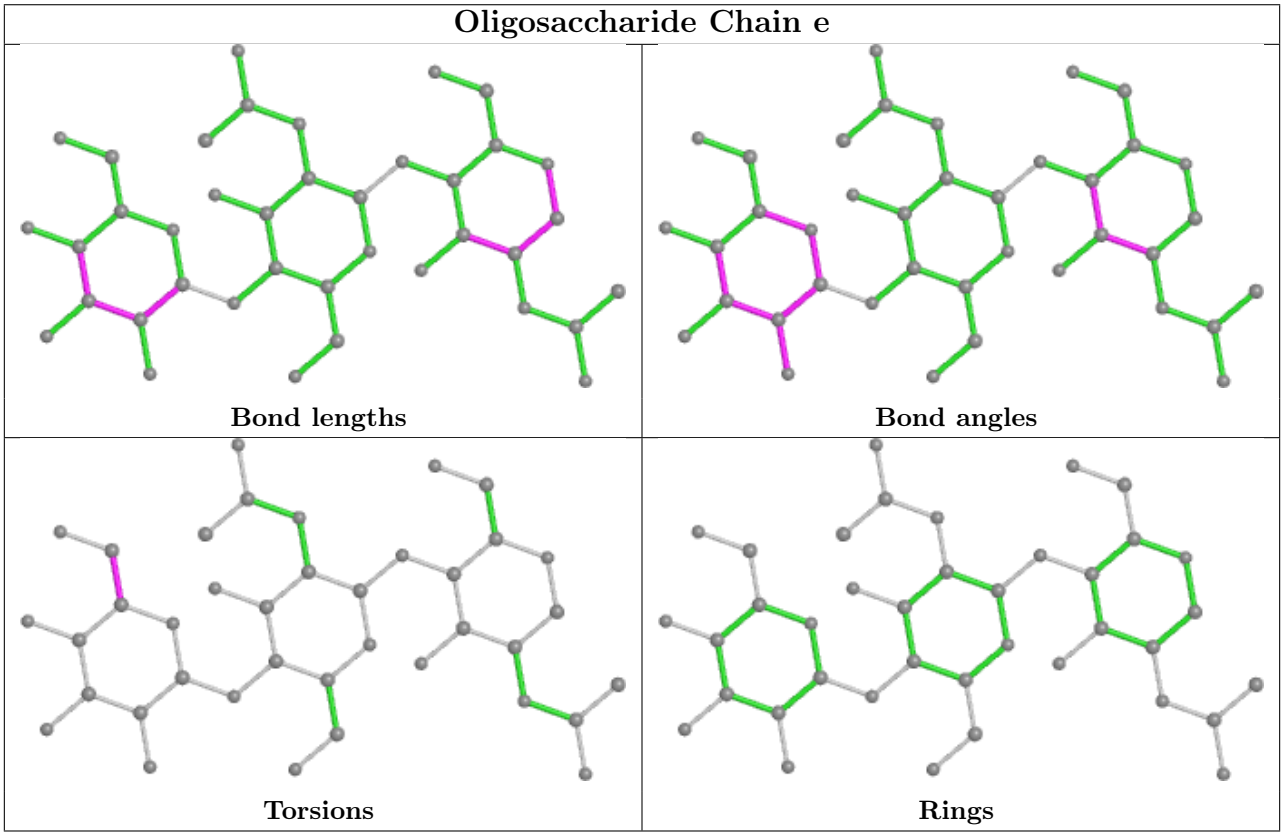
Mol	Chain	Res	Type	Atoms
3	j	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
5	s	3	BMA	O5-C5-C6-O6
3	w	3	BMA	C4-C5-C6-O6
4	t	1	NAG	C4-C5-C6-O6
4	r	2	NAG	C4-C5-C6-O6
3	o	3	BMA	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

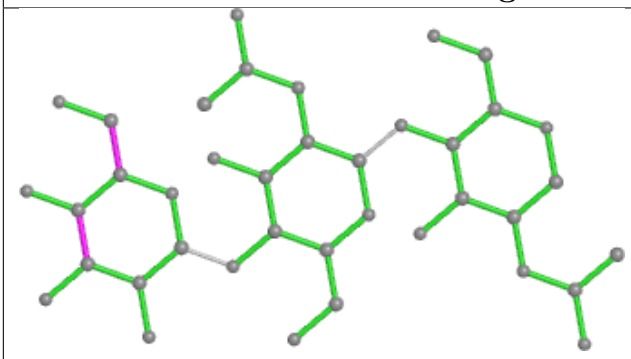
Mol	Chain	Res	Type	Atoms
3	w	3	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

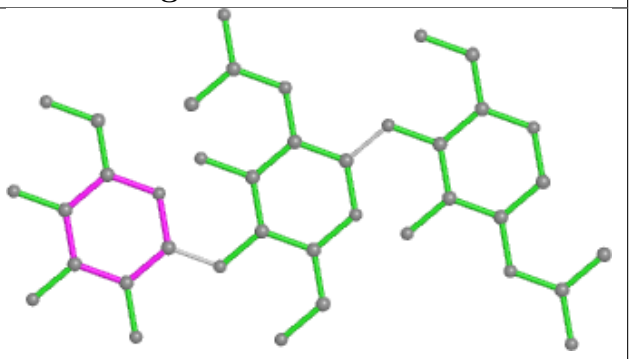
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



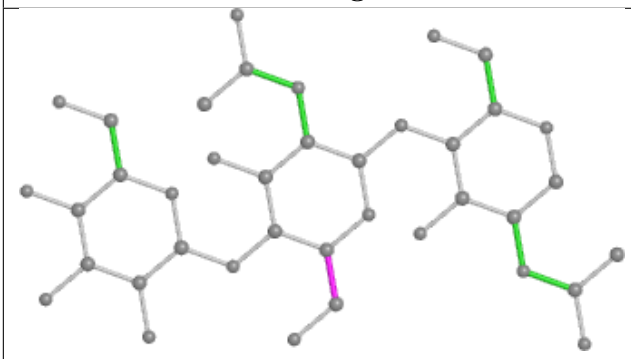
Oligosaccharide Chain g



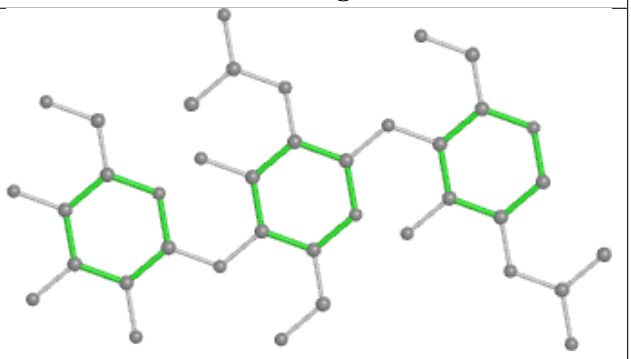
Bond lengths



Bond angles

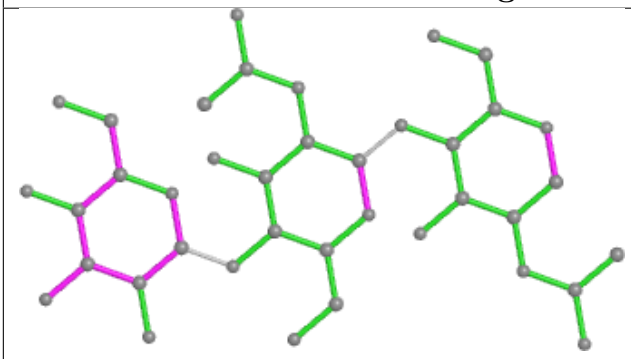


Torsions

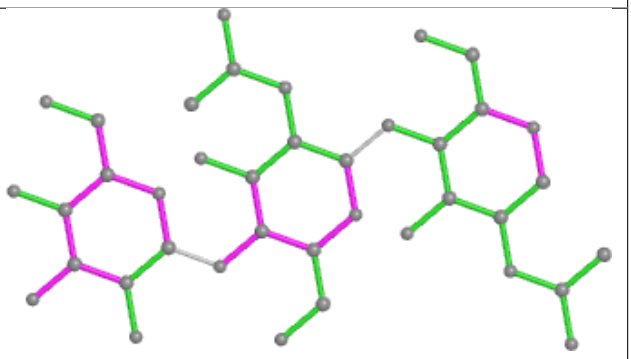


Rings

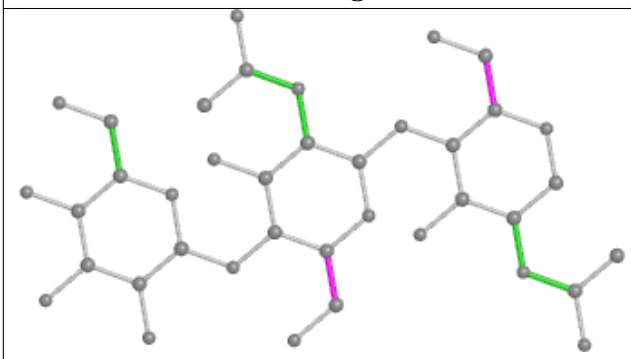
Oligosaccharide Chain h



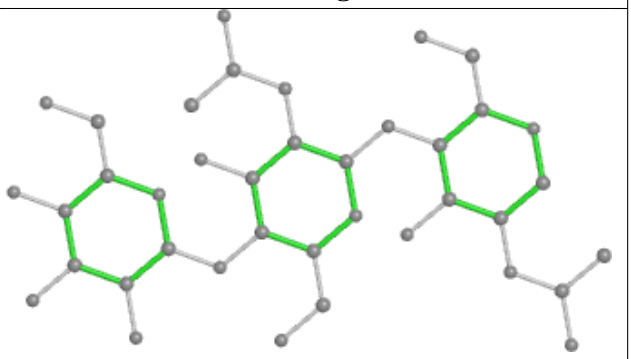
Bond lengths



Bond angles

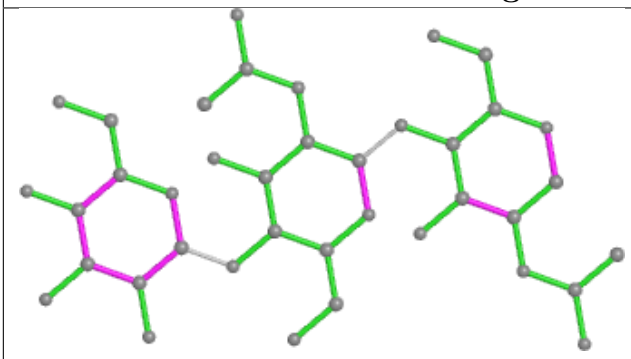


Torsions

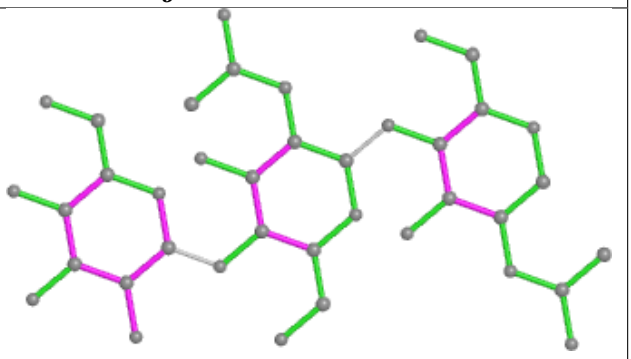


Rings

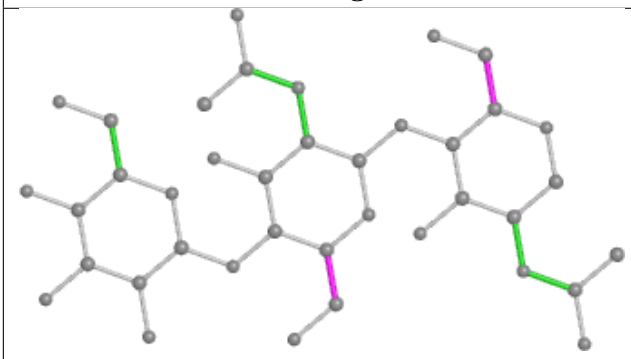
Oligosaccharide Chain j



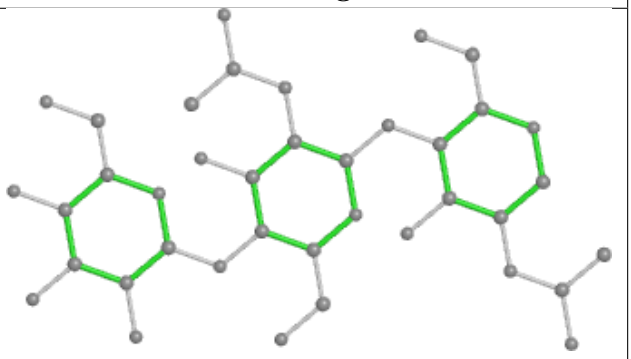
Bond lengths



Bond angles

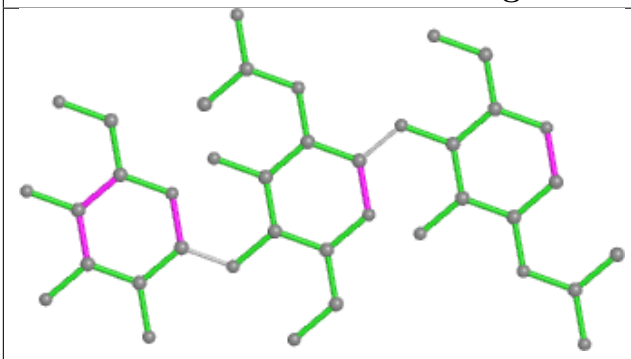


Torsions

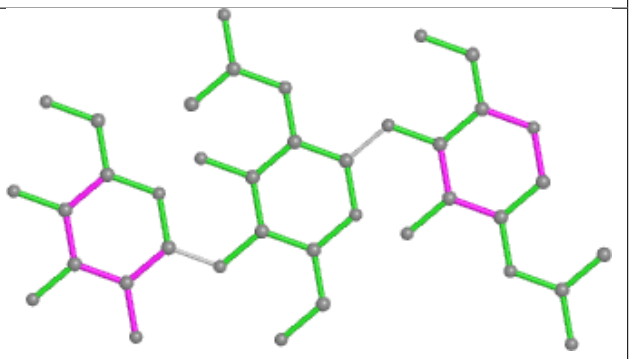


Rings

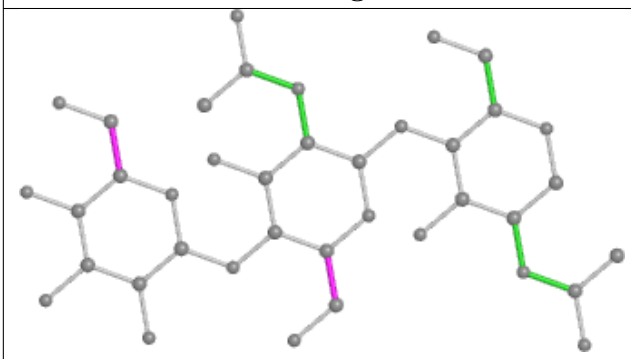
Oligosaccharide Chain l



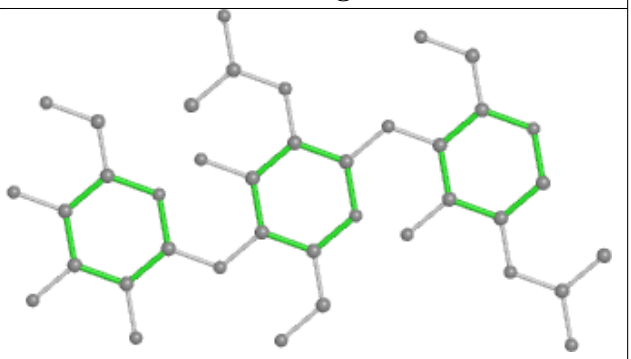
Bond lengths



Bond angles

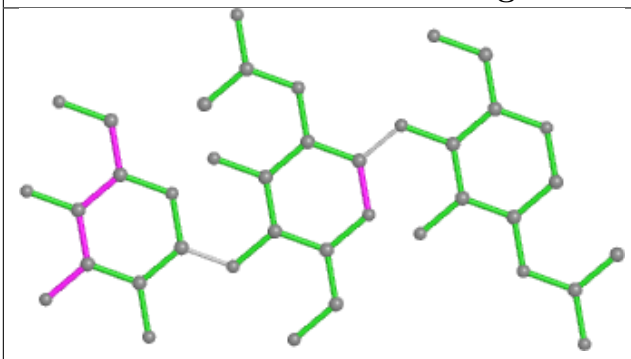


Torsions

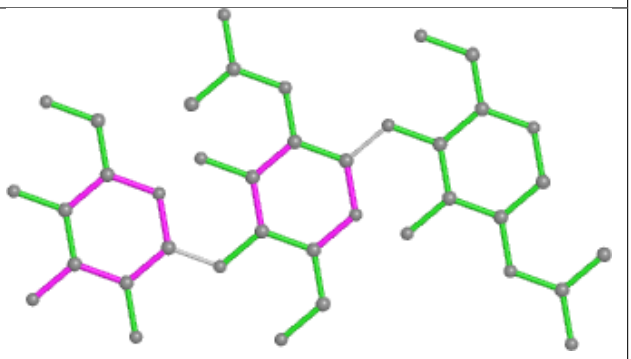


Rings

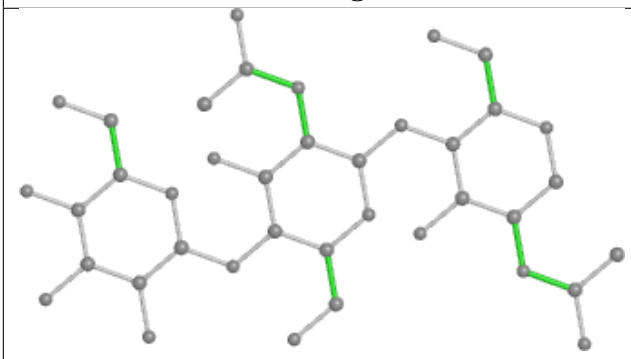
Oligosaccharide Chain n



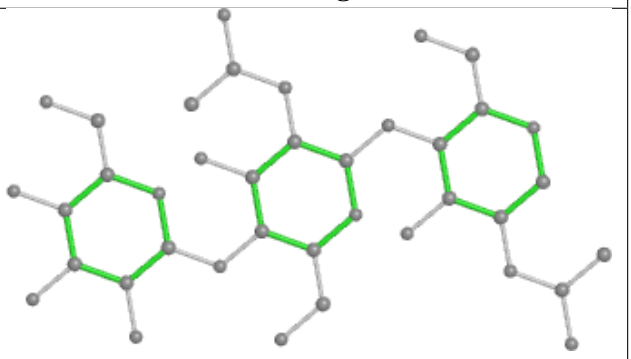
Bond lengths



Bond angles

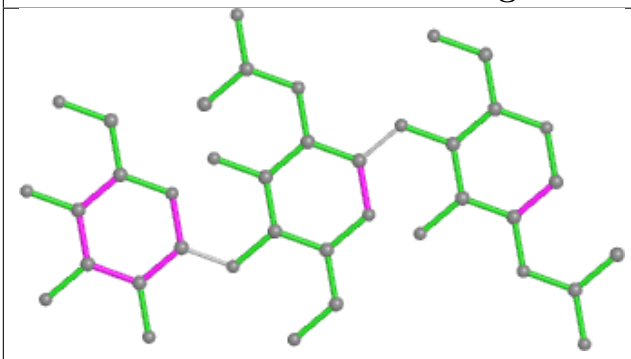


Torsions

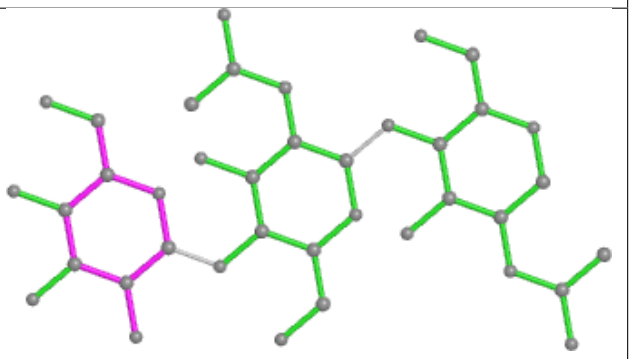


Rings

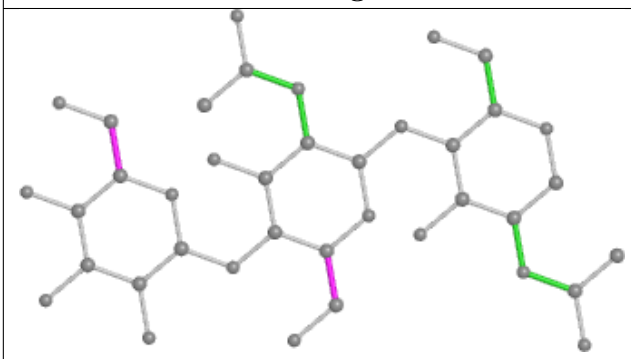
Oligosaccharide Chain o



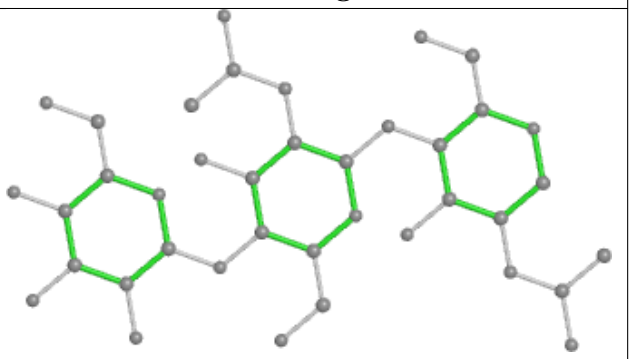
Bond lengths



Bond angles

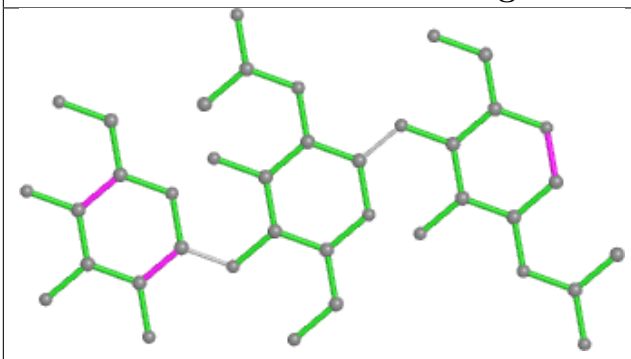


Torsions



Rings

Oligosaccharide Chain q



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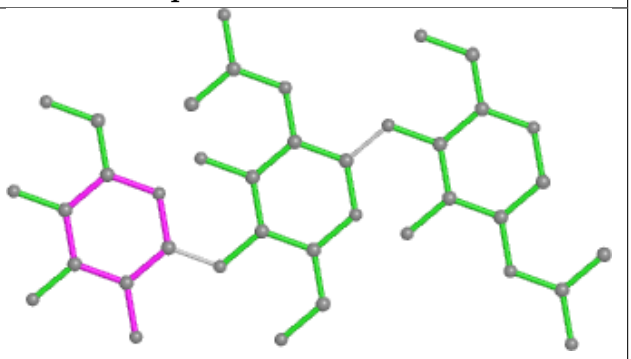

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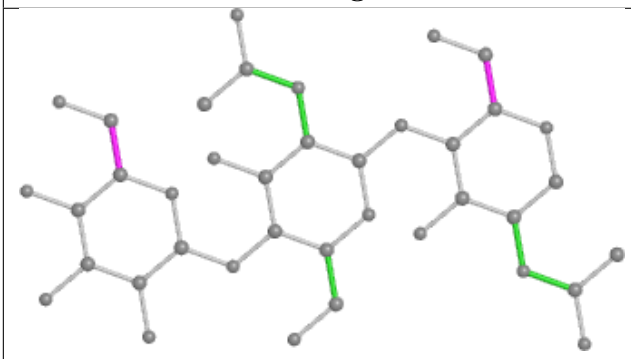

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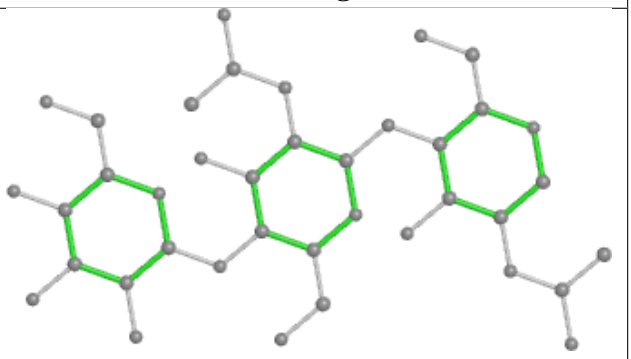
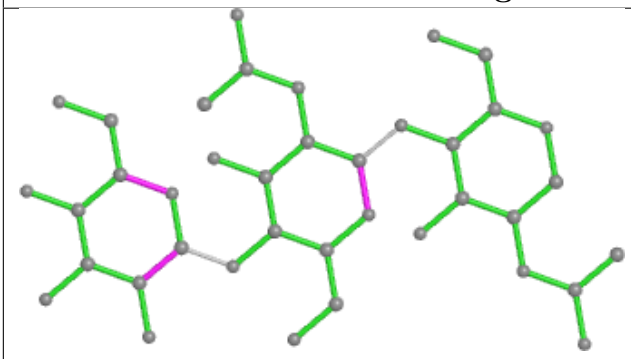


Rings

Oligosaccharide Chain w



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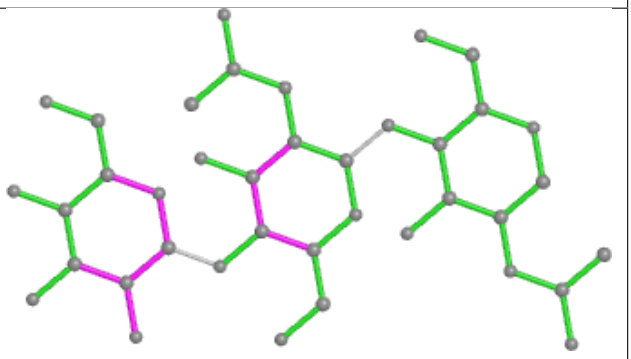

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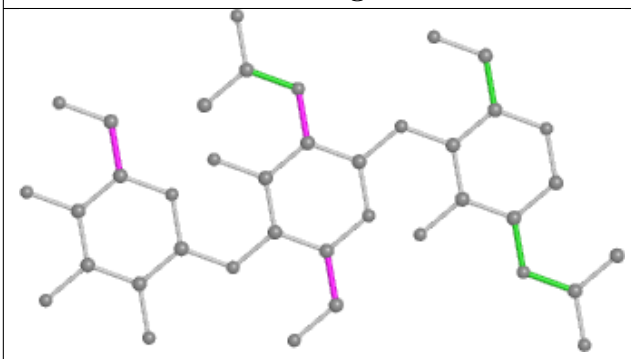

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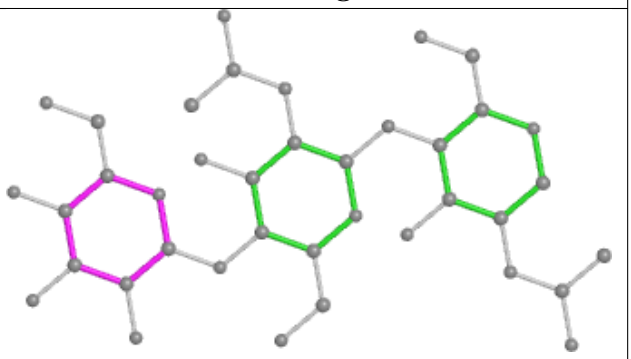
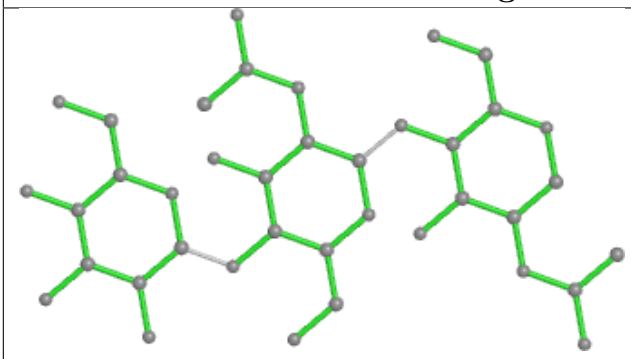


Rings

Oligosaccharide Chain y



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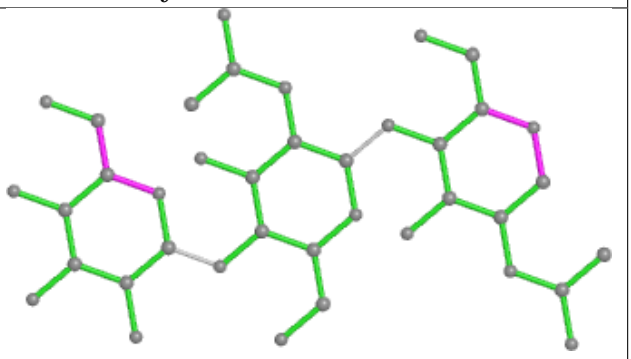
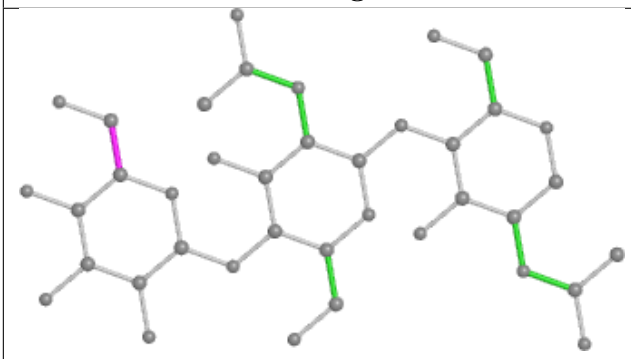


Bond angles



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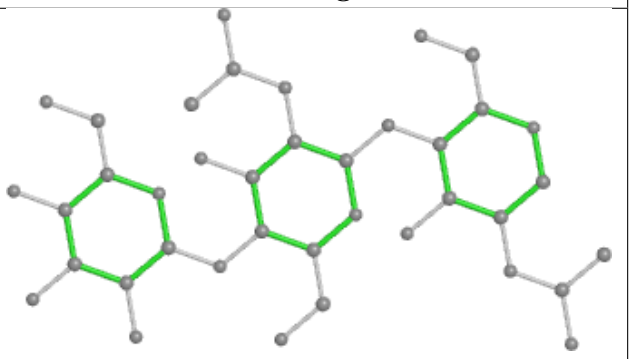
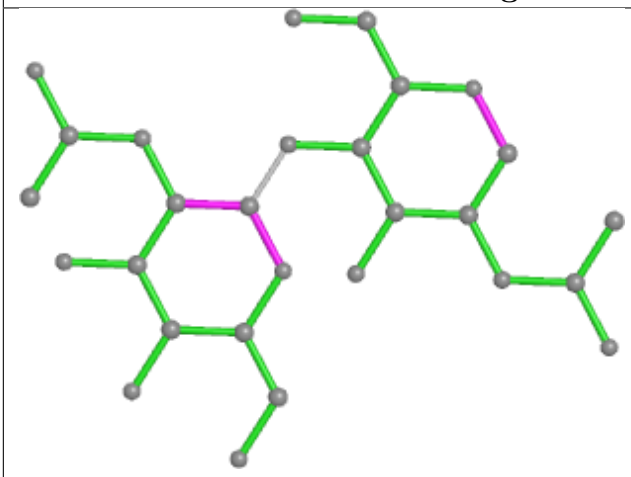


Rings

Oligosaccharide Chain f



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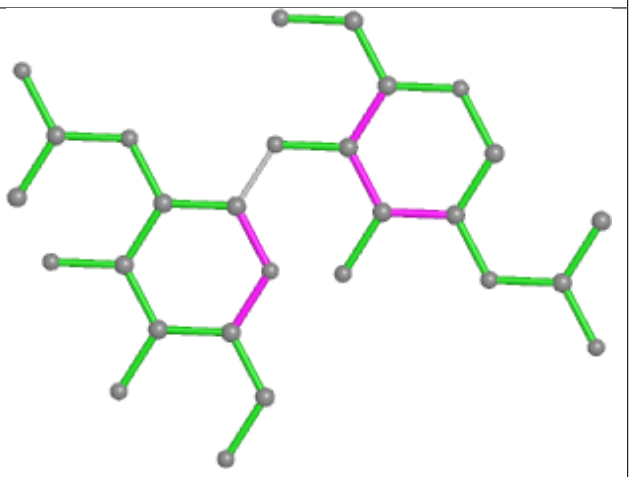

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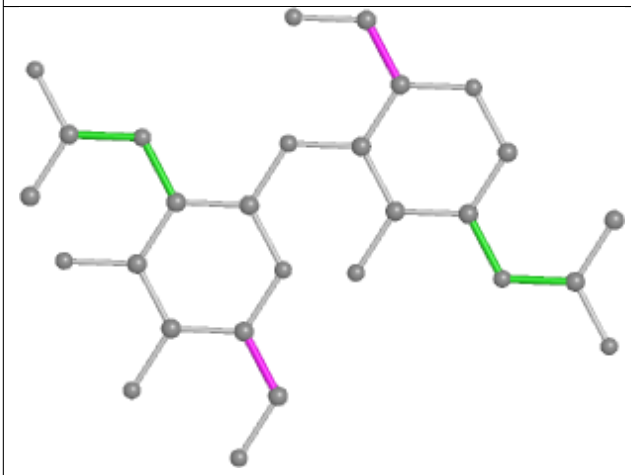

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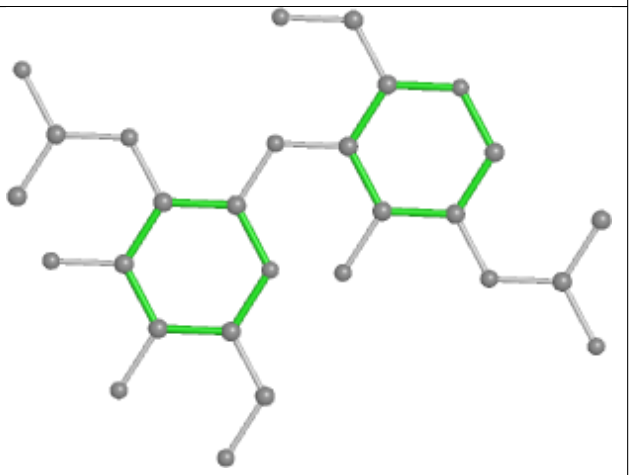
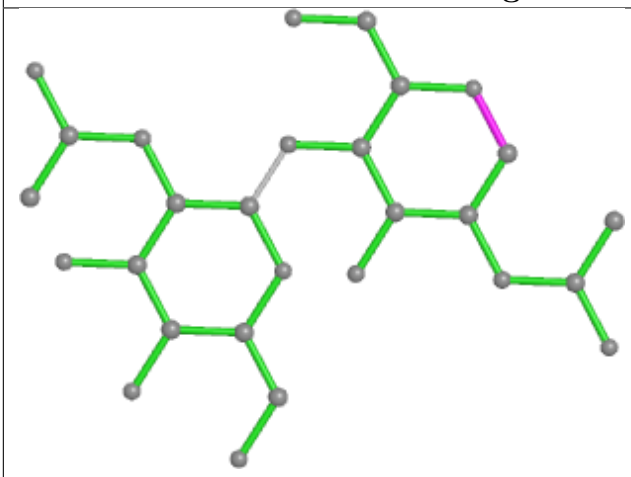


Rings

Oligosaccharide Chain i



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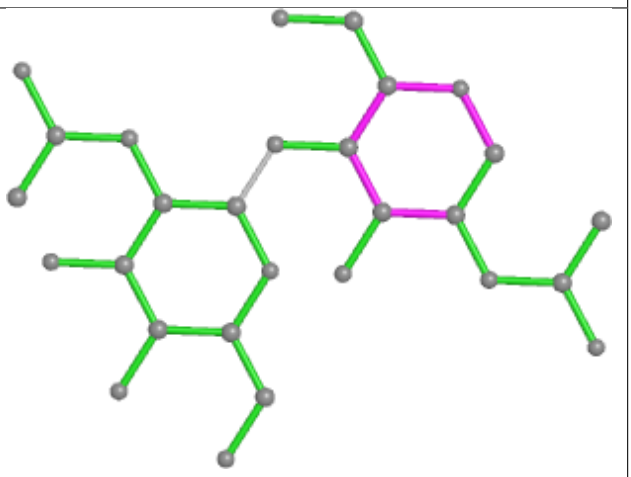
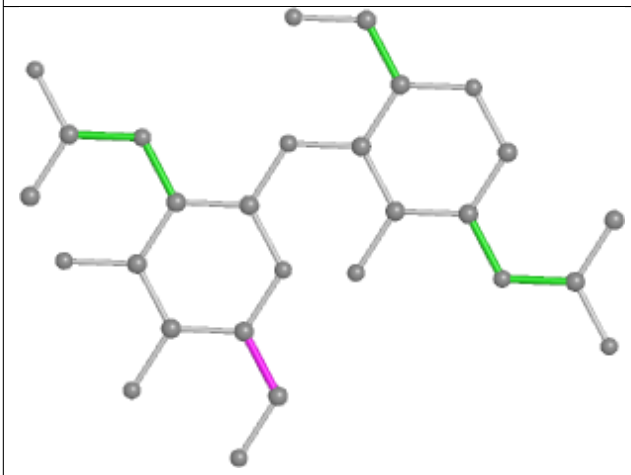


Bond angles



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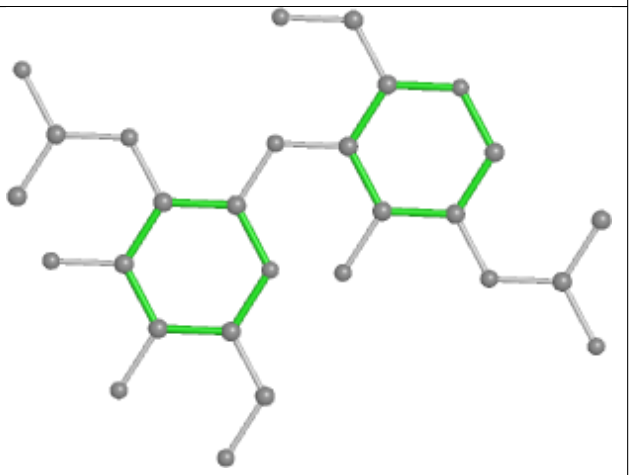
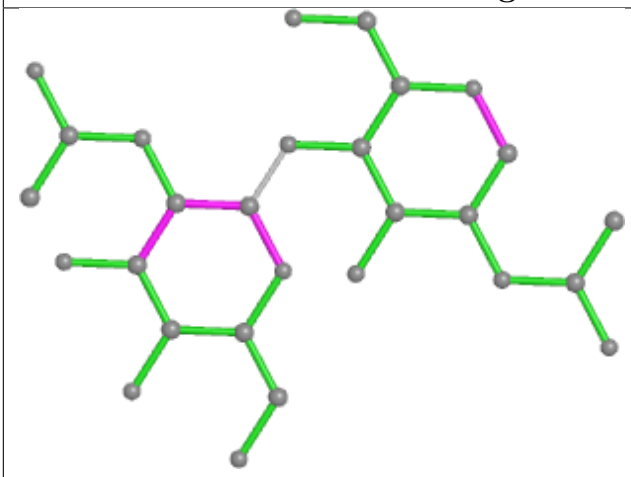


Rings

Oligosaccharide Chain k



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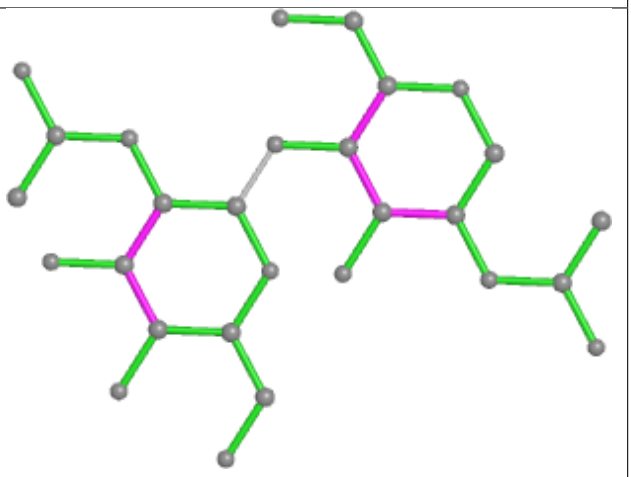
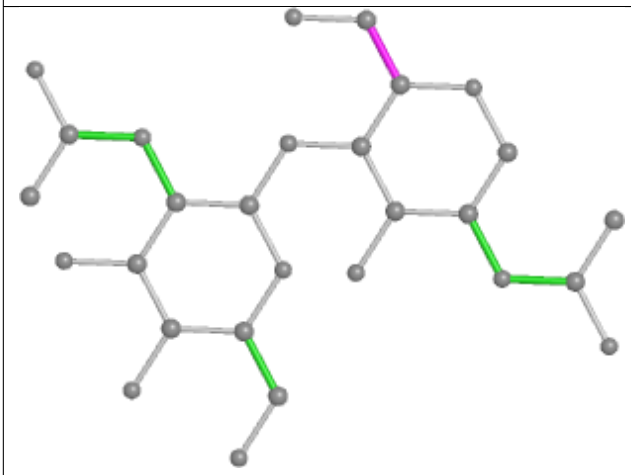


Bond angles



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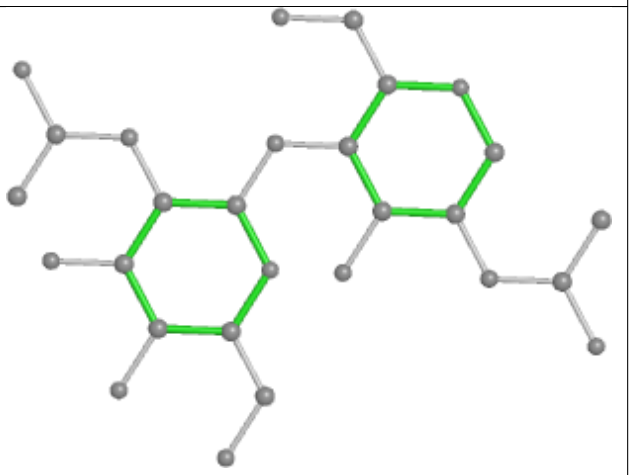
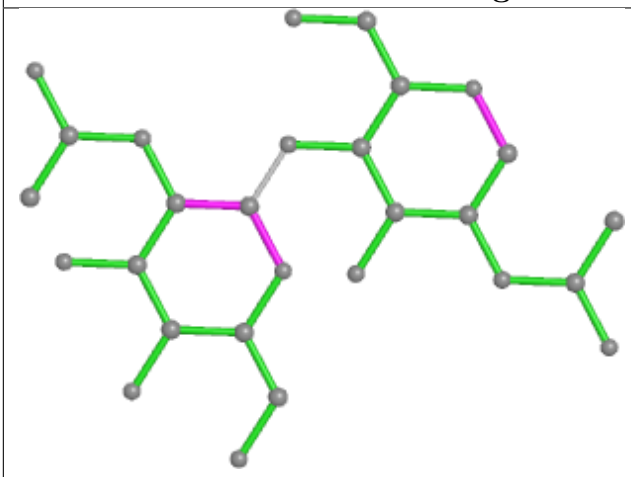


Rings

Oligosaccharide Chain m



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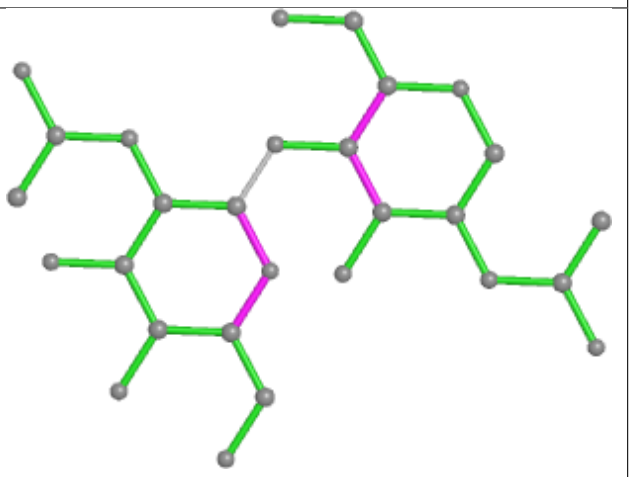
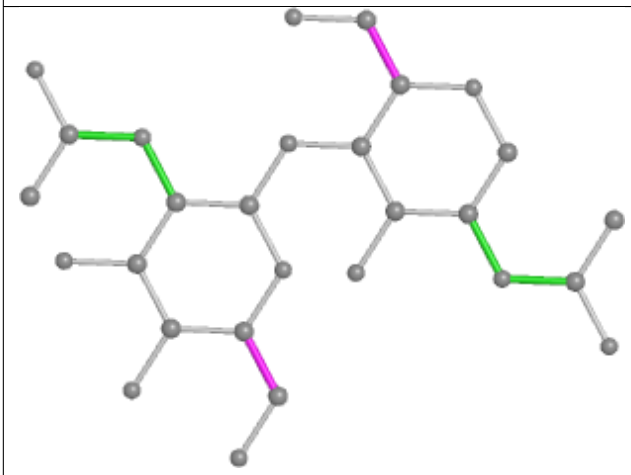


Bond angles



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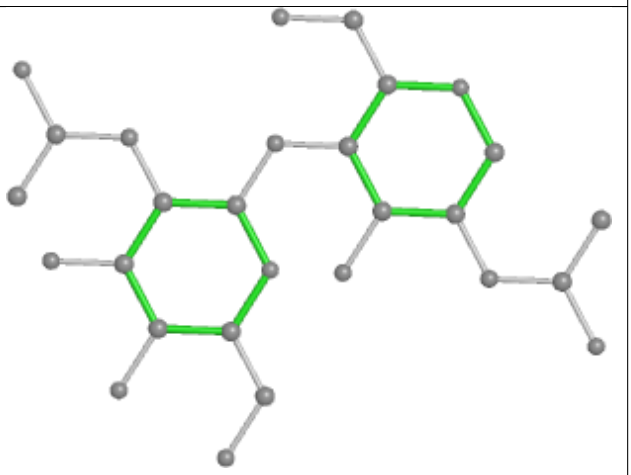
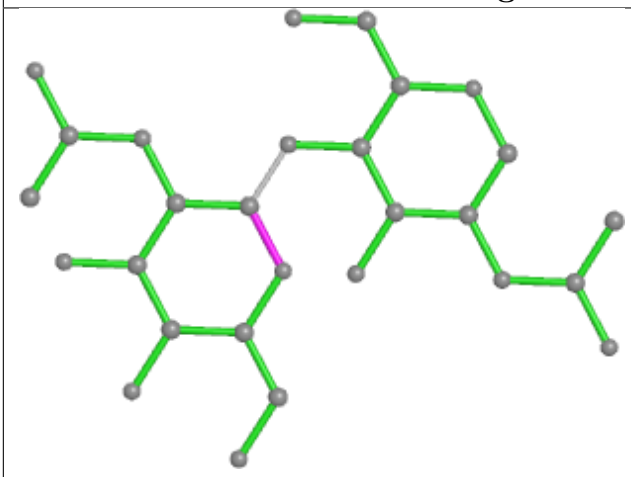


Rings

Oligosaccharide Chain p



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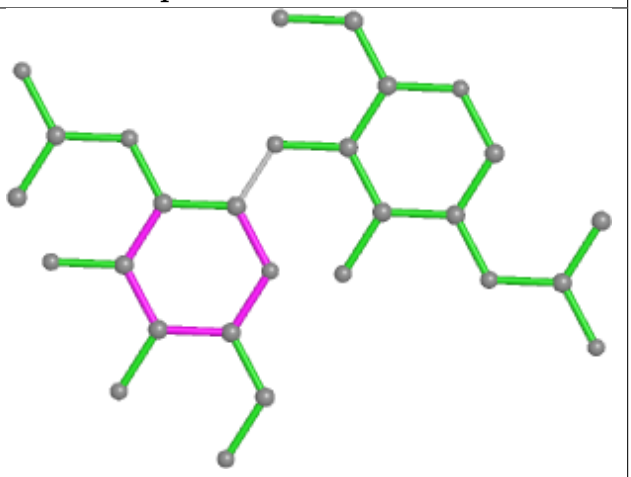
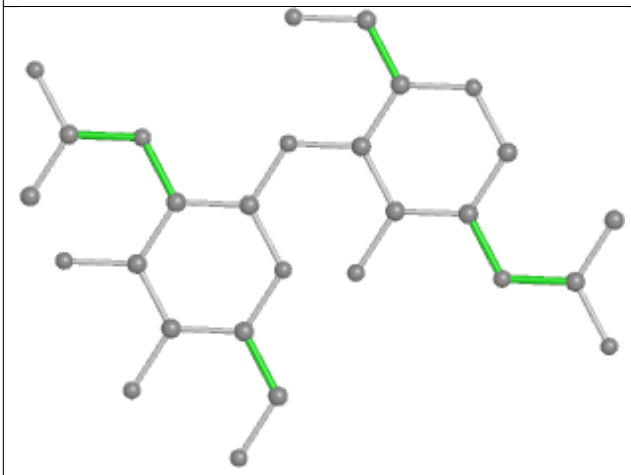


Bond angles



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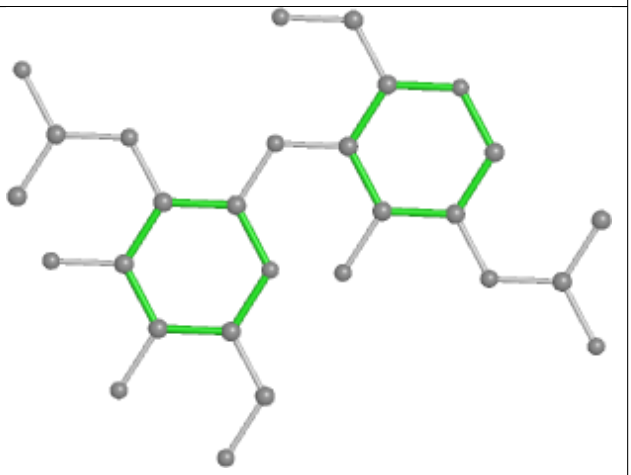
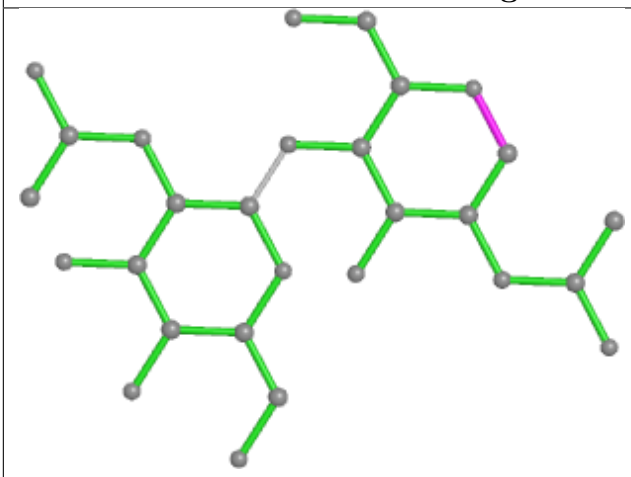


Rings

Oligosaccharide Chain r



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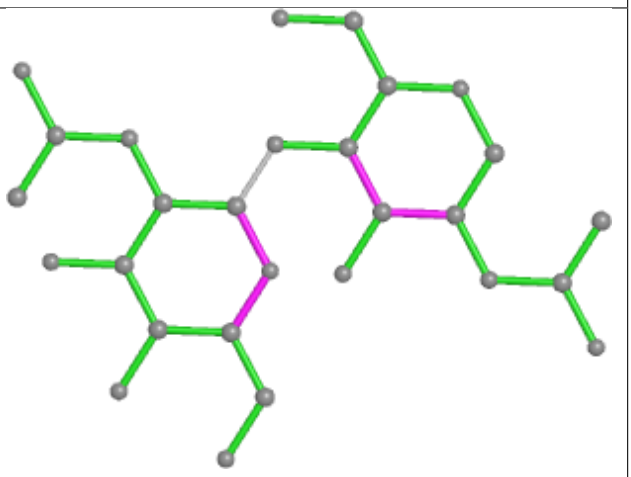

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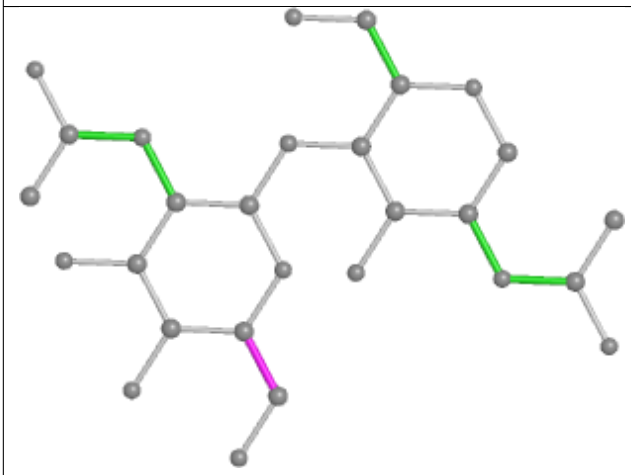

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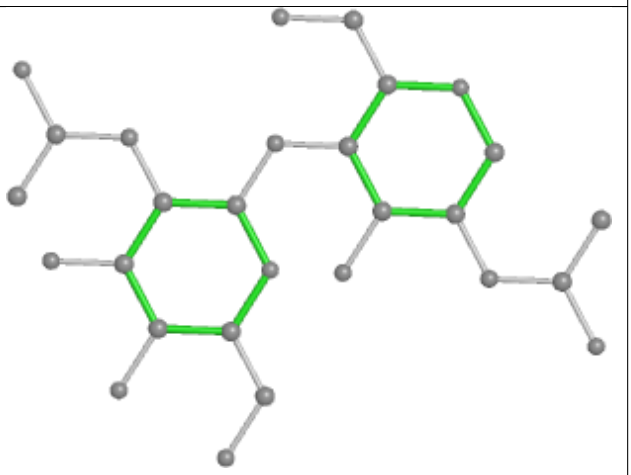
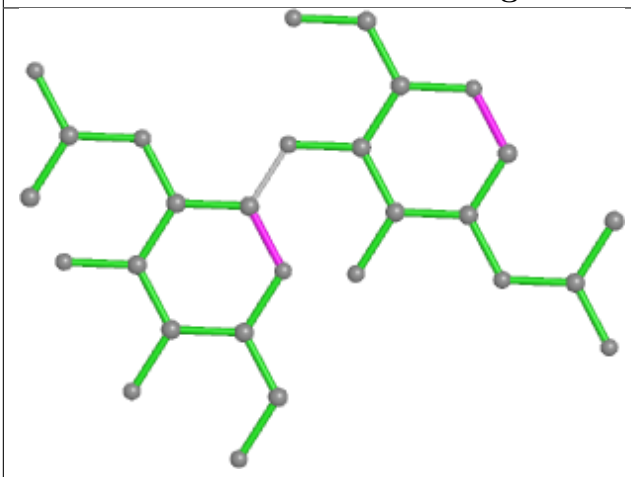


Rings

Oligosaccharide Chain t



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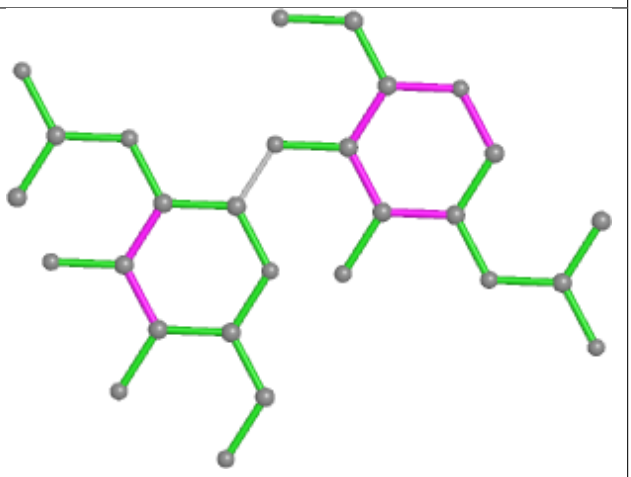

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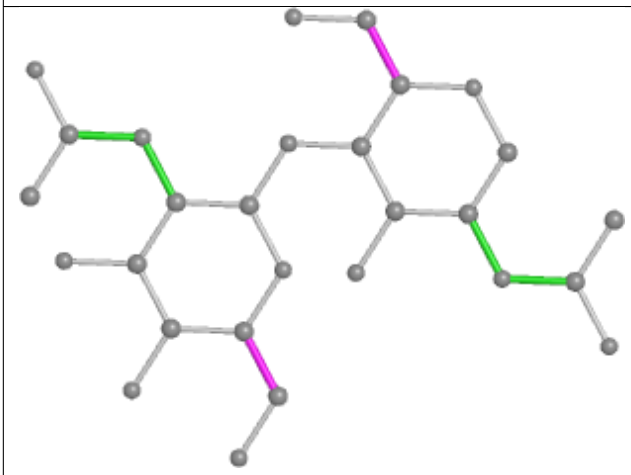

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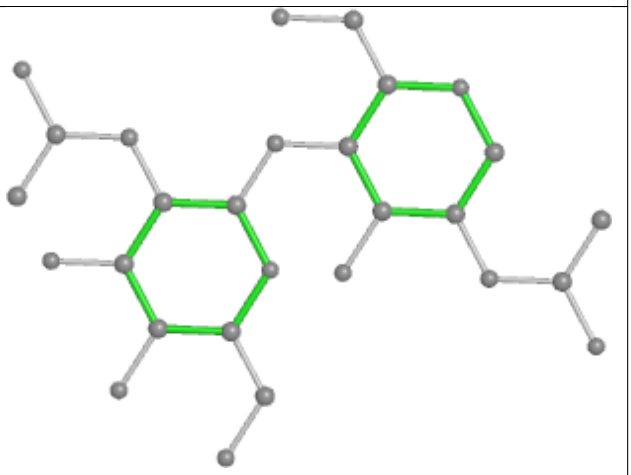
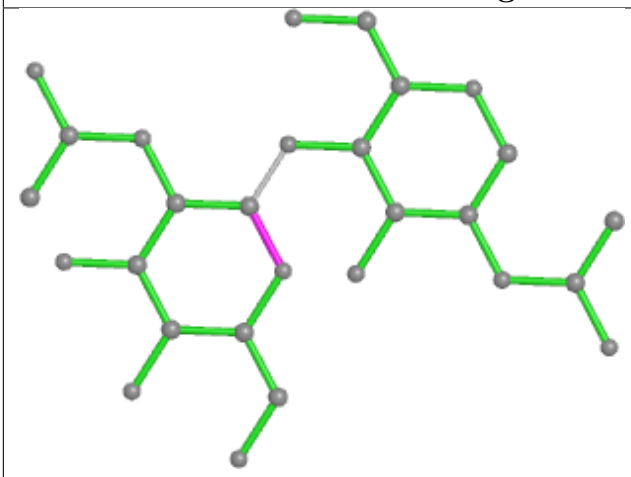


Rings

Oligosaccharide Chain u



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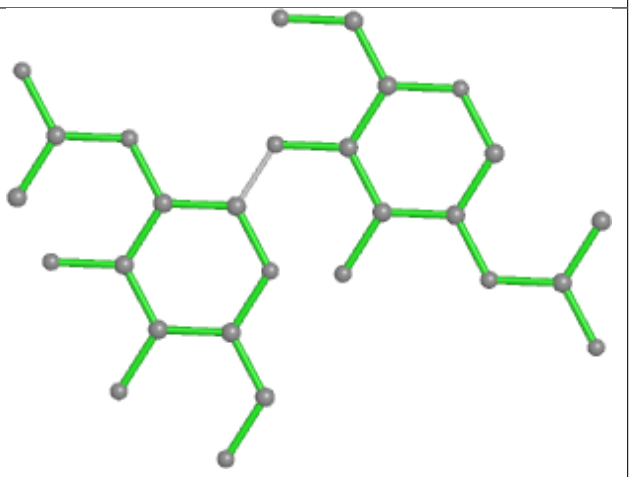
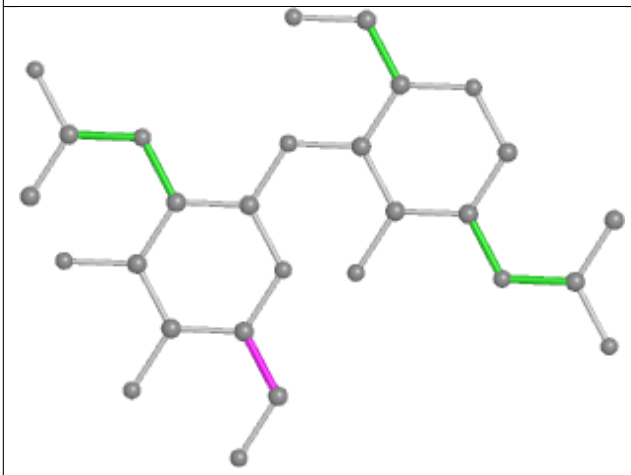


Bond angles



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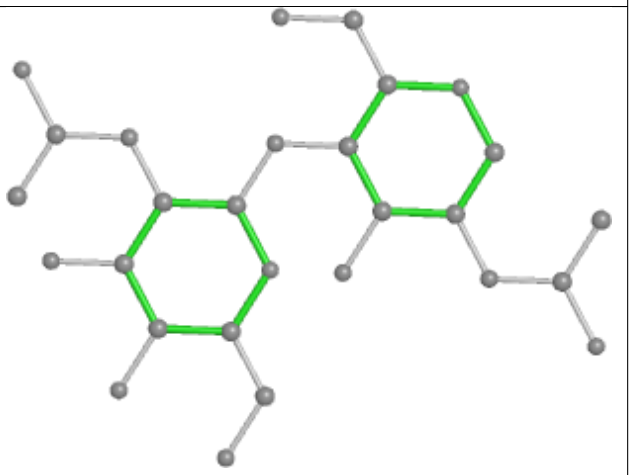
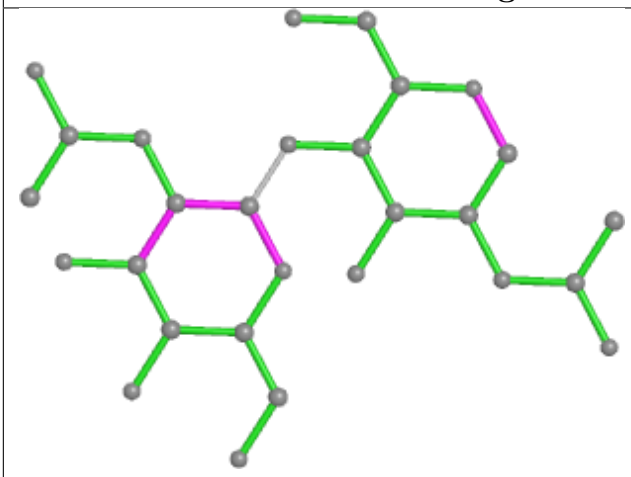


Rings

Oligosaccharide Chain v



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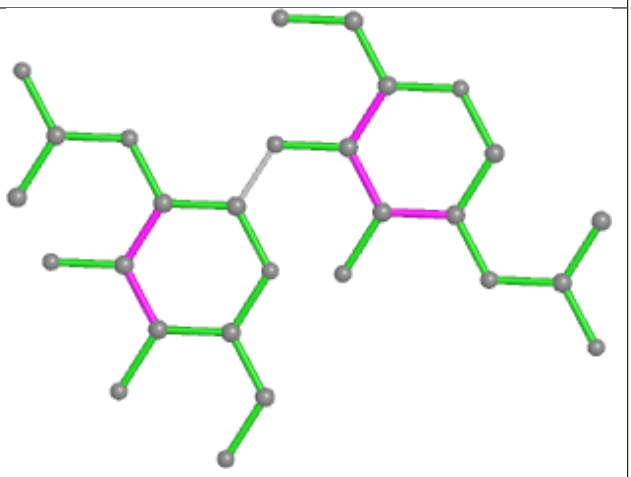
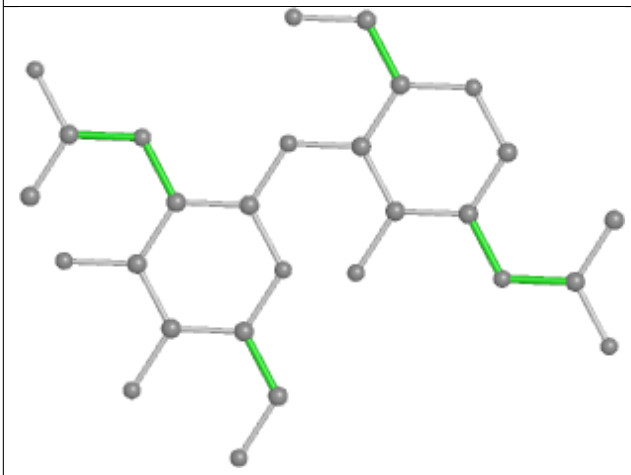


Bond angles



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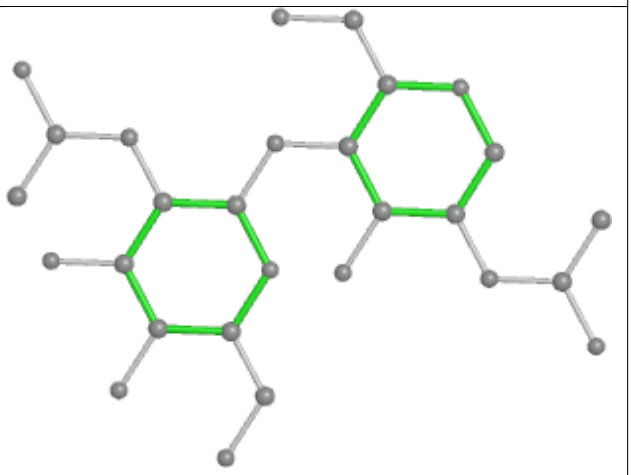
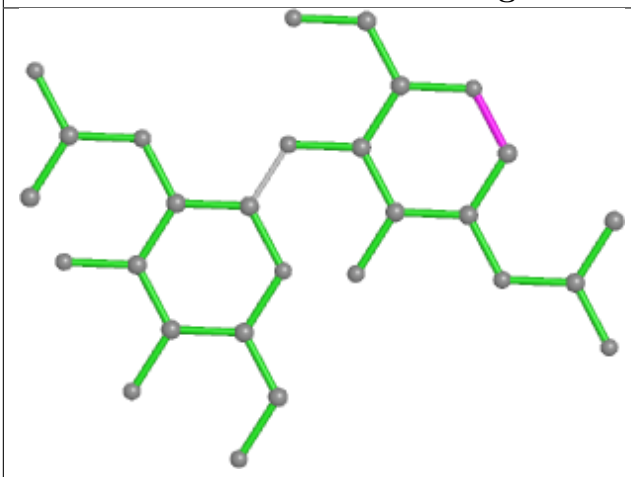


Rings

Oligosaccharide Chain x



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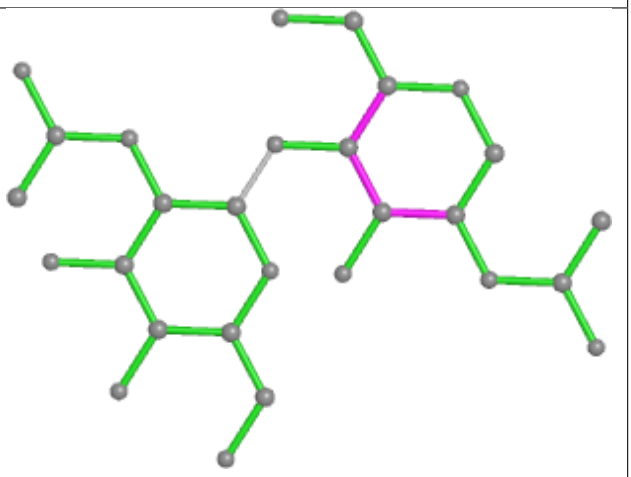
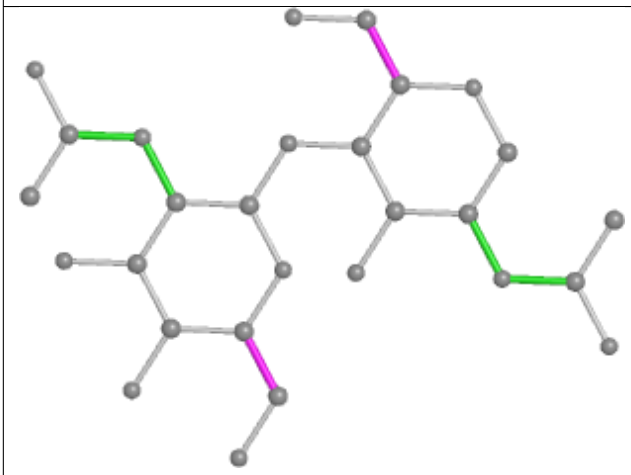


Bond angles



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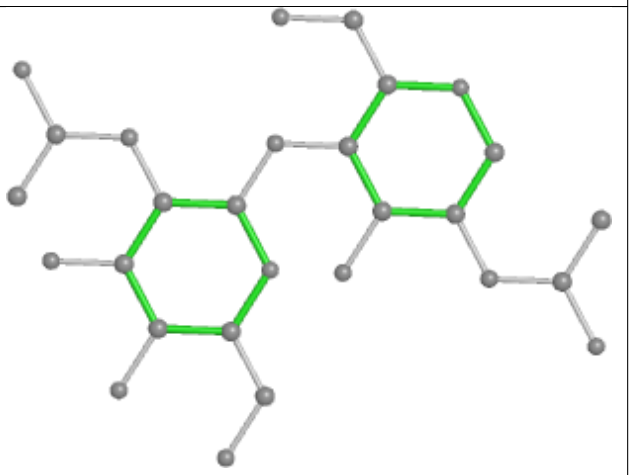
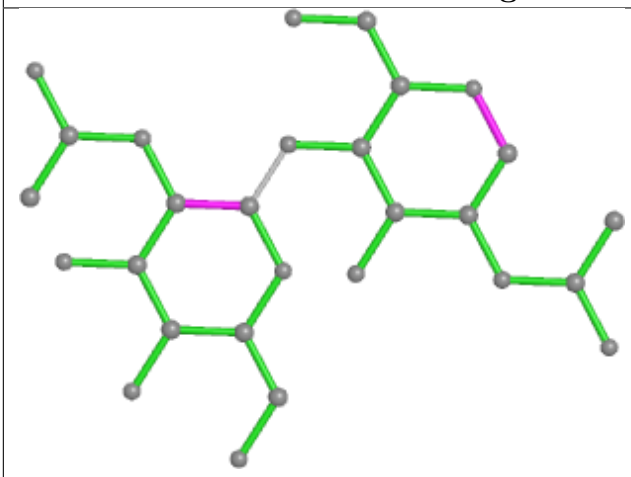
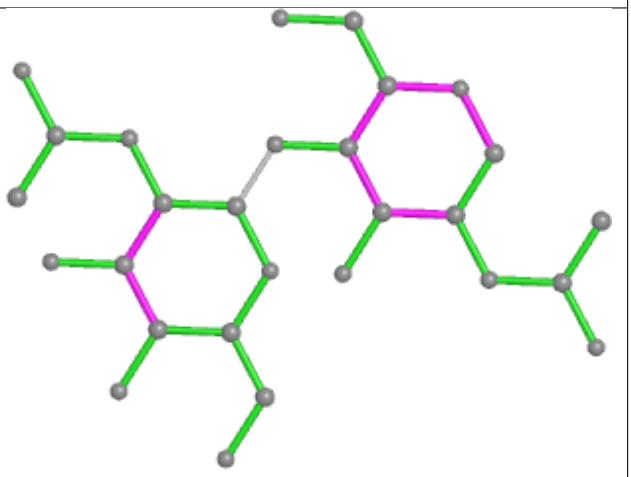


Rings

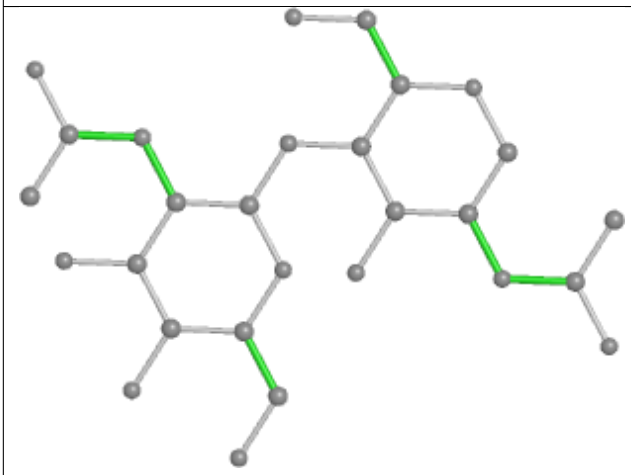
Oligosaccharide Chain z



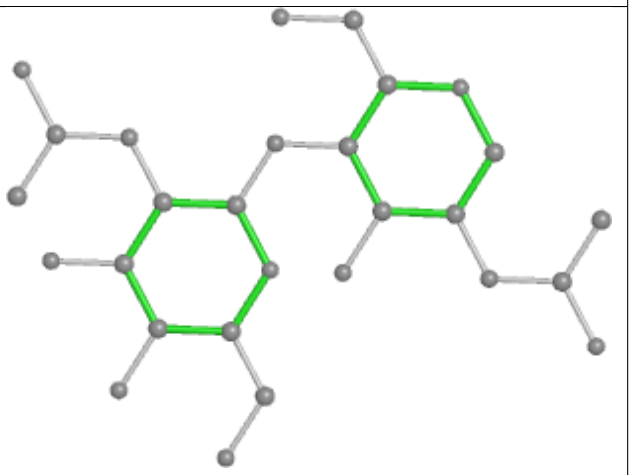
Bond lengths



Bond angles

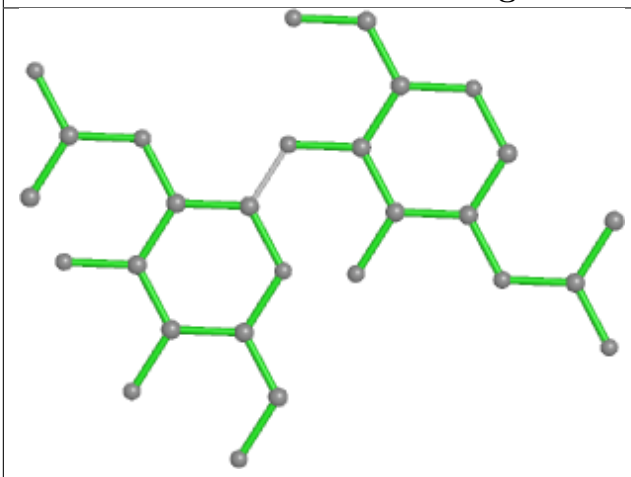


Torsions

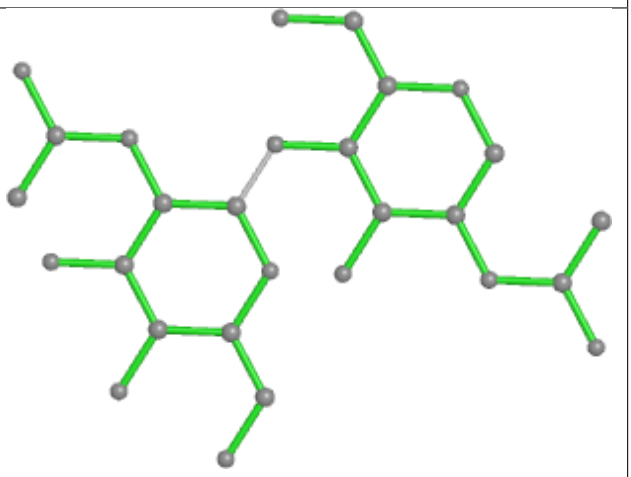


Rings

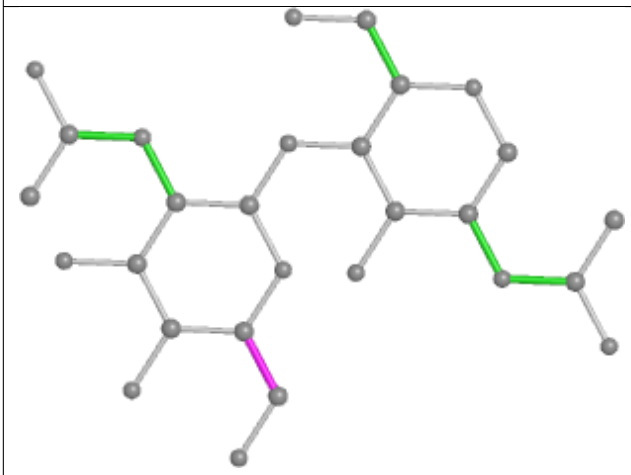
Oligosaccharide Chain 0



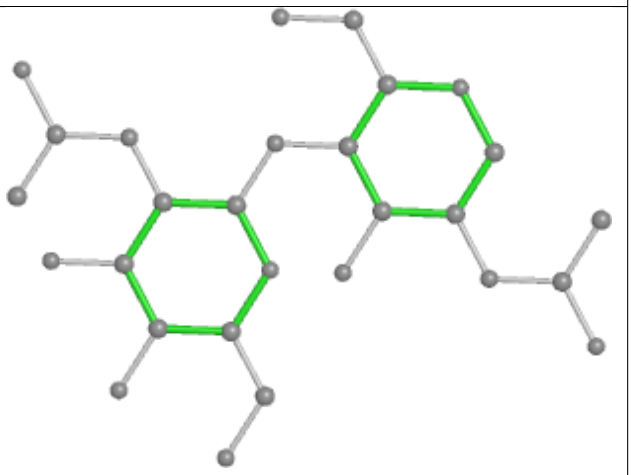
Bond lengths



Bond angles

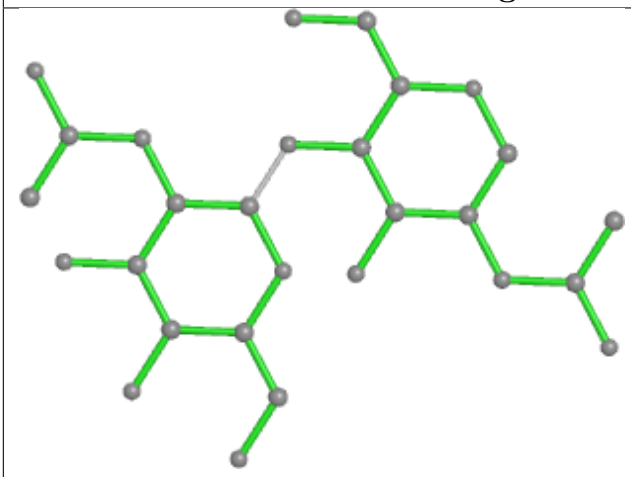


Torsions

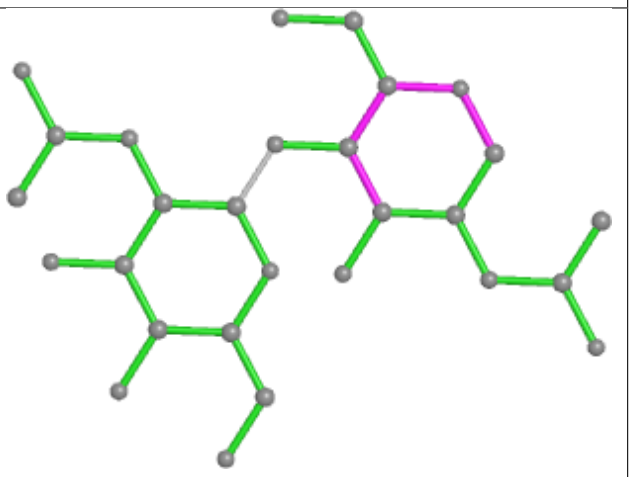


Rings

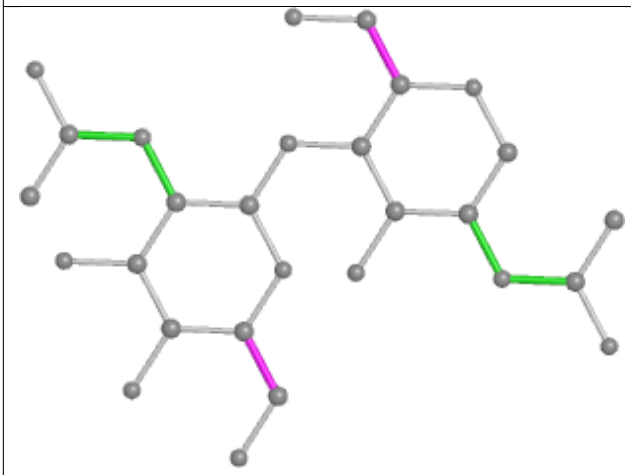
Oligosaccharide Chain 1



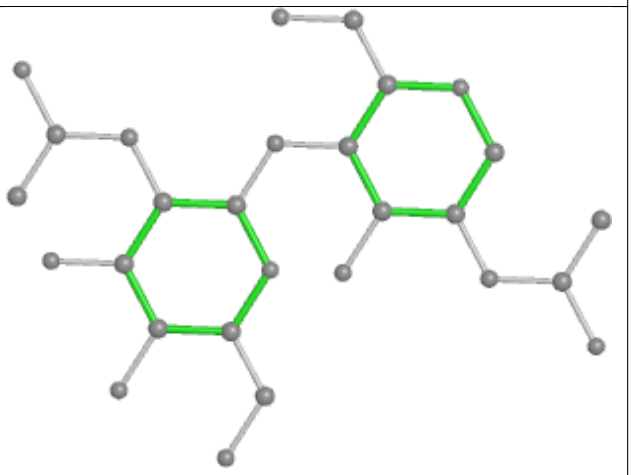
Bond lengths



Bond angles

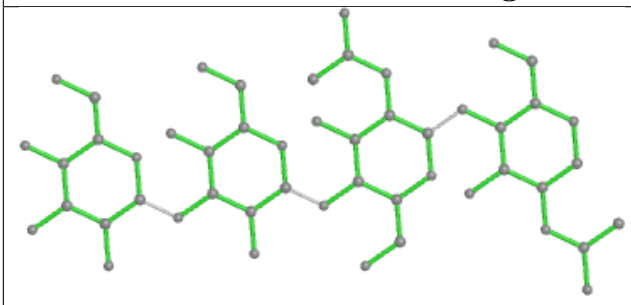


Torsions

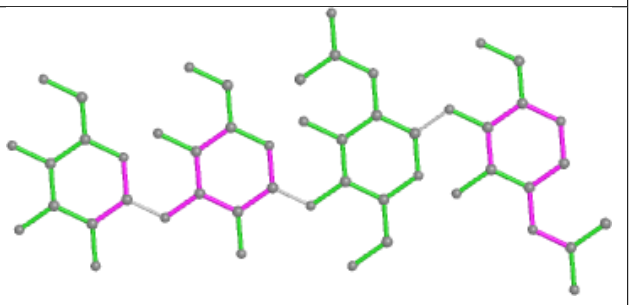


Rings

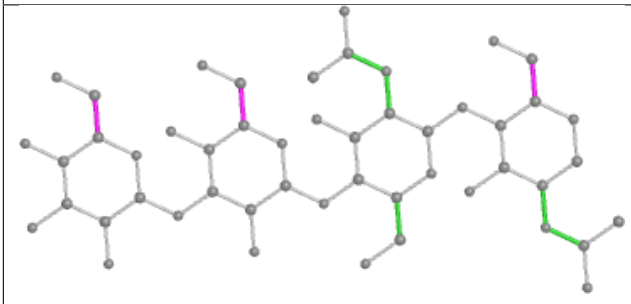
Oligosaccharide Chain s



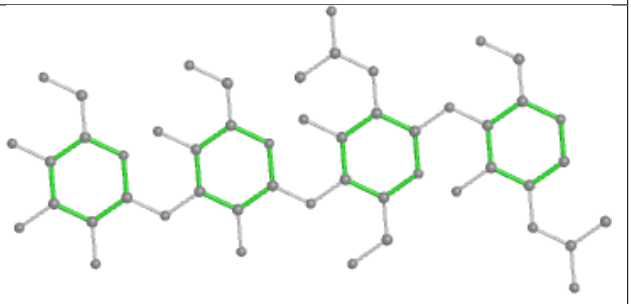
Bond lengths



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.

All (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
6	K	2004	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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

All (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
2	P	140	PHE	11.0
1	O	12	GLN	10.7
1	Q	16	GLY	9.9
2	d	141	TYR	9.9
1	a	16	GLY	9.7
2	P	27	SER	9.6
2	V	157	TYR	9.4
2	d	8	GLY	9.3
2	X	142	HIS	9.0
2	d	153	ARG	9.0
2	R	32	SER	8.8
1	c	23	THR	8.8
2	b	153	ARG	8.7
1	Y	12	GLN	8.6
2	Z	22	TYR	8.5
2	P	32	SER	8.4
2	P	33	GLY	8.3
2	Z	23	GLY	8.3
1	Y	23	THR	8.1
2	d	32	SER	8.1
1	Q	14	CYS	8.1
1	O	14	CYS	8.0
2	N	22	TYR	8.0
2	V	158	ASP	8.0

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Mol	Chain	Res	Type	RSRZ
2	F	157	TYR	8.0
2	Z	157	TYR	8.0
2	V	140	PHE	7.9
2	b	35	ALA	7.8
1	M	9	PRO	7.8
1	a	23	THR	7.7
2	X	27	SER	7.7
2	d	152	VAL	7.6
2	b	37	ASP	7.5
2	V	22	TYR	7.5
1	Q	13	ILE	7.4
2	X	140	PHE	7.4
2	N	29	GLU	7.3
1	S	12	GLN	7.2
2	P	26	HIS	7.2
2	b	130	ALA	7.2
1	K	12	GLN	7.2
1	W	12	GLN	7.1
2	R	22	TYR	7.1
1	M	8	ASP	7.1
2	F	1	GLY	7.0
2	Z	140	PHE	7.0
1	M	16	GLY	7.0
2	Z	152	VAL	7.0
2	Z	153	ARG	6.9
1	M	10	GLY	6.9
1	O	324	PRO	6.9
2	b	142	HIS	6.9
1	M	14	CYS	6.9
2	Z	37	ASP	6.8
1	c	15	ILE	6.8
2	F	140	PHE	6.8
1	Q	12	GLN	6.7
2	Z	35	ALA	6.7
2	b	24	TYR	6.7
2	T	140	PHE	6.7
2	Z	1	GLY	6.7
2	Z	130	ALA	6.7
2	P	25	HIS	6.5
1	O	16	GLY	6.5
2	D	26	HIS	6.5
1	M	13	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
1	Y	14	CYS	6.4
2	N	160	PRO	6.4
2	Z	38	LYS	6.4
1	Q	18	HIS	6.4
1	Y	13	ILE	6.3
2	L	1	GLY	6.3
1	K	13	ILE	6.3
2	Z	159	TYR	6.3
2	V	149	MET	6.2
2	b	23	GLY	6.2
2	R	27	SER	6.2
2	b	1	GLY	6.2
1	M	12	GLN	6.2
2	L	142	HIS	6.2
2	d	24	TYR	6.2
2	b	140	PHE	6.1
2	b	36	ALA	6.1
2	P	31	GLY	6.1
1	U	8	ASP	6.1
1	K	16	GLY	6.1
2	X	143	LYS	6.1
2	d	157	TYR	6.1
2	b	129	ASN	6.0
2	d	37	ASP	6.0
2	N	140	PHE	6.0
2	V	143	LYS	6.0
1	I	324	PRO	6.0
2	b	26	HIS	6.0
2	Z	41	THR	6.0
2	P	22	TYR	6.0
2	R	176	GLY	6.0
1	E	324	PRO	5.9
2	F	158	ASP	5.9
1	Q	320	LEU	5.8
2	d	38	LYS	5.8
2	Z	125	GLN	5.8
1	Y	16	GLY	5.8
2	d	154	ASN	5.7
2	N	27	SER	5.7
2	d	36	ALA	5.7
2	L	138	PHE	5.7
2	L	144	CYS	5.7

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Mol	Chain	Res	Type	RSRZ
2	N	23	GLY	5.7
2	X	22	TYR	5.7
2	L	140	PHE	5.6
2	b	157	TYR	5.6
2	Z	24	TYR	5.6
2	b	143	LYS	5.5
1	O	10	GLY	5.5
2	L	22	TYR	5.5
1	U	13	ILE	5.5
2	b	128	ASP	5.5
1	a	13	ILE	5.5
1	O	11	ASP	5.5
2	V	161	GLN	5.4
1	M	11	ASP	5.4
1	c	14	CYS	5.3
2	X	26	HIS	5.3
2	X	157	TYR	5.3
1	G	324	PRO	5.3
2	V	27	SER	5.3
2	V	35	ALA	5.3
2	V	144	CYS	5.3
2	d	144	CYS	5.3
2	d	143	LYS	5.3
2	X	160	PRO	5.3
2	N	144	CYS	5.3
2	d	156	THR	5.2
2	D	22	TYR	5.2
2	F	33	GLY	5.2
2	b	32	SER	5.2
2	Z	148	CYS	5.2
2	T	22	TYR	5.2
2	d	170	ARG	5.2
2	T	157	TYR	5.2
2	T	35	ALA	5.2
1	Q	10	GLY	5.2
1	c	13	ILE	5.2
1	Y	21[A]	ASN	5.1
2	D	140	PHE	5.1
2	d	16	GLY	5.1
2	d	22	TYR	5.1
2	X	23	GLY	5.0
2	Z	42	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
2	P	23	GLY	5.0
2	b	152	VAL	5.0
2	L	134	GLY	5.0
2	Z	176	GLY	5.0
2	d	155	GLY	4.9
2	P	160	PRO	4.9
2	D	1	GLY	4.9
1	a	11	ASP	4.9
1	C	12	GLN	4.9
2	d	158	ASP	4.9
2	V	24	TYR	4.8
2	P	10	ILE	4.8
2	T	141	TYR	4.8
1	Q	319	GLY	4.8
2	D	144	CYS	4.8
2	d	35	ALA	4.8
2	T	158	ASP	4.8
2	V	141	TYR	4.8
2	d	163	SER	4.8
2	P	29	GLU	4.8
2	d	132	GLU	4.8
2	N	157	TYR	4.7
2	P	144	CYS	4.7
2	F	142	HIS	4.7
1	Y	15	ILE	4.7
2	R	33	GLY	4.7
1	K	15	ILE	4.7
2	R	171	GLU	4.7
1	U	14	CYS	4.7
1	C	13	ILE	4.7
2	T	143	LYS	4.7
2	R	25	HIS	4.7
2	H	175	SER	4.7
2	N	159	TYR	4.7
2	b	160	PRO	4.7
2	Z	36	ALA	4.7
1	a	22	SER	4.6
2	V	148	CYS	4.6
2	X	24	TYR	4.6
2	X	149	MET	4.6
2	T	24	TYR	4.6
2	F	141	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	P	148	CYS	4.6
2	Z	16	GLY	4.6
2	N	24	TYR	4.6
2	b	38	LYS	4.6
2	d	31	GLY	4.6
2	R	160	PRO	4.6
2	N	32	SER	4.5
2	R	31	GLY	4.5
2	R	138	PHE	4.5
1	S	13	ILE	4.5
2	X	32	SER	4.5
2	N	21	TRP	4.5
2	X	158	ASP	4.5
2	L	132	GLU	4.5
2	Z	4	GLY	4.5
2	Z	136	GLY	4.5
1	E	322	ASN	4.5
2	N	176	GLY	4.4
1	c	22	SER	4.4
2	V	156	THR	4.4
2	T	21	TRP	4.4
2	b	144	CYS	4.4
2	d	164	GLU	4.4
2	b	22	TYR	4.4
2	T	38	LYS	4.4
2	b	149	MET	4.4
2	T	144	CYS	4.3
2	b	7	ALA	4.3
2	d	148	CYS	4.3
2	L	133	LEU	4.3
2	X	141	TYR	4.3
2	P	139	GLU	4.3
2	L	145	ASP	4.3
1	Y	323	SER	4.3
2	P	7	ALA	4.3
2	Z	26	HIS	4.3
2	Z	32	SER	4.3
2	R	175	SER	4.3
2	b	148	CYS	4.3
1	Y	22	SER	4.2
2	b	31	GLY	4.2
1	c	320	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	Z	126	LEU	4.2
2	T	149	MET	4.2
2	F	32	SER	4.2
1	O	9	PRO	4.2
1	S	8	ASP	4.2
2	d	168	LEU	4.2
2	d	26	HIS	4.1
2	d	9	PHE	4.1
2	N	46	ASP	4.1
2	Z	128	ASP	4.1
1	K	319	GLY	4.1
2	R	157	TYR	4.1
2	H	177	ARG	4.1
1	I	8	ASP	4.1
2	b	27	SER	4.1
2	b	168	LEU	4.1
2	V	152	VAL	4.1
2	F	126	LEU	4.1
2	b	34	TYR	4.1
1	E	25	GLN	4.1
2	Z	29	GLU	4.1
2	b	138	PHE	4.0
1	C	24	GLU	4.0
2	D	134	GLY	4.0
2	Z	151	SER	4.0
1	c	21[A]	ASN	4.0
2	V	21	TRP	4.0
1	C	324	PRO	4.0
2	P	142	HIS	4.0
2	Z	143	LYS	4.0
2	d	25	HIS	4.0
2	d	27	SER	4.0
2	P	157	TYR	4.0
1	Y	317	ALA	4.0
2	Z	154	ASN	3.9
2	F	22	TYR	3.9
1	G	9	PRO	3.9
1	Q	324	PRO	3.9
1	Q	24	GLU	3.9
2	V	23	GLY	3.9
2	d	15	GLN	3.9
2	H	176	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	33	GLY	3.9
2	P	138	PHE	3.9
2	d	1	GLY	3.9
1	Y	11	ASP	3.9
2	Z	46	ASP	3.9
2	d	121	LYS	3.9
2	D	27	SER	3.9
2	R	140	PHE	3.9
2	R	177	ARG	3.9
1	Y	30	MET	3.9
2	d	172	GLU	3.9
2	T	156	THR	3.9
2	b	33	GLY	3.9
2	N	35	ALA	3.9
2	N	148	CYS	3.8
1	K	324	PRO	3.8
2	Z	40	SER	3.8
2	d	18	VAL	3.8
1	c	20	ASN	3.8
1	a	15	ILE	3.8
2	V	153	ARG	3.8
2	X	156	THR	3.8
2	Z	25	HIS	3.8
1	S	324	PRO	3.8
2	N	142	HIS	3.8
2	N	143	LYS	3.8
1	K	17	TYR	3.8
2	L	141	TYR	3.8
2	T	172	GLU	3.8
1	A	8	ASP	3.7
2	F	177	ARG	3.7
1	K	14	CYS	3.7
2	P	5	ALA	3.7
2	Z	141	TYR	3.7
2	N	25	HIS	3.7
2	X	16	GLY	3.7
1	Q	11	ASP	3.7
2	N	158	ASP	3.7
2	R	26	HIS	3.7
2	X	25	HIS	3.7
2	d	142	HIS	3.7
2	F	38	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	24	TYR	3.7
1	E	24	GLU	3.7
2	Z	39	GLU	3.7
1	c	37	THR	3.7
2	B	176	GLY	3.7
2	R	134	GLY	3.7
2	d	136	GLY	3.7
2	R	19	ASP	3.7
2	D	139	GLU	3.7
2	R	158	ASP	3.7
2	V	126	LEU	3.7
2	X	151	SER	3.7
2	D	157	TYR	3.7
2	P	158	ASP	3.6
2	R	18	VAL	3.6
2	V	139	GLU	3.6
2	X	7	ALA	3.6
1	W	8	ASP	3.6
2	T	26	HIS	3.6
2	F	35	ALA	3.6
1	c	11	ASP	3.6
2	V	151	SER	3.6
2	B	175	SER	3.6
2	D	33	GLY	3.6
2	X	161	GLN	3.6
2	R	1	GLY	3.6
2	V	162	TYR	3.6
2	L	146	ASN	3.6
2	d	166	ALA	3.6
1	E	23	THR	3.6
2	P	6	ILE	3.6
2	X	35	ALA	3.6
2	d	140	PHE	3.5
1	Y	9	PRO	3.5
2	Z	160	PRO	3.5
2	d	171	GLU	3.5
1	W	288	ILE	3.5
2	N	30	GLN	3.5
1	U	9	PRO	3.5
2	b	170	ARG	3.5
2	b	177	ARG	3.5
2	F	21	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
2	Z	127	ARG	3.5
1	U	11	ASP	3.5
1	W	11	ASP	3.5
2	V	155	GLY	3.5
2	V	25	HIS	3.5
1	a	323	SER	3.5
2	P	4	GLY	3.5
2	d	149	MET	3.5
2	b	158	ASP	3.5
1	A	324	PRO	3.5
2	P	162	TYR	3.5
1	a	20	ASN	3.4
2	N	19	ASP	3.4
2	T	27	SER	3.4
2	V	147	GLU	3.4
2	d	106	ARG	3.4
2	V	150	GLU	3.4
2	D	158	ASP	3.4
2	D	25	HIS	3.4
2	B	140	PHE	3.4
2	F	156	THR	3.4
2	F	26	HIS	3.4
2	F	145	ASP	3.4
1	Y	322	ASN	3.4
1	S	9	PRO	3.4
2	N	26	HIS	3.4
2	b	9	PHE	3.4
1	a	63	ASP	3.4
2	F	138	PHE	3.4
2	d	151	SER	3.4
2	R	159	TYR	3.4
2	Z	144	CYS	3.4
1	Q	8	ASP	3.4
2	Z	47	GLY	3.4
2	N	161	GLN	3.3
2	b	156	THR	3.3
2	R	137	CYS	3.3
1	O	34	VAL	3.3
2	F	171	GLU	3.3
2	X	144	CYS	3.3
2	Z	156	THR	3.3
1	E	13	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	Z	13	GLY	3.3
2	X	153	ARG	3.3
2	T	23	GLY	3.3
2	Z	45	ILE	3.3
2	d	29	GLU	3.3
2	Z	131	LYS	3.3
1	c	63	ASP	3.3
2	d	17	MET	3.3
2	F	24	TYR	3.3
1	Y	34	VAL	3.3
2	R	29	GLU	3.3
2	b	132	GLU	3.3
2	D	145	ASP	3.3
1	c	24	GLU	3.3
2	L	177	ARG	3.3
1	O	323	SER	3.3
2	P	156	THR	3.3
2	P	145	ASP	3.3
2	Z	149	MET	3.2
2	Z	175	SER	3.2
2	N	36	ALA	3.2
2	R	141	TYR	3.2
2	X	29	GLU	3.2
1	G	12	GLN	3.2
1	W	16	GLY	3.2
2	X	31	GLY	3.2
2	P	132	GLU	3.2
1	E	16	GLY	3.2
1	Q	20	ASN	3.2
2	T	18	VAL	3.2
2	b	109	ASP	3.2
2	V	26	HIS	3.2
1	Q	9	PRO	3.2
2	P	137	CYS	3.2
1	c	312	ASN	3.2
2	X	162	TYR	3.2
2	B	156	THR	3.2
2	d	130	ALA	3.2
2	R	21	TRP	3.2
2	X	21	TRP	3.2
1	W	13	ILE	3.2
2	V	16	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	176	GLY	3.2
2	L	148	CYS	3.2
2	V	118	LEU	3.1
2	d	135	ASN	3.1
2	T	19	ASP	3.1
2	L	23	GLY	3.1
2	Z	33	GLY	3.1
2	T	161	GLN	3.1
2	Z	34	TYR	3.1
2	Z	171	GLU	3.1
2	L	175	SER	3.1
2	V	125	GLN	3.1
1	U	322	ASN	3.1
2	P	154	ASN	3.1
2	b	163	SER	3.1
2	b	155	GLY	3.1
2	N	146	ASN	3.1
2	F	166	ALA	3.1
2	N	42	GLN	3.1
2	L	168	LEU	3.1
2	b	2	LEU	3.1
2	N	177	ARG	3.1
1	A	9	PRO	3.1
1	G	8	ASP	3.1
2	N	175	SER	3.1
2	D	153	ARG	3.1
2	P	28	ASN	3.1
2	F	144	CYS	3.1
2	P	131	LYS	3.1
2	R	132	GLU	3.1
2	Z	147	GLU	3.1
1	c	17	TYR	3.0
2	F	175	SER	3.0
2	P	155	GLY	3.0
2	P	161	GLN	3.0
1	U	21[A]	ASN	3.0
2	V	29	GLU	3.0
1	I	9	PRO	3.0
1	K	24	GLU	3.0
2	N	44	ALA	3.0
2	F	31	GLY	3.0
1	O	8	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	R	168	LEU	3.0
2	B	177	ARG	3.0
2	N	31	GLY	3.0
2	T	160	PRO	3.0
2	J	38	LYS	3.0
2	X	147	GLU	3.0
2	Z	132	GLU	3.0
1	W	324	PRO	3.0
1	K	10	GLY	3.0
1	E	12	GLN	3.0
1	G	13	ILE	3.0
2	L	158	ASP	3.0
2	b	159	TYR	3.0
1	C	21[A]	ASN	3.0
2	D	32	SER	3.0
2	R	164	GLU	3.0
2	Z	158	ASP	2.9
1	Q	17	TYR	2.9
2	Z	18	VAL	2.9
1	U	22	SER	2.9
2	R	142	HIS	2.9
2	X	33	GLY	2.9
2	P	146	ASN	2.9
2	Z	14	TRP	2.9
2	P	143	LYS	2.9
2	V	160	PRO	2.9
2	L	126	LEU	2.9
2	D	177	ARG	2.9
2	d	111	HIS	2.9
2	Z	142	HIS	2.9
2	R	139	GLU	2.9
2	F	127	ARG	2.9
2	d	33	GLY	2.9
2	L	21	TRP	2.9
2	P	46	ASP	2.9
2	d	134	GLY	2.9
2	B	16	GLY	2.9
1	S	21[A]	ASN	2.8
2	L	139	GLU	2.8
2	P	177	ARG	2.8
2	V	38	LYS	2.8
2	T	168	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	149	MET	2.8
2	T	142	HIS	2.8
2	T	173	ILE	2.8
2	V	145	ASP	2.8
1	K	31	GLU	2.8
1	Y	324	PRO	2.8
2	L	157	TYR	2.8
2	P	130	ALA	2.8
1	Y	20	ASN	2.8
2	T	16	GLY	2.8
2	D	126	LEU	2.8
2	L	31	GLY	2.8
2	V	142	HIS	2.8
1	c	12	GLN	2.8
2	R	144	CYS	2.8
2	V	154	ASN	2.8
2	L	143	LYS	2.8
2	d	131	LYS	2.8
2	L	38	LYS	2.8
2	N	1	GLY	2.8
2	P	34	TYR	2.8
2	b	25	HIS	2.8
1	U	34	VAL	2.8
1	W	21[A]	ASN	2.8
2	b	164	GLU	2.8
2	L	27	SER	2.8
1	C	23	THR	2.8
1	K	23	THR	2.8
2	P	153	ARG	2.8
2	d	34	TYR	2.8
2	T	25	HIS	2.8
1	S	323	SER	2.7
1	Q	322	ASN	2.7
2	R	166	ALA	2.7
1	G	85	SER	2.7
1	a	317	ALA	2.7
1	c	19	ALA	2.7
2	D	31	GLY	2.7
2	T	171	GLU	2.7
2	P	134	GLY	2.7
2	J	177	ARG	2.7
2	b	145	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	126	LEU	2.7
2	d	14	TRP	2.7
2	L	166	ALA	2.7
2	P	159	TYR	2.7
1	a	21[A]	ASN	2.7
2	F	19	ASP	2.7
2	b	8	GLY	2.7
2	N	34	TYR	2.7
2	P	47	GLY	2.7
2	d	28	ASN	2.7
2	P	44	ALA	2.7
2	D	143	LYS	2.7
2	R	4	GLY	2.7
2	N	145	ASP	2.7
1	U	294	PHE	2.7
2	T	33	GLY	2.7
2	P	35	ALA	2.7
2	L	131	LYS	2.7
2	T	29	GLU	2.7
2	T	36	ALA	2.7
2	Z	137	CYS	2.7
1	a	17	TYR	2.6
2	F	173	ILE	2.7
2	L	152	VAL	2.6
2	H	22	TYR	2.6
1	Q	36	VAL	2.6
2	X	148	CYS	2.6
1	C	15	ILE	2.6
2	T	42	GLN	2.6
2	T	166	ALA	2.6
1	W	318	THR	2.6
2	V	177	ARG	2.6
1	O	320	LEU	2.6
2	T	153	ARG	2.6
2	R	34	TYR	2.6
2	F	146	ASN	2.6
2	R	135	ASN	2.6
2	Z	170	ARG	2.6
2	X	145	ASP	2.6
2	V	146	ASN	2.6
1	E	320	LEU	2.6
2	b	124	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	22	SER	2.6
2	T	165	GLU	2.6
2	N	28	ASN	2.6
2	T	146	ASN	2.6
2	B	142	HIS	2.6
2	Z	49	THR	2.6
2	P	30	GLN	2.5
2	Z	48	VAL	2.5
2	X	1	GLY	2.5
1	Q	323	SER	2.5
2	T	9	PHE	2.5
2	R	170	ARG	2.5
2	d	42	GLN	2.5
2	D	21	TRP	2.5
2	B	38	LYS	2.5
2	b	29	GLU	2.5
2	F	168	LEU	2.5
1	Y	63	ASP	2.5
2	P	19	ASP	2.5
2	T	34	TYR	2.5
2	F	120	ASP	2.5
2	J	140	PHE	2.5
2	T	162	TYR	2.5
1	E	323	SER	2.5
2	F	153	ARG	2.4
1	Y	31	GLU	2.4
2	d	10	ILE	2.4
2	Z	174	SER	2.4
1	K	320	LEU	2.4
1	U	23	THR	2.4
1	W	20	ASN	2.4
1	A	12	GLN	2.4
2	L	149	MET	2.4
2	R	23	GLY	2.4
2	P	24	TYR	2.4
1	M	21[A]	ASN	2.4
2	F	37	ASP	2.4
2	P	1	GLY	2.4
2	d	139	GLU	2.4
1	Y	35	THR	2.4
2	N	17	MET	2.4
2	d	160	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	162	TYR	2.4
1	Y	17	TYR	2.4
2	D	148	CYS	2.4
1	E	51	LEU	2.4
2	R	156	THR	2.4
2	Z	8	GLY	2.4
1	c	95	ASN	2.4
2	N	16	GLY	2.4
2	F	152	VAL	2.4
2	Z	106	ARG	2.4
1	a	324	PRO	2.4
2	T	152	VAL	2.4
2	d	173	ILE	2.4
1	I	12	GLN	2.3
1	Q	25	GLN	2.3
2	d	162	TYR	2.3
2	F	18	VAL	2.3
2	R	155	GLY	2.3
2	d	41	THR	2.3
1	S	25	GLN	2.3
2	b	125	GLN	2.3
2	Z	27	SER	2.3
2	F	139	GLU	2.3
2	H	142	HIS	2.3
1	C	14	CYS	2.3
2	D	35	ALA	2.3
2	d	45	ILE	2.3
2	D	23	GLY	2.3
2	H	140	PHE	2.3
2	Z	163	SER	2.3
2	b	167	ARG	2.3
2	V	30	GLN	2.3
2	T	44	ALA	2.3
2	Z	122	VAL	2.3
1	E	18	HIS	2.3
2	R	42	GLN	2.3
2	X	146	ASN	2.3
2	Z	164	GLU	2.3
1	c	311	SER	2.3
1	Q	21[A]	ASN	2.3
2	L	33	GLY	2.3
2	Z	161	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	8	GLY	2.3
2	T	148	CYS	2.3
2	Z	21	TRP	2.3
2	N	168	LEU	2.3
1	a	280	LYS	2.3
2	P	21	TRP	2.2
1	Y	95	ASN	2.2
2	F	169	LYS	2.2
2	D	132	GLU	2.2
2	d	6	ILE	2.2
2	D	36	ALA	2.2
2	X	19	ASP	2.2
2	Z	50	ASN	2.2
2	b	135	ASN	2.2
1	c	39	ALA	2.2
1	S	50	LYS	2.2
1	E	22	SER	2.2
1	a	312	ASN	2.2
1	c	48	ASN	2.2
2	L	120	ASP	2.2
2	Z	7	ALA	2.2
2	P	18	VAL	2.2
2	F	109	ASP	2.2
2	T	20	GLY	2.2
1	U	25	GLN	2.2
2	d	133	LEU	2.2
1	W	18	HIS	2.2
2	T	151	SER	2.2
1	C	22	SER	2.2
1	C	36	VAL	2.2
2	D	113	SER	2.2
1	C	16	GLY	2.2
1	U	307	LYS	2.2
2	D	24	TYR	2.2
2	F	34	TYR	2.2
2	H	174	SER	2.2
2	V	163	SER	2.2
1	a	14	CYS	2.2
1	K	25	GLN	2.2
1	a	32	LYS	2.2
2	H	26	HIS	2.2
2	N	126	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	126	LEU	2.1
2	d	57	ASP	2.1
2	d	109	ASP	2.1
1	E	17	TYR	2.1
2	N	14	TRP	2.1
2	b	171	GLU	2.1
1	W	319	GLY	2.1
2	R	153	ARG	2.1
2	b	28	ASN	2.1
1	U	15	ILE	2.1
2	T	147	GLU	2.1
1	U	319	GLY	2.1
2	L	32	SER	2.1
2	N	149	MET	2.1
1	U	10	GLY	2.1
1	Q	19	ALA	2.1
2	F	112	ASP	2.1
2	Z	115	VAL	2.1
2	T	30	GLN	2.1
1	U	323	SER	2.1
2	b	162	TYR	2.1
2	N	37	ASP	2.1
2	b	121	LYS	2.1
2	b	131	LYS	2.1
2	R	37	ASP	2.1
2	X	20	GLY	2.1
2	Z	44	ALA	2.1
2	d	39	GLU	2.1
1	W	281	CYS	2.1
2	L	45	ILE	2.1
1	S	10	GLY	2.1
1	U	40	GLN	2.0
2	Z	31	GLY	2.0
2	b	176	GLY	2.0
2	F	111	HIS	2.0
2	N	163	SER	2.0
2	X	9	PHE	2.0
2	Z	150	GLU	2.0
1	E	34	VAL	2.0
1	M	17	TYR	2.0
1	S	34	VAL	2.0
1	A	13	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	a	30	MET	2.0
2	P	149	MET	2.0
1	Y	8	ASP	2.0
1	Y	85	SER	2.0
2	F	132	GLU	2.0
2	R	146	ASN	2.0
2	T	154	ASN	2.0
1	a	36	VAL	2.0
2	N	153	ARG	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
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

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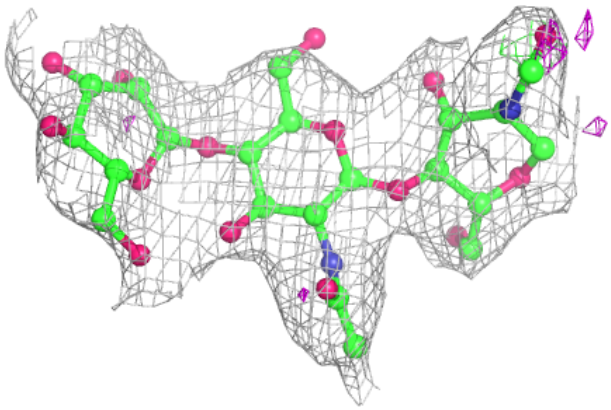
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	z	1	14/15	0.81	0.23	145,151,158,159	0
4	NAG	m	1	14/15	0.81	0.20	94,108,117,122	0
3	BMA	l	3	11/12	0.81	0.39	83,95,103,110	0
4	NAG	r	2	14/15	0.81	0.20	138,149,152,152	0
4	NAG	x	1	14/15	0.82	0.15	141,148,158,159	0
5	NAG	s	1	14/15	0.82	0.23	68,80,90,103	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
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

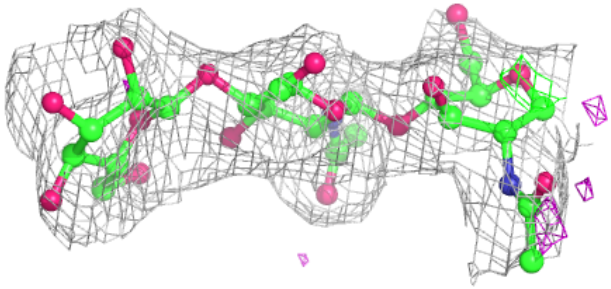
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

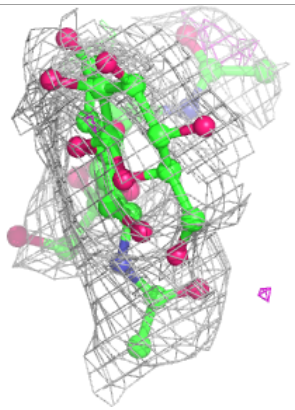
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

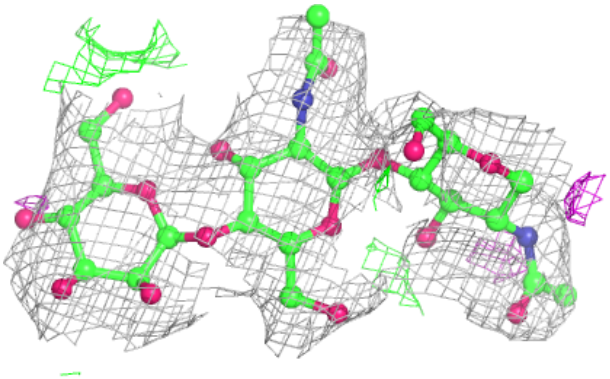


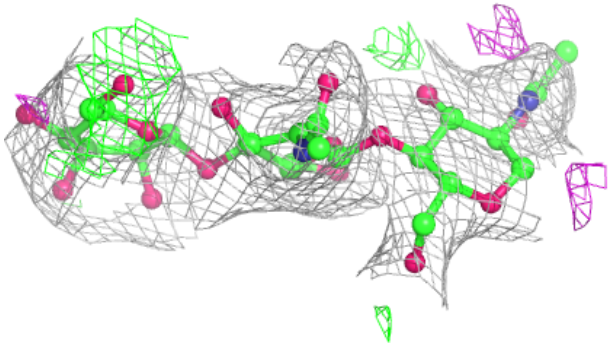


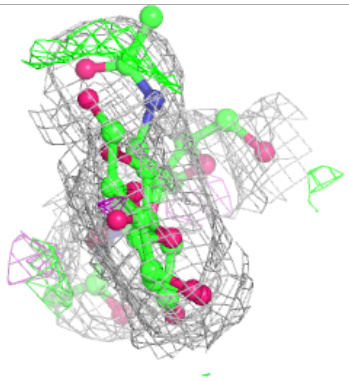


Electron density around Chain g:

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

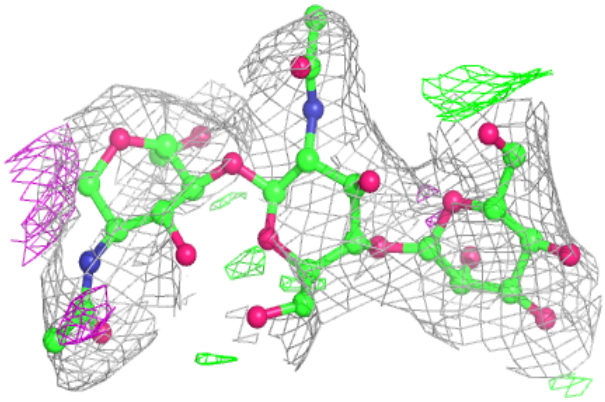


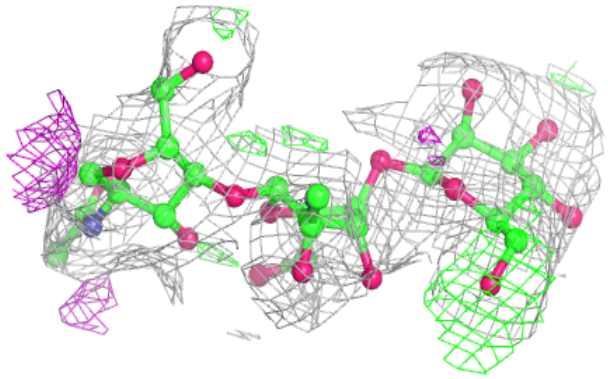


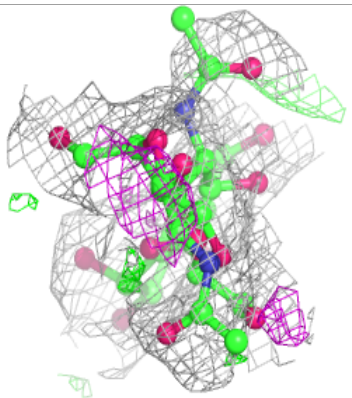


Electron density around Chain h:

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

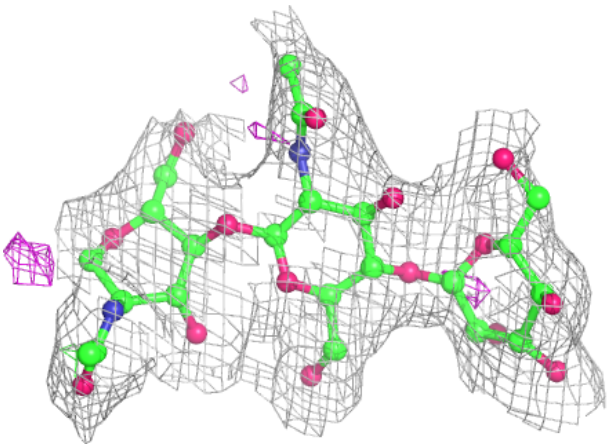


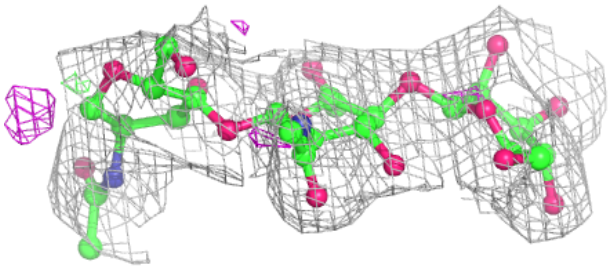


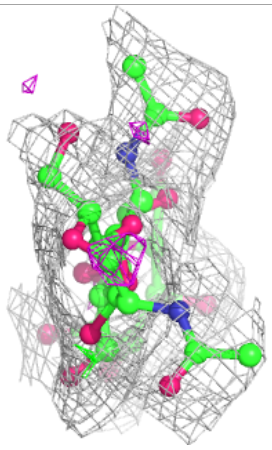


Electron density around Chain j:

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

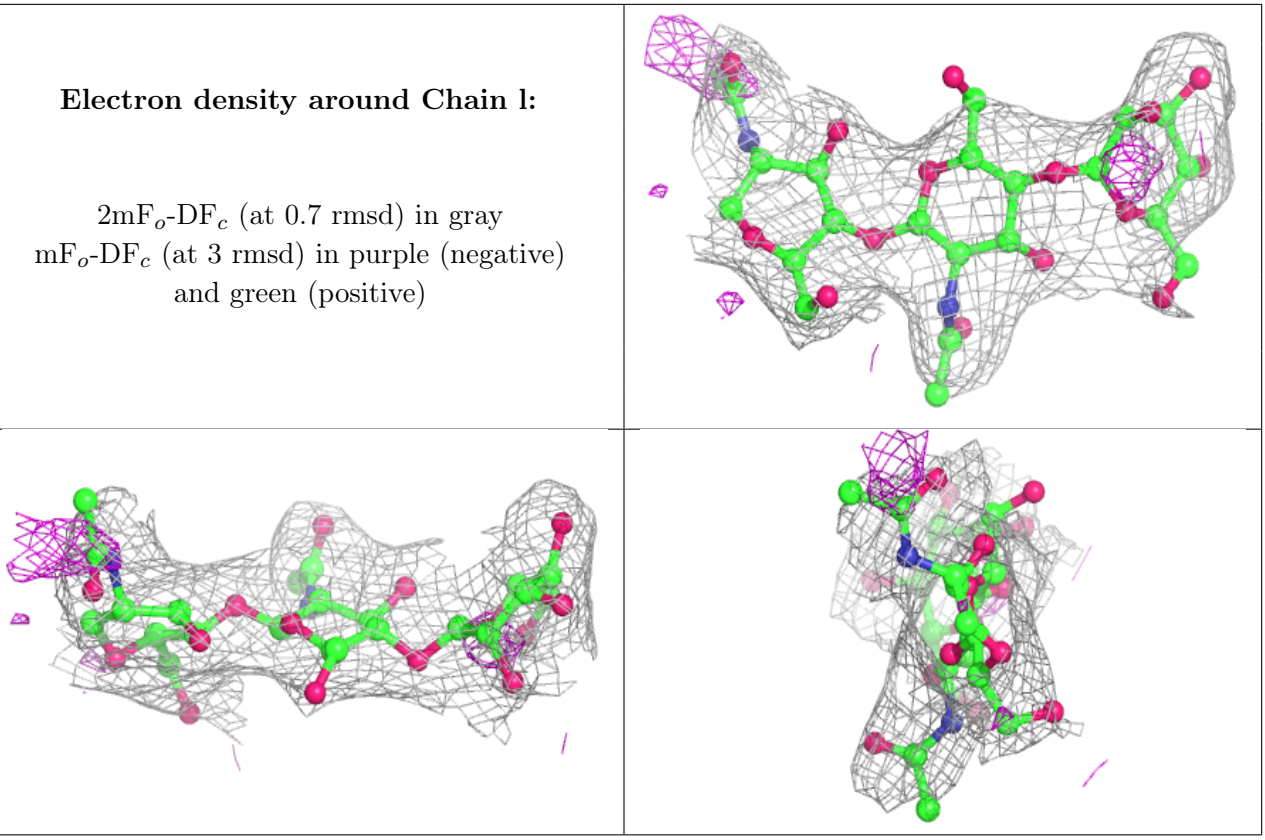






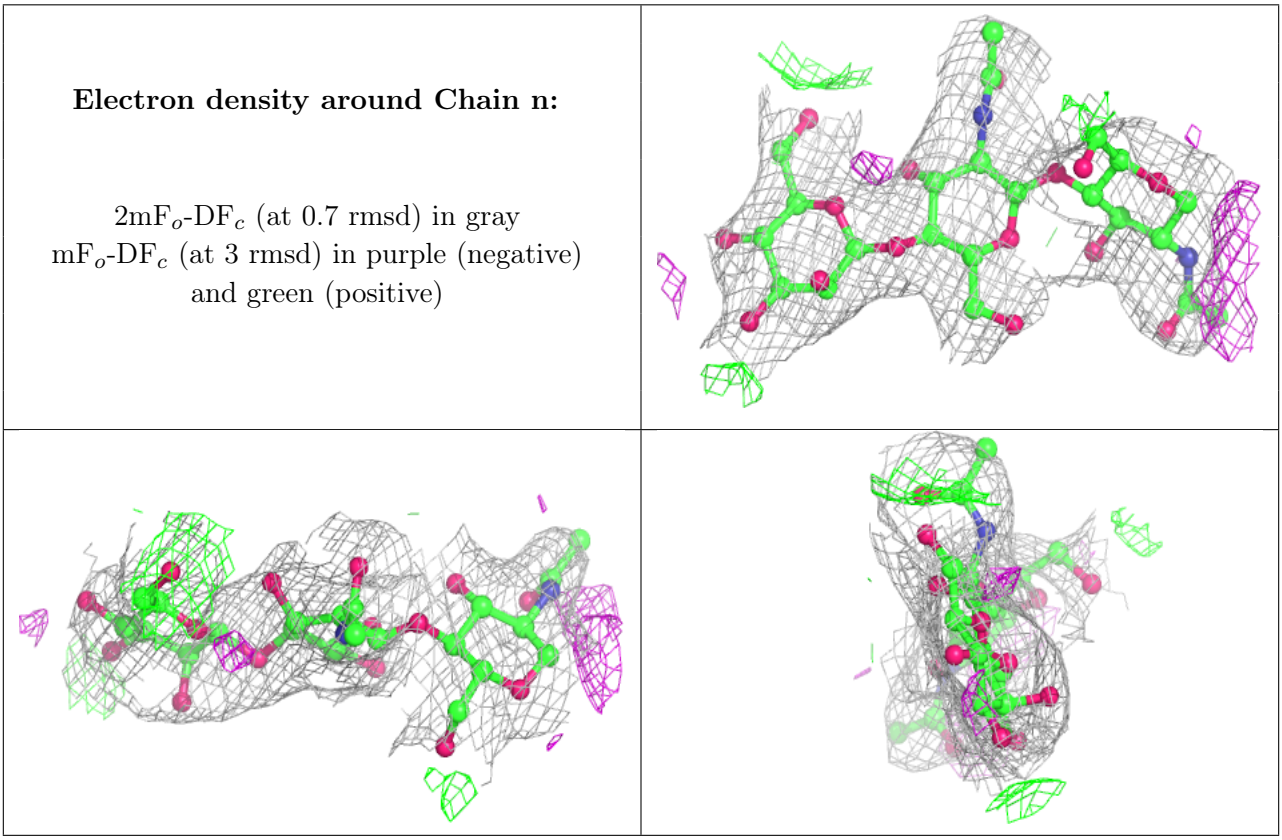
Electron density around Chain l:

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



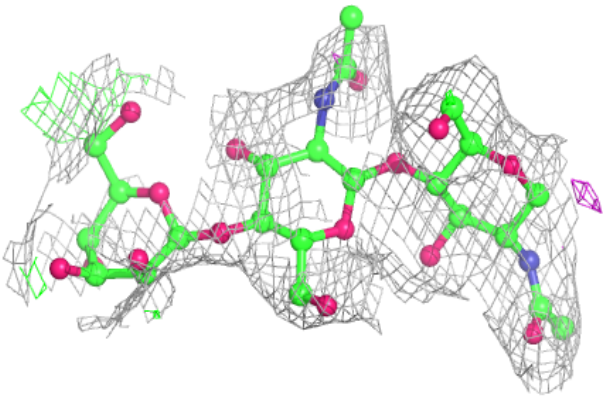
Electron density around Chain n:

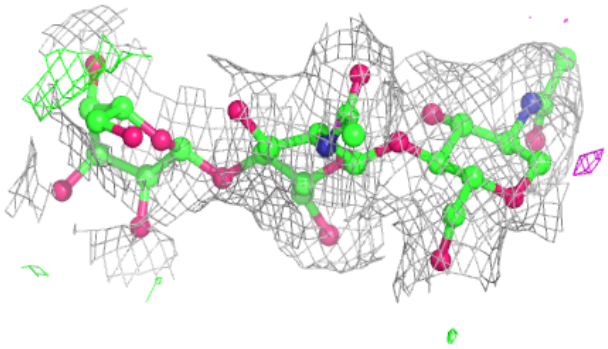
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

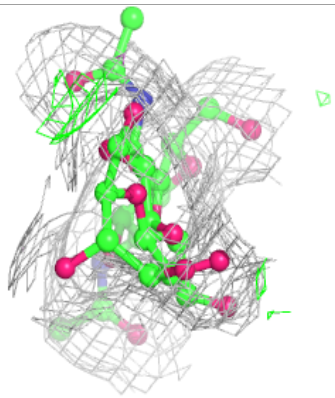


Electron density around Chain o:

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

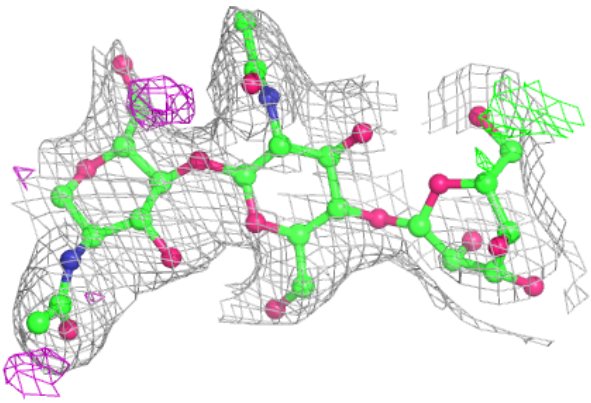


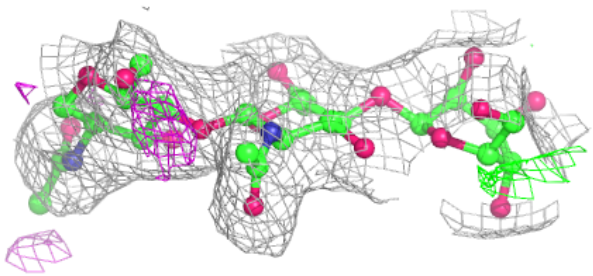


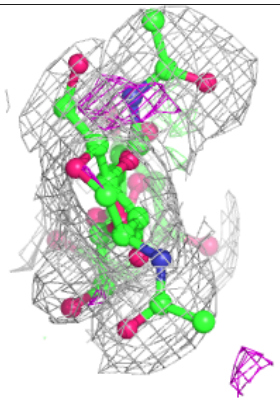


Electron density around Chain q:

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

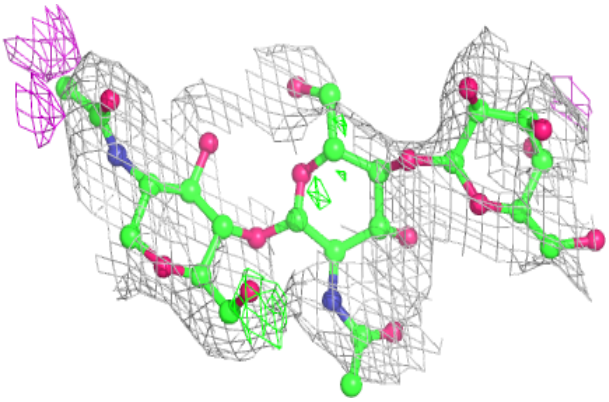


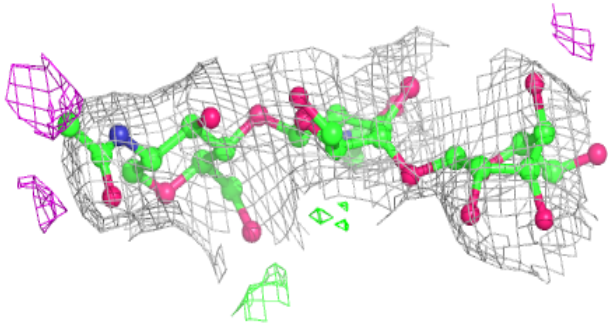


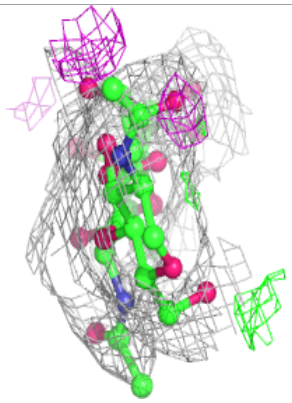


Electron density around Chain w:

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

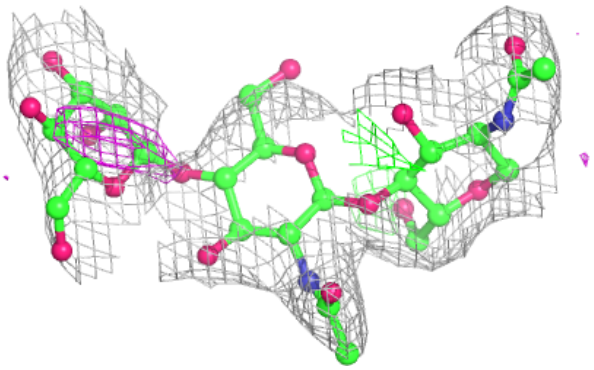


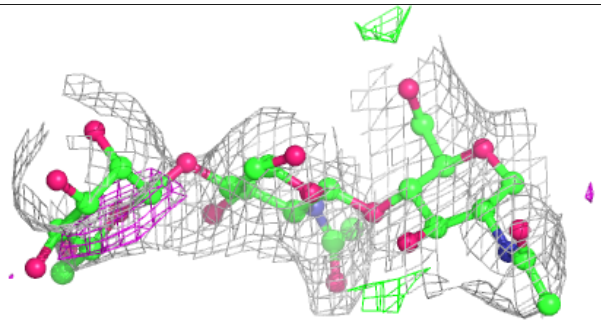


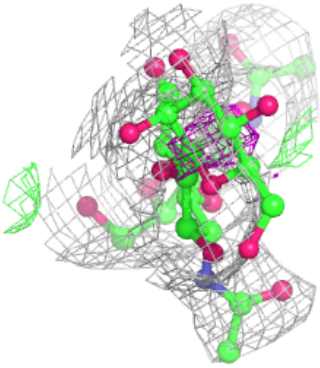


Electron density around Chain y:

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

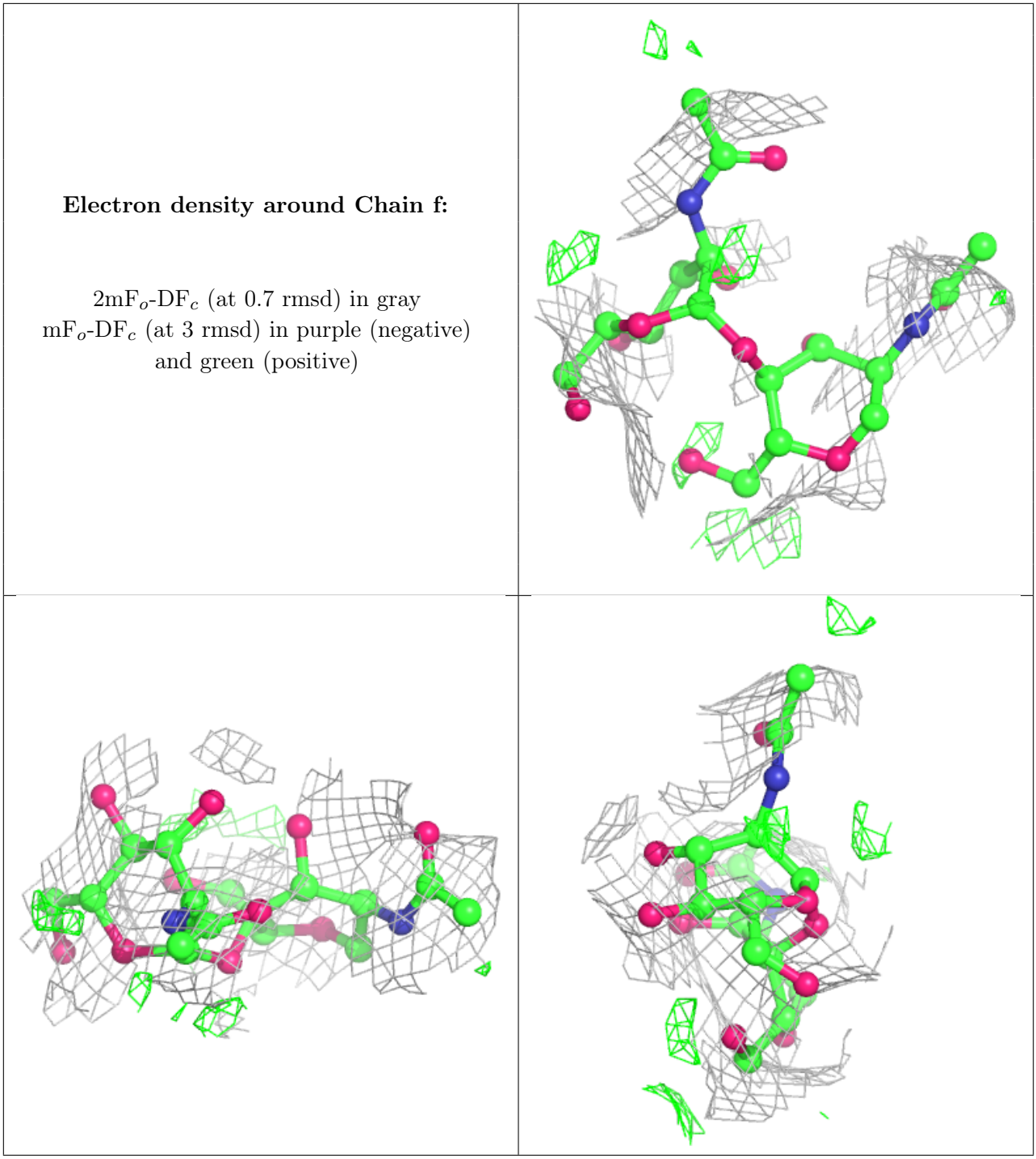






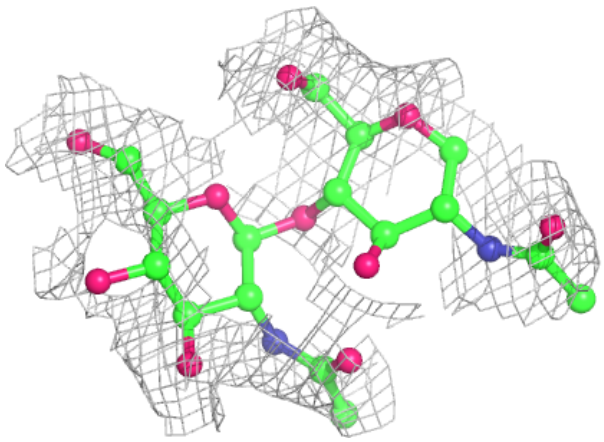
Electron density around Chain f:

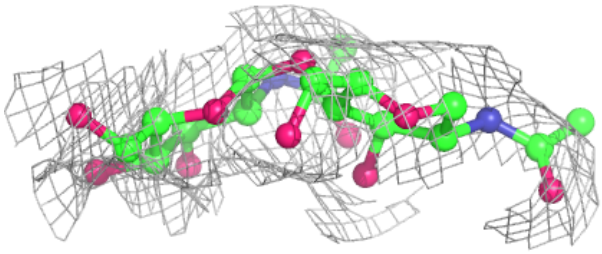
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

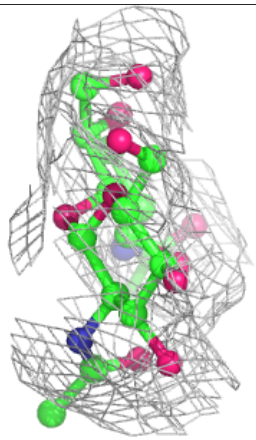


Electron density around Chain i:

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

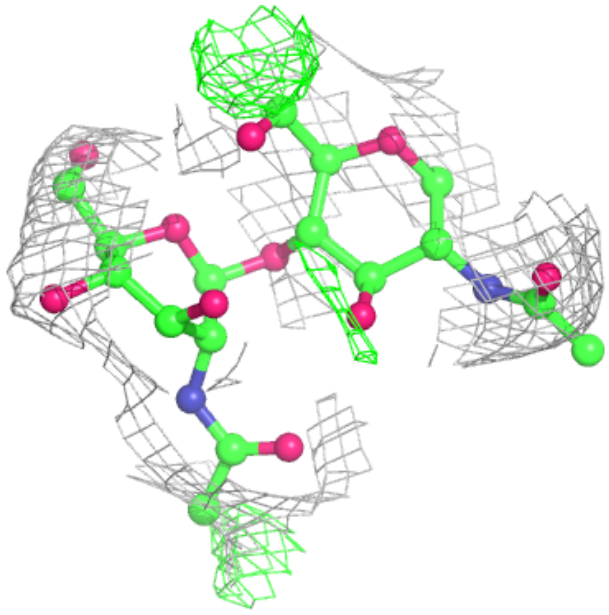


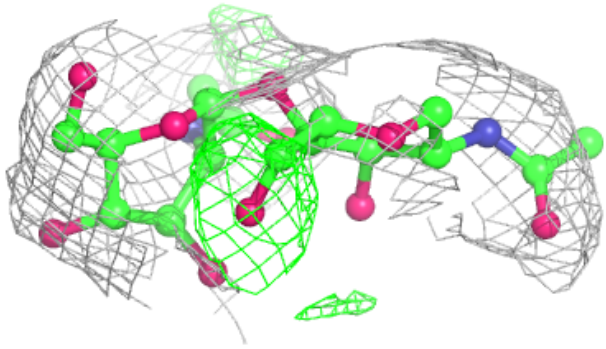


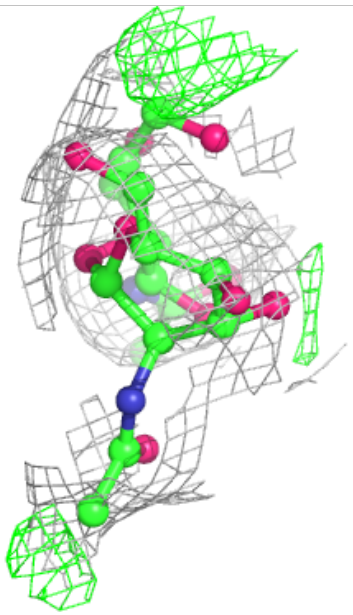


Electron density around Chain k:

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

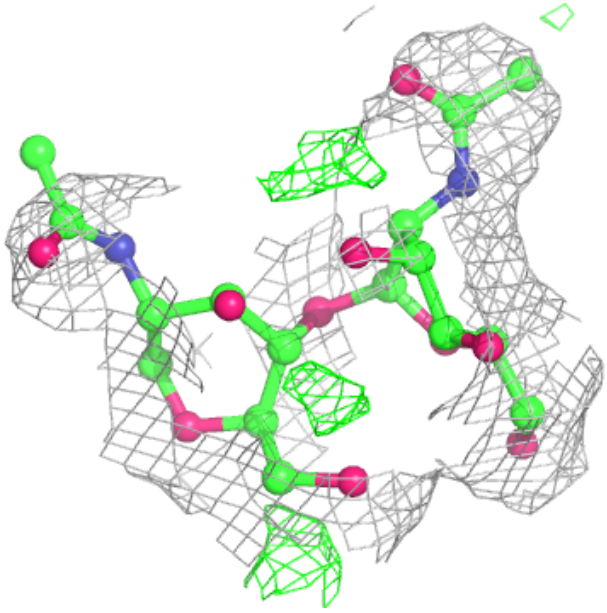


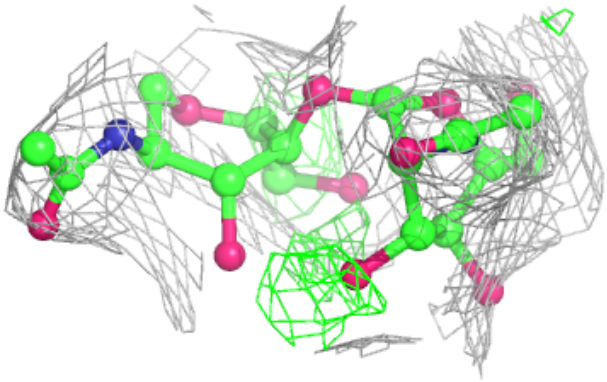


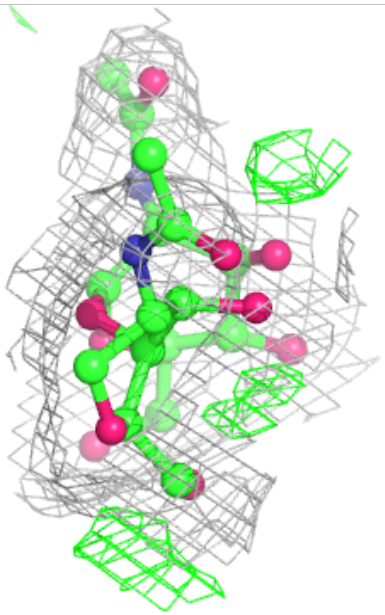


Electron density around Chain m:

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

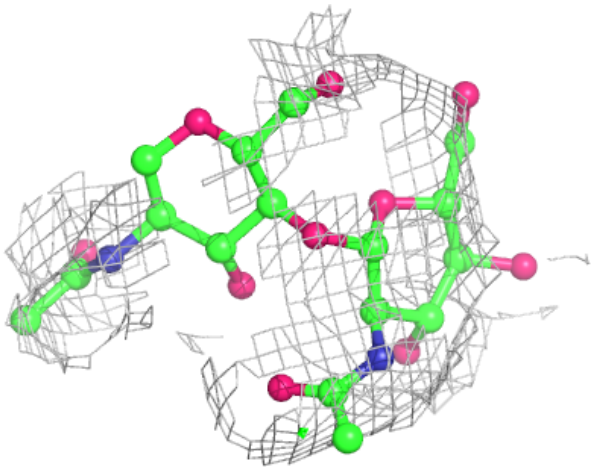


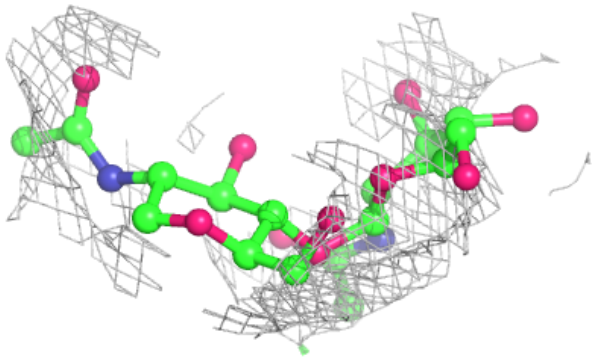


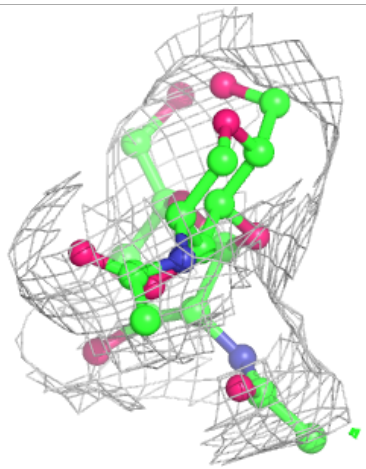


Electron density around Chain p:

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

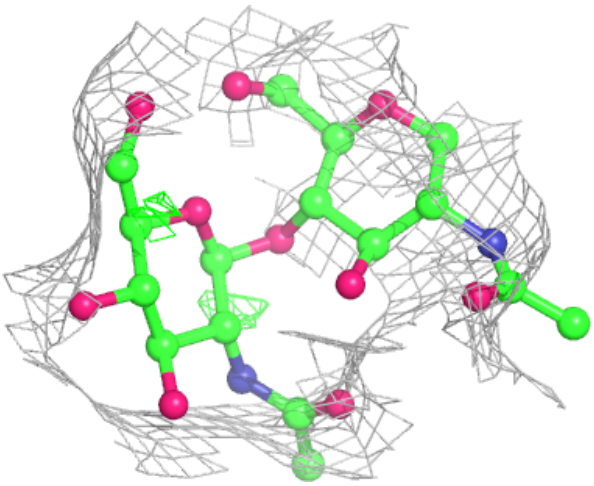


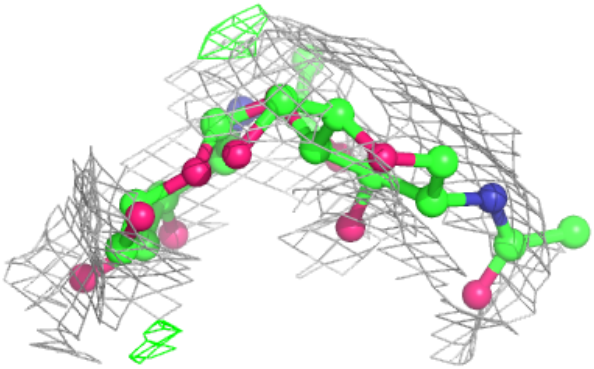


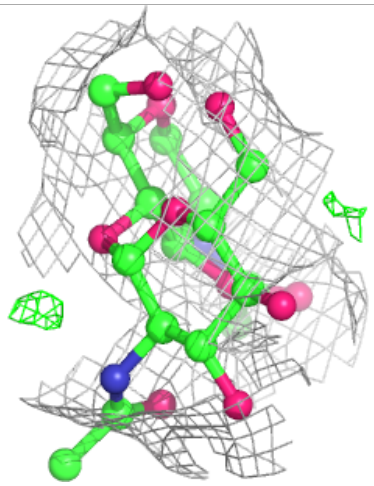


Electron density around Chain r:

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

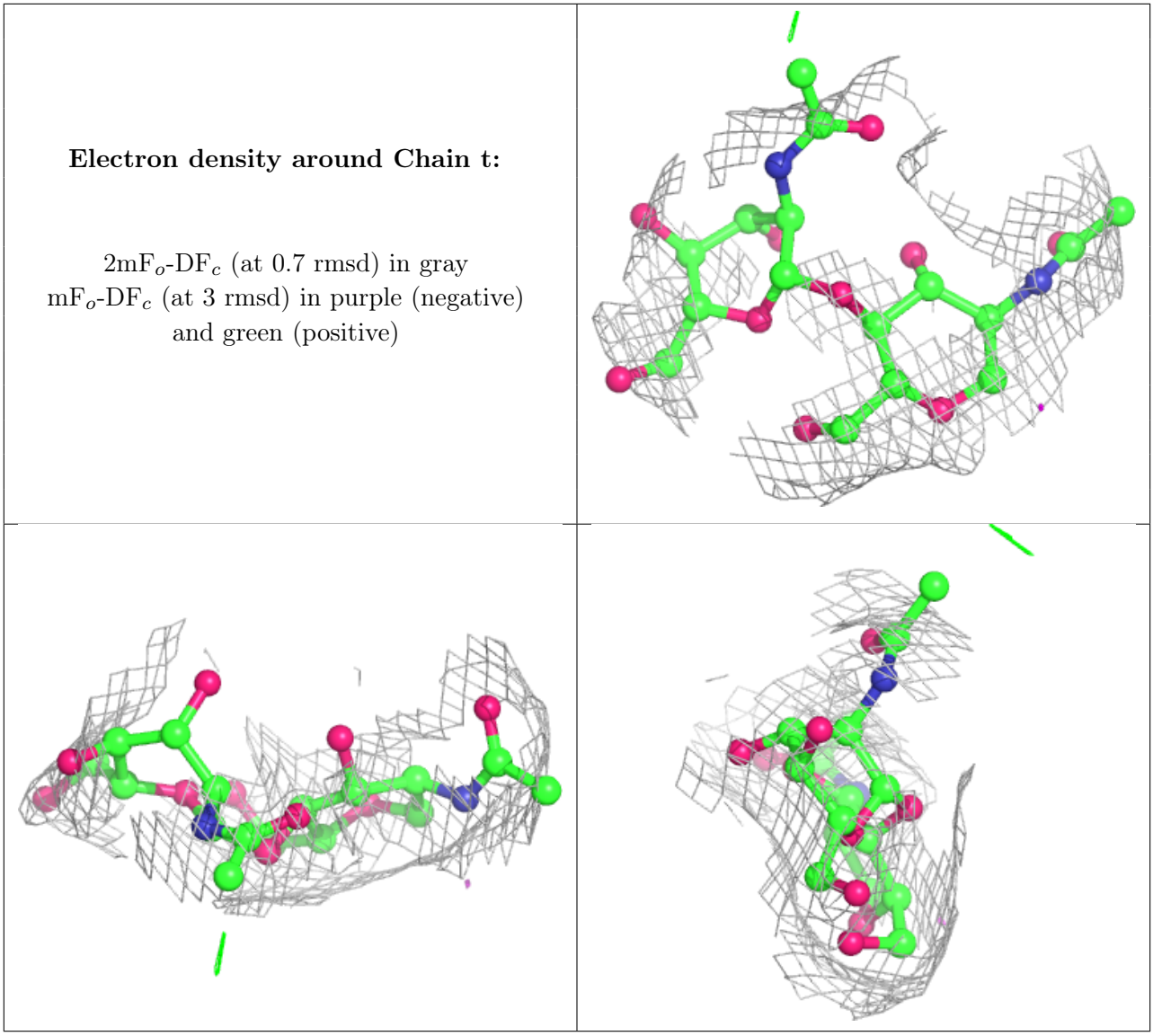






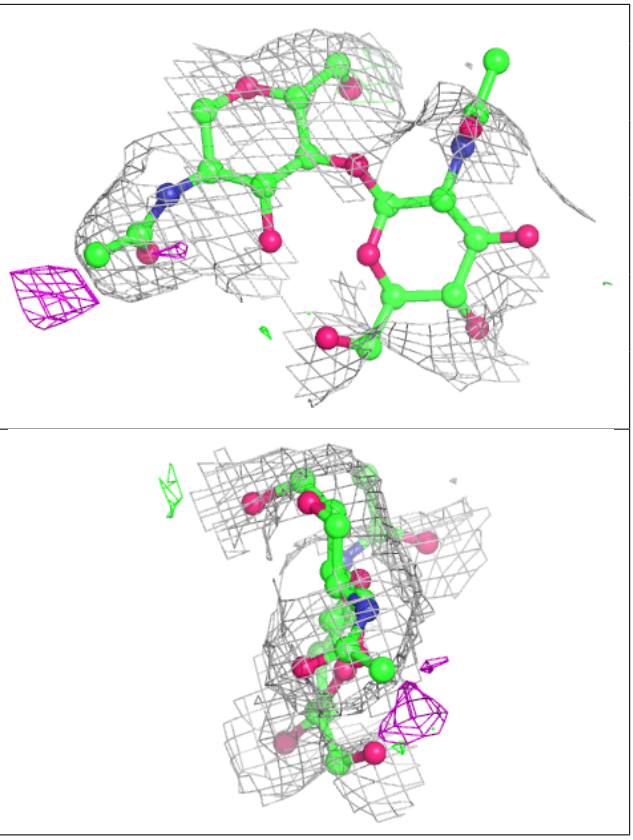
Electron density around Chain t:

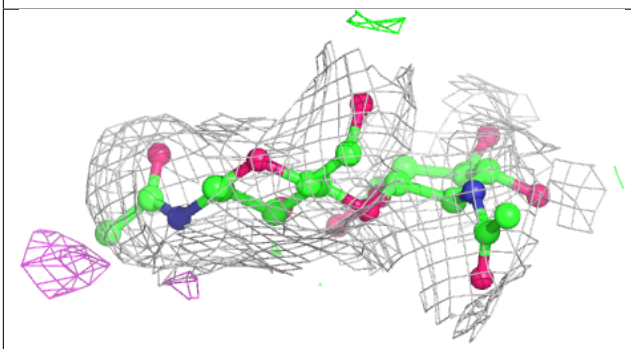
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain u:

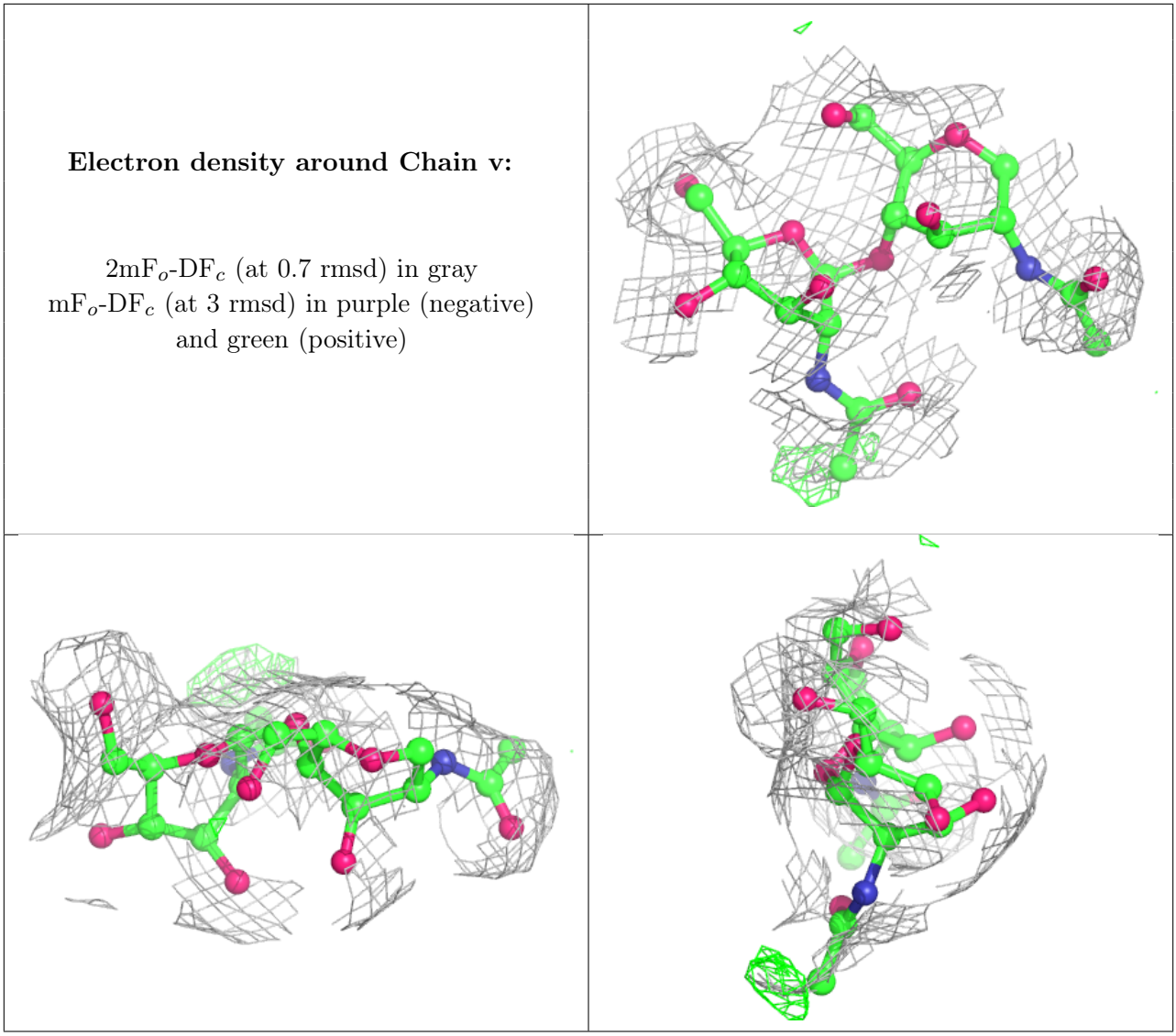
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





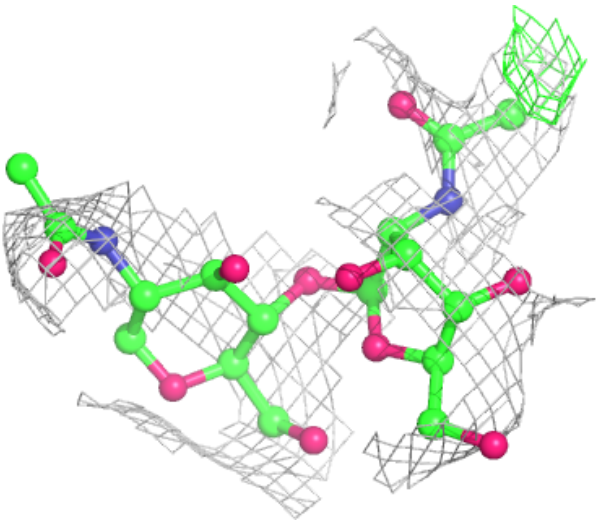
Electron density around Chain v:

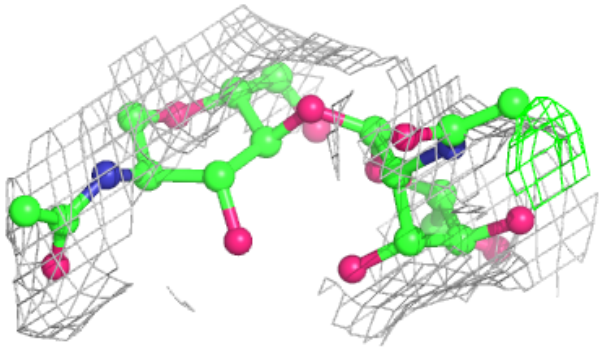
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

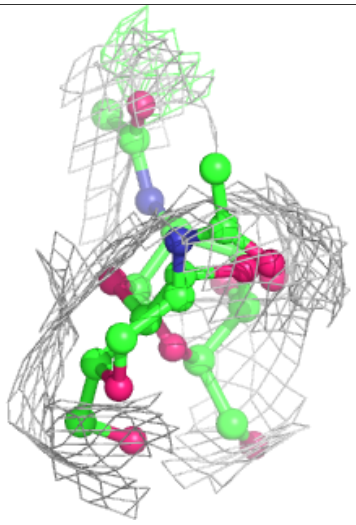


Electron density around Chain x:

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

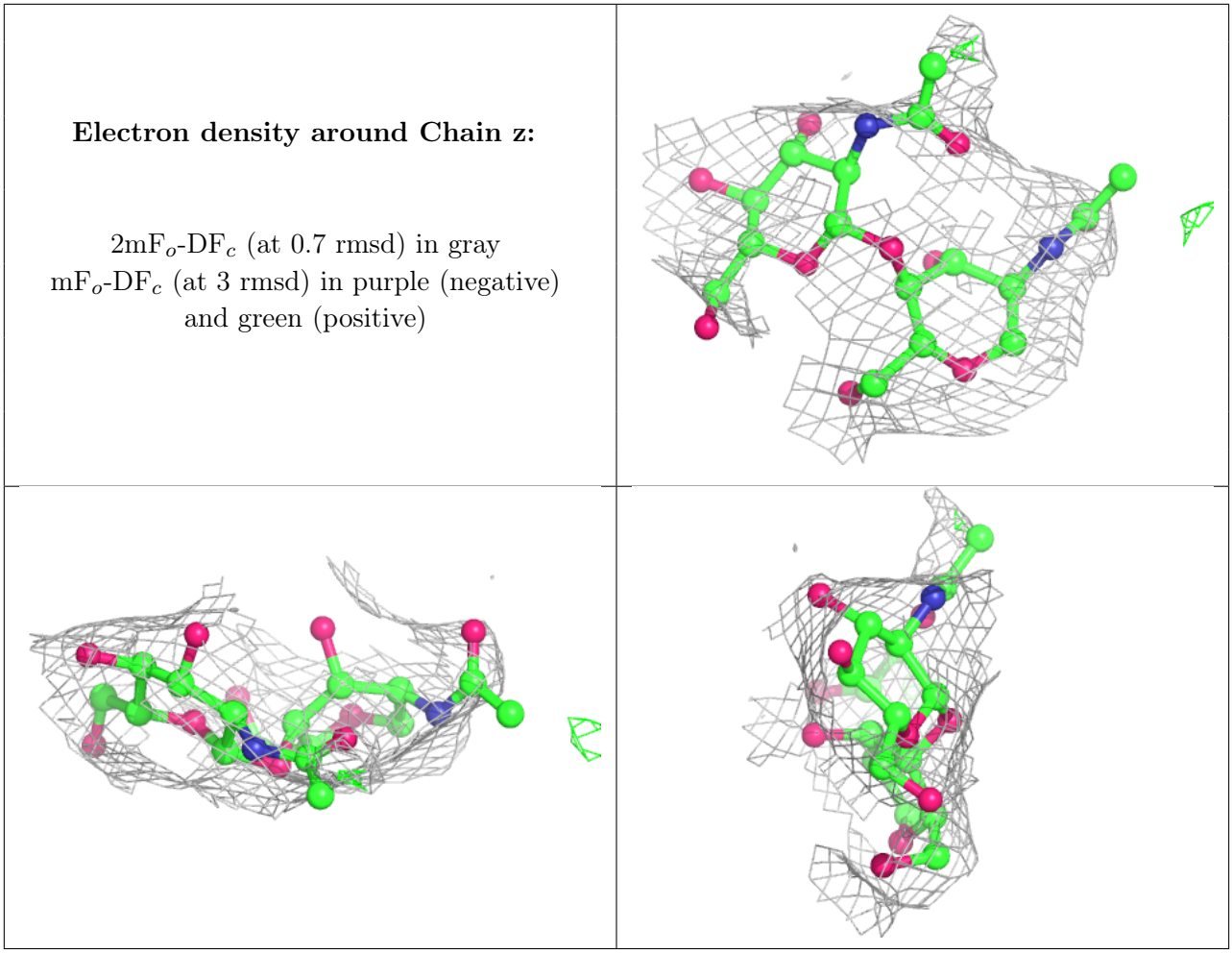






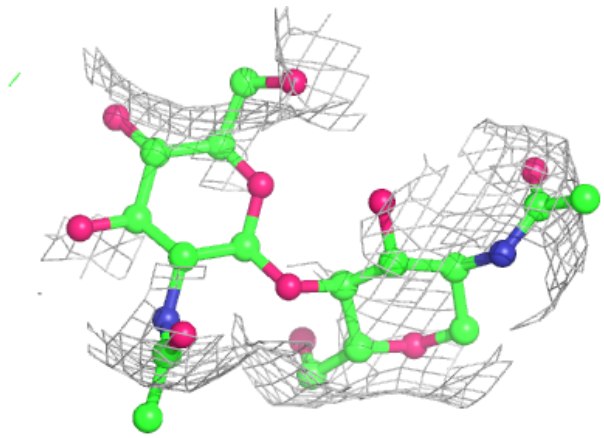
Electron density around Chain z:

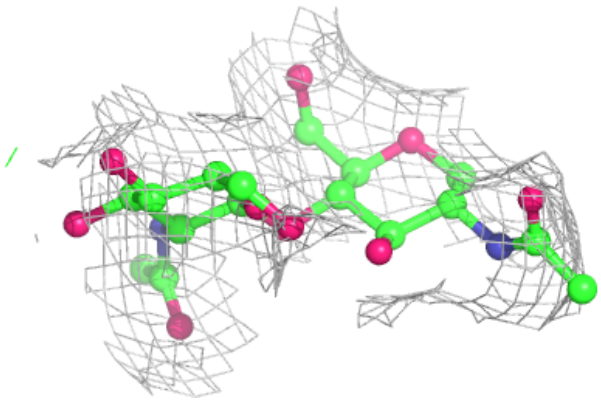
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

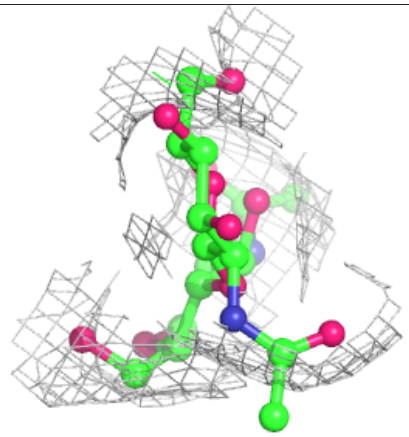


Electron density around Chain 0:

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

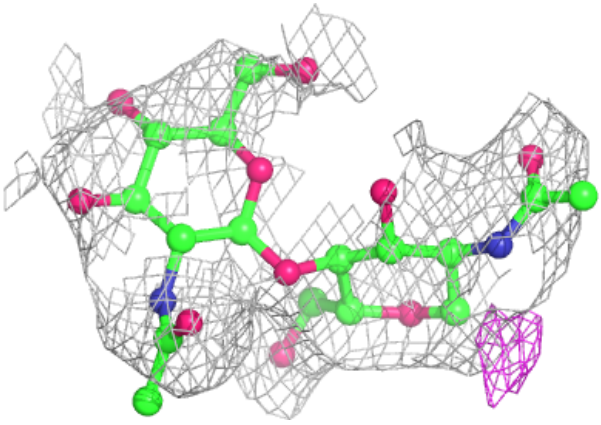


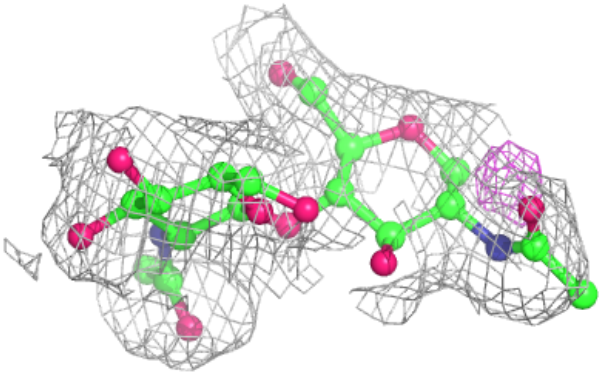




Electron density around Chain 1:

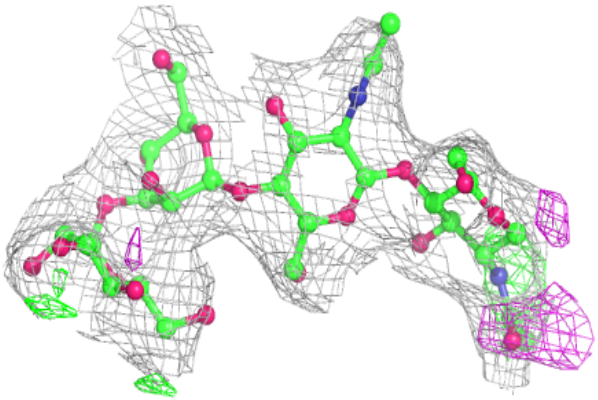
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

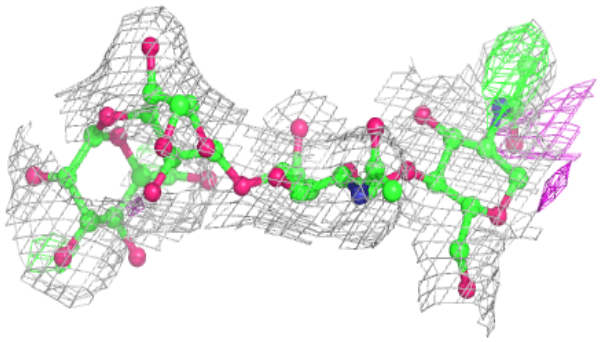


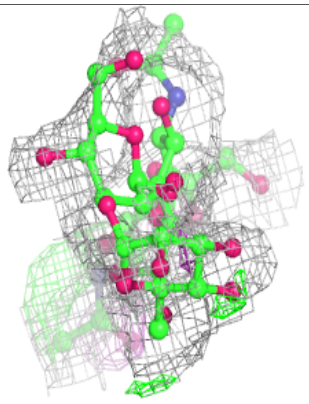


Electron density around Chain s:

$2mF_o$-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, 95^{th} 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.