Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 08:07 PM EDT

PDB ID	:	4N5Z
Title	:	Crystal structure of aerosol transmissible influenza H5 hemagglutinin mutant (N158D, N224K, Q226L and T318I) from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-10-10
Resolution	:	2.95 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 (i) symbol.

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

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

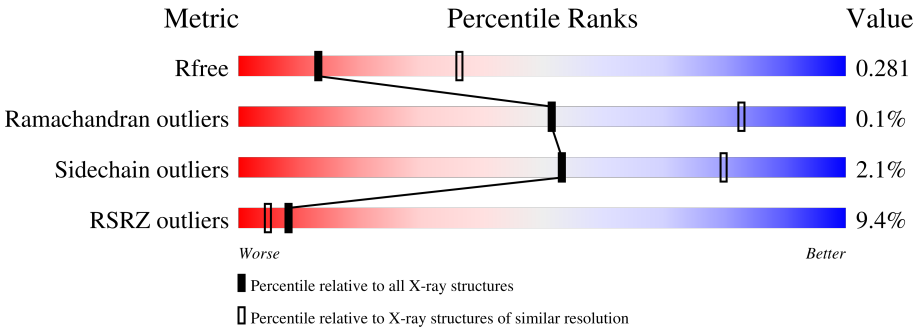
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	94%
1	C	334	3% 95%
1	E	334	95%
1	G	334	2% 93%
1	I	334	92% 5%
1	K	334	2% 94%

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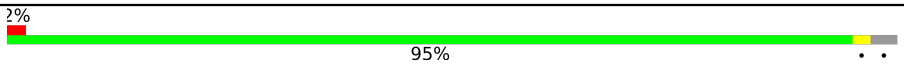
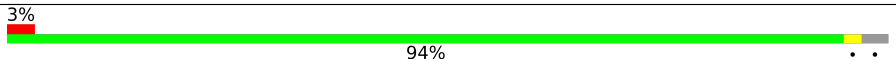
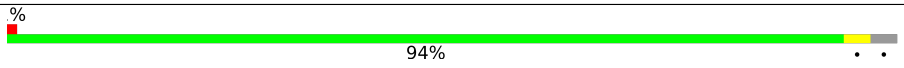
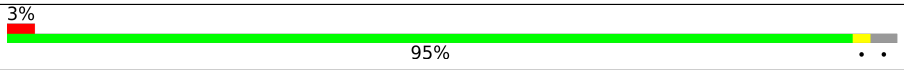
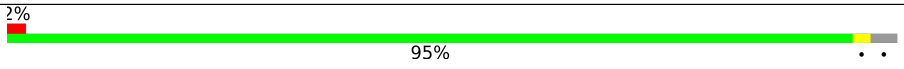
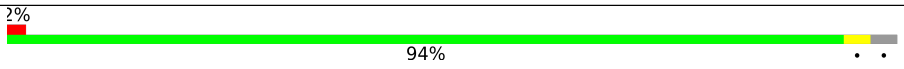
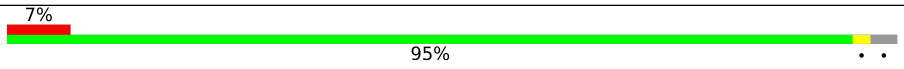
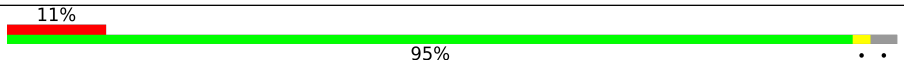
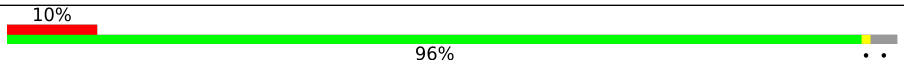
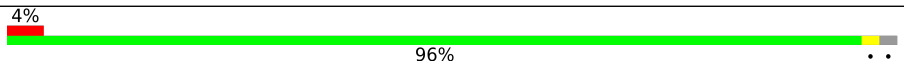
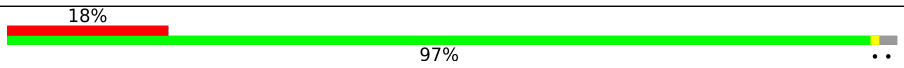
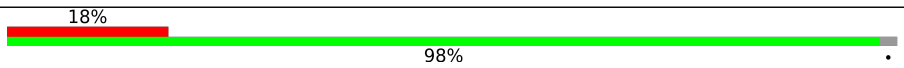
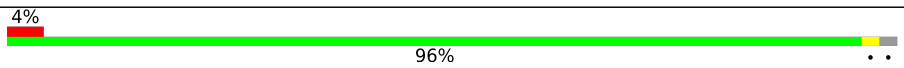
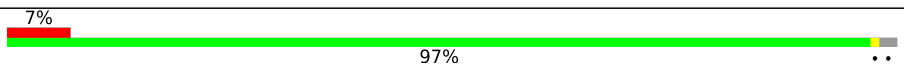
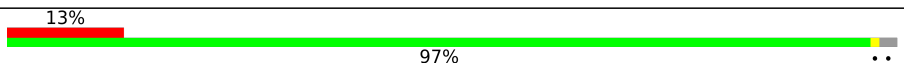
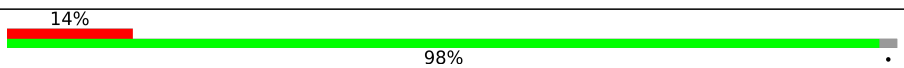
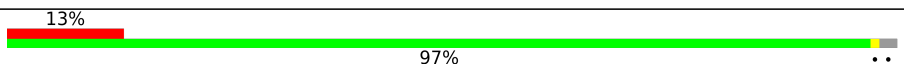
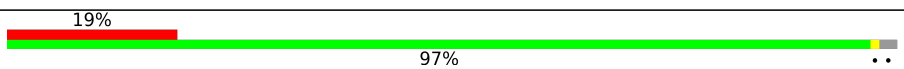
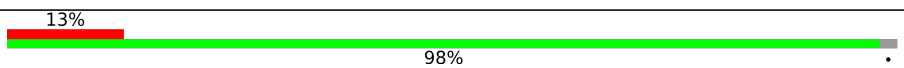
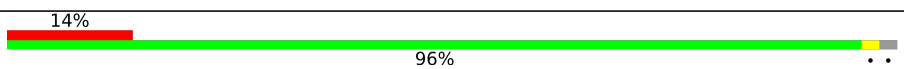
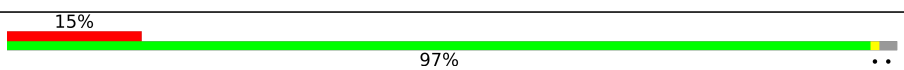
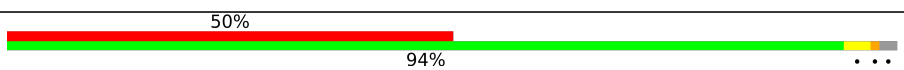
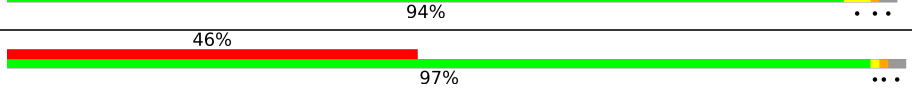
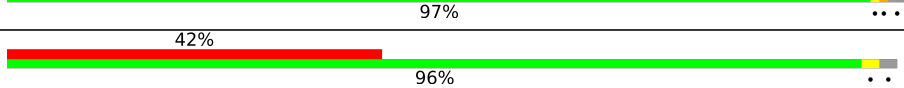
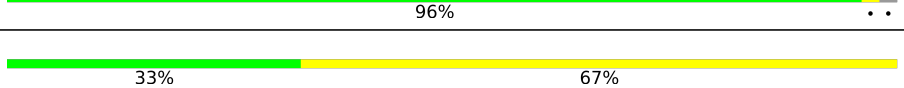
Mol	Chain	Length	Quality of chain
1	M	334	
1	O	334	
1	Q	334	
1	S	334	
1	U	334	
1	W	334	
1	Y	334	
1	a	334	
1	c	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
2	T	181	
2	V	181	
2	X	181	
2	Z	181	
2	b	181	
2	d	181	
3	e	3	

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 60979 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
			2574	1630	442	487	15			
1	C	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	E	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	G	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	I	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	K	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	M	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	O	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	S	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	U	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	W	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	a	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	c	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			

There are 120 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
A	318	ILE	THR	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
C	318	ILE	THR	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
E	318	ILE	THR	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
G	318	ILE	THR	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
I	318	ILE	THR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
K	318	ILE	THR	engineered mutation	UNP Q6DQ33
M	7	ALA	-	expression tag	UNP Q6DQ33
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
M	318	ILE	THR	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
O	318	ILE	THR	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
Q	318	ILE	THR	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
S	318	ILE	THR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
U	224	LYS	ASN	engineered mutation	UNP Q6DQ33
U	226	LEU	GLN	engineered mutation	UNP Q6DQ33
U	318	ILE	THR	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
W	318	ILE	THR	engineered mutation	UNP Q6DQ33
Y	7	ALA	-	expression tag	UNP Q6DQ33
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
Y	318	ILE	THR	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
a	318	ILE	THR	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
c	318	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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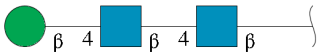
Chain	Residue	Modelled	Actual	Comment	Reference
b	181	ARG	-	expression tag	UNP Q6DQ33
d	175	SER	-	expression tag	UNP Q6DQ33
d	176	GLY	-	expression tag	UNP Q6DQ33
d	177	ARG	-	expression tag	UNP Q6DQ33
d	178	LEU	-	expression tag	UNP Q6DQ33
d	179	VAL	-	expression tag	UNP Q6DQ33
d	180	PRO	-	expression tag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

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

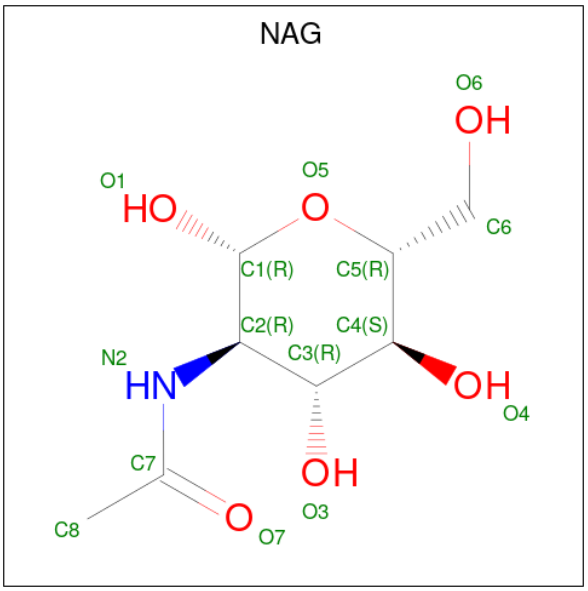


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	e	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	g	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	n	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	o	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	p	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	t	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	v	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	x	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

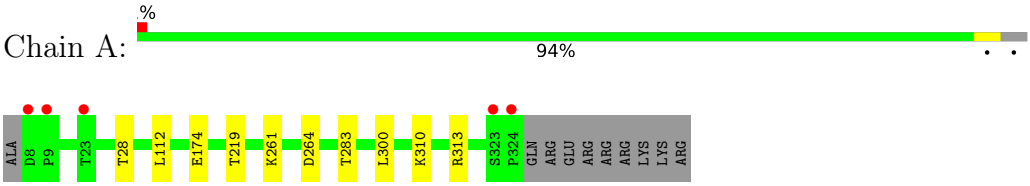


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	K	1	Total C N O 14 8 1 5	0	0
5	M	1	Total C N O 14 8 1 5	0	0
5	O	1	Total C N O 14 8 1 5	0	0
5	Y	1	Total C N O 14 8 1 5	0	0
5	a	1	Total C N O 14 8 1 5	0	0
5	c	1	Total C N O 14 8 1 5	0	0

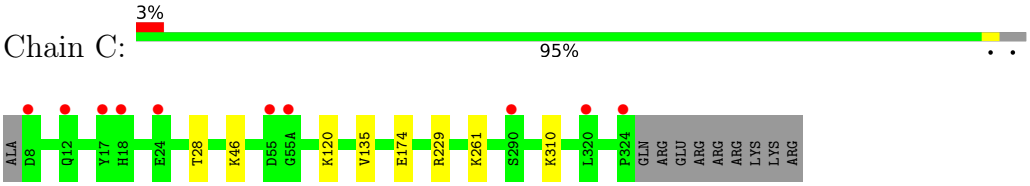
3 Residue-property plots (i)

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.

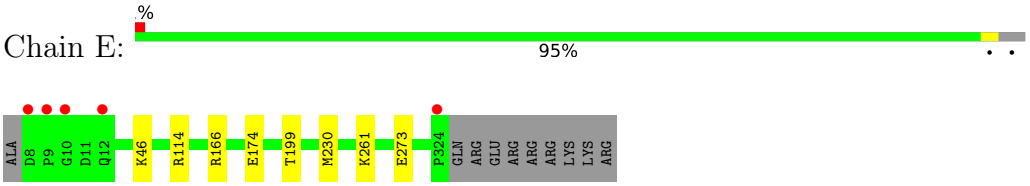
• Molecule 1: Hemagglutinin HA1 chain



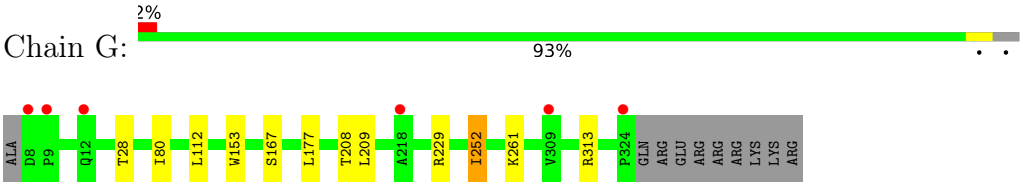
• Molecule 1: Hemagglutinin HA1 chain



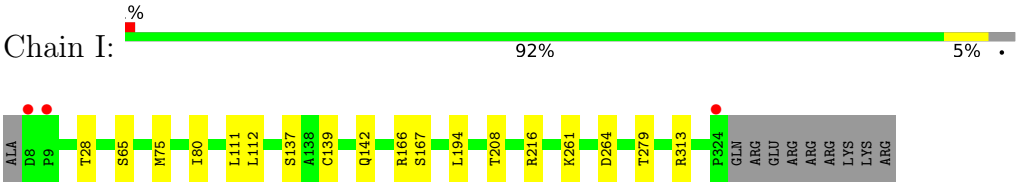
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

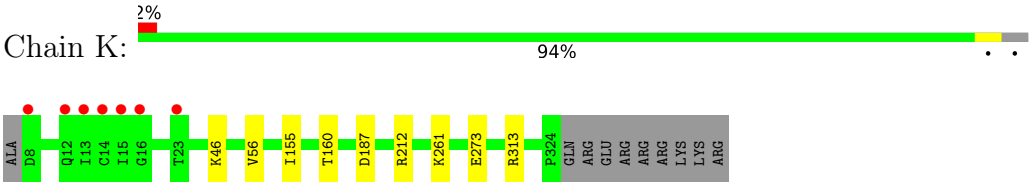


• Molecule 1: Hemagglutinin HA1 chain



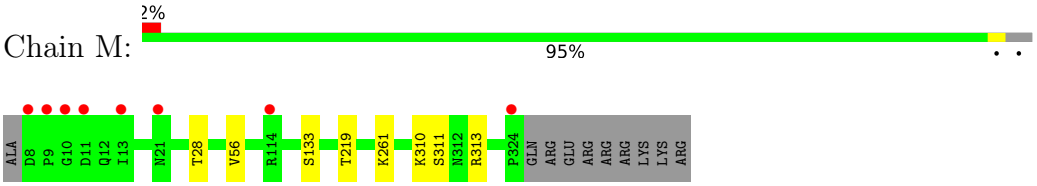
• Molecule 1: Hemagglutinin HA1 chain

Chain K:



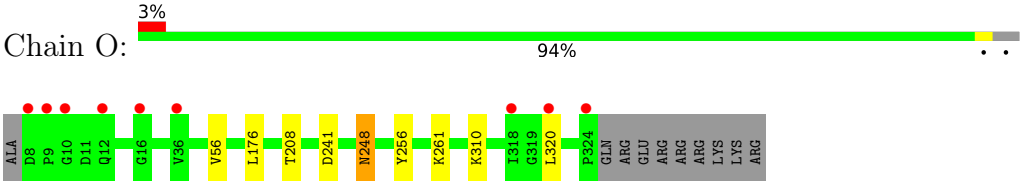
• Molecule 1: Hemagglutinin HA1 chain

Chain M:



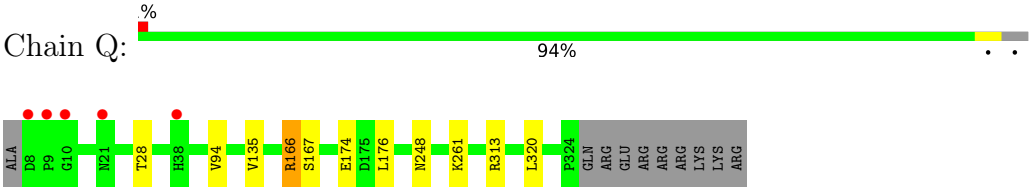
• Molecule 1: Hemagglutinin HA1 chain

Chain O:



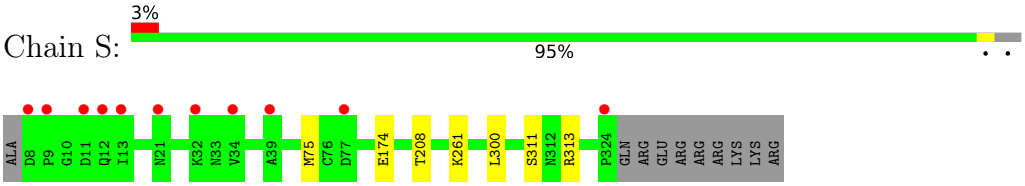
• Molecule 1: Hemagglutinin HA1 chain

Chain Q:



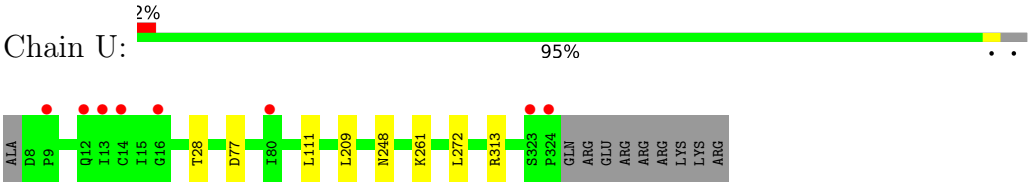
• Molecule 1: Hemagglutinin HA1 chain

Chain S:



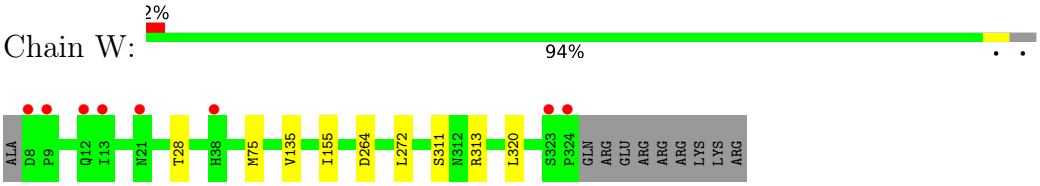
• Molecule 1: Hemagglutinin HA1 chain

Chain U:



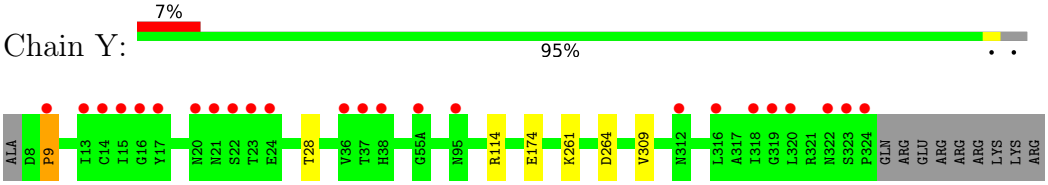
• Molecule 1: Hemagglutinin HA1 chain

Chain W:



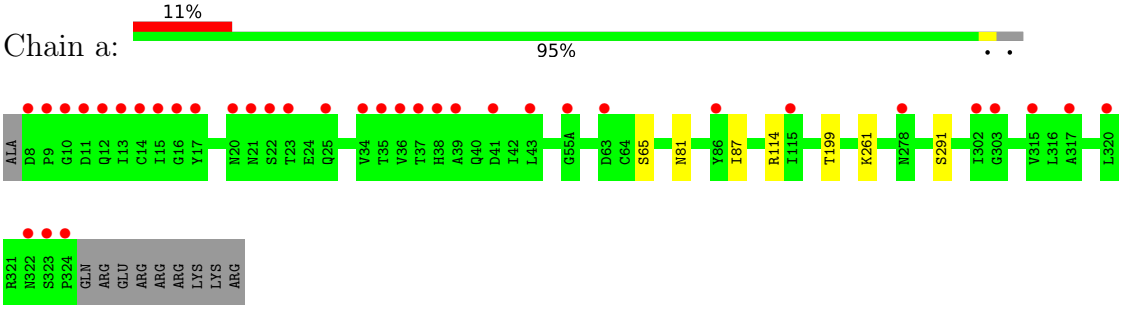
• Molecule 1: Hemagglutinin HA1 chain

Chain Y:



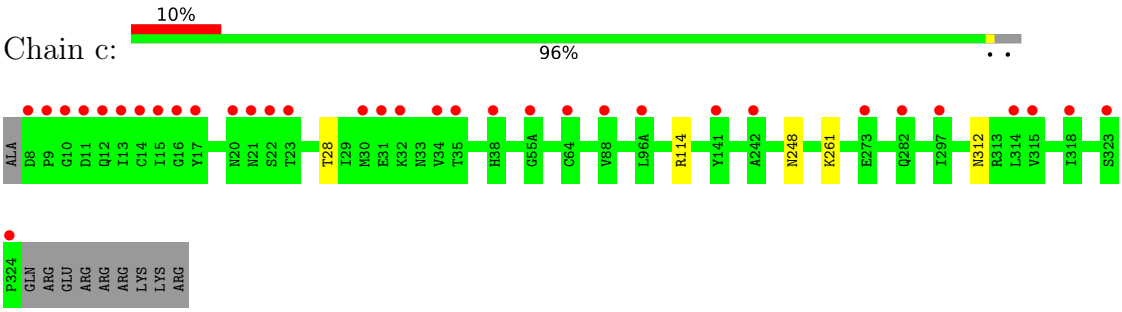
• Molecule 1: Hemagglutinin HA1 chain

Chain a:



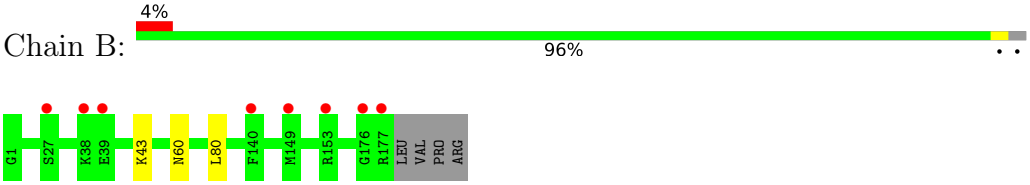
• Molecule 1: Hemagglutinin HA1 chain

Chain c:



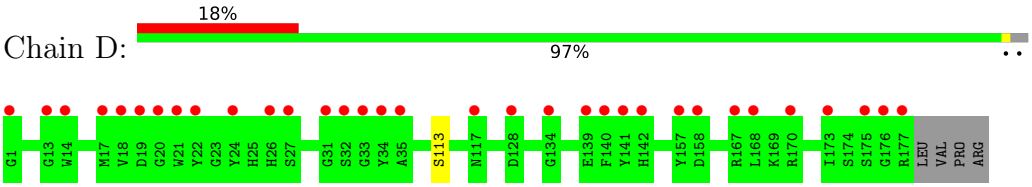
• Molecule 2: Hemagglutinin

Chain B:



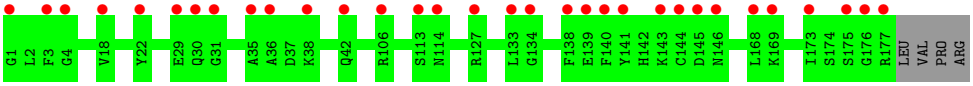
• Molecule 2: Hemagglutinin

Chain D:



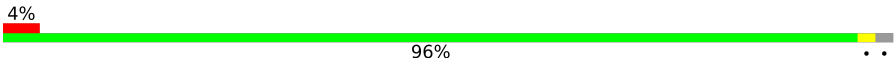
• Molecule 2: Hemagglutinin

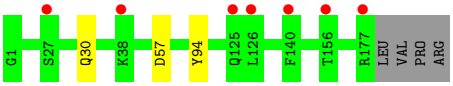
Chain F:



• Molecule 2: Hemagglutinin

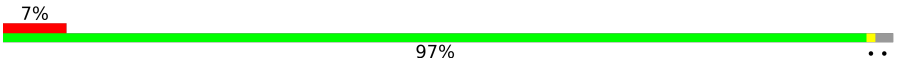
Chain H:

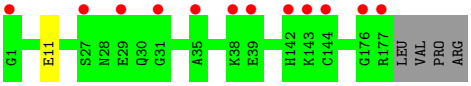




• Molecule 2: Hemagglutinin

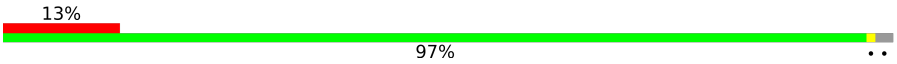
Chain J:

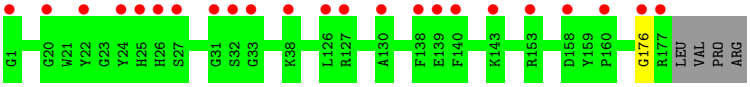




• Molecule 2: Hemagglutinin

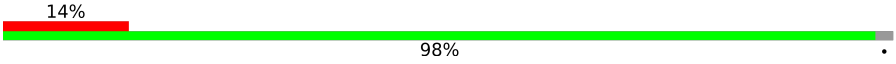
Chain L:

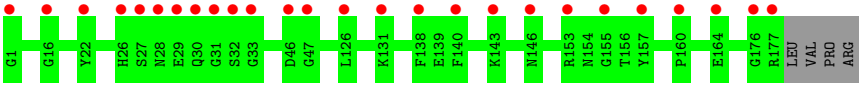




• Molecule 2: Hemagglutinin

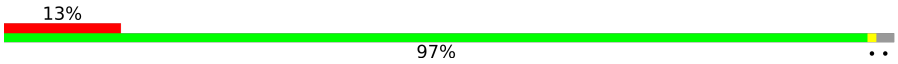
Chain N:

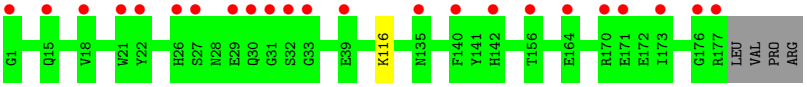




• Molecule 2: Hemagglutinin

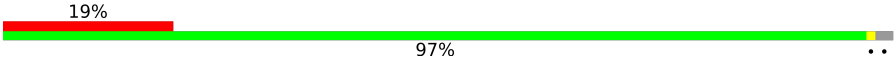
Chain P:

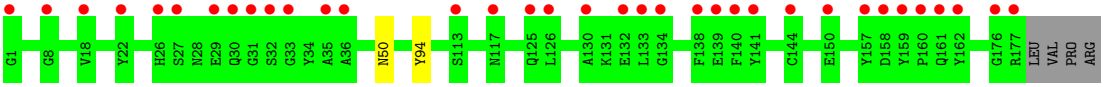




• Molecule 2: Hemagglutinin

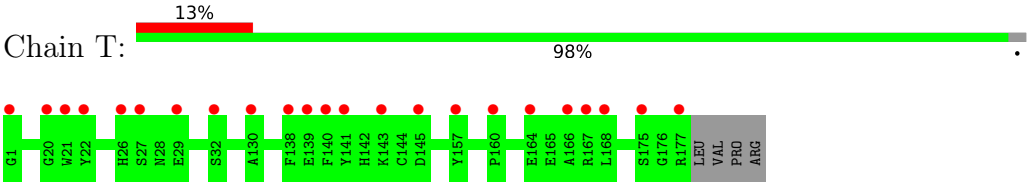
Chain R:





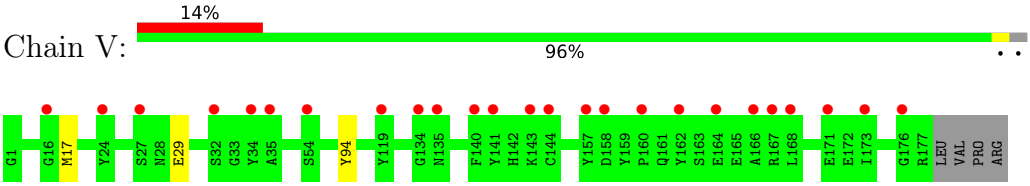
• Molecule 2: Hemagglutinin

Chain T:



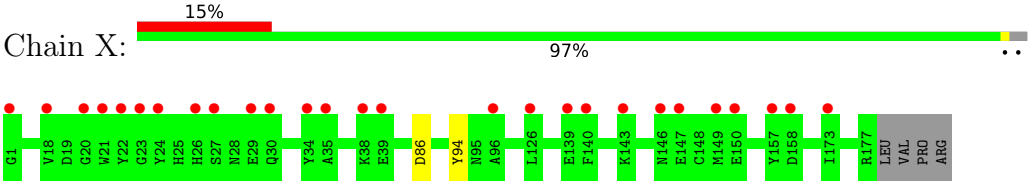
• Molecule 2: Hemagglutinin

Chain V:



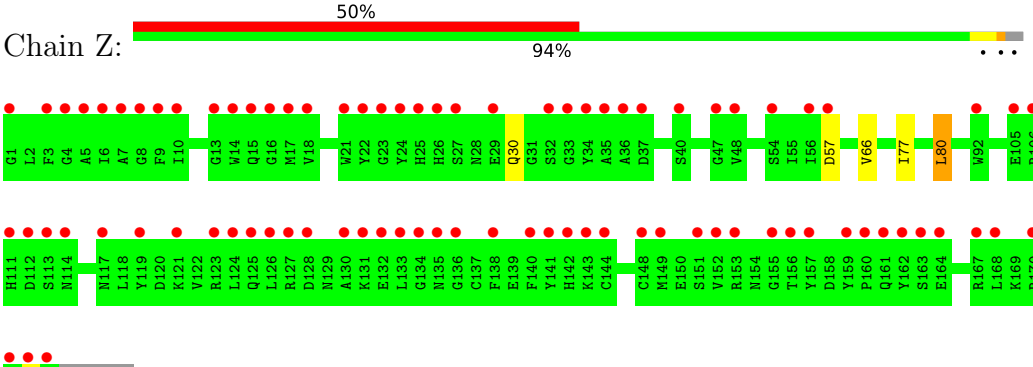
• Molecule 2: Hemagglutinin

Chain X:



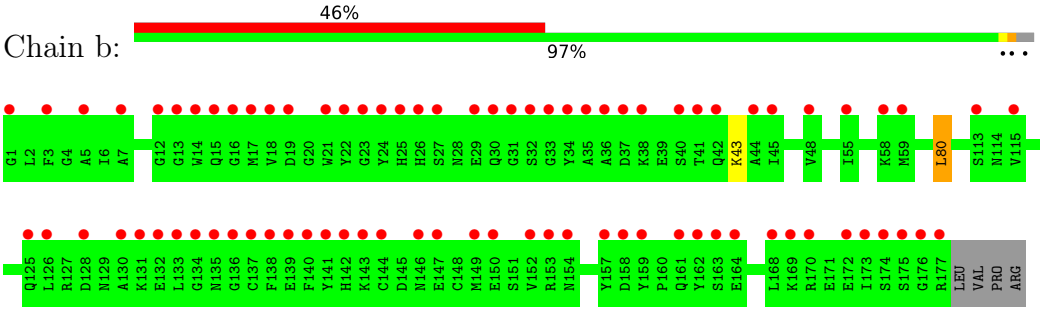
• Molecule 2: Hemagglutinin

Chain Z:



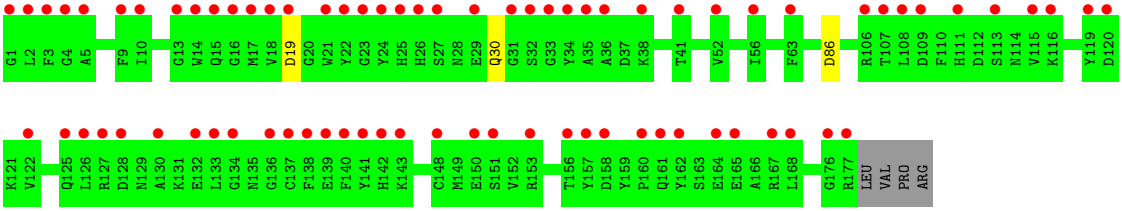
• Molecule 2: Hemagglutinin

Chain b:



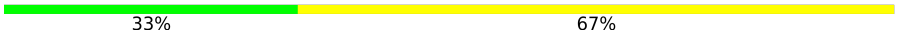
• Molecule 2: Hemagglutinin

Chain d:



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

Chain e:

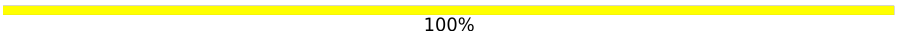


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

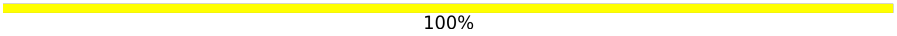
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



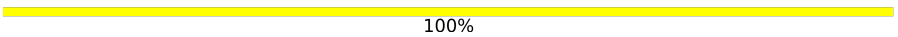
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



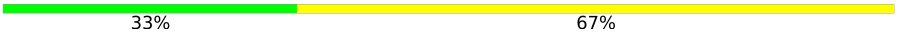
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



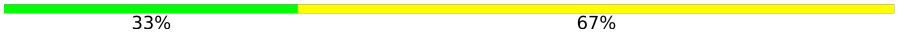
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



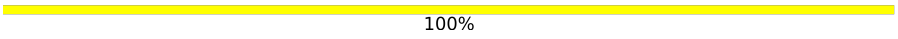
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



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

Chain p:

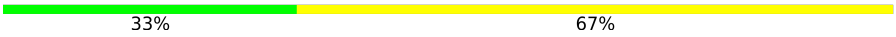


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

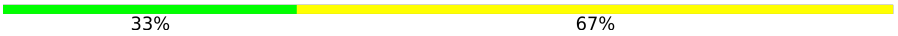
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



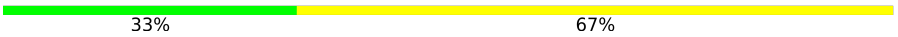
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



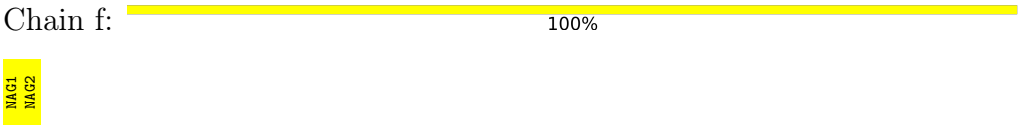
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



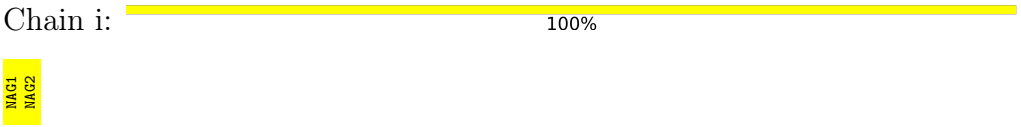
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain i:

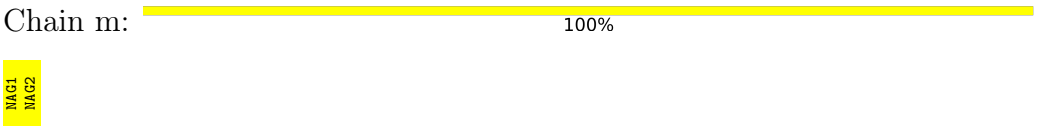


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

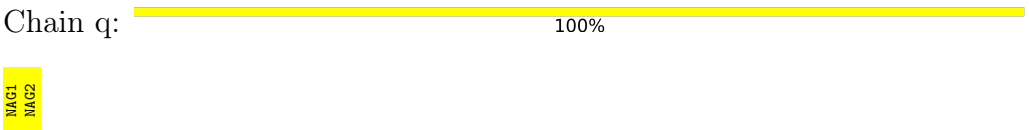
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



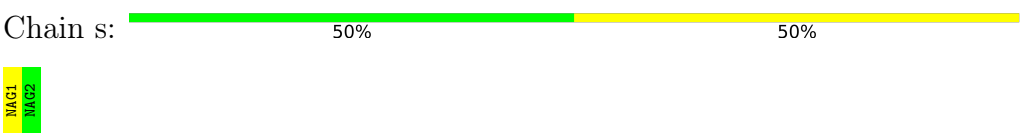
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



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

Chain s:

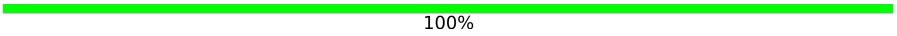


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

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

Chain w:



• Molecule 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 z:

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

Chain 0:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	117.24Å 118.94Å 273.41Å 88.43° 89.68° 60.26°	Depositor
Resolution (Å)	47.75 – 2.95 48.12 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.75-2.95) 87.8 (48.12-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.281 0.234 , 0.281	Depositor DCC
R_{free} test set	11860 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.013 for k,-h+k,l 0.013 for h-k,h,l 0.055 for -h+k,-h,l 0.055 for -k,h-k,l 0.067 for h,h-k,-l 0.027 for -k,-h,-l 0.012 for -h,-k,l 0.026 for -h+k,k,-l 0.017 for h-k,-k,-l 0.011 for -h,-h+k,-l 0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	60979	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.14% 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: 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	0.66	0/2640	0.83	0/3585
1	C	0.56	0/2640	0.75	1/3585 (0.0%)
1	E	0.59	0/2640	0.76	0/3585
1	G	0.68	1/2640 (0.0%)	0.86	6/3585 (0.2%)
1	I	0.69	1/2640 (0.0%)	0.87	2/3585 (0.1%)
1	K	0.61	0/2640	0.75	1/3585 (0.0%)
1	M	0.66	0/2640	0.80	0/3585
1	O	0.64	0/2640	0.79	1/3585 (0.0%)
1	Q	0.64	0/2640	0.82	1/3585 (0.0%)
1	S	0.57	0/2640	0.75	0/3585
1	U	0.57	0/2640	0.74	1/3585 (0.0%)
1	W	0.58	1/2640 (0.0%)	0.74	0/3585
1	Y	0.46	0/2640	0.65	1/3585 (0.0%)
1	a	0.44	0/2640	0.64	0/3585
1	c	0.44	0/2640	0.63	0/3585
2	B	0.50	0/1460	0.69	1/1961 (0.1%)
2	D	0.41	0/1460	0.56	0/1961
2	F	0.40	0/1460	0.56	0/1961
2	H	0.49	0/1460	0.64	0/1961
2	J	0.50	0/1460	0.67	0/1961
2	L	0.42	0/1460	0.54	0/1961
2	N	0.42	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.44	0/1460	0.57	0/1961
2	T	0.39	0/1460	0.57	0/1961
2	V	0.42	0/1460	0.58	0/1961
2	X	0.40	0/1460	0.59	0/1961
2	Z	0.35	0/1460	0.60	1/1961 (0.1%)
2	b	0.33	0/1460	0.56	1/1961 (0.1%)
2	d	0.36	0/1460	0.55	0/1961
All	All	0.54	3/61500 (0.0%)	0.71	17/83190 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	135	VAL	CB-CG2	-5.53	1.41	1.52
1	I	139	CYS	CB-SG	-5.52	1.72	1.81
1	G	153	TRP	CB-CG	5.50	1.60	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	166	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	Y	9	PRO	CA-N-CD	-7.79	100.59	111.50
1	G	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	Z	80	LEU	CA-CB-CG	7.16	131.78	115.30
1	G	229	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	U	209	LEU	CA-CB-CG	6.60	130.49	115.30
2	b	80	LEU	CA-CB-CG	6.20	129.56	115.30
1	G	252	ILE	CG1-CB-CG2	-5.68	98.90	111.40
1	G	80	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	G	177	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	I	112	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	G	209	LEU	CA-CB-CG	5.30	127.50	115.30
1	K	212	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	O	241	ASP	CB-CG-OD1	5.17	122.96	118.30
1	I	216	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	B	80	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	C	229	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	9	PRO	Peptide

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%)	301 (93%)	22 (7%)	0	100	100
1	C	323/334 (97%)	305 (94%)	18 (6%)	0	100	100
1	E	323/334 (97%)	302 (94%)	21 (6%)	0	100	100
1	G	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	I	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	K	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	M	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	O	323/334 (97%)	303 (94%)	19 (6%)	1 (0%)	41	73
1	Q	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	41	73
1	S	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	U	323/334 (97%)	305 (94%)	16 (5%)	2 (1%)	25	60
1	W	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	Y	323/334 (97%)	303 (94%)	20 (6%)	0	100	100
1	a	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	c	323/334 (97%)	301 (93%)	21 (6%)	1 (0%)	41	73
2	B	175/181 (97%)	166 (95%)	8 (5%)	1 (1%)	25	60
2	D	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	F	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
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%)	164 (94%)	10 (6%)	1 (1%)	25	60

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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%)	165 (94%)	10 (6%)	0	100 100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100 100
2	T	175/181 (97%)	166 (95%)	9 (5%)	0	100 100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100 100
2	X	175/181 (97%)	164 (94%)	11 (6%)	0	100 100
2	Z	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	25 60
2	b	175/181 (97%)	165 (94%)	10 (6%)	0	100 100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100 100
All	All	7470/7725 (97%)	7003 (94%)	459 (6%)	8 (0%)	51 83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	O	248	ASN
1	Q	248	ASN
1	c	248	ASN
2	B	60	ASN
2	Z	176	GLY
1	U	248	ASN
2	L	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%)	282 (97%)	10 (3%)	37 69
1	C	292/300 (97%)	285 (98%)	7 (2%)	49 77
1	E	292/300 (97%)	284 (97%)	8 (3%)	44 74
1	G	292/300 (97%)	285 (98%)	7 (2%)	49 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	292/300 (97%)	277 (95%)	15 (5%)	24 56
1	K	292/300 (97%)	284 (97%)	8 (3%)	44 74
1	M	292/300 (97%)	284 (97%)	8 (3%)	44 74
1	O	292/300 (97%)	284 (97%)	8 (3%)	44 74
1	Q	292/300 (97%)	282 (97%)	10 (3%)	37 69
1	S	292/300 (97%)	285 (98%)	7 (2%)	49 77
1	U	292/300 (97%)	287 (98%)	5 (2%)	60 83
1	W	292/300 (97%)	284 (97%)	8 (3%)	44 74
1	Y	292/300 (97%)	286 (98%)	6 (2%)	53 80
1	a	292/300 (97%)	285 (98%)	7 (2%)	49 77
1	c	292/300 (97%)	288 (99%)	4 (1%)	67 86
2	B	151/155 (97%)	150 (99%)	1 (1%)	84 93
2	D	151/155 (97%)	150 (99%)	1 (1%)	84 93
2	F	151/155 (97%)	151 (100%)	0	100 100
2	H	151/155 (97%)	148 (98%)	3 (2%)	55 80
2	J	151/155 (97%)	150 (99%)	1 (1%)	84 93
2	L	151/155 (97%)	151 (100%)	0	100 100
2	N	151/155 (97%)	151 (100%)	0	100 100
2	P	151/155 (97%)	150 (99%)	1 (1%)	84 93
2	R	151/155 (97%)	149 (99%)	2 (1%)	69 87
2	T	151/155 (97%)	151 (100%)	0	100 100
2	V	151/155 (97%)	148 (98%)	3 (2%)	55 80
2	X	151/155 (97%)	149 (99%)	2 (1%)	69 87
2	Z	151/155 (97%)	146 (97%)	5 (3%)	38 70
2	b	151/155 (97%)	149 (99%)	2 (1%)	69 87
2	d	151/155 (97%)	148 (98%)	3 (2%)	55 80
All	All	6645/6825 (97%)	6503 (98%)	142 (2%)	53 80

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	174	GLU
1	A	219	THR
1	A	261	LYS
1	A	264	ASP
1	A	283	THR
1	A	300	LEU
1	A	310	LYS
1	A	313	ARG
1	C	28	THR
1	C	46	LYS
1	C	120	LYS
1	C	135	VAL
1	C	174	GLU
1	C	261	LYS
1	C	310	LYS
1	E	46	LYS
1	E	114	ARG
1	E	166	ARG
1	E	174	GLU
1	E	199	THR
1	E	230	MET
1	E	261	LYS
1	E	273	GLU
1	G	28	THR
1	G	112	LEU
1	G	167	SER
1	G	208	THR
1	G	252	ILE
1	G	261	LYS
1	G	313	ARG
1	I	28	THR
1	I	65	SER
1	I	75	MET
1	I	80	ILE
1	I	111	LEU
1	I	137	SER
1	I	142	GLN
1	I	166	ARG
1	I	167	SER
1	I	194	LEU
1	I	208	THR
1	I	261	LYS

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Mol	Chain	Res	Type
1	I	264	ASP
1	I	279	THR
1	I	313	ARG
1	K	46	LYS
1	K	56	VAL
1	K	155	ILE
1	K	160	THR
1	K	187	ASP
1	K	261	LYS
1	K	273	GLU
1	K	313	ARG
1	M	28	THR
1	M	56	VAL
1	M	133	SER
1	M	219	THR
1	M	261	LYS
1	M	310	LYS
1	M	311	SER
1	M	313	ARG
1	O	56	VAL
1	O	176	LEU
1	O	208	THR
1	O	248	ASN
1	O	256	TYR
1	O	261	LYS
1	O	310	LYS
1	O	320	LEU
1	Q	28	THR
1	Q	94	VAL
1	Q	135	VAL
1	Q	166	ARG
1	Q	167	SER
1	Q	174	GLU
1	Q	176	LEU
1	Q	261	LYS
1	Q	313	ARG
1	Q	320	LEU
1	S	75	MET
1	S	174	GLU
1	S	208	THR
1	S	261	LYS
1	S	300	LEU

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Mol	Chain	Res	Type
1	S	311	SER
1	S	313	ARG
1	U	28	THR
1	U	111	LEU
1	U	261	LYS
1	U	272	LEU
1	U	313	ARG
1	W	28	THR
1	W	75	MET
1	W	155	ILE
1	W	264	ASP
1	W	272	LEU
1	W	311	SER
1	W	313	ARG
1	W	320	LEU
1	Y	28	THR
1	Y	114	ARG
1	Y	174	GLU
1	Y	261	LYS
1	Y	264	ASP
1	Y	309	VAL
1	a	65	SER
1	a	81	ASN
1	a	87	ILE
1	a	114	ARG
1	a	199	THR
1	a	261	LYS
1	a	291	SER
1	c	28	THR
1	c	114	ARG
1	c	261	LYS
1	c	312	ASN
2	B	43	LYS
2	D	113	SER
2	H	30	GLN
2	H	57	ASP
2	H	94	TYR
2	J	11	GLU
2	P	116	LYS
2	R	50	ASN
2	R	94	TYR
2	V	17	MET

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Mol	Chain	Res	Type
2	V	29	GLU
2	V	94	TYR
2	X	86	ASP
2	X	94	TYR
2	Z	30	GLN
2	Z	57	ASP
2	Z	66	VAL
2	Z	77	ILE
2	Z	80	LEU
2	b	43	LYS
2	b	80	LEU
2	d	19	ASP
2	d	30	GLN
2	d	86	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	C	122	GLN
1	E	110	HIS
1	E	197	ASN
1	G	117	HIS
1	G	210	ASN
1	I	122	GLN
1	I	150	ASN
1	K	196	GLN
1	K	197	ASN
1	M	12	GLN
1	M	197	ASN
1	M	322	ASN
1	O	150	ASN
1	Q	117	HIS
1	Q	196	GLN
1	S	110	HIS
1	S	122	GLN
1	U	122	GLN
1	W	150	ASN
1	Y	38	HIS
1	Y	197	ASN
1	c	18	HIS
2	L	62	GLN

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Mol	Chain	Res	Type
2	P	142	HIS
2	V	117	ASN
2	b	142	HIS
2	d	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

58 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	1,4	14,14,15	0.62	0	17,19,21	1.00	1 (5%)
4	NAG	0	2	4	14,14,15	0.43	0	17,19,21	0.43	0
3	NAG	e	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	1.10	2 (11%)
3	NAG	e	2	3	14,14,15	0.31	0	17,19,21	0.51	0
3	BMA	e	3	3	11,11,12	1.69	3 (27%)	15,15,17	1.43	3 (20%)
4	NAG	f	1	1,4	14,14,15	1.03	1 (7%)	17,19,21	1.21	2 (11%)
4	NAG	f	2	4	14,14,15	1.43	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	g	1	3,1	14,14,15	0.34	0	17,19,21	0.56	0
3	NAG	g	2	3	14,14,15	0.60	0	17,19,21	0.64	0
3	BMA	g	3	3	11,11,12	2.17	5 (45%)	15,15,17	1.60	3 (20%)
3	NAG	h	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	h	2	3	14,14,15	1.27	1 (7%)	17,19,21	1.27	2 (11%)
3	BMA	h	3	3	11,11,12	1.62	1 (9%)	15,15,17	1.75	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	i	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.39	3 (17%)
4	NAG	i	2	4	14,14,15	0.65	1 (7%)	17,19,21	0.46	0
3	NAG	j	1	3,1	14,14,15	1.69	2 (14%)	17,19,21	1.36	2 (11%)
3	NAG	j	2	3	14,14,15	0.90	1 (7%)	17,19,21	0.79	0
3	BMA	j	3	3	11,11,12	2.01	4 (36%)	15,15,17	1.23	2 (13%)
4	NAG	k	1	1,4	14,14,15	1.31	1 (7%)	17,19,21	1.37	2 (11%)
4	NAG	k	2	4	14,14,15	0.64	0	17,19,21	0.39	0
3	NAG	l	1	3,1	14,14,15	1.45	1 (7%)	17,19,21	1.27	2 (11%)
3	NAG	l	2	3	14,14,15	1.03	1 (7%)	17,19,21	0.81	1 (5%)
3	BMA	l	3	3	11,11,12	2.43	4 (36%)	15,15,17	1.68	4 (26%)
4	NAG	m	1	1,4	14,14,15	0.79	1 (7%)	17,19,21	1.13	2 (11%)
4	NAG	m	2	4	14,14,15	1.61	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	n	1	3,1	14,14,15	0.61	1 (7%)	17,19,21	0.69	0
3	NAG	n	2	3	14,14,15	0.45	0	17,19,21	0.80	0
3	BMA	n	3	3	11,11,12	2.26	4 (36%)	15,15,17	1.67	2 (13%)
3	NAG	o	1	3,1	14,14,15	0.59	0	17,19,21	0.68	0
3	NAG	o	2	3	14,14,15	0.95	1 (7%)	17,19,21	0.83	1 (5%)
3	BMA	o	3	3	11,11,12	2.01	3 (27%)	15,15,17	1.59	2 (13%)
3	NAG	p	1	3,1	14,14,15	0.36	0	17,19,21	0.90	1 (5%)
3	NAG	p	2	3	14,14,15	0.66	1 (7%)	17,19,21	0.35	0
3	BMA	p	3	3	11,11,12	1.65	3 (27%)	15,15,17	1.39	3 (20%)
4	NAG	q	1	1,4	14,14,15	1.21	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	q	2	4	14,14,15	0.43	0	17,19,21	0.69	1 (5%)
3	NAG	r	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	r	2	3	14,14,15	0.23	0	17,19,21	0.52	0
3	BMA	r	3	3	11,11,12	0.72	0	15,15,17	1.96	4 (26%)
4	NAG	s	1	1,4	14,14,15	1.18	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	s	2	4	14,14,15	0.50	0	17,19,21	0.51	0
3	NAG	t	1	3,1	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
3	NAG	t	2	3	14,14,15	0.47	0	17,19,21	0.82	0
3	BMA	t	3	3	11,11,12	1.97	3 (27%)	15,15,17	1.97	5 (33%)
4	NAG	u	1	1,4	14,14,15	0.55	0	17,19,21	0.70	0
4	NAG	u	2	4	14,14,15	1.57	3 (21%)	17,19,21	1.19	1 (5%)
3	NAG	v	1	3,1	14,14,15	0.44	0	17,19,21	0.55	0
3	NAG	v	2	3	14,14,15	1.53	2 (14%)	17,19,21	1.08	1 (5%)
3	BMA	v	3	3	11,11,12	1.18	0	15,15,17	1.75	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	w	1	1,4	14,14,15	0.47	0	17,19,21	0.52	0
4	NAG	w	2	4	14,14,15	0.40	0	17,19,21	0.39	0
3	NAG	x	1	3,1	14,14,15	0.63	0	17,19,21	0.97	1 (5%)
3	NAG	x	2	3	14,14,15	0.61	0	17,19,21	0.92	0
3	BMA	x	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
4	NAG	y	1	1,4	14,14,15	1.37	1 (7%)	17,19,21	1.40	2 (11%)
4	NAG	y	2	4	14,14,15	0.69	0	17,19,21	0.71	0
4	NAG	z	1	1,4	14,14,15	0.36	0	17,19,21	0.40	0
4	NAG	z	2	4	14,14,15	0.35	0	17,19,21	0.51	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
4	NAG	0	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	0	2	4	-	2/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	BMA	e	3	3	-	0/2/19/22	0/1/1/1
4	NAG	f	1	1,4	-	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	-	2/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
4	NAG	k	1	1,4	-	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	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1
3	BMA	l	3	3	-	0/2/19/22	0/1/1/1
4	NAG	m	1	1,4	-	1/6/23/26	0/1/1/1

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

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	1	NAG	O5-C1	-5.82	1.34	1.43
3	v	2	NAG	O5-C1	-5.03	1.35	1.43
4	u	2	NAG	O5-C1	-4.96	1.35	1.43
3	l	1	NAG	O5-C1	-4.94	1.35	1.43
4	y	1	NAG	O5-C1	-4.80	1.36	1.43
3	l	3	BMA	C4-C3	4.70	1.64	1.52
4	m	2	NAG	O5-C1	4.66	1.51	1.43
4	k	1	NAG	O5-C1	-4.62	1.36	1.43
4	i	1	NAG	O5-C1	-4.49	1.36	1.43
3	g	3	BMA	C4-C5	4.45	1.62	1.53
3	l	3	BMA	C4-C5	4.39	1.62	1.53
3	t	3	BMA	C2-C3	4.35	1.58	1.52
3	h	2	NAG	O5-C1	-4.31	1.36	1.43
3	n	3	BMA	C4-C3	4.26	1.63	1.52
3	o	3	BMA	C4-C5	4.24	1.62	1.53
4	s	1	NAG	O5-C1	-4.14	1.37	1.43
3	t	3	BMA	C1-C2	4.04	1.61	1.52
4	q	1	NAG	O5-C1	-4.03	1.37	1.43
3	n	3	BMA	C4-C5	3.93	1.61	1.53
3	j	3	BMA	C4-C3	3.93	1.62	1.52
4	f	2	NAG	C1-C2	3.90	1.58	1.52
3	e	3	BMA	C1-C2	3.81	1.60	1.52
3	h	3	BMA	C1-C2	3.76	1.60	1.52
3	l	2	NAG	O5-C1	-3.63	1.37	1.43
4	m	2	NAG	C1-C2	3.59	1.57	1.52
4	f	1	NAG	O5-C1	-3.59	1.38	1.43
3	p	3	BMA	C4-C5	3.47	1.60	1.53
3	o	3	BMA	C4-C3	3.36	1.60	1.52
4	f	2	NAG	O5-C1	3.31	1.49	1.43
3	e	1	NAG	C1-C2	3.27	1.57	1.52
3	j	2	NAG	O5-C1	-3.27	1.38	1.43
3	g	3	BMA	C4-C3	3.21	1.60	1.52
3	g	3	BMA	C1-C2	3.15	1.59	1.52
3	j	3	BMA	C4-C5	2.98	1.59	1.53
3	p	3	BMA	O5-C1	-2.73	1.39	1.43
3	o	2	NAG	O5-C1	-2.64	1.39	1.43
3	n	3	BMA	C6-C5	2.63	1.60	1.51
3	n	3	BMA	O3-C3	2.63	1.49	1.43
4	m	1	NAG	O5-C1	-2.60	1.39	1.43
3	e	3	BMA	C4-C3	2.59	1.58	1.52
3	l	3	BMA	C1-C2	2.55	1.58	1.52
3	h	1	NAG	O5-C1	2.47	1.47	1.43
3	j	3	BMA	C2-C3	2.46	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	o	3	BMA	O5-C1	-2.44	1.39	1.43
3	g	3	BMA	O3-C3	2.35	1.48	1.43
3	r	1	NAG	O5-C1	-2.31	1.40	1.43
4	i	2	NAG	C1-C2	2.28	1.55	1.52
3	p	3	BMA	C4-C3	2.28	1.58	1.52
3	e	3	BMA	C2-C3	2.28	1.55	1.52
3	v	2	NAG	C1-C2	2.18	1.55	1.52
3	l	3	BMA	O2-C2	2.17	1.47	1.43
4	u	2	NAG	C1-C2	2.15	1.55	1.52
3	j	3	BMA	C1-C2	2.12	1.57	1.52
3	g	3	BMA	C6-C5	2.12	1.59	1.51
3	p	2	NAG	O5-C1	-2.10	1.40	1.43
3	n	1	NAG	C1-C2	2.09	1.55	1.52
4	u	2	NAG	C3-C2	2.09	1.57	1.52
3	j	1	NAG	C3-C2	2.06	1.56	1.52
3	t	3	BMA	C4-C3	2.01	1.57	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	v	3	BMA	C1-O5-C5	4.85	118.76	112.19
4	f	2	NAG	C1-O5-C5	4.40	118.15	112.19
3	t	3	BMA	C1-C2-C3	4.39	115.07	109.67
3	j	1	NAG	C4-C3-C2	4.25	117.25	111.02
3	r	3	BMA	C3-C4-C5	4.23	117.78	110.24
4	k	1	NAG	C3-C4-C5	4.05	117.46	110.24
3	o	3	BMA	C3-C4-C5	3.94	117.28	110.24
3	h	2	NAG	C3-C4-C5	3.94	117.27	110.24
4	u	2	NAG	C4-C3-C2	3.88	116.71	111.02
3	n	3	BMA	C1-O5-C5	3.85	117.40	112.19
3	l	3	BMA	C3-C4-C5	3.83	117.07	110.24
3	h	3	BMA	O2-C2-C1	3.78	116.88	109.15
4	y	1	NAG	C3-C4-C5	3.77	116.97	110.24
4	f	1	NAG	C3-C4-C5	3.70	116.83	110.24
4	y	1	NAG	C4-C3-C2	3.60	116.30	111.02
4	i	1	NAG	C4-C3-C2	3.55	116.22	111.02
3	r	3	BMA	O5-C1-C2	-3.49	105.39	110.77
4	m	1	NAG	C3-C4-C5	3.47	116.44	110.24
3	l	1	NAG	C4-C3-C2	3.45	116.08	111.02
3	h	1	NAG	C1-O5-C5	3.41	116.81	112.19
3	t	3	BMA	O5-C1-C2	3.30	115.87	110.77
3	r	3	BMA	O3-C3-C4	-3.28	102.78	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	r	3	BMA	O3-C3-C2	3.24	116.19	109.99
4	m	2	NAG	C1-O5-C5	3.20	116.53	112.19
4	k	1	NAG	C4-C3-C2	3.12	115.59	111.02
3	p	1	NAG	C1-O5-C5	3.06	116.34	112.19
4	i	1	NAG	C3-C4-C5	3.00	115.60	110.24
3	h	3	BMA	C1-O5-C5	2.90	116.12	112.19
3	l	3	BMA	O2-C2-C1	2.87	115.03	109.15
4	q	1	NAG	C4-C3-C2	2.81	115.14	111.02
3	e	3	BMA	O5-C1-C2	2.81	115.11	110.77
3	l	3	BMA	C2-C3-C4	2.75	115.65	110.89
3	x	3	BMA	O5-C5-C6	2.70	111.43	107.20
3	h	3	BMA	O2-C2-C3	-2.66	104.80	110.14
3	t	3	BMA	C1-O5-C5	2.63	115.75	112.19
3	t	3	BMA	C2-C3-C4	2.63	115.44	110.89
3	j	1	NAG	C3-C4-C5	2.61	114.90	110.24
3	e	1	NAG	C1-O5-C5	2.61	115.73	112.19
3	r	1	NAG	C1-O5-C5	2.58	115.69	112.19
3	v	2	NAG	C4-C3-C2	2.54	114.74	111.02
3	v	3	BMA	O2-C2-C3	-2.53	105.06	110.14
3	g	3	BMA	O2-C2-C1	2.52	114.32	109.15
3	h	2	NAG	C4-C3-C2	2.52	114.72	111.02
4	f	1	NAG	C4-C3-C2	2.52	114.70	111.02
3	o	2	NAG	C1-O5-C5	-2.51	108.78	112.19
4	0	1	NAG	C4-C3-C2	2.43	114.58	111.02
3	g	3	BMA	O2-C2-C3	-2.41	105.32	110.14
4	i	1	NAG	C1-O5-C5	-2.40	108.94	112.19
3	p	3	BMA	C1-O5-C5	2.38	115.42	112.19
4	m	1	NAG	C4-C3-C2	2.37	114.50	111.02
3	n	3	BMA	O2-C2-C3	-2.36	105.40	110.14
3	e	3	BMA	C1-C2-C3	2.36	112.57	109.67
3	g	3	BMA	C3-C4-C5	2.34	114.41	110.24
3	t	3	BMA	O2-C2-C1	2.33	113.91	109.15
4	q	1	NAG	C1-O5-C5	-2.32	109.04	112.19
4	q	2	NAG	C1-O5-C5	2.29	115.29	112.19
3	e	3	BMA	O2-C2-C1	2.28	113.82	109.15
3	l	1	NAG	C1-O5-C5	-2.21	109.19	112.19
3	p	3	BMA	C3-C4-C5	2.21	114.19	110.24
3	x	1	NAG	C1-O5-C5	2.21	115.19	112.19
3	o	3	BMA	O2-C2-C3	-2.17	105.79	110.14
3	j	3	BMA	C3-C4-C5	2.15	114.08	110.24
3	j	3	BMA	O5-C5-C6	2.15	110.58	107.20
3	e	1	NAG	O5-C1-C2	-2.13	107.92	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	s	1	NAG	C4-C3-C2	2.09	114.09	111.02
3	p	3	BMA	C1-C2-C3	-2.08	107.11	109.67
3	t	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	l	3	BMA	O5-C1-C2	2.07	113.96	110.77
3	v	3	BMA	O5-C1-C2	2.05	113.94	110.77
3	l	2	NAG	C1-O5-C5	-2.04	109.42	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	x	3	BMA	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	s	1	NAG	C4-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
3	v	2	NAG	O5-C5-C6-O6
3	v	3	BMA	O5-C5-C6-O6
4	s	1	NAG	O5-C5-C6-O6
3	v	2	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	p	3	BMA	O5-C5-C6-O6
3	x	3	BMA	C4-C5-C6-O6
4	s	2	NAG	O5-C5-C6-O6
4	0	1	NAG	O5-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
4	0	1	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	s	2	NAG	C4-C5-C6-O6
4	z	1	NAG	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
3	p	1	NAG	C4-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	p	3	BMA	C4-C5-C6-O6
3	v	3	BMA	C4-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
4	0	2	NAG	C4-C5-C6-O6
4	z	1	NAG	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6

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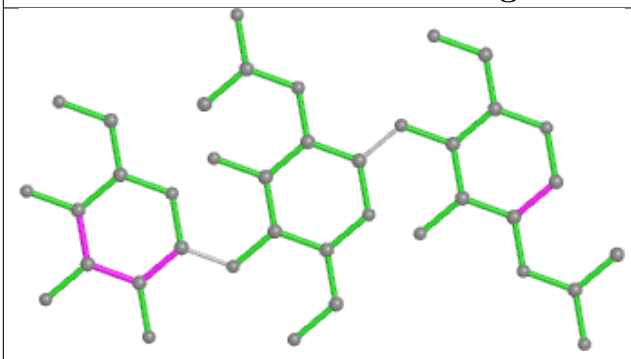
Mol	Chain	Res	Type	Atoms
4	w	1	NAG	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
3	p	1	NAG	O5-C5-C6-O6
3	l	1	NAG	C4-C5-C6-O6
3	r	3	BMA	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
3	r	2	NAG	C4-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
4	w	1	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	w	2	NAG	O5-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	t	1	NAG	C4-C5-C6-O6
4	k	1	NAG	C4-C5-C6-O6
3	r	3	BMA	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	p	2	NAG	C4-C5-C6-O6
4	z	2	NAG	C4-C5-C6-O6
4	u	1	NAG	C4-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6
3	v	2	NAG	C1-C2-N2-C7
3	o	3	BMA	C4-C5-C6-O6
4	q	1	NAG	C1-C2-N2-C7
3	h	2	NAG	C4-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6

There are no ring outliers.

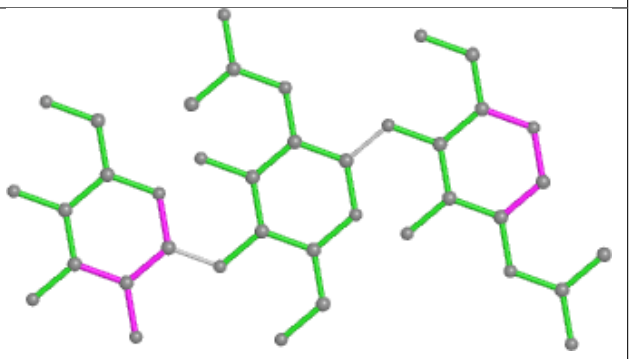
No monomer is involved in short contacts.

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

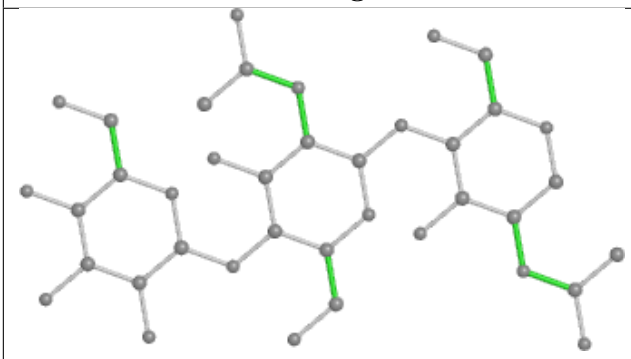
Oligosaccharide Chain e



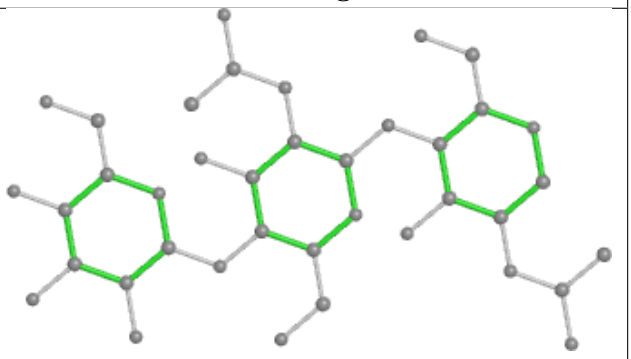
Bond lengths



Bond angles

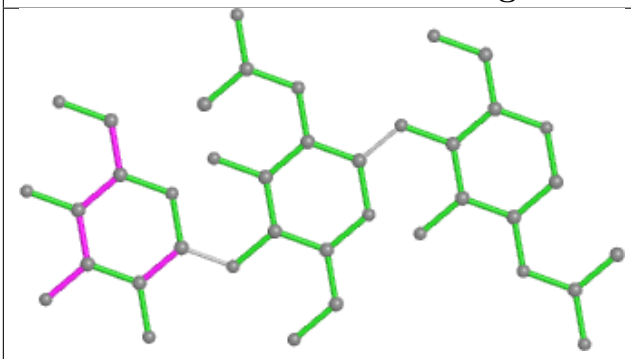


Torsions

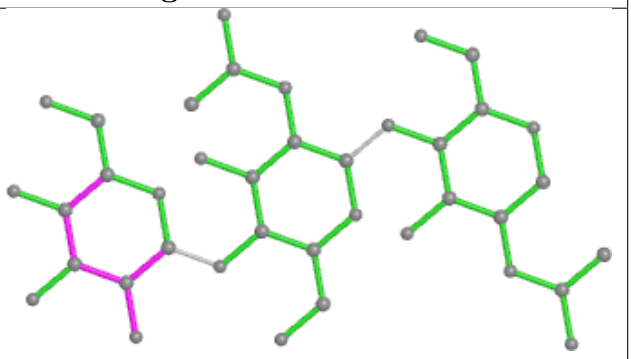


Rings

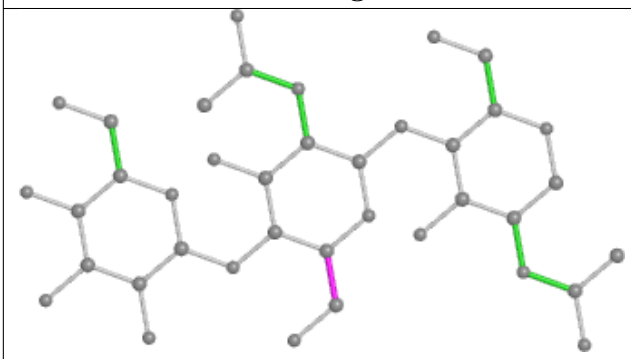
Oligosaccharide Chain g



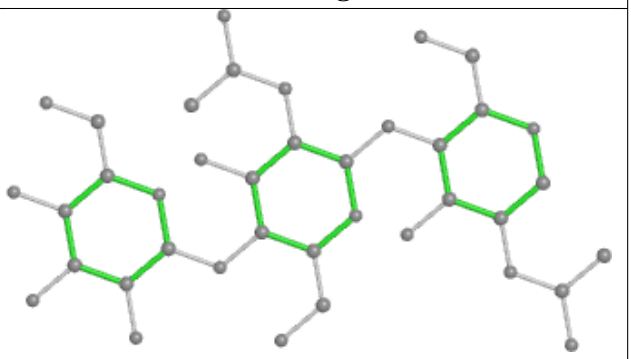
Bond lengths



Bond angles

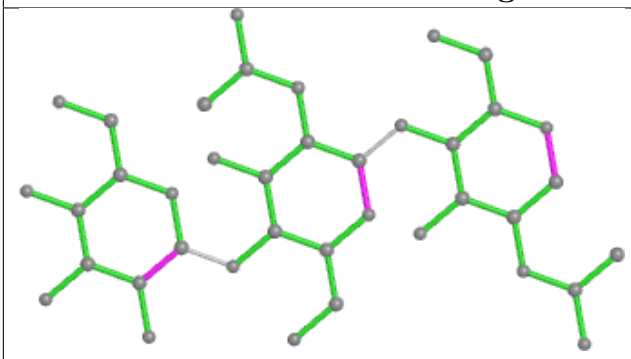


Torsions

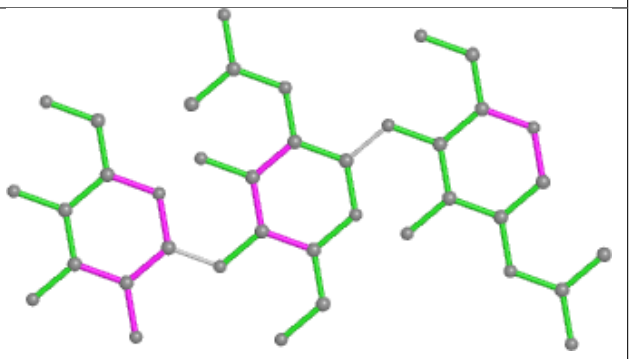


Rings

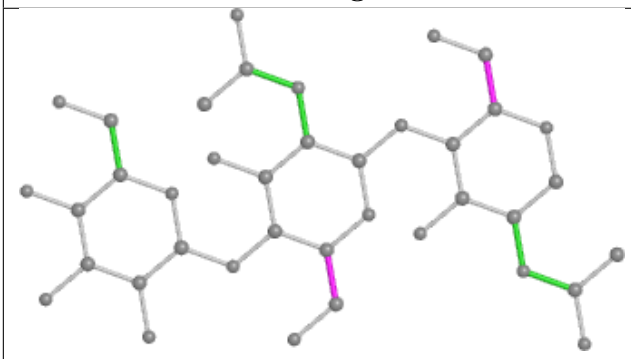
Oligosaccharide Chain h



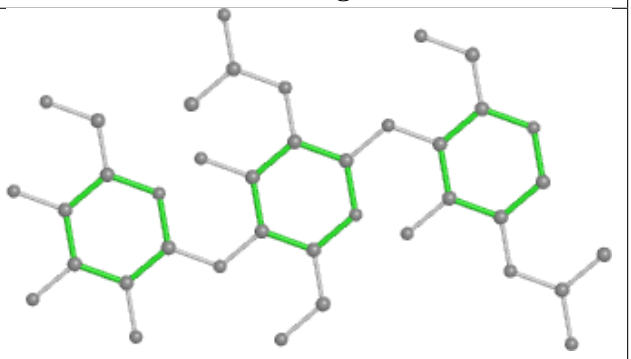
Bond lengths



Bond angles

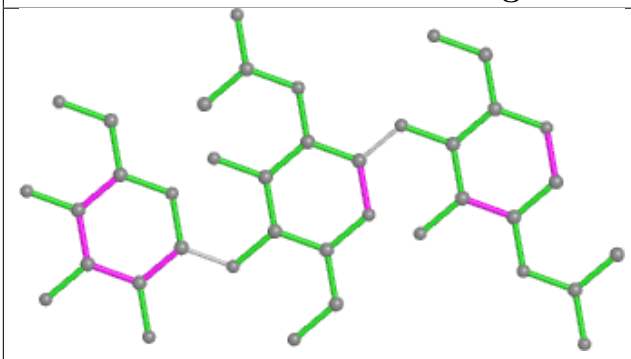


Torsions

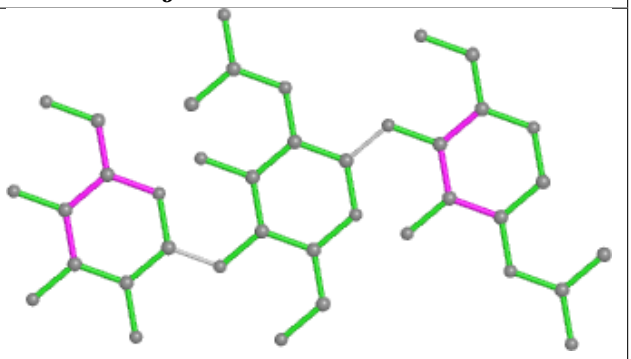


Rings

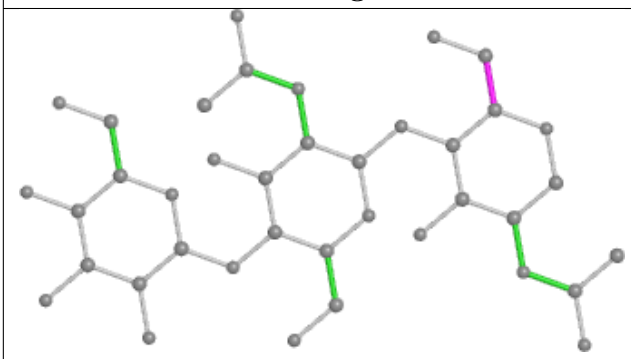
Oligosaccharide Chain j



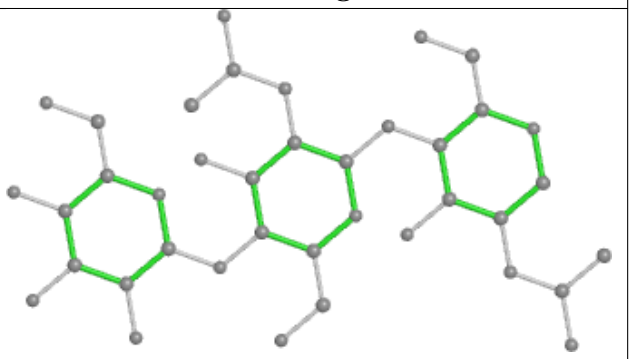
Bond lengths



Bond angles

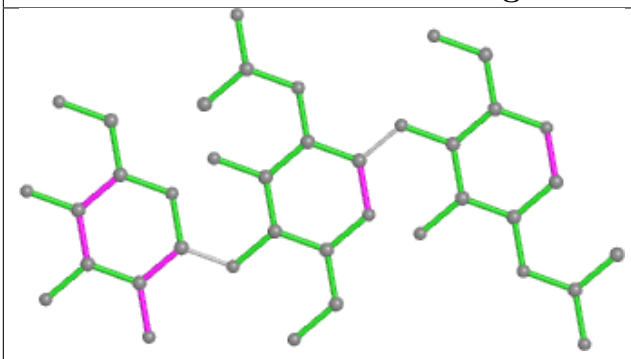


Torsions



Rings

Oligosaccharide Chain l



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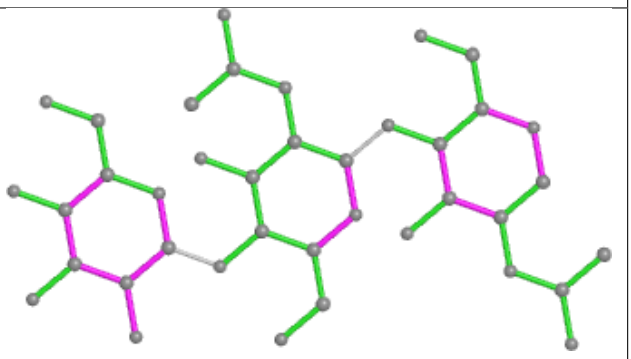

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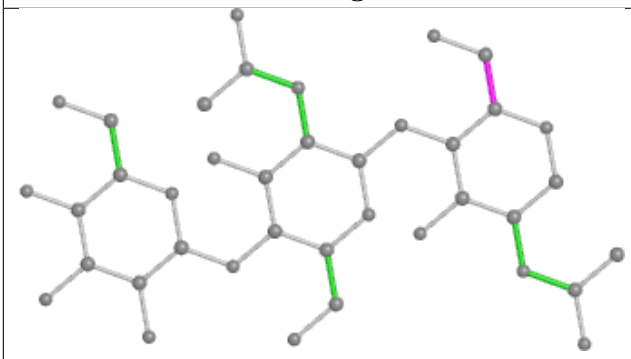

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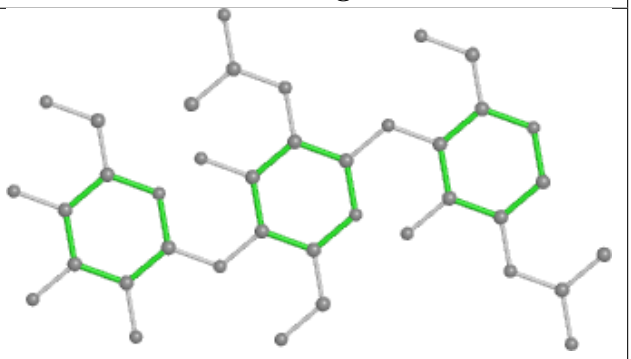
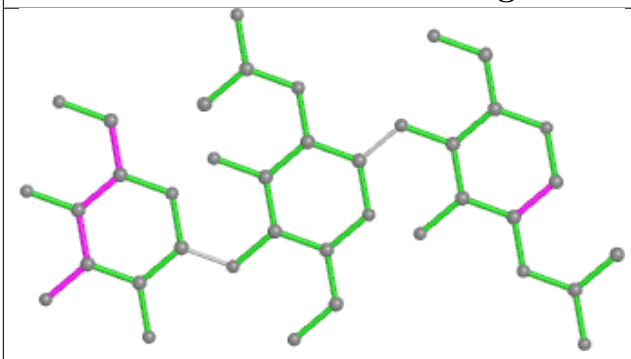


Rings

Oligosaccharide Chain n



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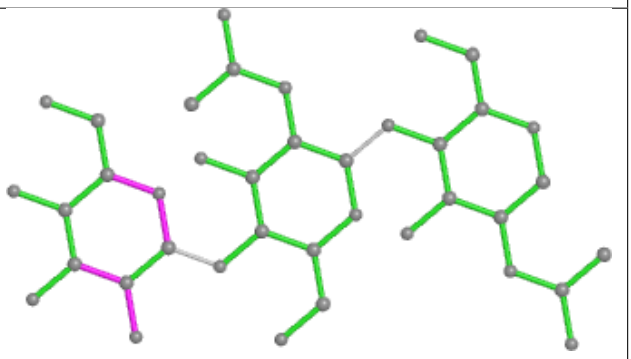

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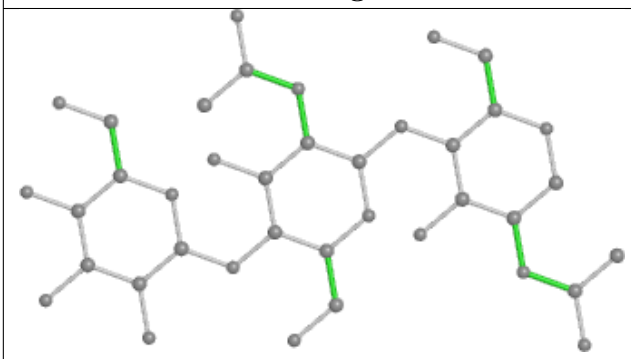

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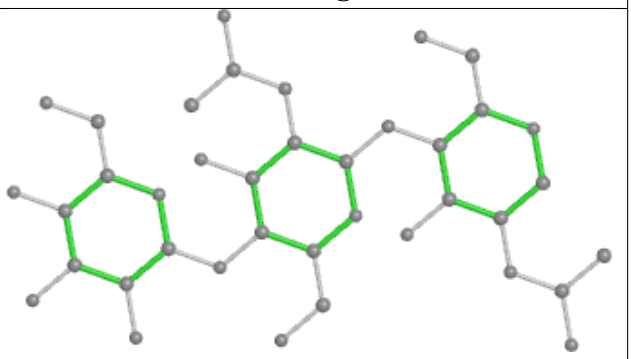
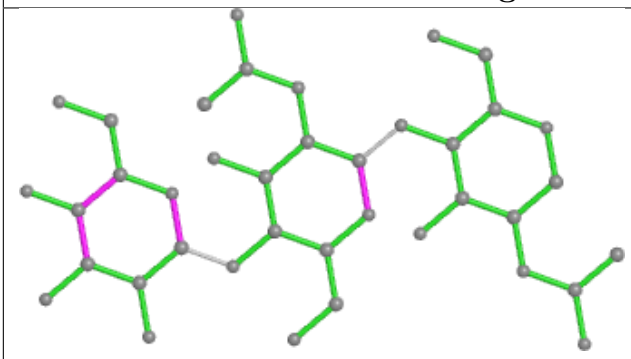


Rings

Oligosaccharide Chain o



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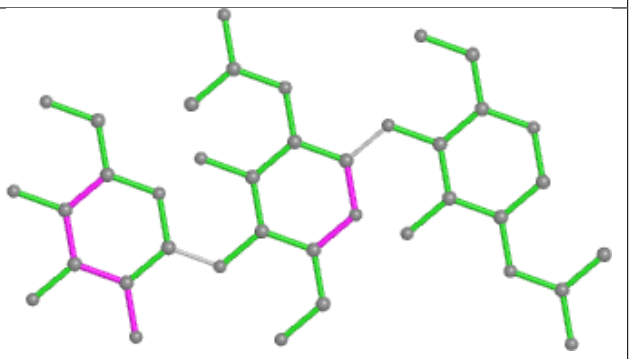

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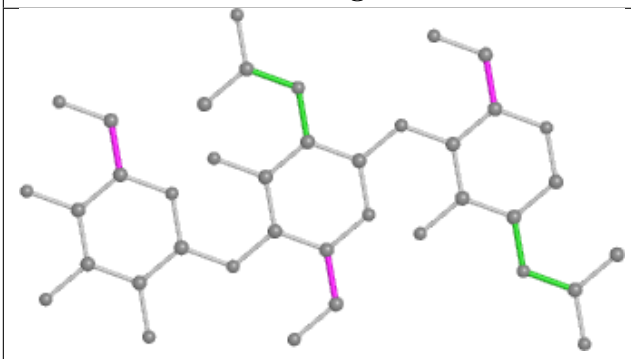

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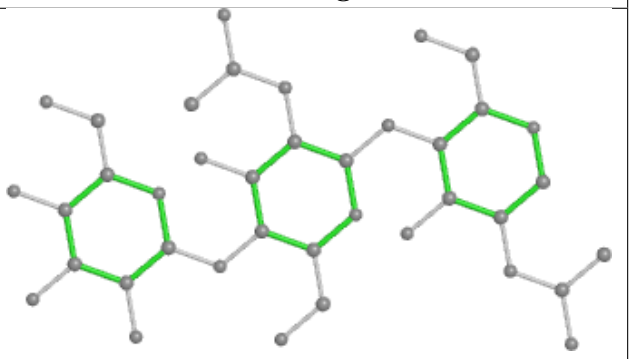
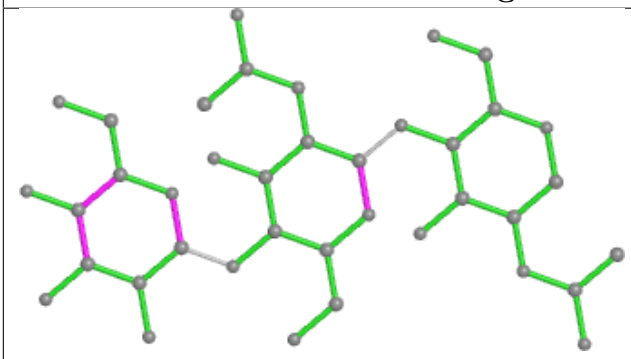


Rings

Oligosaccharide Chain p



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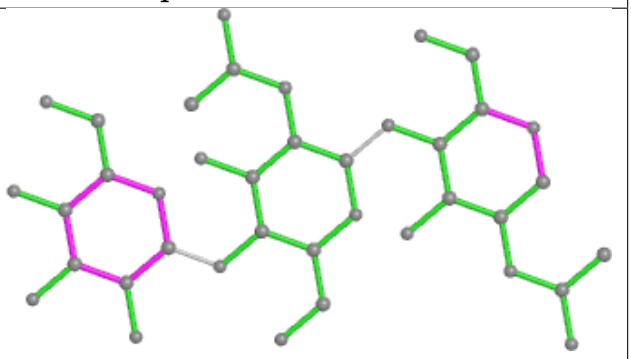

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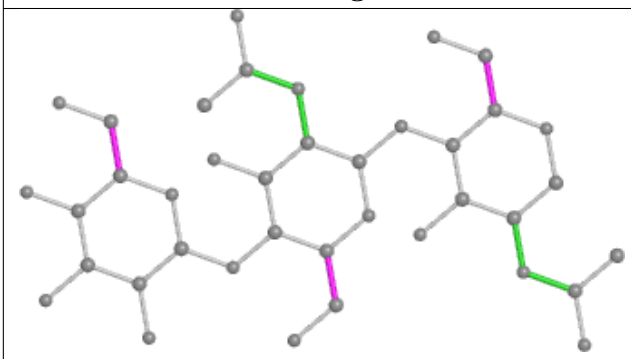

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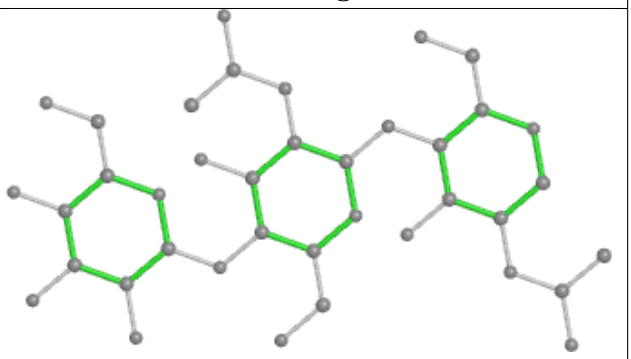
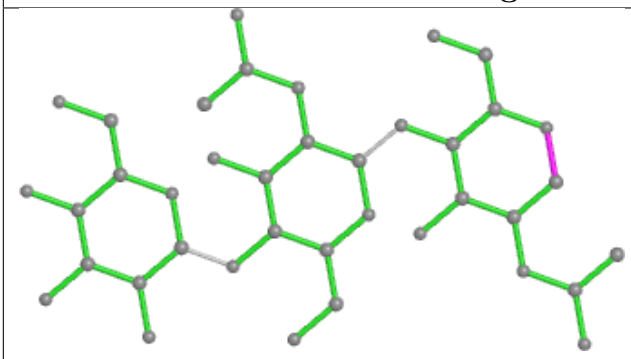


Rings

Oligosaccharide Chain r



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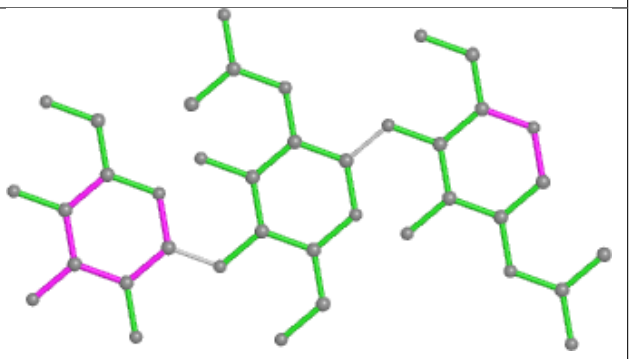

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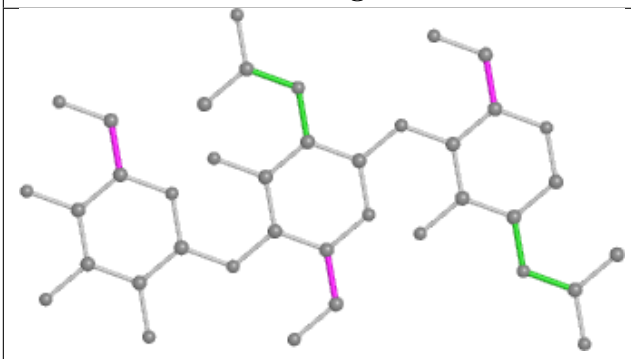

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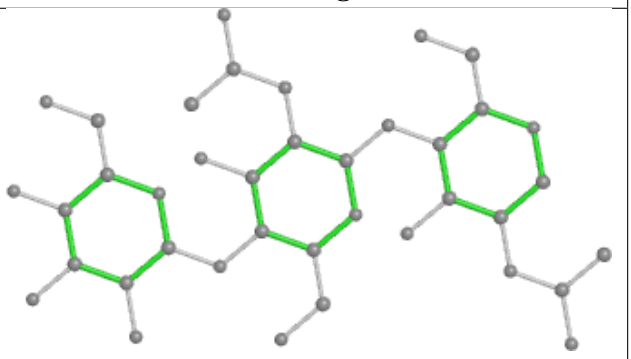
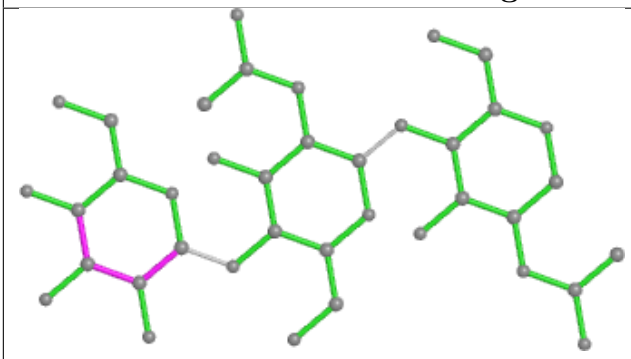


Rings

Oligosaccharide Chain t



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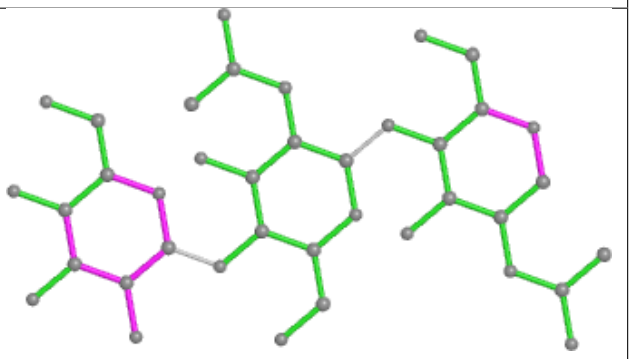

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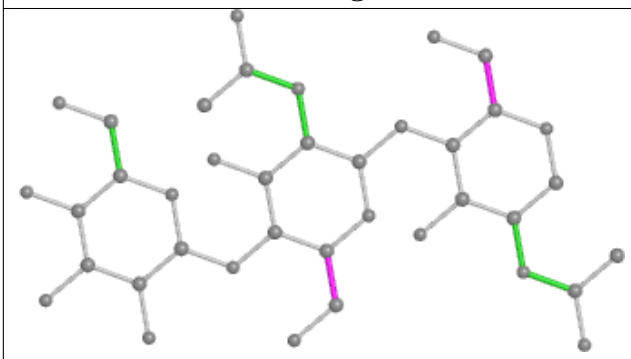

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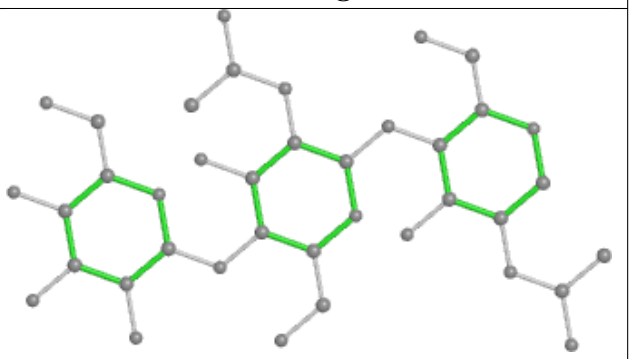
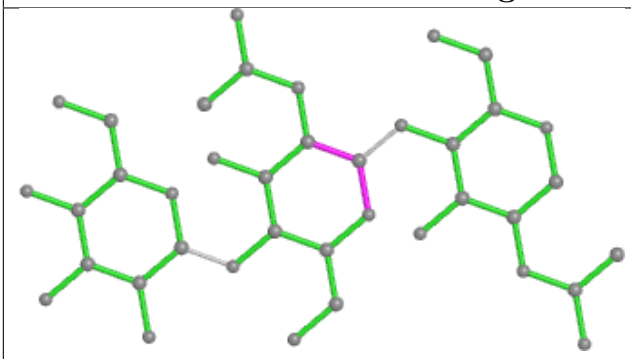


Rings

Oligosaccharide Chain v



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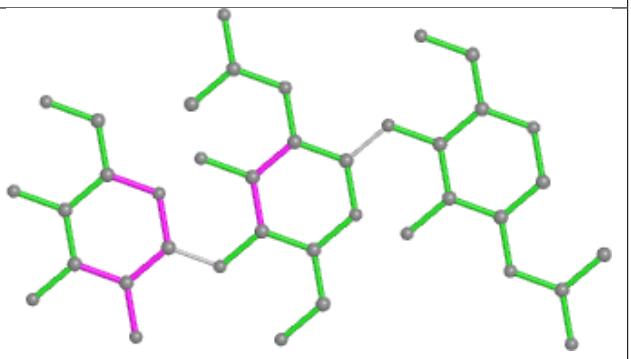

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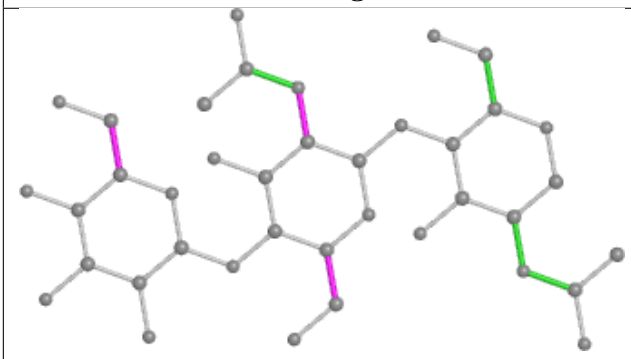

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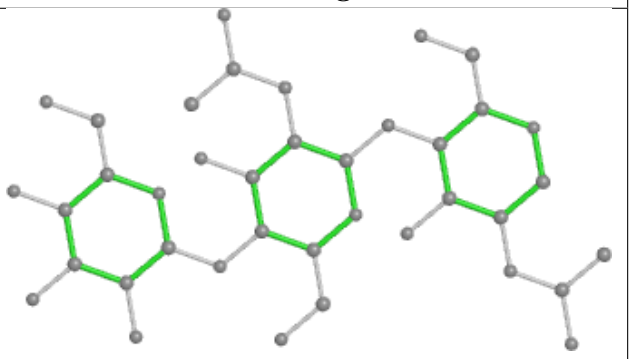
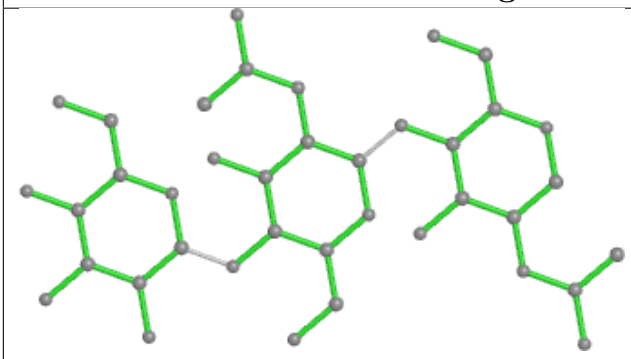


Rings

Oligosaccharide Chain x



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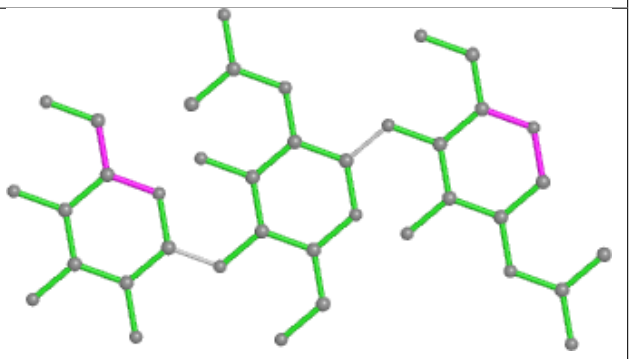

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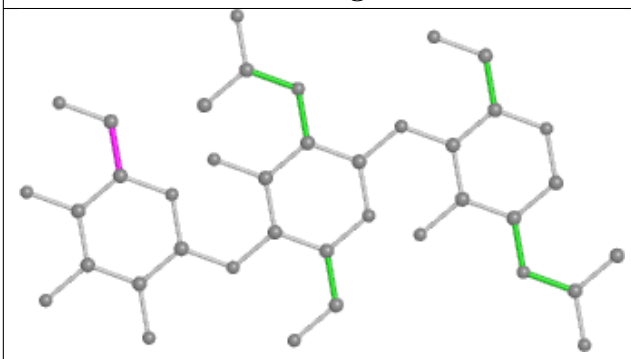

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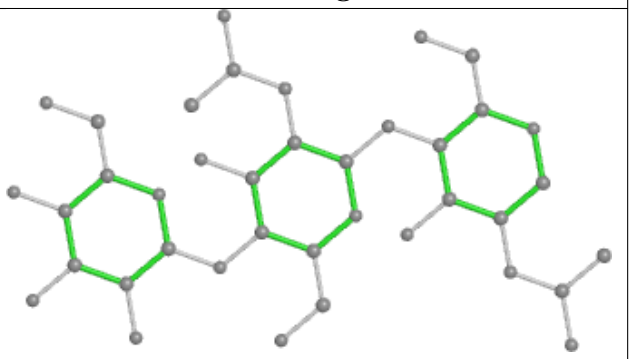
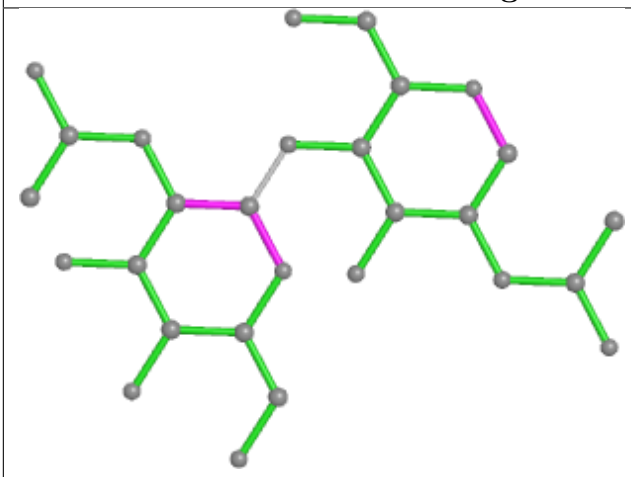


Rings

Oligosaccharide Chain f



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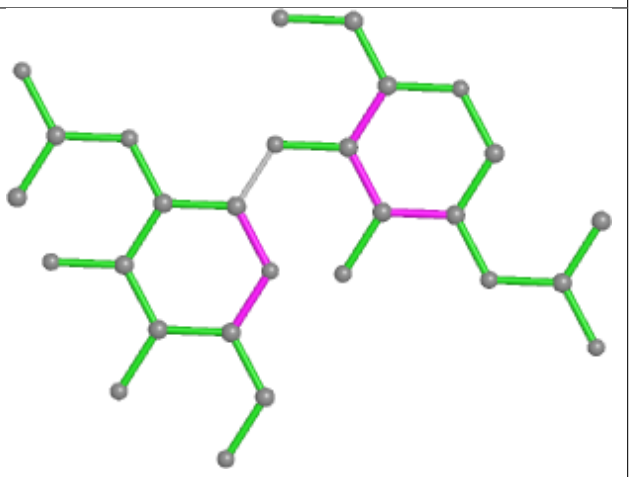

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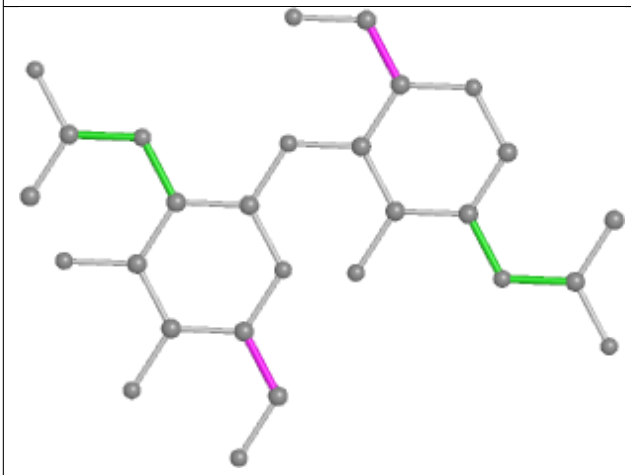

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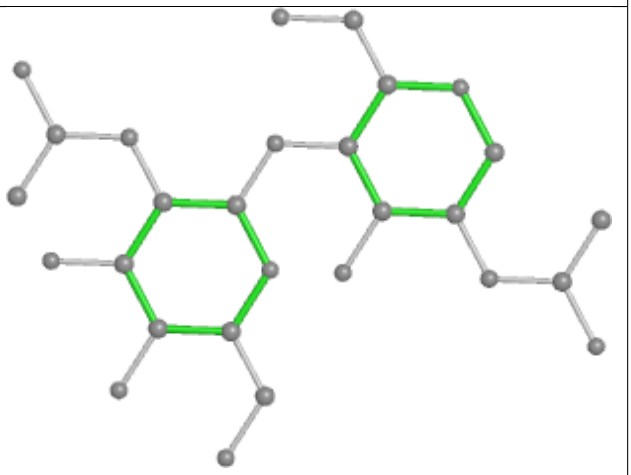
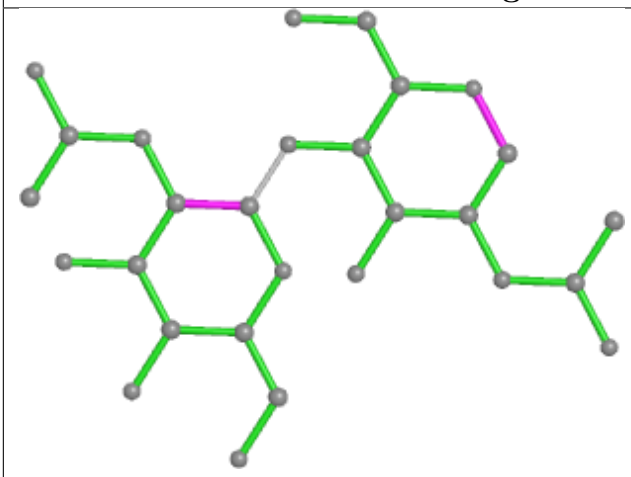


Rings

Oligosaccharide Chain i



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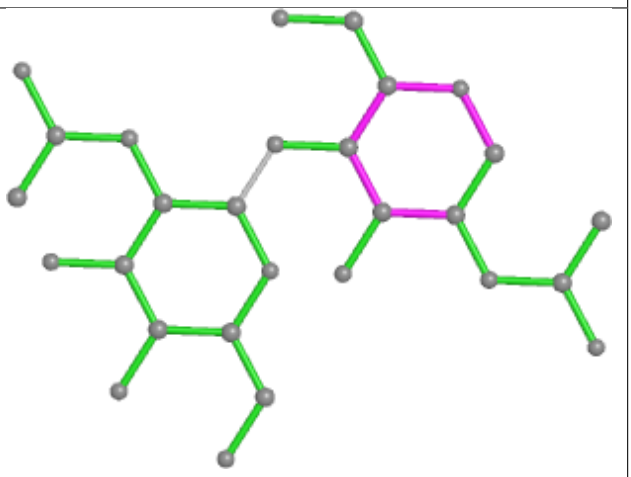

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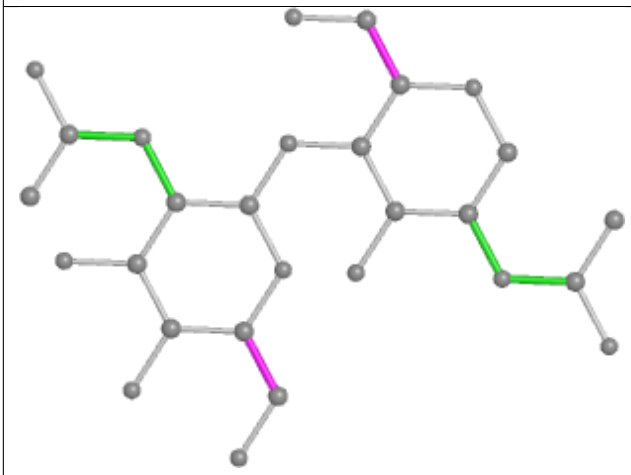

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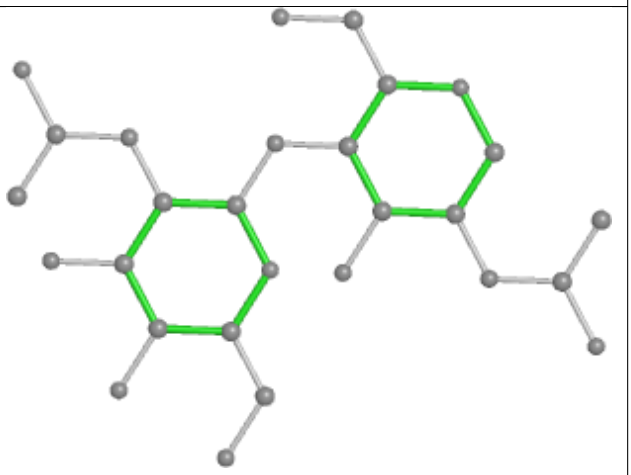
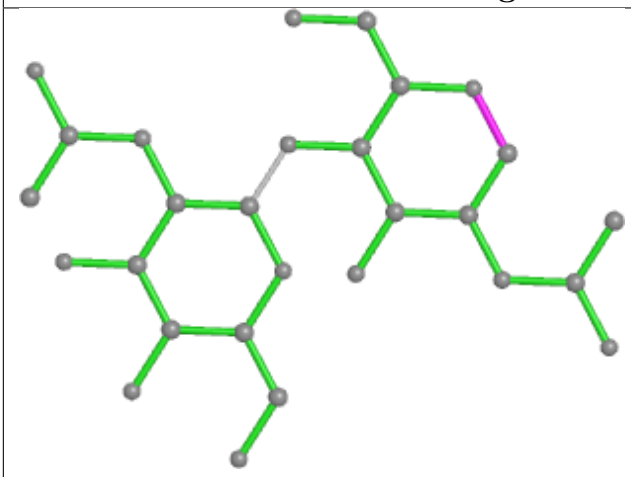


Rings

Oligosaccharide Chain k



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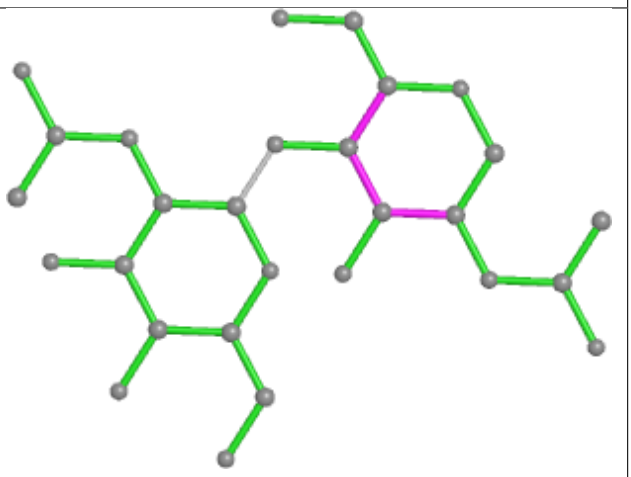
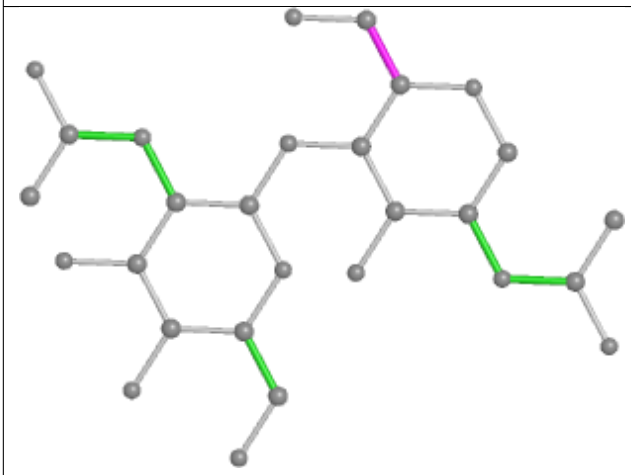


Bond angles



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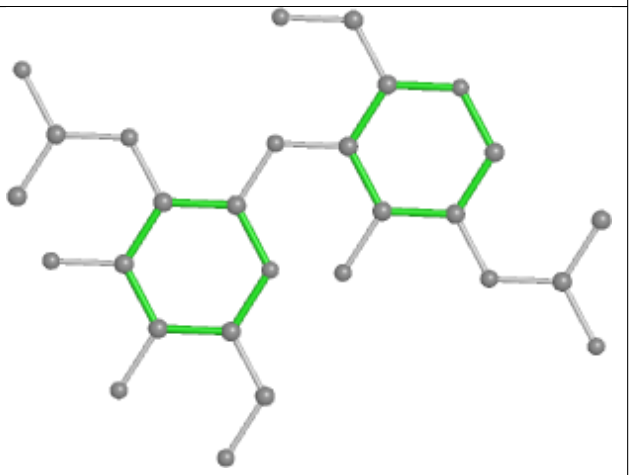
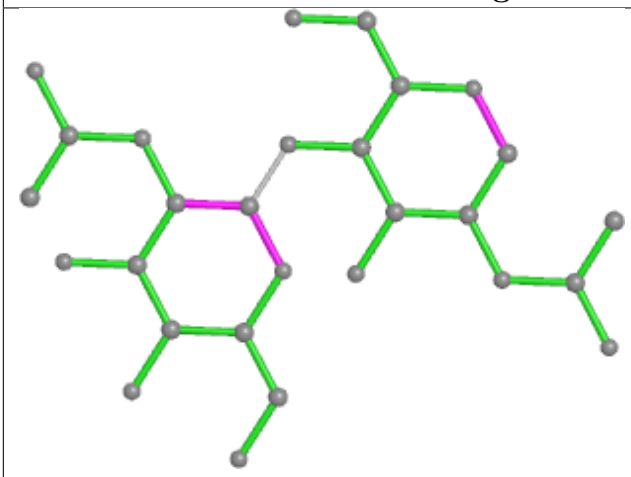


Rings

Oligosaccharide Chain m



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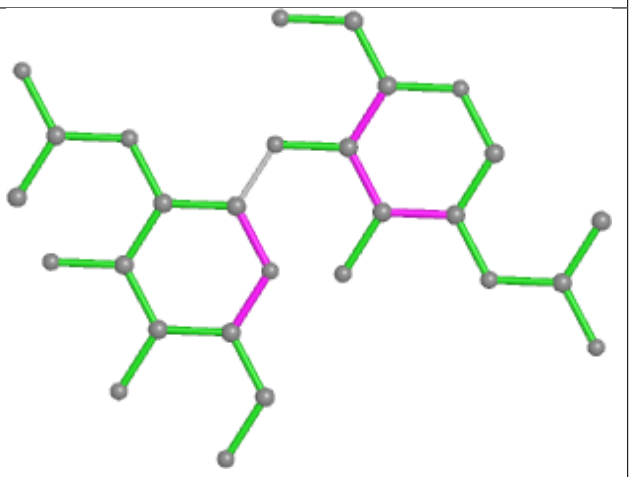
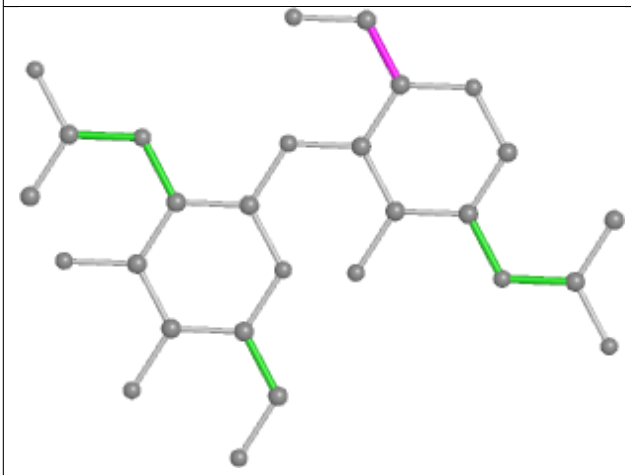


Bond angles



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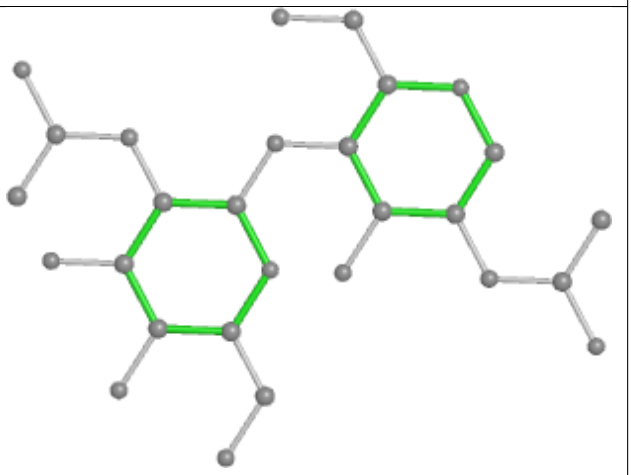
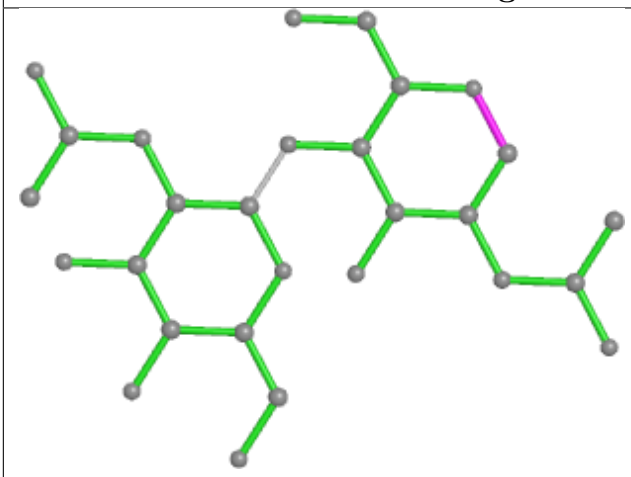


Rings

Oligosaccharide Chain q



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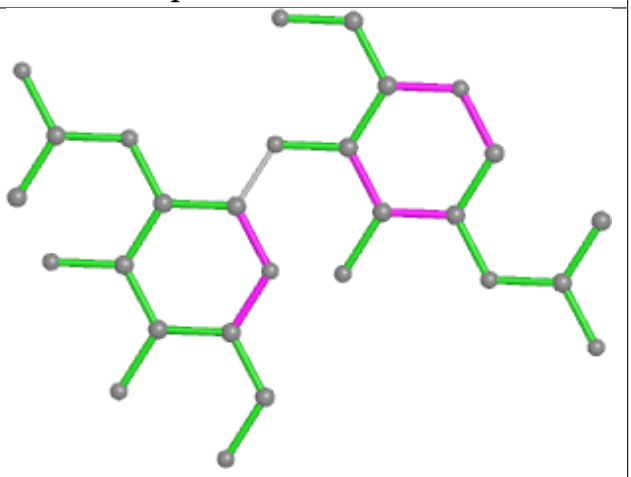
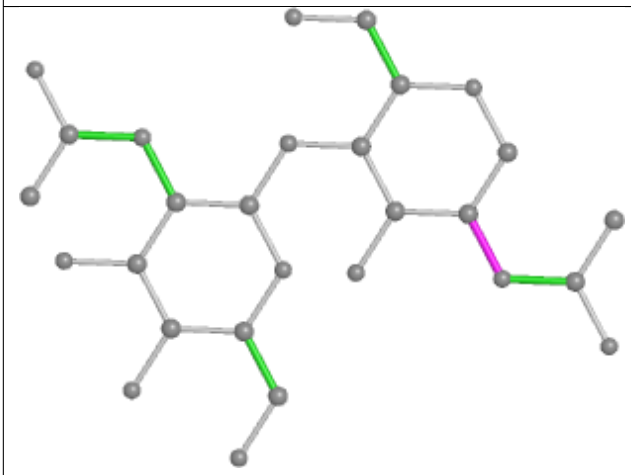


Bond angles



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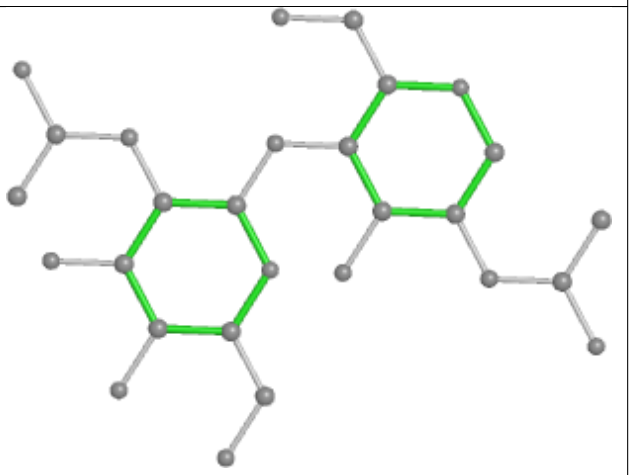
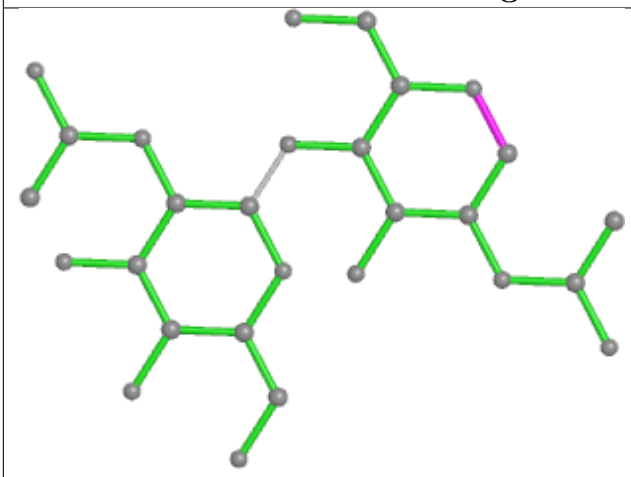
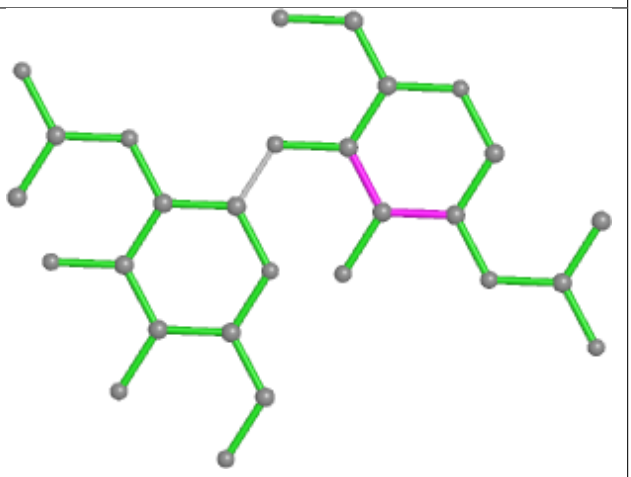


Rings

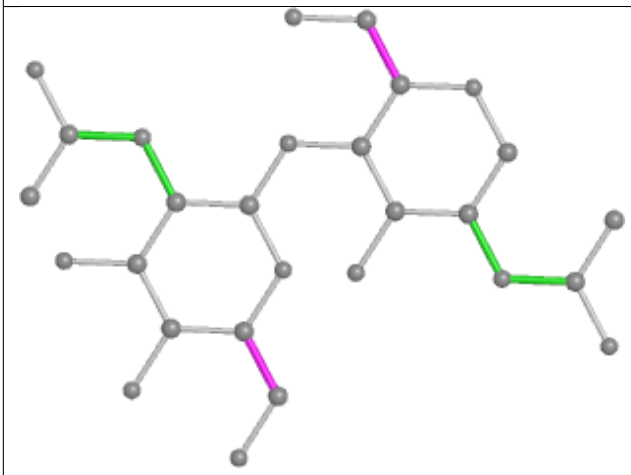
Oligosaccharide Chain s



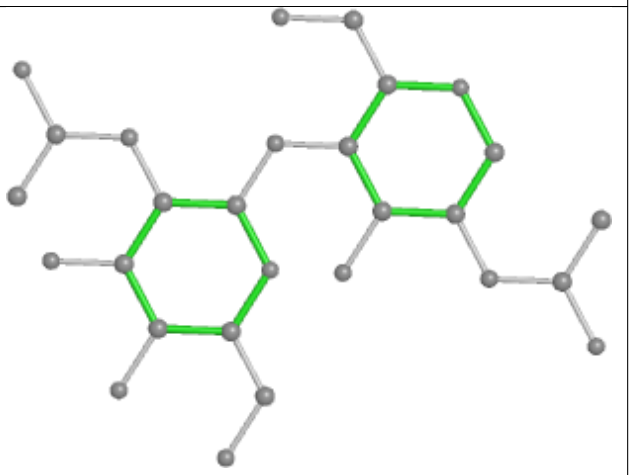
Bond lengths



Bond angles

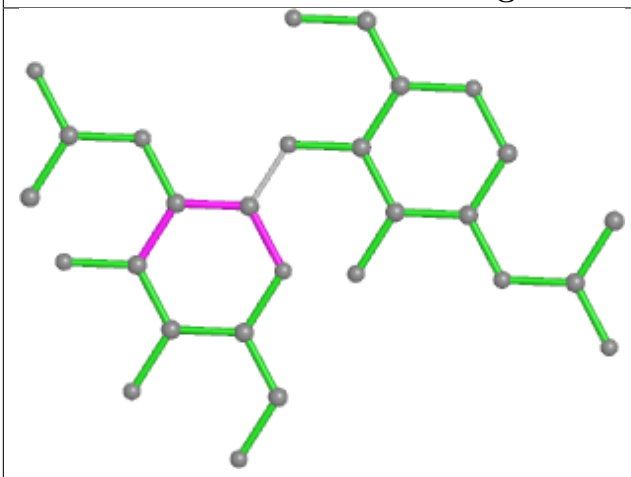


Torsions

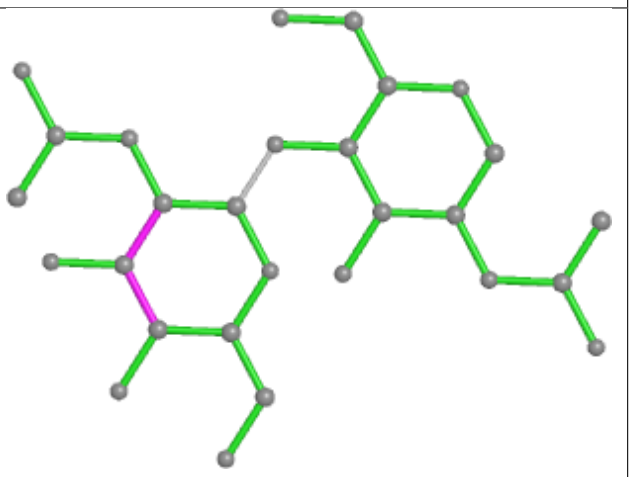


Rings

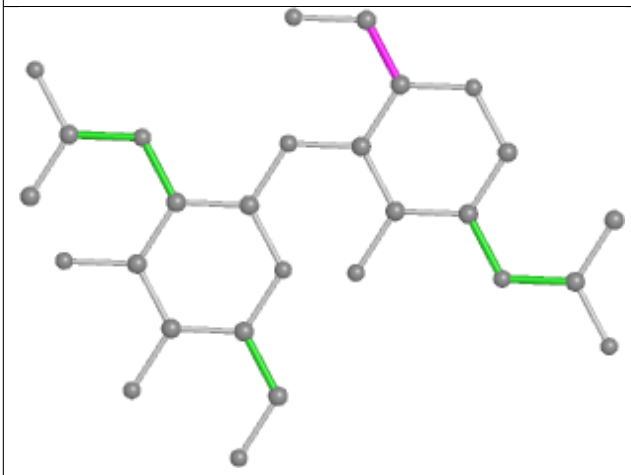
Oligosaccharide Chain u



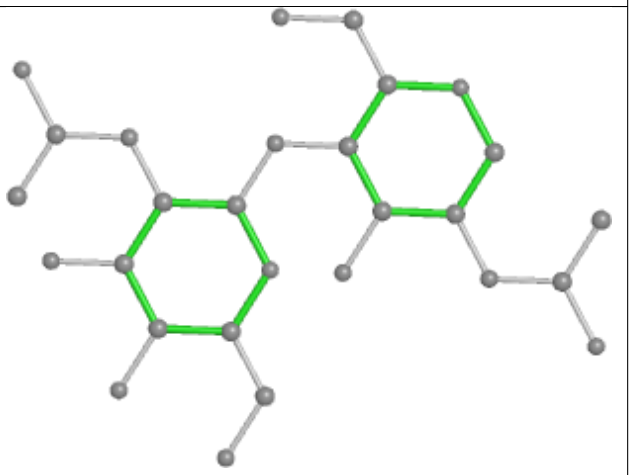
Bond lengths



Bond angles

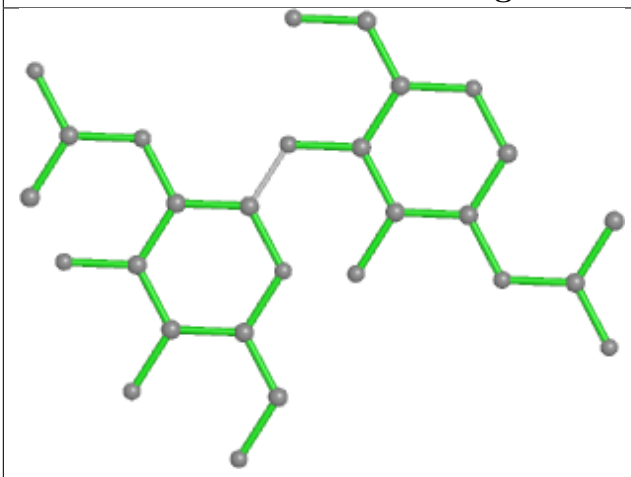


Torsions

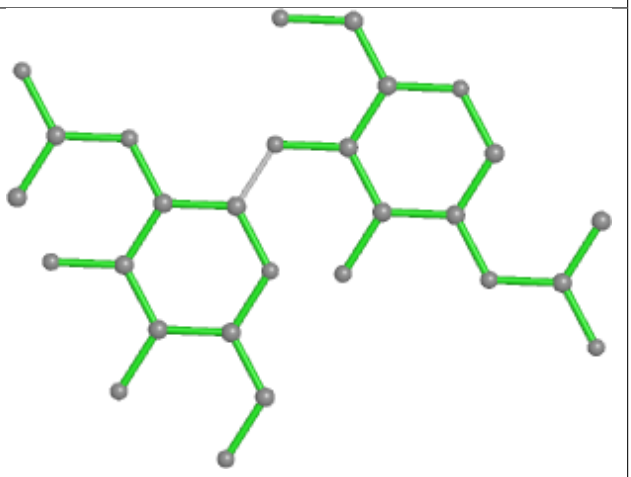


Rings

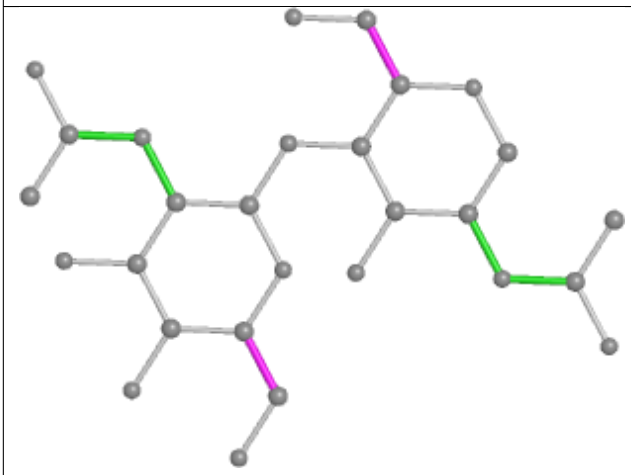
Oligosaccharide Chain w



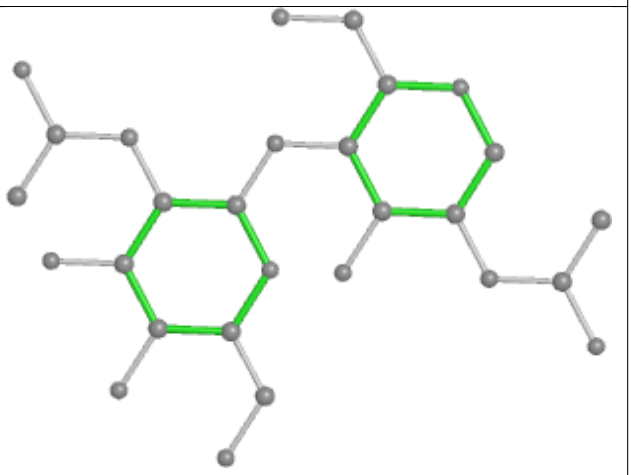
Bond lengths



Bond angles

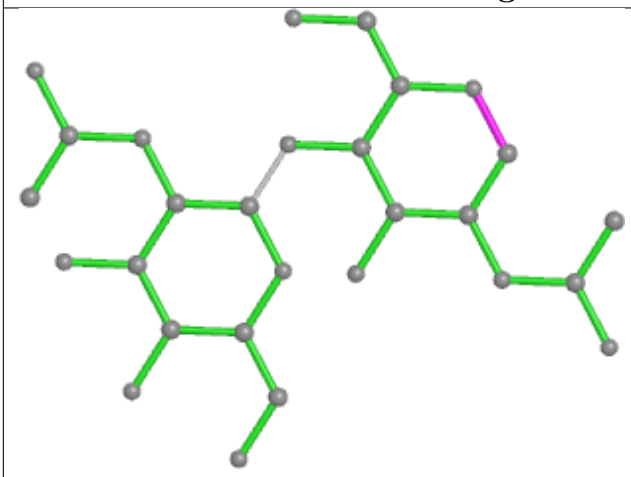


Torsions

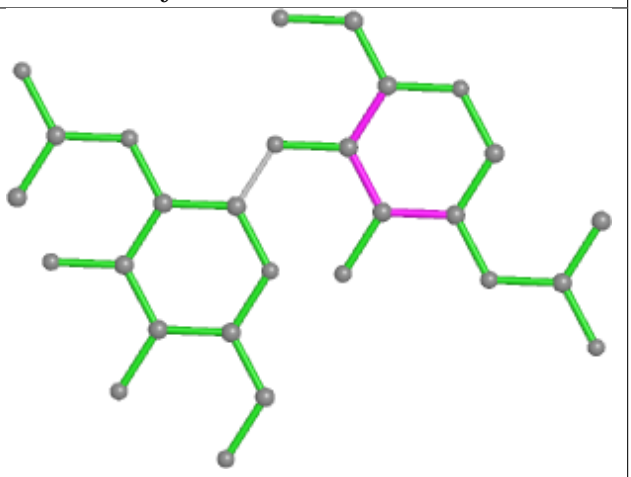


Rings

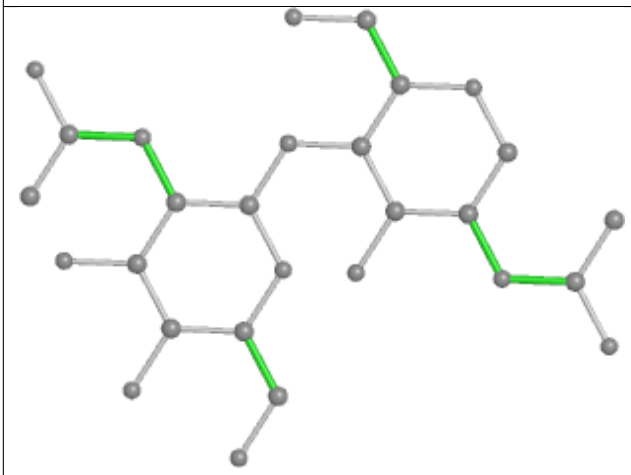
Oligosaccharide Chain y



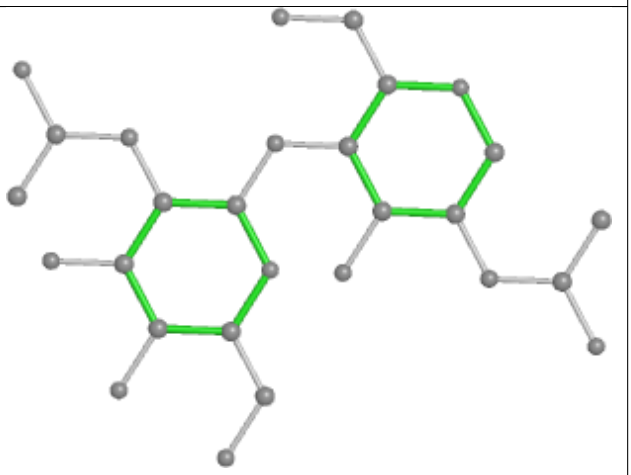
Bond lengths



Bond angles

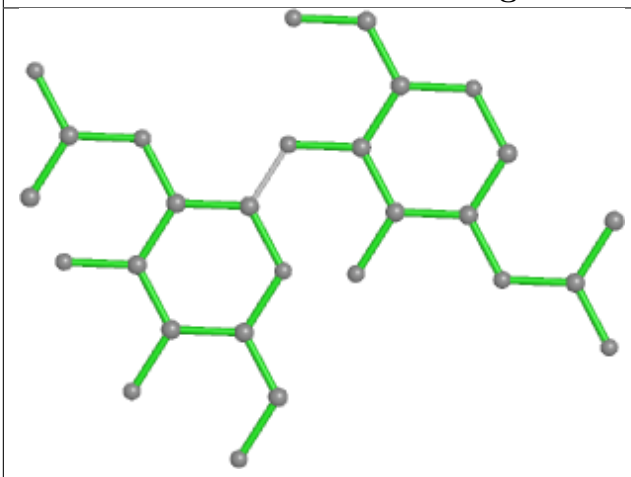


Torsions

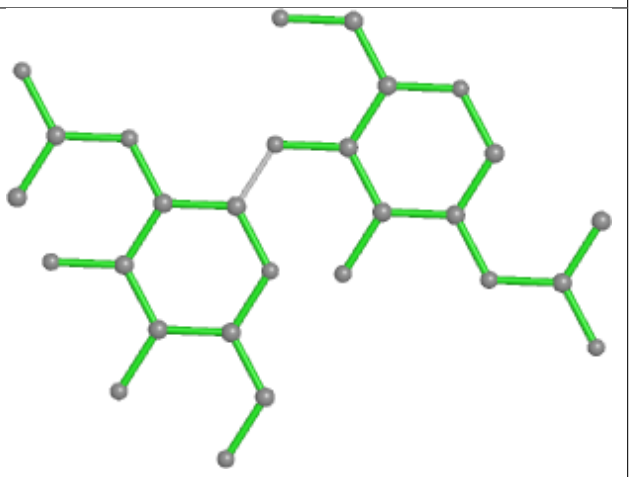


Rings

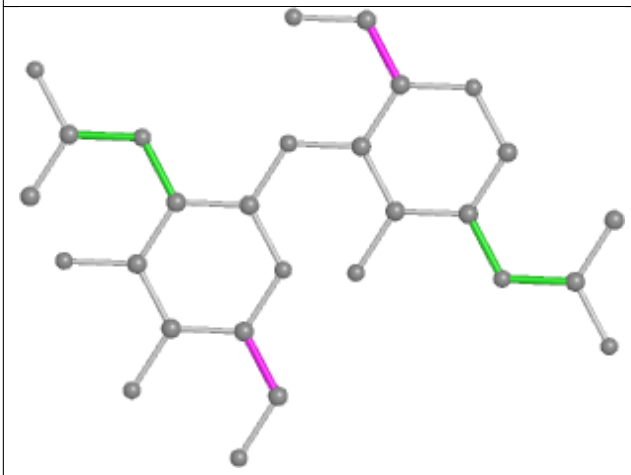
Oligosaccharide Chain z



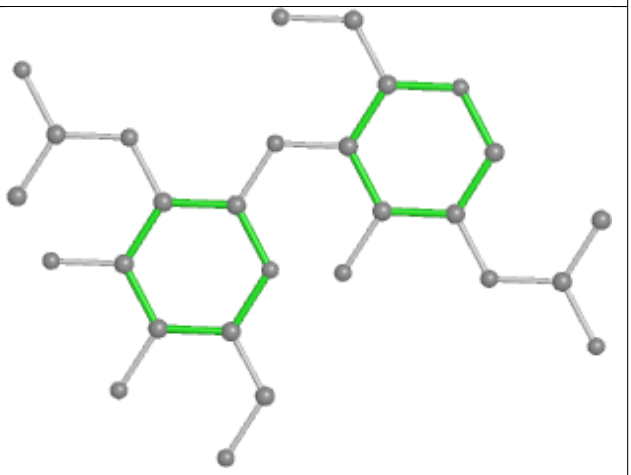
Bond lengths



Bond angles

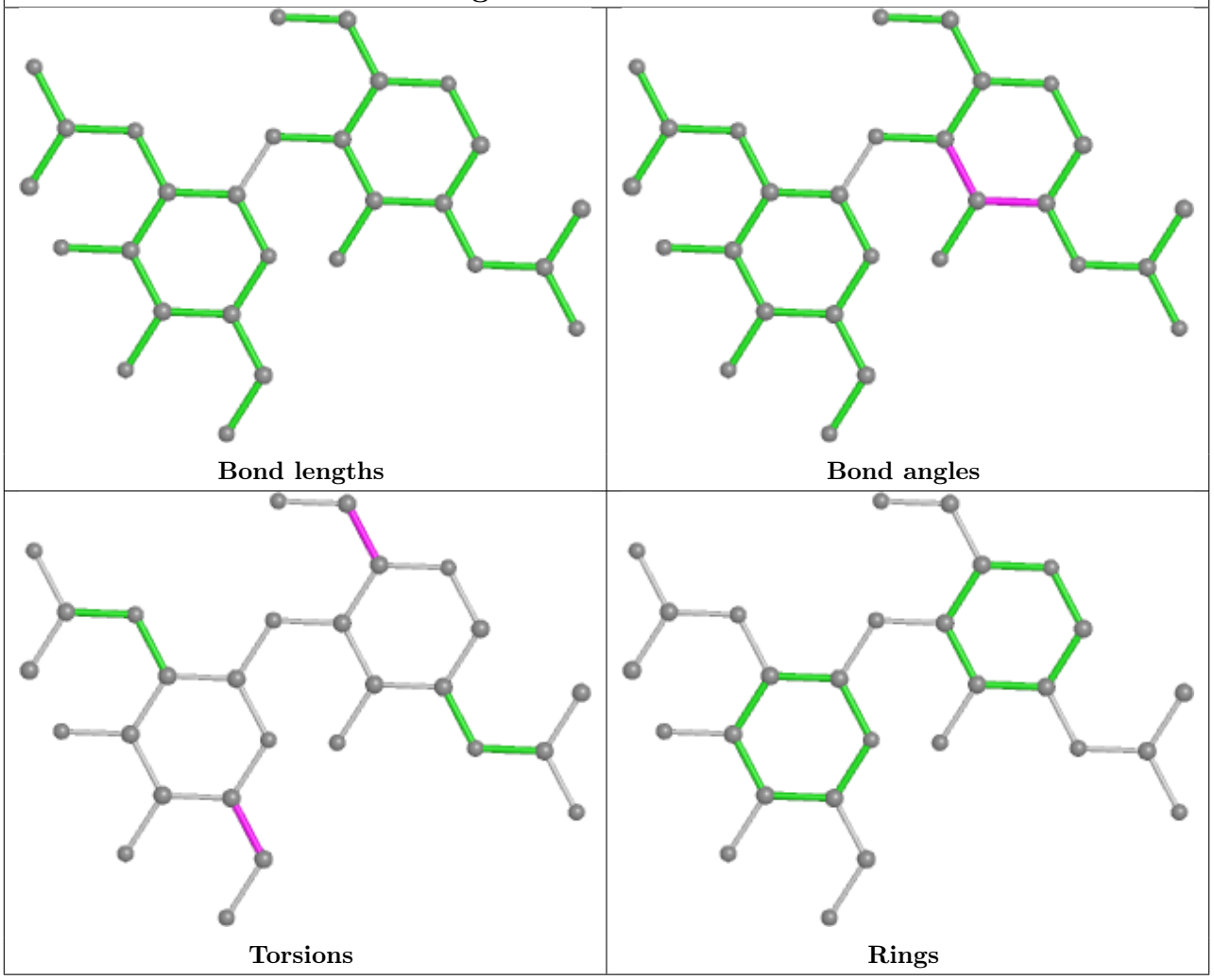


Torsions



Rings

Oligosaccharide Chain 0



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
5	NAG	Y	2001	1	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
5	NAG	M	2004	1	14,14,15	0.31	0	17,19,21	0.43	0
5	NAG	c	2001	1	14,14,15	0.65	1 (7%)	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	O	2006	1	14,14,15	1.02	1 (7%)	17,19,21	0.99	2 (11%)
5	NAG	C	2004	1	14,14,15	0.89	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	K	2004	1	14,14,15	0.64	0	17,19,21	0.57	0
5	NAG	a	2001	1	14,14,15	0.61	0	17,19,21	0.67	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
5	NAG	Y	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	M	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	O	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	a	2001	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2006	NAG	O5-C1	-3.07	1.38	1.43
5	C	2004	NAG	O5-C1	-2.57	1.39	1.43
5	c	2001	NAG	O5-C1	-2.21	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	2001	NAG	C1-O5-C5	3.45	116.86	112.19
5	O	2006	NAG	C4-C3-C2	2.76	115.06	111.02
5	O	2006	NAG	C3-C4-C5	2.30	114.34	110.24
5	a	2001	NAG	C1-O5-C5	2.18	115.15	112.19
5	C	2004	NAG	C4-C3-C2	2.18	114.21	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2006	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	a	2001	NAG	O5-C5-C6-O6
5	O	2006	NAG	O5-C5-C6-O6
5	a	2001	NAG	C4-C5-C6-O6
5	M	2004	NAG	C4-C5-C6-O6
5	M	2004	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.21	5 (1%) 73 57	32, 52, 87, 162	0
1	C	324/334 (97%)	-0.00	10 (3%) 49 32	38, 63, 124, 185	0
1	E	324/334 (97%)	-0.07	5 (1%) 73 57	36, 58, 115, 196	0
1	G	324/334 (97%)	-0.19	6 (1%) 66 49	28, 51, 92, 170	0
1	I	324/334 (97%)	-0.15	3 (0%) 84 71	27, 49, 94, 166	0
1	K	324/334 (97%)	-0.08	7 (2%) 62 45	37, 59, 112, 178	0
1	M	324/334 (97%)	-0.18	8 (2%) 57 40	28, 54, 114, 206	0
1	O	324/334 (97%)	-0.10	9 (2%) 53 36	32, 54, 117, 190	0
1	Q	324/334 (97%)	-0.19	5 (1%) 73 57	34, 53, 116, 181	0
1	S	324/334 (97%)	-0.17	11 (3%) 45 29	37, 62, 128, 177	0
1	U	324/334 (97%)	-0.04	8 (2%) 57 40	36, 66, 124, 186	0
1	W	324/334 (97%)	0.03	8 (2%) 57 40	41, 64, 125, 183	0
1	Y	324/334 (97%)	0.54	24 (7%) 14 8	57, 83, 178, 247	0
1	a	324/334 (97%)	0.59	36 (11%) 5 3	59, 86, 197, 263	0
1	c	324/334 (97%)	0.57	34 (10%) 6 4	55, 87, 184, 267	0
2	B	177/181 (97%)	0.26	8 (4%) 33 21	36, 94, 134, 165	0
2	D	177/181 (97%)	0.96	33 (18%) 1 0	42, 124, 175, 199	0
2	F	177/181 (97%)	0.85	32 (18%) 1 1	45, 123, 173, 182	0
2	H	177/181 (97%)	0.22	7 (3%) 38 25	35, 97, 139, 151	0
2	J	177/181 (97%)	0.36	12 (6%) 17 10	36, 95, 136, 152	0
2	L	177/181 (97%)	0.81	23 (12%) 3 2	42, 122, 163, 171	0
2	N	177/181 (97%)	0.78	26 (14%) 2 1	37, 123, 176, 197	0
2	P	177/181 (97%)	0.74	23 (12%) 3 2	31, 120, 174, 185	0
2	R	177/181 (97%)	0.98	35 (19%) 1 0	42, 122, 189, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
2	T	177/181 (97%)	0.64	23 (12%)	3 2	48, 123, 166, 184	0
2	V	177/181 (97%)	0.73	25 (14%)	2 1	45, 123, 167, 180	0
2	X	177/181 (97%)	0.84	27 (15%)	2 1	46, 123, 171, 182	0
2	Z	177/181 (97%)	2.52	90 (50%)	0 0	68, 193, 265, 299	0
2	b	177/181 (97%)	2.71	84 (47%)	0 0	74, 189, 251, 272	0
2	d	177/181 (97%)	2.31	76 (42%)	0 0	68, 193, 239, 274	0
All	All	7515/7725 (97%)	0.39	703 (9%)	8 5	27, 75, 185, 299	0

All (703) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	16	GLY	34.9
2	Z	23	GLY	28.4
2	b	16	GLY	26.4
2	Z	35	ALA	14.6
1	c	16	GLY	14.4
2	b	141	TYR	14.4
1	a	9	PRO	14.2
1	a	16	GLY	14.1
2	Z	24	TYR	13.8
1	Y	15	ILE	12.7
2	d	26	HIS	12.7
2	d	36	ALA	11.7
2	b	18	VAL	11.7
2	d	22	TYR	11.2
1	a	21[A]	ASN	10.9
2	d	35	ALA	10.8
2	b	153	ARG	10.6
2	b	176	GLY	10.6
1	a	8	ASP	10.5
2	Z	141	TYR	10.2
2	b	152	VAL	9.9
2	Z	136	GLY	9.5
2	d	130	ALA	9.5
2	Z	36	ALA	9.3
1	a	10	GLY	9.2
1	M	9	PRO	9.2
1	c	21[A]	ASN	9.2
2	d	16	GLY	9.0
2	b	157	TYR	8.9

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Mol	Chain	Res	Type	RSRZ
1	I	8	ASP	8.9
1	c	15	ILE	8.9
1	Q	8	ASP	8.8
1	W	324	PRO	8.7
2	Z	163	SER	8.7
2	d	15	GLN	8.6
2	b	140	PHE	8.5
1	Y	323	SER	8.4
2	d	141	TYR	8.3
1	E	324	PRO	8.2
2	L	140	PHE	8.2
1	O	9	PRO	8.1
2	b	133	LEU	8.0
1	c	8	ASP	8.0
2	N	27	SER	7.9
2	d	138	PHE	7.9
1	M	8	ASP	7.8
2	b	35	ALA	7.8
2	T	140	PHE	7.7
1	a	15	ILE	7.7
1	Y	324	PRO	7.6
2	Z	175	SER	7.6
2	Z	128	ASP	7.5
2	R	177	ARG	7.2
2	b	34	TYR	7.2
2	d	33	GLY	7.1
2	Z	22	TYR	7.1
2	d	157	TYR	7.0
1	I	324	PRO	7.0
1	U	324	PRO	7.0
1	Y	22	SER	6.9
2	Z	37	ASP	6.9
2	P	31	GLY	6.8
2	b	13	GLY	6.8
2	d	38	LYS	6.8
2	b	44	ALA	6.8
1	A	8	ASP	6.8
2	b	131	LYS	6.6
2	P	176	GLY	6.6
2	T	141	TYR	6.6
2	b	168	LEU	6.6
1	c	9	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
2	Z	57	ASP	6.5
2	D	177	ARG	6.5
1	c	10	GLY	6.4
1	S	8	ASP	6.4
2	Z	134	GLY	6.4
2	N	22	TYR	6.4
2	Z	16	GLY	6.4
1	Y	23	THR	6.4
2	X	22	TYR	6.3
2	Z	164	GLU	6.2
2	Z	160	PRO	6.1
1	a	323	SER	6.1
1	a	324	PRO	6.1
2	Z	10	ILE	6.1
2	b	48	VAL	6.1
2	R	158	ASP	6.0
2	P	32	SER	6.0
2	b	33	GLY	6.0
1	a	14	CYS	6.0
1	Y	319	GLY	5.9
2	b	24	TYR	5.8
1	Q	9	PRO	5.8
2	R	126	LEU	5.8
2	b	143	LYS	5.7
2	Z	168	LEU	5.7
2	b	38	LYS	5.7
2	b	169	LYS	5.7
2	d	143	LYS	5.7
2	d	34	TYR	5.7
2	d	139	GLU	5.7
2	N	140	PHE	5.7
2	d	111	HIS	5.7
2	d	140	PHE	5.6
2	Z	152	VAL	5.6
2	N	160	PRO	5.5
2	N	26	HIS	5.5
2	L	32	SER	5.4
2	D	21	TRP	5.4
2	d	23	GLY	5.4
1	c	22	SER	5.3
2	b	1	GLY	5.3
2	Z	138	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	K	12	GLN	5.3
1	I	9	PRO	5.3
2	b	21	TRP	5.3
2	b	32	SER	5.3
2	N	176	GLY	5.2
1	a	23	THR	5.2
2	N	32	SER	5.2
2	d	24	TYR	5.2
2	b	37	ASP	5.2
2	d	125	GLN	5.2
2	R	22	TYR	5.1
1	O	8	ASP	5.1
1	c	13	ILE	5.1
2	Z	148	CYS	5.1
2	N	177	ARG	5.0
1	E	12	GLN	5.0
2	d	126	LEU	5.0
2	d	107	THR	5.0
1	a	17	TYR	5.0
2	R	140	PHE	5.0
2	b	139	GLU	5.0
1	E	8	ASP	5.0
2	Z	177	ARG	5.0
2	R	36	ALA	5.0
2	D	32	SER	4.9
1	U	323	SER	4.9
2	b	174	SER	4.9
2	d	132	GLU	4.8
1	A	9	PRO	4.8
2	N	31	GLY	4.8
2	d	122	VAL	4.8
1	Y	21[A]	ASN	4.8
2	b	119	TYR	4.8
2	Z	7	ALA	4.8
2	d	128	ASP	4.8
1	a	35	THR	4.8
1	a	12	GLN	4.7
2	d	1	GLY	4.7
1	Y	17	TYR	4.7
2	b	149	MET	4.7
1	E	9	PRO	4.7
1	W	8	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	F	177	ARG	4.7
2	d	168	LEU	4.6
2	b	22	TYR	4.6
2	b	41	THR	4.6
2	b	138	PHE	4.6
2	b	125	GLN	4.6
1	Y	20	ASN	4.5
1	K	13	ILE	4.5
2	L	33	GLY	4.5
2	b	173	ILE	4.5
2	L	22	TYR	4.5
2	R	18	VAL	4.5
2	Z	132	GLU	4.5
1	M	10	GLY	4.5
2	D	31	GLY	4.5
2	b	27	SER	4.5
2	d	127	ARG	4.5
2	b	26	HIS	4.4
2	b	12	GLY	4.4
2	b	170	ARG	4.4
2	d	32	SER	4.4
1	G	9	PRO	4.4
2	d	17	MET	4.4
1	c	34	VAL	4.4
2	b	23	GLY	4.4
1	O	10	GLY	4.4
1	a	39	ALA	4.4
2	D	22	TYR	4.4
2	D	176	GLY	4.4
2	P	170	ARG	4.4
2	b	177	ARG	4.3
1	c	11	ASP	4.3
1	c	14	CYS	4.3
2	X	20	GLY	4.3
2	F	1	GLY	4.3
2	L	31	GLY	4.3
1	c	23	THR	4.3
2	b	142	HIS	4.3
1	a	22	SER	4.3
2	b	175	SER	4.3
2	Z	5	ALA	4.3
1	c	324	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
2	b	36	ALA	4.2
2	V	141	TYR	4.2
2	X	23	GLY	4.2
2	Z	9	PHE	4.2
2	R	161	GLN	4.2
2	D	173	ILE	4.2
2	R	32	SER	4.1
2	B	177	ARG	4.1
2	Z	143	LYS	4.1
2	F	139	GLU	4.1
2	d	133	LEU	4.1
2	b	25	HIS	4.1
2	L	138	PHE	4.1
2	d	158	ASP	4.1
2	Z	119	TYR	4.1
1	Y	318	ILE	4.1
1	a	322	ASN	4.0
2	P	177	ARG	4.0
1	C	324	PRO	4.0
2	d	153	ARG	4.0
2	b	132	GLU	4.0
2	P	27	SER	4.0
2	F	140	PHE	4.0
2	X	24	TYR	4.0
2	P	173	ILE	3.9
2	N	164	GLU	3.9
2	X	35	ALA	3.9
2	D	33	GLY	3.9
2	Z	157	TYR	3.9
2	V	160	PRO	3.9
2	Z	54	SER	3.9
2	Z	34	TYR	3.9
2	R	29	GLU	3.9
2	b	154	ASN	3.9
2	d	164	GLU	3.9
2	F	127	ARG	3.9
2	V	34	TYR	3.9
2	d	165	GLU	3.9
2	d	31	GLY	3.9
2	b	29	GLU	3.9
2	b	126	LEU	3.8
1	c	12	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	1	GLY	3.8
2	b	17	MET	3.8
1	a	36	VAL	3.8
2	d	106	ARG	3.8
2	L	27	SER	3.8
1	c	323	SER	3.8
2	Z	127	ARG	3.8
2	D	1	GLY	3.8
1	K	15	ILE	3.8
2	P	156	THR	3.8
1	Y	320	LEU	3.8
1	C	12	GLN	3.8
2	R	176	GLY	3.8
2	d	27	SER	3.7
2	P	1	GLY	3.7
2	H	140	PHE	3.7
2	X	21	TRP	3.7
2	X	38	LYS	3.7
2	b	158	ASP	3.7
2	X	150	GLU	3.7
2	V	173	ILE	3.7
2	d	115	VAL	3.7
2	J	39	GLU	3.6
2	R	35	ALA	3.6
2	b	134	GLY	3.6
1	E	10	GLY	3.6
1	Y	322	ASN	3.6
2	R	133	LEU	3.6
1	C	55(A)	GLY	3.6
2	F	29	GLU	3.6
2	b	7	ALA	3.6
2	X	147	GLU	3.6
2	T	22	TYR	3.6
2	Z	124	LEU	3.6
2	N	46	ASP	3.6
2	R	138	PHE	3.5
1	c	35	THR	3.5
2	B	38	LYS	3.5
2	T	32	SER	3.5
2	D	128	ASP	3.5
2	N	16	GLY	3.5
2	d	25	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	1	GLY	3.5
2	T	26	HIS	3.5
2	D	34	TYR	3.5
2	d	156	THR	3.5
2	R	159	TYR	3.5
2	R	162	TYR	3.5
2	Z	17	MET	3.4
2	d	3	PHE	3.4
2	X	143	LYS	3.4
2	b	136	GLY	3.4
2	Z	32	SER	3.4
2	d	137	CYS	3.4
2	L	38	LYS	3.4
1	S	77	ASP	3.4
2	R	1	GLY	3.4
2	Z	1	GLY	3.4
2	D	35	ALA	3.4
2	Z	6	ILE	3.4
2	d	109	ASP	3.4
2	Z	25	HIS	3.4
2	V	162	TYR	3.4
2	d	14	TRP	3.4
2	d	176	GLY	3.4
2	X	139	GLU	3.4
2	d	177	ARG	3.4
2	b	150	GLU	3.4
2	Z	159	TYR	3.3
1	c	282	GLN	3.3
2	Z	125	GLN	3.3
2	J	144	CYS	3.3
1	W	323	SER	3.3
2	F	141	TYR	3.3
2	V	167	ARG	3.3
2	Z	14	TRP	3.3
2	F	175	SER	3.3
2	D	140	PHE	3.3
1	S	9	PRO	3.3
2	T	139	GLU	3.3
2	D	14	TRP	3.3
2	P	30	GLN	3.3
2	Z	142	HIS	3.3
2	V	140	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	c	32	LYS	3.3
2	b	15	GLN	3.3
2	Z	140	PHE	3.3
1	Y	13	ILE	3.2
2	b	162	TYR	3.2
2	R	160	PRO	3.2
2	b	137	CYS	3.2
1	a	11	ASP	3.2
1	Q	21[A]	ASN	3.2
1	Y	37	THR	3.2
2	J	38	LYS	3.2
2	d	5	ALA	3.2
1	M	324	PRO	3.2
2	F	4	GLY	3.2
1	Y	24	GLU	3.2
1	A	324	PRO	3.2
1	W	38	HIS	3.2
2	X	157	TYR	3.2
1	Y	9	PRO	3.2
2	Z	126	LEU	3.1
2	b	40	SER	3.1
1	O	16	GLY	3.1
2	X	1	GLY	3.1
2	d	162	TYR	3.1
2	L	177	ARG	3.1
2	T	160	PRO	3.1
2	J	176	GLY	3.1
1	a	43	LEU	3.1
1	K	8	ASP	3.1
2	b	146	ASN	3.1
2	V	166	ALA	3.1
2	N	138	PHE	3.1
2	Z	149	MET	3.1
2	R	31	GLY	3.1
2	d	116	LYS	3.1
2	F	144	CYS	3.1
1	A	323	SER	3.1
2	d	18	VAL	3.1
2	b	3	PHE	3.1
2	V	158	ASP	3.0
1	Y	55(A)	GLY	3.0
2	D	139	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	Z	131	LYS	3.0
2	F	138	PHE	3.0
2	d	150	GLU	3.0
1	c	55(A)	GLY	3.0
2	d	113	SER	3.0
1	c	31	GLU	3.0
2	b	45	ILE	3.0
2	b	5	ALA	3.0
2	Z	109	ASP	3.0
1	W	9	PRO	3.0
1	a	315	VAL	3.0
2	D	24	TYR	3.0
2	Z	170	ARG	3.0
2	N	143	LYS	3.0
2	L	26	HIS	3.0
1	U	9	PRO	3.0
2	J	143	LYS	3.0
2	N	131	LYS	3.0
2	Z	29	GLU	3.0
2	V	168	LEU	3.0
2	R	8	GLY	3.0
2	P	29	GLU	3.0
2	P	18	VAL	3.0
2	V	24	TYR	3.0
2	D	20	GLY	3.0
2	Z	106	ARG	3.0
2	N	29	GLU	3.0
2	L	126	LEU	2.9
2	b	144	CYS	2.9
2	D	19	ASP	2.9
1	G	8	ASP	2.9
2	b	135	ASN	2.9
2	X	173	ILE	2.9
2	Z	156	THR	2.9
2	D	141	TYR	2.9
2	H	177	ARG	2.9
1	c	20	ASN	2.9
2	D	18	VAL	2.9
2	T	177	ARG	2.9
1	c	273	GLU	2.9
2	R	33	GLY	2.9
2	R	144	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	Z	13	GLY	2.9
2	D	168	LEU	2.9
2	N	126	LEU	2.9
1	M	11	ASP	2.9
2	Z	171	GLU	2.9
2	b	19	ASP	2.9
2	P	15	GLN	2.8
2	V	157	TYR	2.8
2	N	33	GLY	2.8
2	Z	135	ASN	2.8
2	H	27	SER	2.8
1	a	20	ASN	2.8
2	Z	15	GLN	2.8
2	T	27	SER	2.8
2	Z	173	ILE	2.8
2	D	157	TYR	2.8
2	V	35	ALA	2.8
2	V	171	GLU	2.8
2	Z	114	ASN	2.8
2	d	148	CYS	2.8
2	P	21	TRP	2.8
2	P	22	TYR	2.8
2	d	21	TRP	2.8
2	X	149	MET	2.8
2	Z	113	SER	2.8
2	X	39	GLU	2.8
1	M	21[A]	ASN	2.8
1	W	21[A]	ASN	2.8
2	T	1	GLY	2.8
2	Z	8	GLY	2.8
1	O	318	ILE	2.8
1	S	32	LYS	2.8
2	T	168	LEU	2.8
2	d	4	GLY	2.7
1	C	8	ASP	2.7
2	b	159	TYR	2.7
2	b	128	ASP	2.7
2	D	170	ARG	2.7
2	b	14	TRP	2.7
1	Q	38	HIS	2.7
1	S	12	GLN	2.7
2	L	127	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	10	GLY	2.7
2	Z	21	TRP	2.7
2	T	130	ALA	2.7
2	J	29	GLU	2.7
2	d	108	LEU	2.7
2	Z	121	LYS	2.7
2	d	63	PHE	2.7
1	a	320	LEU	2.7
1	C	24	GLU	2.7
2	b	115	VAL	2.7
2	b	172	GLU	2.7
2	F	176	GLY	2.7
2	D	142	HIS	2.7
1	c	315	VAL	2.7
2	T	21	TRP	2.6
1	Y	14	CYS	2.6
2	D	158	ASP	2.6
2	b	120	ASP	2.6
2	V	32	SER	2.6
2	R	134	GLY	2.6
2	Z	3	PHE	2.6
2	F	173	ILE	2.6
1	c	318	ILE	2.6
2	F	42	GLN	2.6
2	F	133	LEU	2.6
2	d	119	TYR	2.6
1	c	242	ALA	2.6
2	T	138	PHE	2.6
2	R	125	GLN	2.6
2	Z	162	TYR	2.6
1	G	324	PRO	2.6
2	Z	123	ARG	2.6
2	F	106	ARG	2.6
1	a	13	ILE	2.6
2	X	26	HIS	2.6
2	F	145	ASP	2.6
2	X	34	TYR	2.6
2	Z	174	SER	2.6
2	Z	144	CYS	2.6
2	R	26	HIS	2.6
2	Z	4	GLY	2.6
2	D	167	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	157	TYR	2.6
2	F	3	PHE	2.6
2	N	28	ASN	2.6
1	a	25	GLN	2.5
2	H	156	THR	2.5
1	U	14	CYS	2.5
1	c	64	CYS	2.5
2	L	158	ASP	2.5
2	B	27	SER	2.5
2	T	20	GLY	2.5
2	Z	105	GLU	2.5
2	d	2	LEU	2.5
1	c	17	TYR	2.5
2	J	35	ALA	2.5
2	B	39	GLU	2.5
2	H	126	LEU	2.5
2	R	157	TYR	2.5
2	T	29	GLU	2.5
1	c	96(A)	LEU	2.5
2	D	26	HIS	2.5
2	B	176	GLY	2.5
2	R	141	TYR	2.5
2	V	176	GLY	2.5
2	b	147	GLU	2.5
2	Z	161	GLN	2.5
2	L	143	LYS	2.5
2	F	18	VAL	2.5
2	Z	40	SER	2.5
2	F	114	ASN	2.5
2	F	146	ASN	2.5
2	L	153	ARG	2.5
2	d	19	ASP	2.5
2	L	176	GLY	2.5
2	V	144	CYS	2.5
2	Z	47	GLY	2.5
1	c	141	TYR	2.5
2	D	13	GLY	2.4
2	Z	155	GLY	2.4
2	b	161	GLN	2.4
1	C	17	TYR	2.4
2	D	175	SER	2.4
2	F	38	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	303	GLY	2.4
2	N	30	GLN	2.4
1	C	18	HIS	2.4
1	W	13	ILE	2.4
2	Z	151	SER	2.4
1	U	16	GLY	2.4
1	S	13	ILE	2.4
2	L	25	HIS	2.4
2	T	157	TYR	2.4
2	b	122	VAL	2.4
2	T	166	ALA	2.4
2	Z	130	ALA	2.4
2	b	55	ILE	2.4
1	O	36	VAL	2.4
2	F	113	SER	2.4
2	Z	112	ASP	2.4
1	O	324	PRO	2.4
2	V	134	GLY	2.4
1	a	38	HIS	2.4
2	d	142	HIS	2.4
2	L	160	PRO	2.4
2	V	143	LYS	2.4
1	a	37	THR	2.4
2	V	54	SER	2.4
2	B	140	PHE	2.4
1	a	55(A)	GLY	2.4
2	d	136	GLY	2.4
1	A	23	THR	2.3
2	H	38	LYS	2.3
2	d	29	GLU	2.3
1	Y	38	HIS	2.3
2	R	30	GLN	2.3
2	d	160	PRO	2.3
1	M	13	ILE	2.3
1	Y	312	ASN	2.3
2	V	27	SER	2.3
2	V	135	ASN	2.3
2	Z	176	GLY	2.3
1	M	114	ARG	2.3
2	X	29	GLU	2.3
2	X	126	LEU	2.3
2	R	117	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	139	GLU	2.3
1	a	302	ILE	2.3
2	b	113	SER	2.3
2	d	9	PHE	2.3
2	Z	26	HIS	2.3
2	Z	111	HIS	2.3
2	F	143	LYS	2.3
2	X	96	ALA	2.3
2	J	142	HIS	2.3
2	P	171	GLU	2.3
1	a	86	TYR	2.3
1	c	314	LEU	2.3
2	B	149	MET	2.3
1	c	88	VAL	2.3
2	T	175	SER	2.3
2	d	161	GLN	2.3
2	b	164	GLU	2.3
1	K	16	GLY	2.3
2	V	16	GLY	2.3
2	d	56	ILE	2.3
2	b	30	GLN	2.3
2	D	27	SER	2.3
2	N	155	GLY	2.3
2	Z	110	PHE	2.3
1	K	23	THR	2.2
2	B	153	ARG	2.2
2	J	31	GLY	2.2
2	X	30	GLN	2.2
2	Z	107	THR	2.2
2	b	58	LYS	2.2
2	d	120	ASP	2.2
2	R	130	ALA	2.2
1	U	13	ILE	2.2
2	P	39	GLU	2.2
2	T	164	GLU	2.2
2	X	158	ASP	2.2
2	d	134	GLY	2.2
2	R	132	GLU	2.2
1	a	34	VAL	2.2
2	F	169	LYS	2.2
1	S	21[A]	ASN	2.2
1	C	290	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	R	27	SER	2.2
2	b	31	GLY	2.2
2	T	143	LYS	2.2
2	D	134	GLY	2.2
2	Z	18	VAL	2.2
2	P	164	GLU	2.2
2	Z	153	ARG	2.2
1	G	218	ALA	2.2
1	U	80	ILE	2.2
1	a	317	ALA	2.2
2	P	140	PHE	2.2
2	X	140	PHE	2.2
2	b	163	SER	2.2
1	U	12	GLN	2.2
2	P	26	HIS	2.2
2	F	35	ALA	2.2
2	b	59	MET	2.2
2	L	139	GLU	2.2
2	F	134	GLY	2.1
2	T	145	ASP	2.1
2	H	125	GLN	2.1
2	b	42	GLN	2.1
2	P	142	HIS	2.1
2	d	167	ARG	2.1
2	F	31	GLY	2.1
2	N	47	GLY	2.1
2	P	33	GLY	2.1
1	S	39	ALA	2.1
1	Y	95	ASN	2.1
2	Z	48	VAL	2.1
2	F	22	TYR	2.1
2	L	24	TYR	2.1
2	V	119	TYR	2.1
2	F	168	LEU	2.1
2	F	30	GLN	2.1
2	X	27	SER	2.1
2	Z	27	SER	2.1
1	K	14	CYS	2.1
2	J	27	SER	2.1
2	T	167	ARG	2.1
2	R	150	GLU	2.1
2	Z	133	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	Z	167	ARG	2.1
2	N	153	ARG	2.1
2	d	10	ILE	2.1
2	D	117	ASN	2.1
2	X	146	ASN	2.1
1	G	309	VAL	2.1
2	V	164	GLU	2.1
2	d	151	SER	2.1
1	O	12	GLN	2.1
1	S	11	ASP	2.1
1	a	63	ASP	2.1
2	X	18	VAL	2.1
1	G	12	GLN	2.1
1	C	55	ASP	2.1
2	b	130	ALA	2.1
2	L	20	GLY	2.1
1	S	34	VAL	2.1
1	a	115	ILE	2.0
2	L	130	ALA	2.0
1	S	324	PRO	2.0
1	a	278	ASN	2.0
2	N	1	GLY	2.0
2	d	41	THR	2.0
1	Y	36	VAL	2.0
1	c	30	MET	2.0
2	N	146	ASN	2.0
1	W	12	GLN	2.0
1	Y	316	LEU	2.0
2	J	177	ARG	2.0
1	a	41	ASP	2.0
2	R	113	SER	2.0
2	d	13	GLY	2.0
2	Z	92	TRP	2.0
2	D	17	MET	2.0
1	C	320	LEU	2.0
2	P	135	ASN	2.0
2	Z	117	ASN	2.0
1	c	38	HIS	2.0
1	c	297	ILE	2.0
2	F	36	ALA	2.0
2	Z	33	GLY	2.0
2	Z	56	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	d	52	VAL	2.0
1	O	320	LEU	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
4	NAG	f	2	14/15	0.62	0.17	112,122,129,132	0
3	BMA	o	3	11/12	0.63	0.22	105,121,134,135	0
3	BMA	t	3	11/12	0.65	0.24	110,125,137,139	0
4	NAG	z	2	14/15	0.65	0.21	159,180,187,187	0
3	BMA	h	3	11/12	0.67	0.22	74,81,103,103	0
4	NAG	q	2	14/15	0.68	0.21	117,139,146,146	0
4	NAG	0	2	14/15	0.69	0.26	168,181,188,188	0
3	BMA	v	3	11/12	0.70	0.35	114,127,131,133	0
3	BMA	x	3	11/12	0.74	0.21	113,124,130,135	0
4	NAG	s	2	14/15	0.75	0.28	120,148,158,161	0
4	NAG	w	1	14/15	0.76	0.16	130,142,151,153	0
3	BMA	n	3	11/12	0.78	0.20	67,77,85,86	0
4	NAG	u	1	14/15	0.79	0.17	128,150,163,163	0
3	NAG	x	2	14/15	0.79	0.25	77,96,107,119	0
4	NAG	u	2	14/15	0.81	0.16	150,164,166,166	0
3	BMA	p	3	11/12	0.81	0.14	119,127,132,132	0
4	NAG	y	1	14/15	0.81	0.18	114,128,139,141	0
4	NAG	y	2	14/15	0.81	0.16	122,134,141,141	0
3	NAG	h	2	14/15	0.81	0.32	103,121,127,128	0
4	NAG	q	1	14/15	0.81	0.14	123,134,139,143	0
3	NAG	v	2	14/15	0.82	0.18	89,104,121,126	0
3	BMA	j	3	11/12	0.82	0.17	63,85,93,95	0
3	BMA	l	3	11/12	0.82	0.18	56,83,91,91	0
3	NAG	t	2	14/15	0.82	0.18	87,110,127,135	0
3	BMA	g	3	11/12	0.82	0.25	48,70,90,94	0
4	NAG	i	2	14/15	0.83	0.22	106,128,134,134	0

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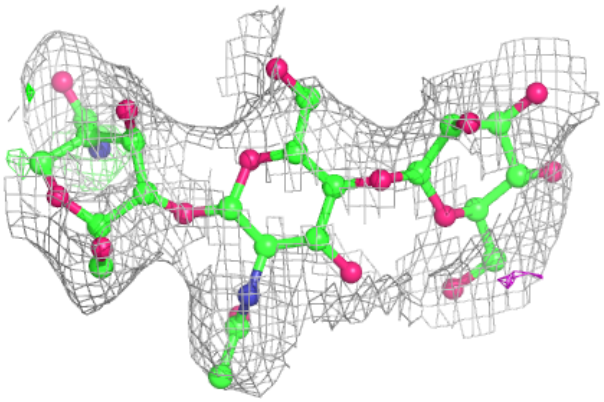
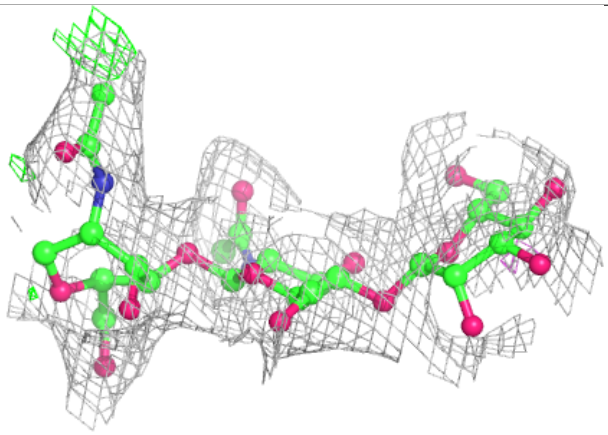
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	m	2	14/15	0.83	0.14	111,117,124,133	0
3	BMA	e	3	11/12	0.83	0.17	81,83,101,101	0
3	BMA	r	3	11/12	0.83	0.14	116,120,126,127	0
4	NAG	f	1	14/15	0.83	0.16	93,112,119,119	0
3	NAG	p	2	14/15	0.83	0.19	83,102,117,123	0
4	NAG	s	1	14/15	0.84	0.14	101,118,133,146	0
4	NAG	z	1	14/15	0.84	0.16	155,161,168,175	0
4	NAG	w	2	14/15	0.84	0.19	136,154,160,165	0
3	NAG	o	2	14/15	0.84	0.22	76,91,113,128	0
3	NAG	x	1	14/15	0.85	0.16	64,71,80,92	0
3	NAG	n	1	14/15	0.85	0.20	56,78,99,101	0
3	NAG	g	2	14/15	0.86	0.35	98,106,110,110	0
4	NAG	0	1	14/15	0.86	0.21	159,180,187,188	0
4	NAG	k	2	14/15	0.86	0.14	106,120,127,128	0
4	NAG	k	1	14/15	0.87	0.13	102,107,113,114	0
3	NAG	v	1	14/15	0.88	0.20	59,71,87,99	0
3	NAG	p	1	14/15	0.89	0.16	58,72,90,97	0
4	NAG	i	1	14/15	0.89	0.10	112,124,125,126	0
3	NAG	n	2	14/15	0.90	0.27	81,97,102,102	0
3	NAG	g	1	14/15	0.90	0.25	70,89,102,112	0
4	NAG	m	1	14/15	0.90	0.18	89,94,103,109	0
3	NAG	e	1	14/15	0.91	0.13	49,69,79,82	0
3	NAG	j	2	14/15	0.92	0.14	49,63,83,84	0
3	NAG	e	2	14/15	0.92	0.14	59,82,94,97	0
3	NAG	r	2	14/15	0.93	0.10	67,88,103,115	0
3	NAG	h	1	14/15	0.93	0.22	74,93,116,124	0
3	NAG	j	1	14/15	0.93	0.16	57,65,73,85	0
3	NAG	l	1	14/15	0.93	0.14	50,58,78,80	0
3	NAG	o	1	14/15	0.94	0.14	50,58,79,79	0
3	NAG	r	1	14/15	0.94	0.12	52,67,75,77	0
3	NAG	t	1	14/15	0.94	0.13	57,81,97,97	0
3	NAG	l	2	14/15	0.95	0.13	44,57,67,71	0

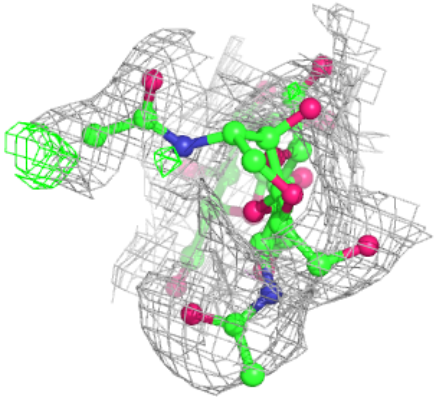
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain e:

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

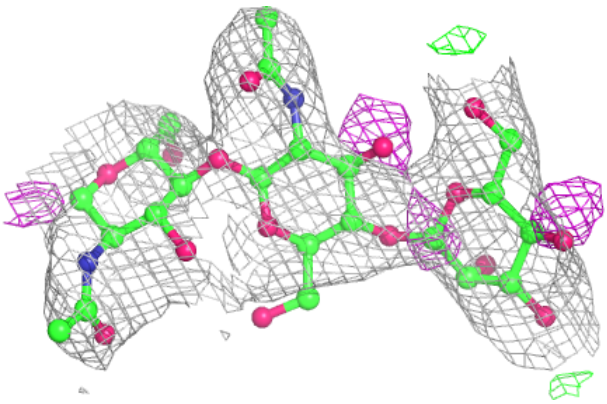


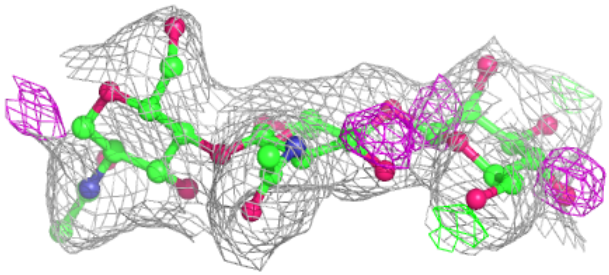


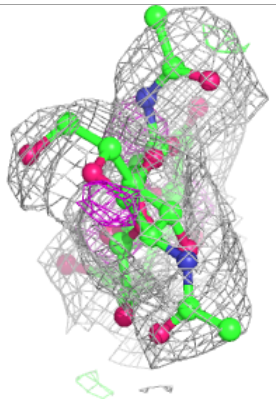


Electron density around Chain g:

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

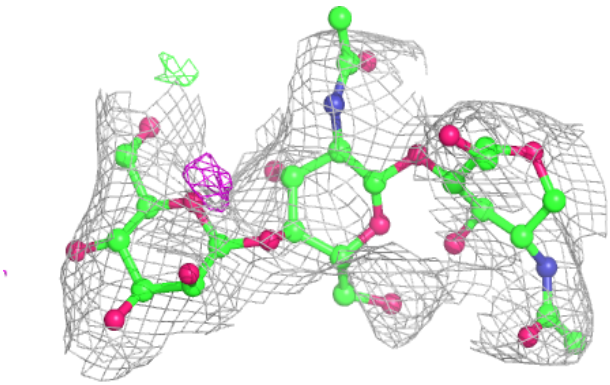


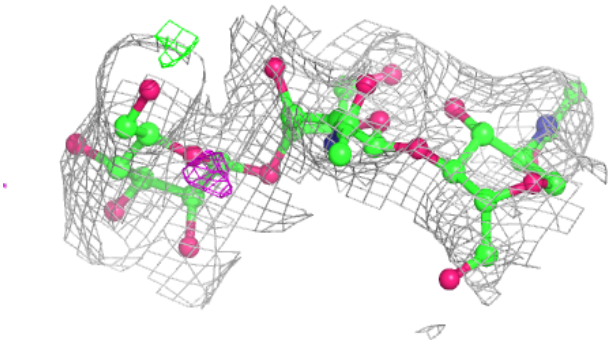


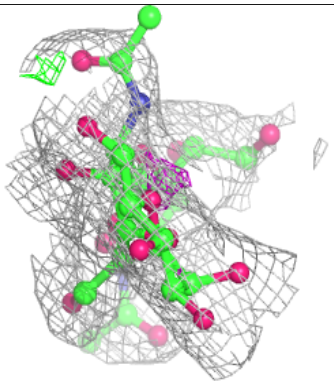


Electron density around Chain h:

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

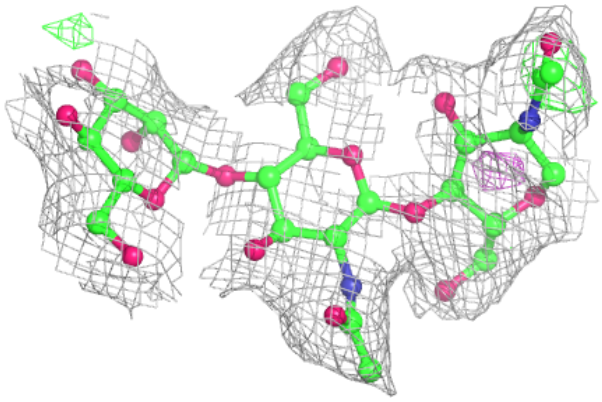


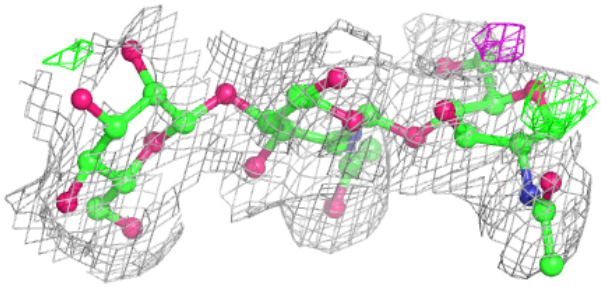


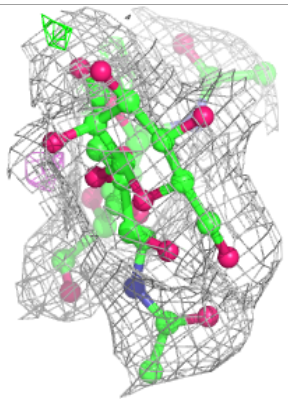


Electron density around Chain j:

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

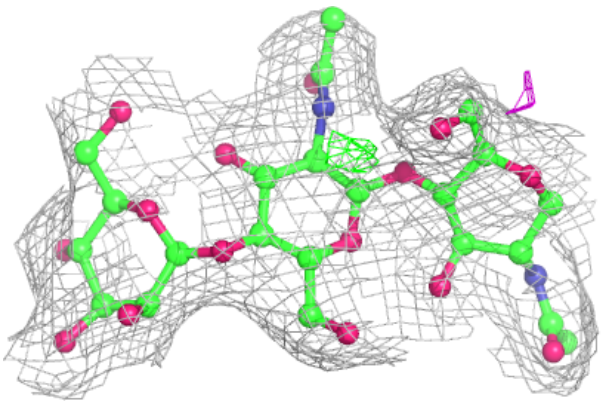


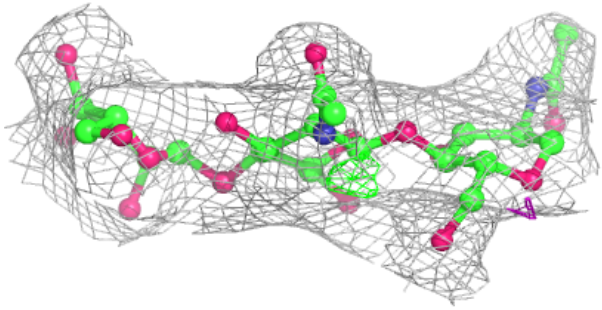


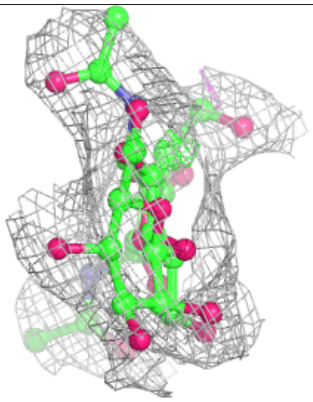


Electron density around Chain l:

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

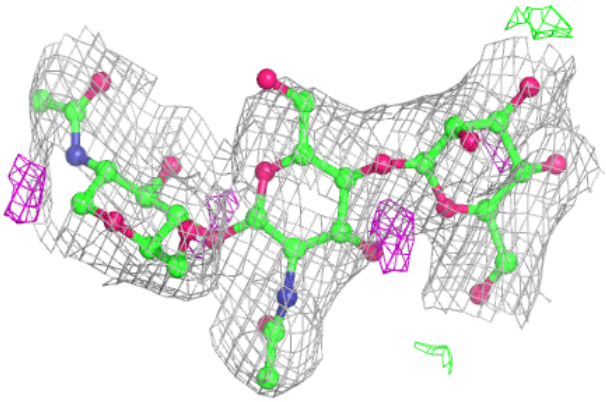


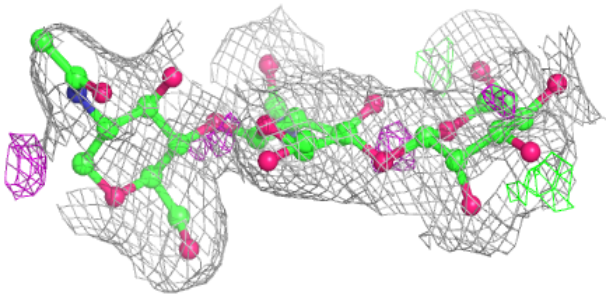


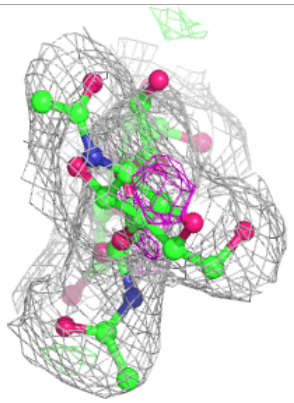


Electron density around Chain n:

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

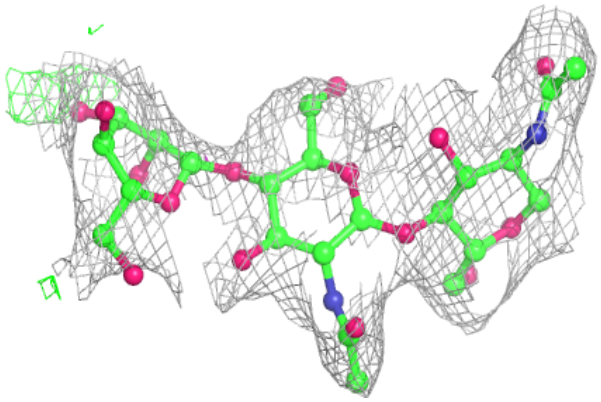


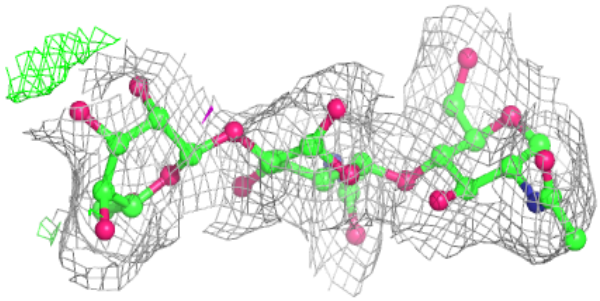


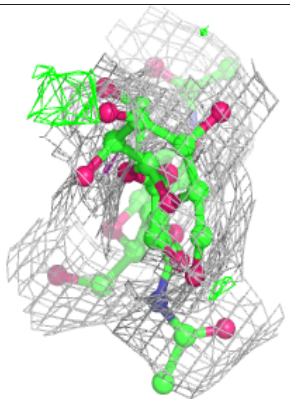


Electron density around Chain o:

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

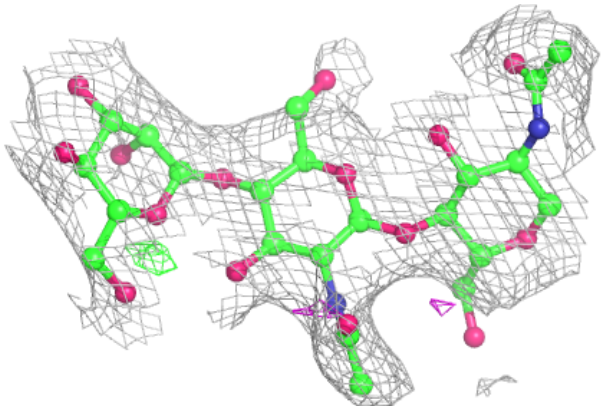


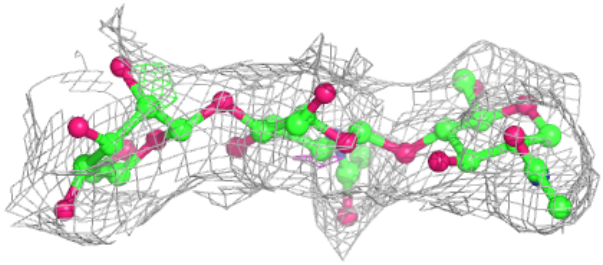


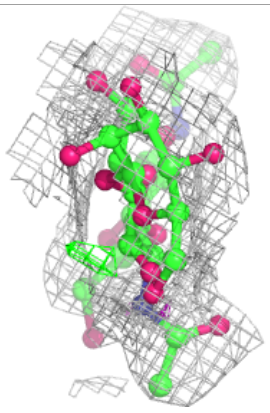


Electron density around Chain p:

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

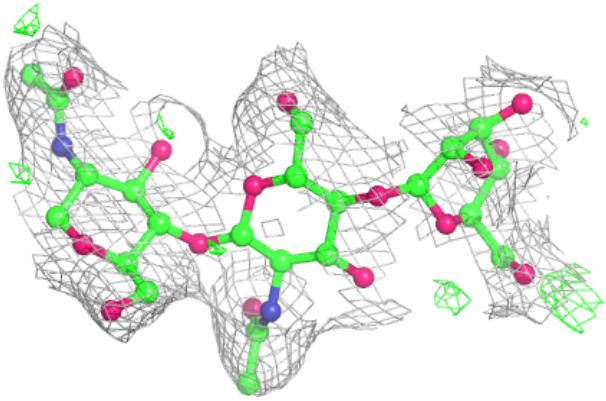


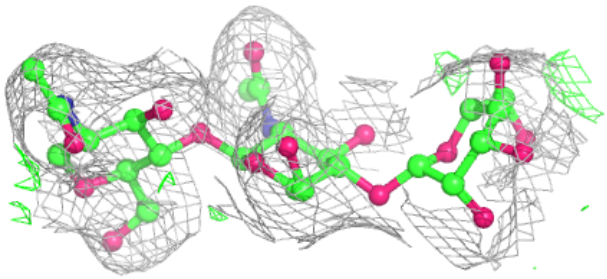


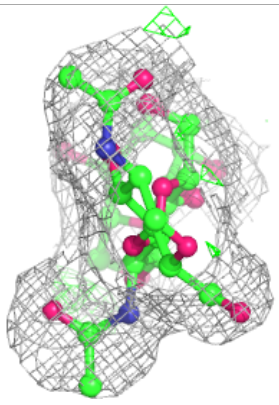


Electron density around Chain r:

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

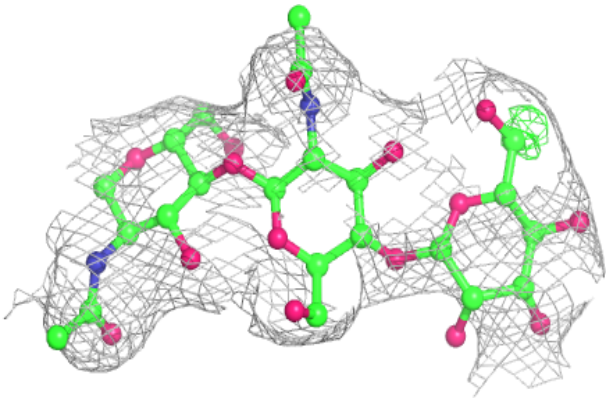


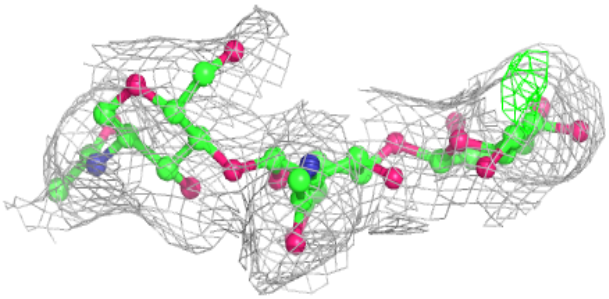


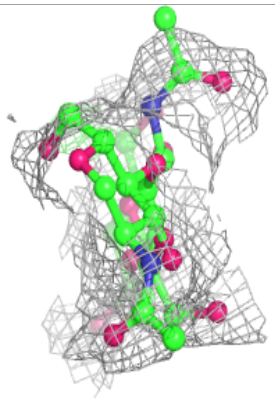


Electron density around Chain t:

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

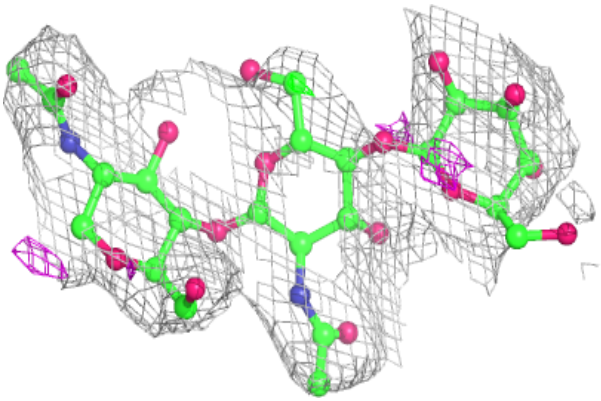


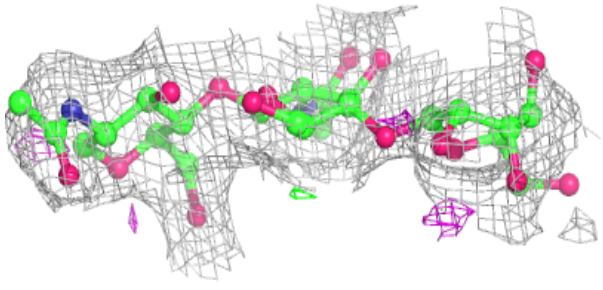


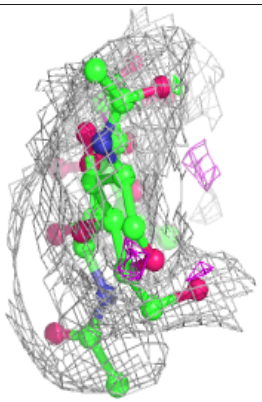


Electron density around Chain v:

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

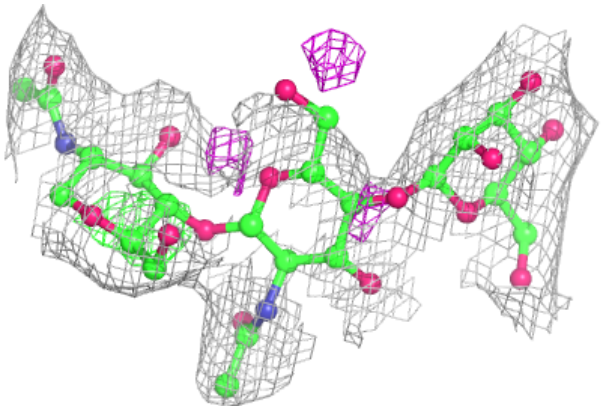


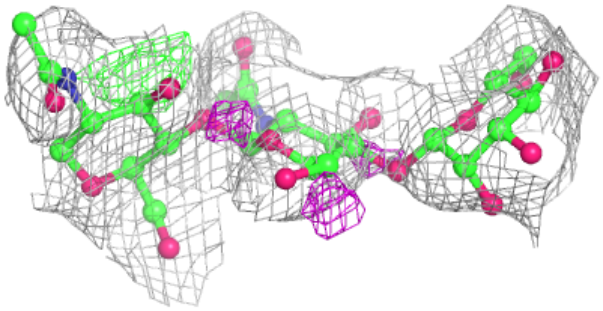


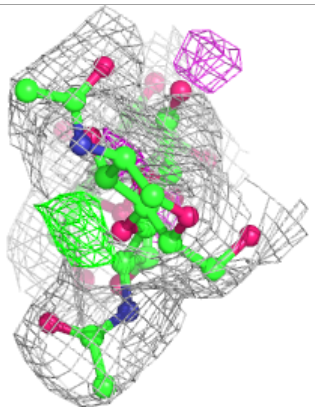


Electron density around Chain x:

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

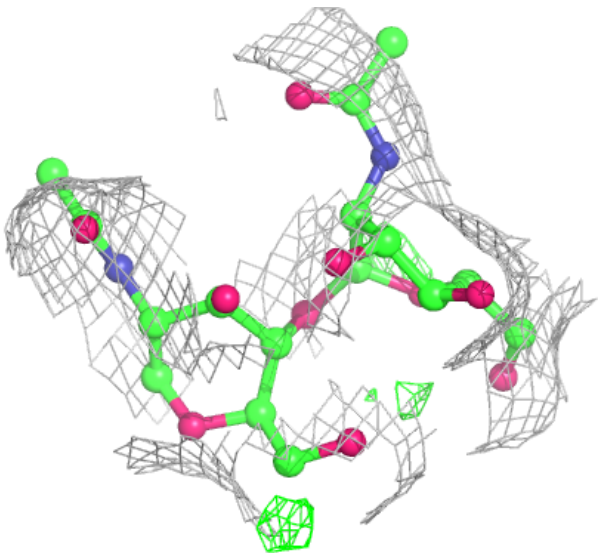


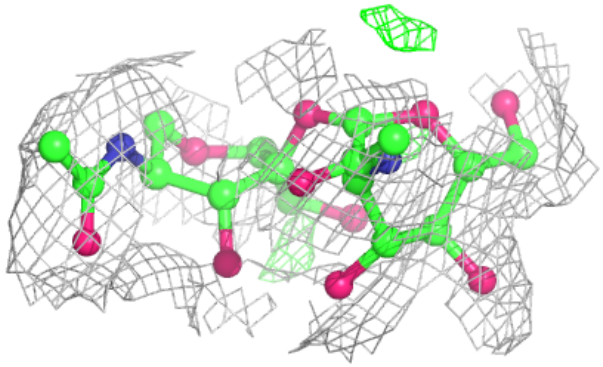


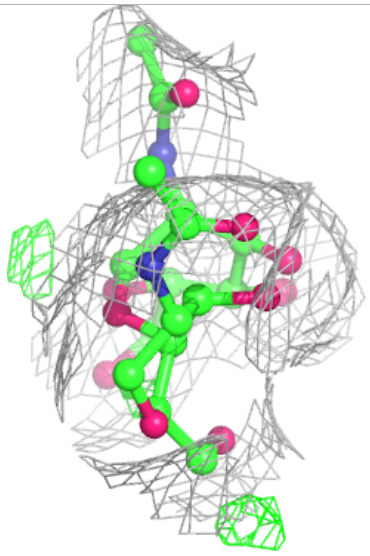


Electron density around Chain f:

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

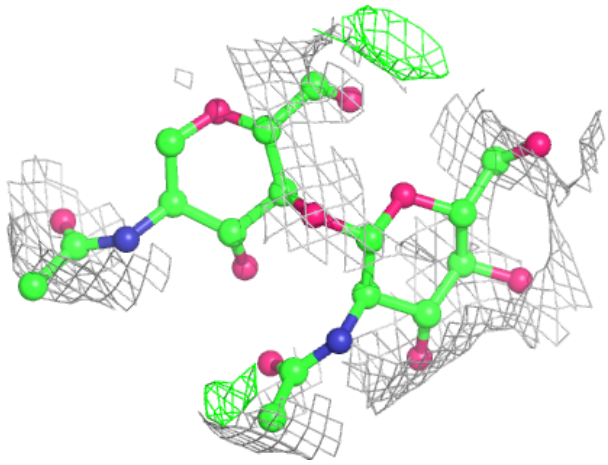


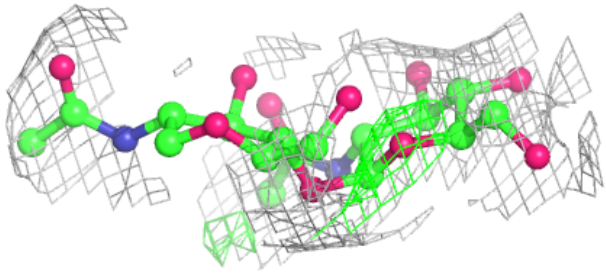


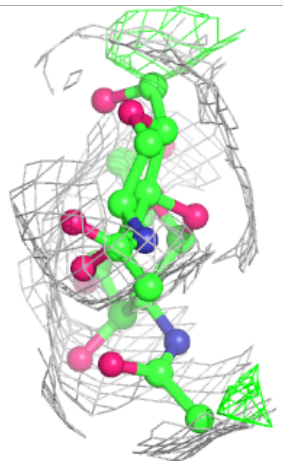


Electron density around Chain i:

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

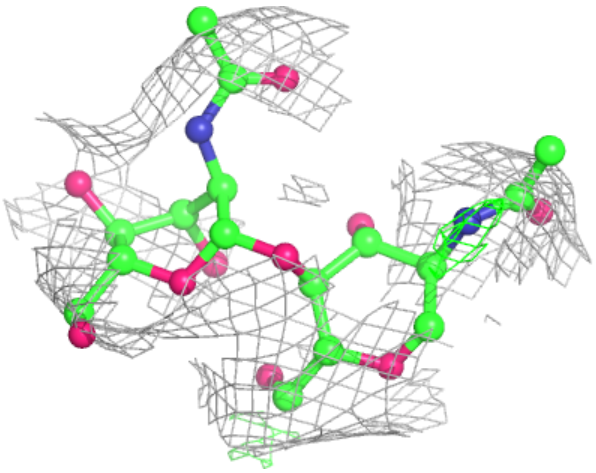


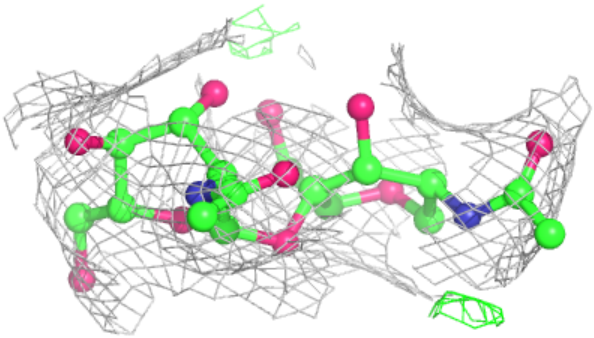


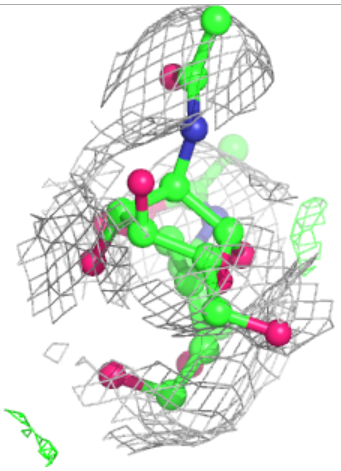


Electron density around Chain k:

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

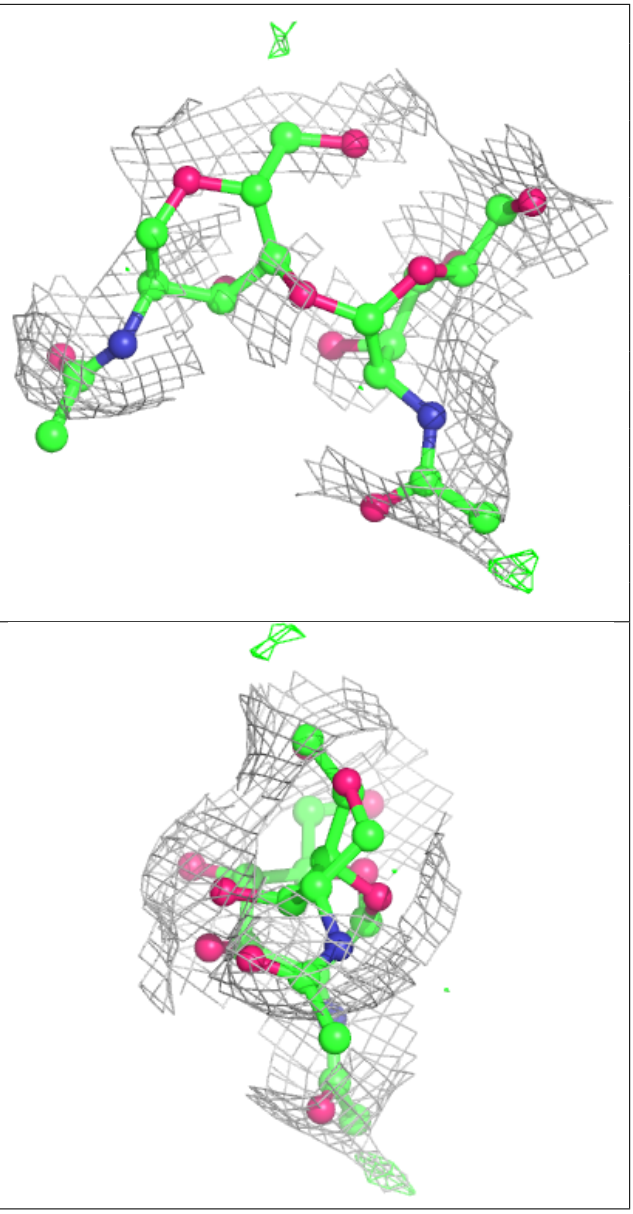


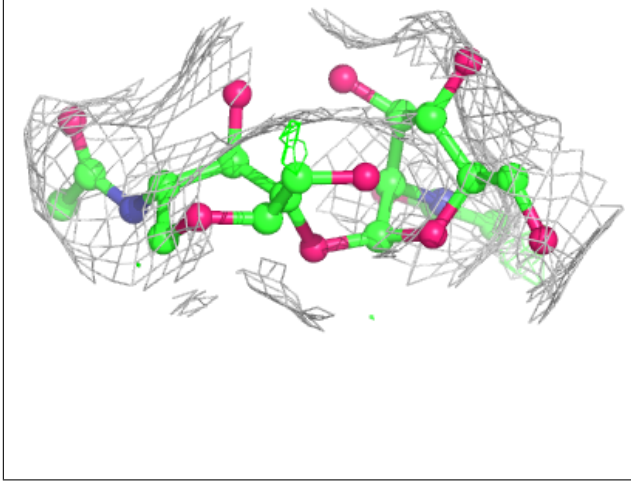




Electron density around Chain m:

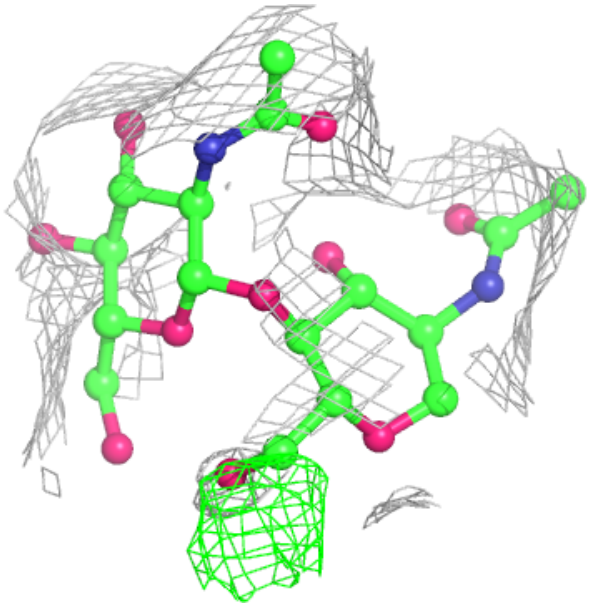
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

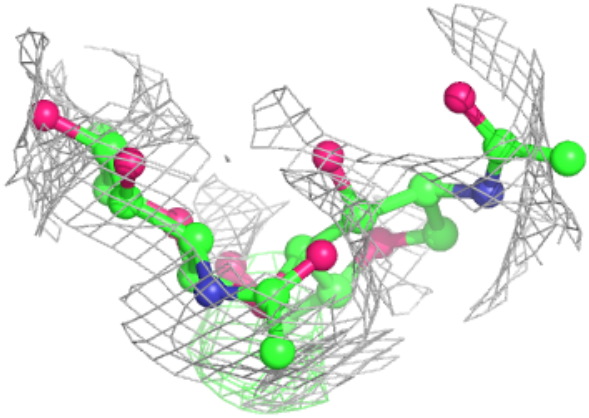


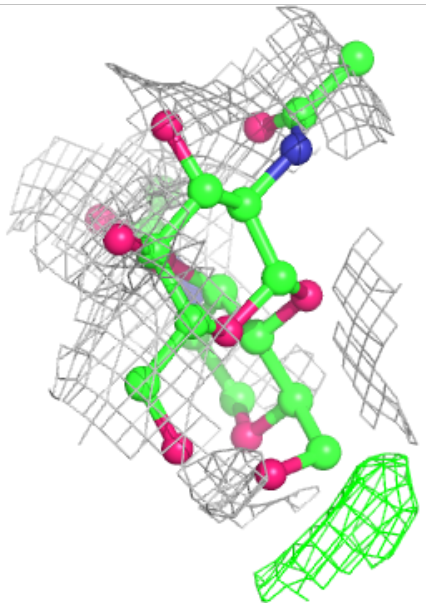


Electron density around Chain q:

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

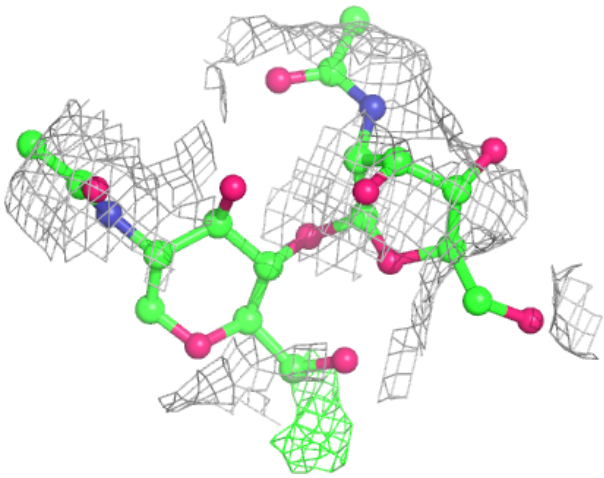


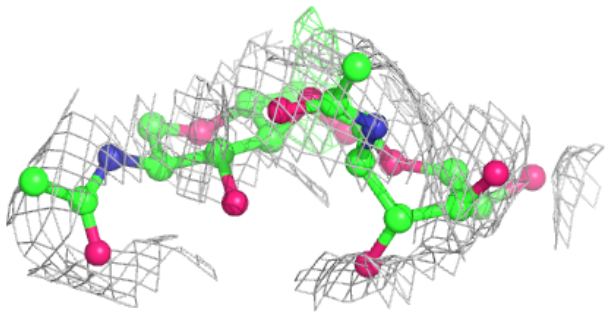


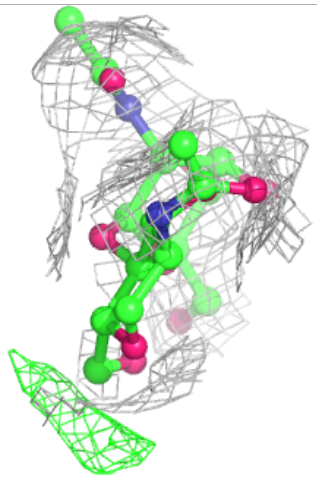


Electron density around Chain s:

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

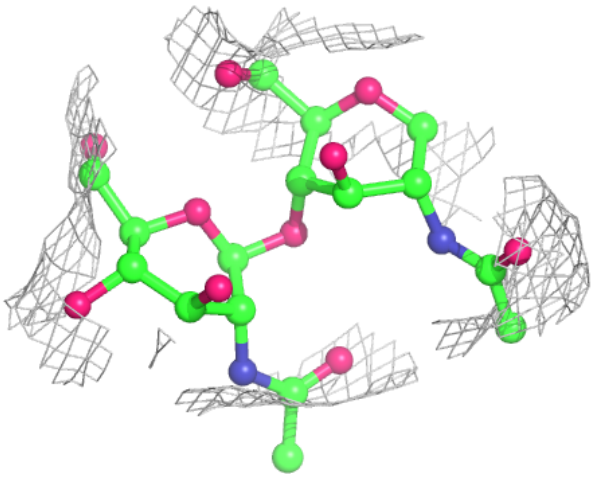


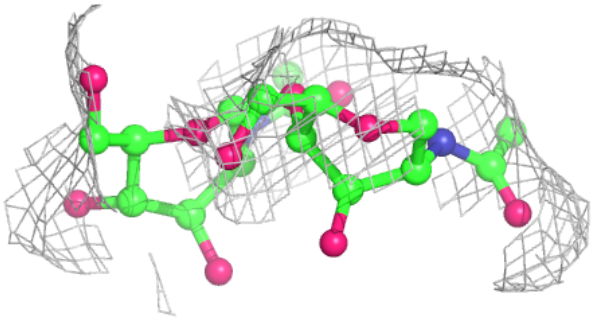


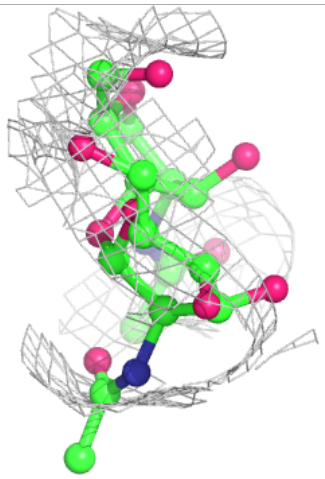


Electron density around Chain u:

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

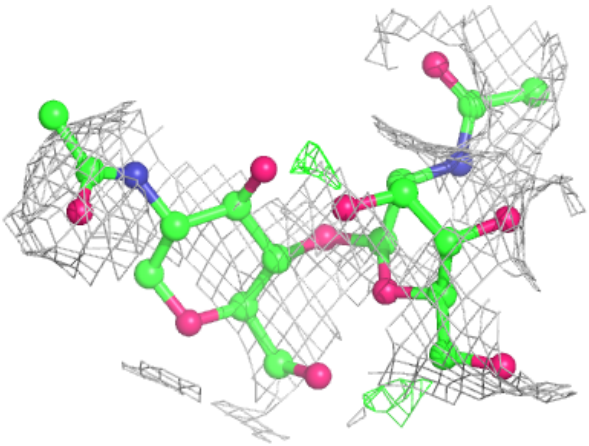


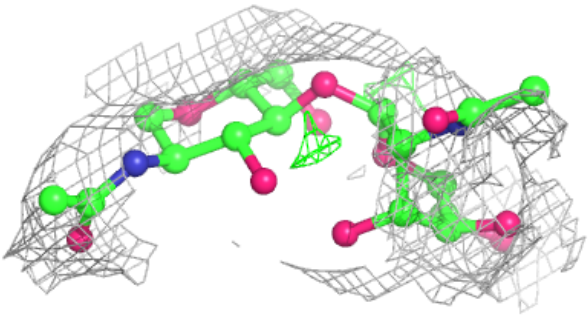


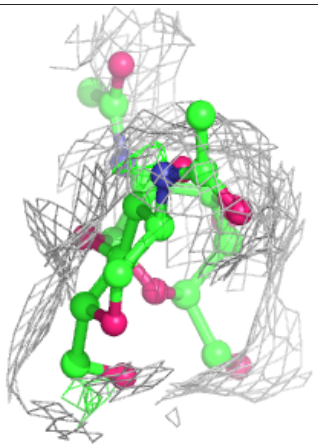


Electron density around Chain w:

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

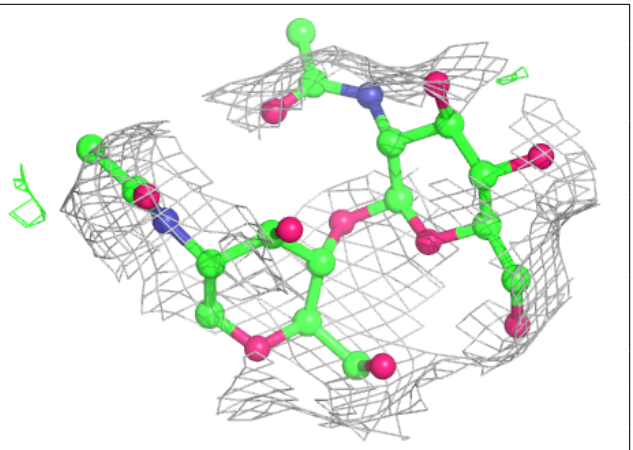


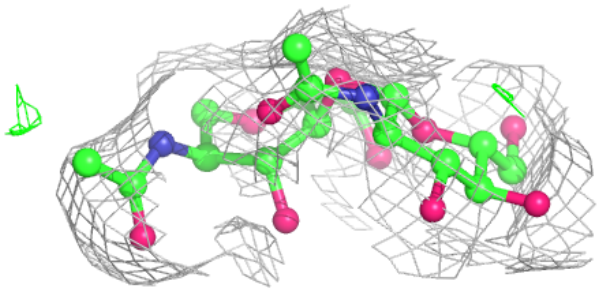


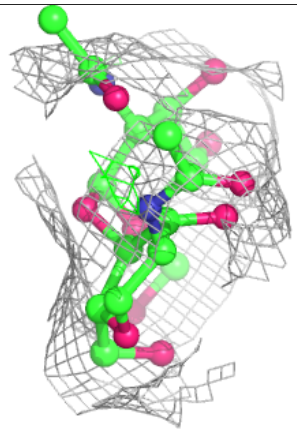


Electron density around Chain y:

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

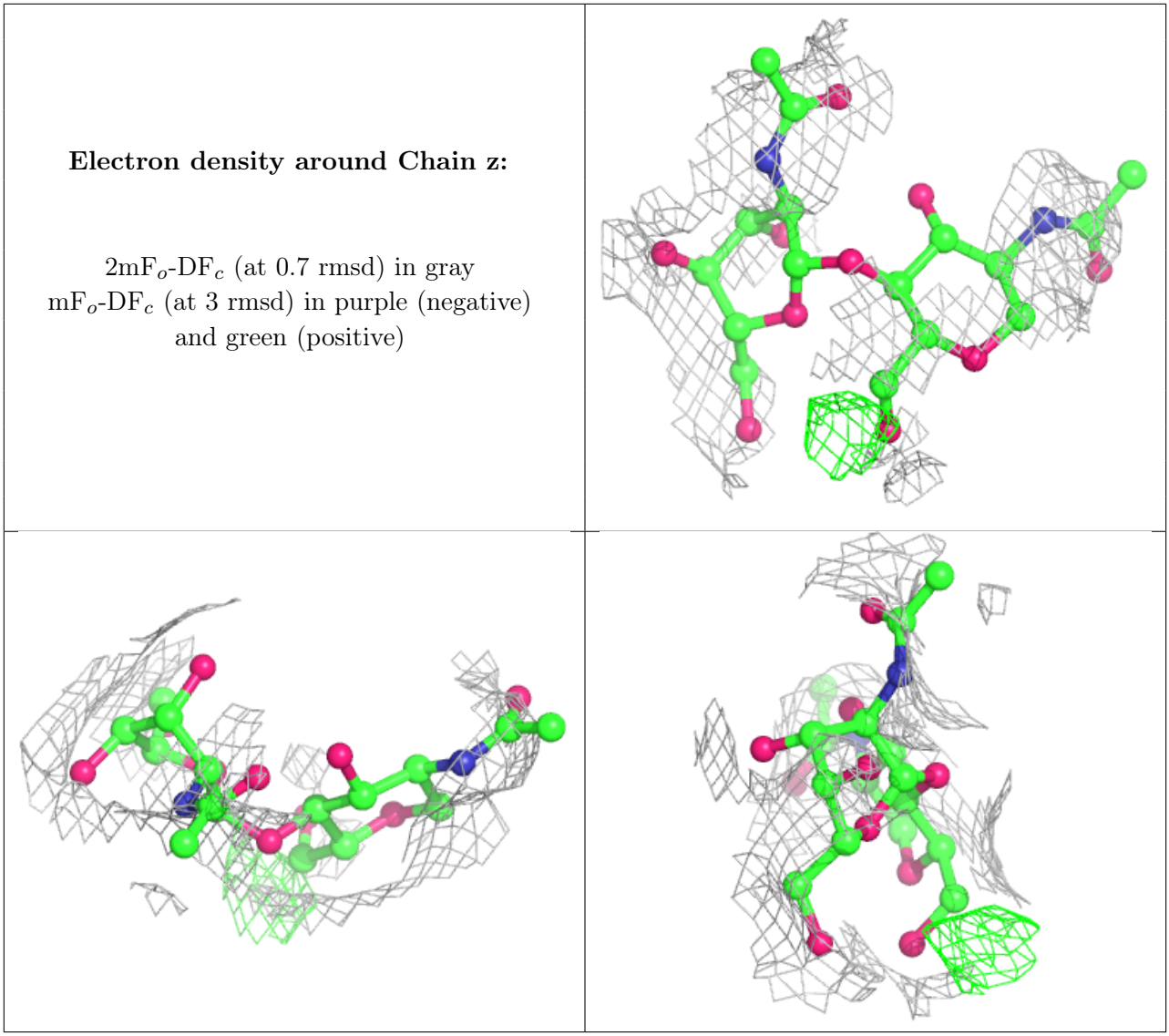






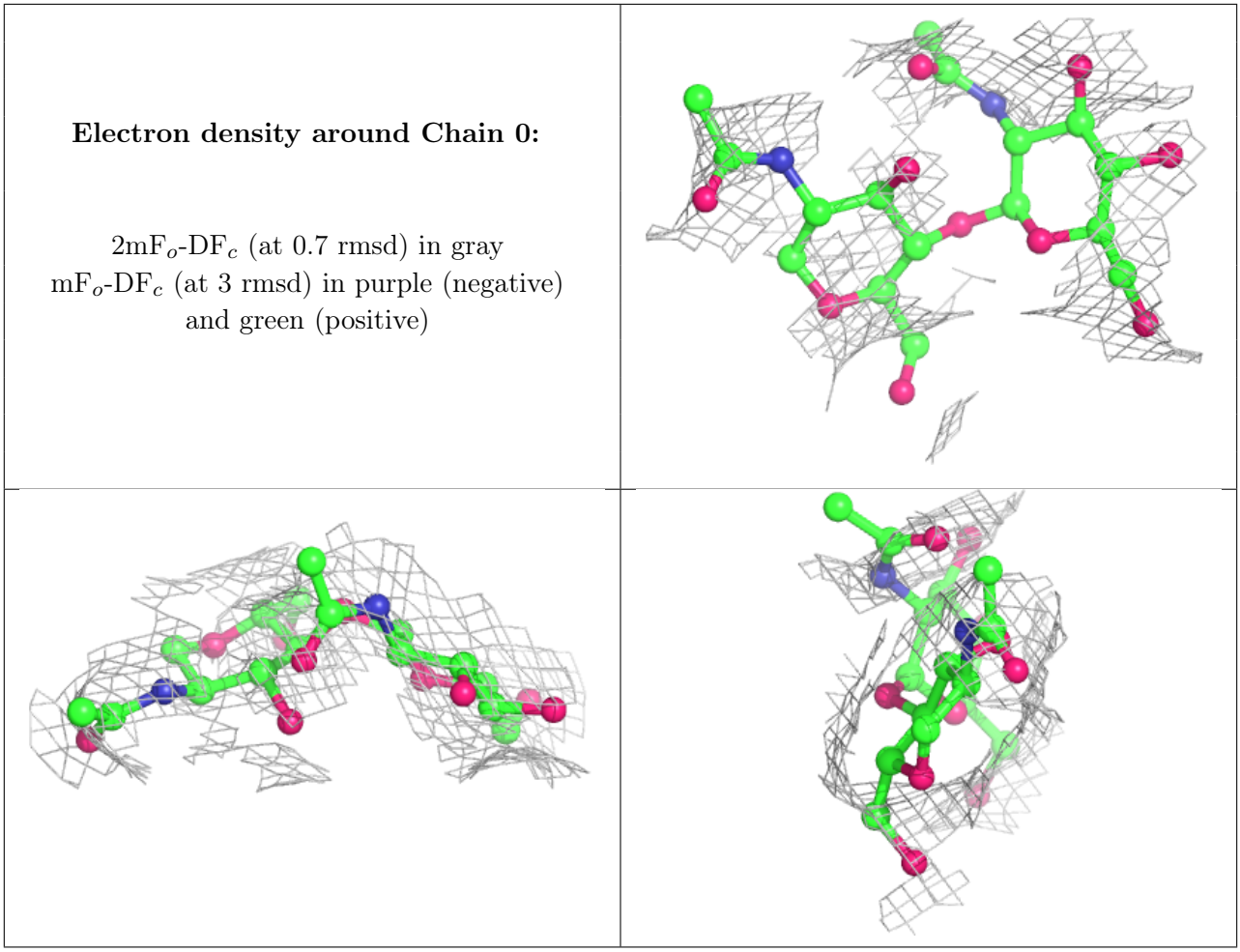
Electron density around Chain z:

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



Electron density around Chain 0:

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



6.4 Ligands

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
5	NAG	C	2004	14/15	0.80	0.16	125,149,153,153	0
5	NAG	a	2001	14/15	0.82	0.20	92,112,119,128	0
5	NAG	Y	2001	14/15	0.85	0.19	75,93,108,120	0
5	NAG	K	2004	14/15	0.85	0.11	127,135,145,149	0
5	NAG	M	2004	14/15	0.87	0.11	119,135,154,161	0
5	NAG	O	2006	14/15	0.87	0.27	96,105,117,126	0
5	NAG	c	2001	14/15	0.89	0.20	91,102,120,122	0

6.5 Other polymers (i)

There are no such residues in this entry.