wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 05:39 AM EDT

PDB ID	:	4FQM
Title	:	Structure of B/Brisbane/60/2008 Influenza Hemagglutinin
Authors	:	Dreyfus, C.; Laursen, N.S.; Wilson, I.A.
Deposited on	:	2012-06-25
Resolution	:	3.45 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

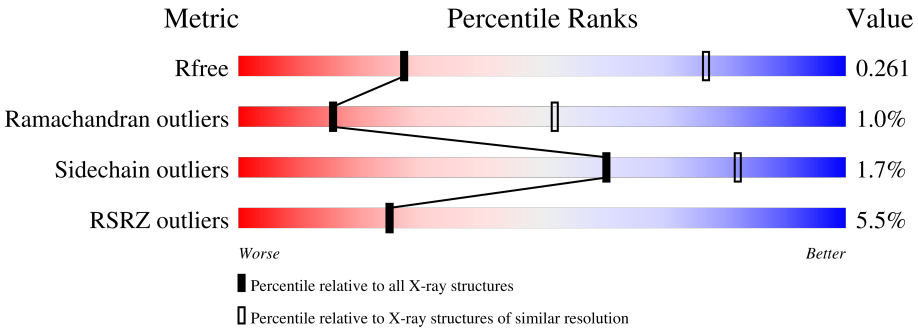
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	347	4% 95%
1	C	347	3% 96%
1	E	347	3% 96%
1	G	347	3% 95%
1	I	347	2% 96%
1	K	347	5% 95%

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Mol	Chain	Length	Quality of chain
2	B	179	7% 93% 6%
2	D	179	11% 93% 6%
2	F	179	8% 92% 6%
2	H	179	13% 93% 6%
2	J	179	7% 94% 6%
2	L	179	12% 93% 6%
3	M	3	100%
3	P	3	100%
3	Q	3	100%
3	R	3	100%
3	T	3	100%
3	U	3	100%
3	V	3	100%
3	Y	3	100%
3	Z	3	100%
3	a	3	100%
3	d	3	100%
3	i	3	100%
3	j	3	100%
3	k	3	100%
3	n	3	100%
3	o	3	100%
4	N	2	100%
4	O	2	50% 50%
4	S	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	W	2	100%
4	X	2	50% 50%
4	b	2	100%
4	c	2	50% 50%
4	e	2	100%
4	f	2	100%
4	g	2	100%
4	h	2	50% 50%
4	l	2	100%
4	m	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	Q	2	-	-	-	X
3	NAG	U	2	-	-	-	X
3	BMA	U	3	-	-	-	X
3	NAG	Z	2	-	-	-	X
3	NAG	a	2	-	-	-	X
3	BMA	j	3	-	-	-	X
3	NAG	o	2	-	-	-	X
4	NAG	e	2	-	-	-	X
4	NAG	f	2	-	-	-	X
5	NAG	C	414	-	-	-	X
5	NAG	D	600	-	-	-	X
5	NAG	E	411	-	-	-	X
5	NAG	I	410	-	-	-	X
5	NAG	I	414	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24446 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	C	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	E	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	G	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	I	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	K	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	F	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	H	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	J	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	L	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	linker	UNP C0LT38

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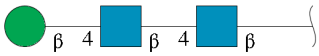
Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	linker	UNP C0LT38
B	526	ARG	-	linker	UNP C0LT38
D	524	SER	-	linker	UNP C0LT38
D	525	GLY	-	linker	UNP C0LT38
D	526	ARG	-	linker	UNP C0LT38
F	524	SER	-	linker	UNP C0LT38
F	525	GLY	-	linker	UNP C0LT38
F	526	ARG	-	linker	UNP C0LT38
H	524	SER	-	linker	UNP C0LT38
H	525	GLY	-	linker	UNP C0LT38
H	526	ARG	-	linker	UNP C0LT38
J	524	SER	-	linker	UNP C0LT38
J	525	GLY	-	linker	UNP C0LT38
J	526	ARG	-	linker	UNP C0LT38
L	524	SER	-	linker	UNP C0LT38
L	525	GLY	-	linker	UNP C0LT38
L	526	ARG	-	linker	UNP C0LT38

- 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	M	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	Q	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	U	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	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Z	3	Total C N O 39 22 2 15	0	0	0
3	a	3	Total C N O 39 22 2 15	0	0	0
3	d	3	Total C N O 39 22 2 15	0	0	0
3	i	3	Total C N O 39 22 2 15	0	0	0
3	j	3	Total C N O 39 22 2 15	0	0	0
3	k	3	Total C N O 39 22 2 15	0	0	0
3	n	3	Total C N O 39 22 2 15	0	0	0
3	o	3	Total C N O 39 22 2 15	0	0	0

- 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	N	2	Total C N O 28 16 2 10	0	0	0
4	O	2	Total C N O 28 16 2 10	0	0	0
4	S	2	Total C N O 28 16 2 10	0	0	0
4	W	2	Total C N O 28 16 2 10	0	0	0
4	X	2	Total C N O 28 16 2 10	0	0	0
4	b	2	Total C N O 28 16 2 10	0	0	0
4	c	2	Total C N O 28 16 2 10	0	0	0
4	e	2	Total C N O 28 16 2 10	0	0	0
4	f	2	Total C N O 28 16 2 10	0	0	0

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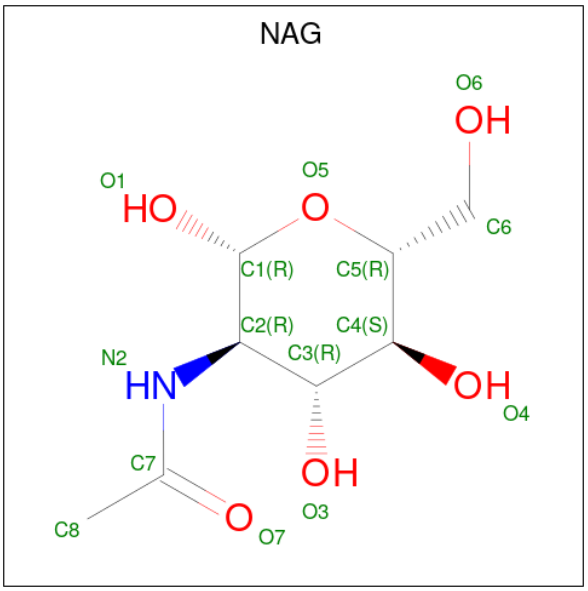
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	g	2	Total C N O 28 16 2 10	0	0	0
4	h	2	Total C N O 28 16 2 10	0	0	0
4	l	2	Total C N O 28 16 2 10	0	0	0
4	m	2	Total C N O 28 16 2 10	0	0	0

- 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	A	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	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

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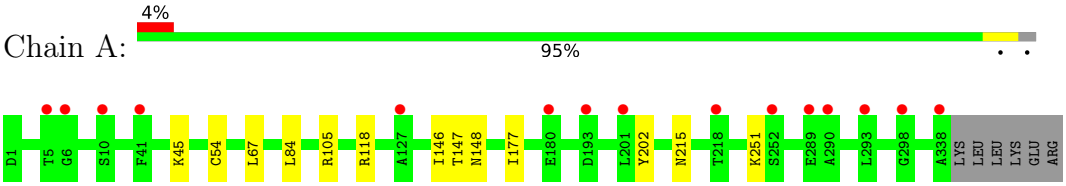
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

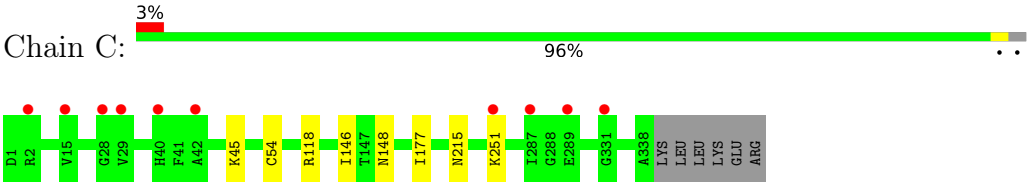
• Molecule 1: Hemagglutinin HA1

Chain A:



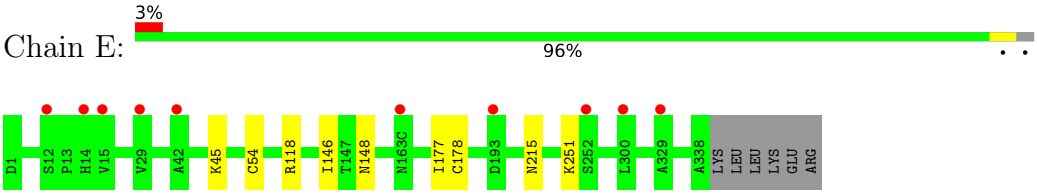
• Molecule 1: Hemagglutinin HA1

Chain C:



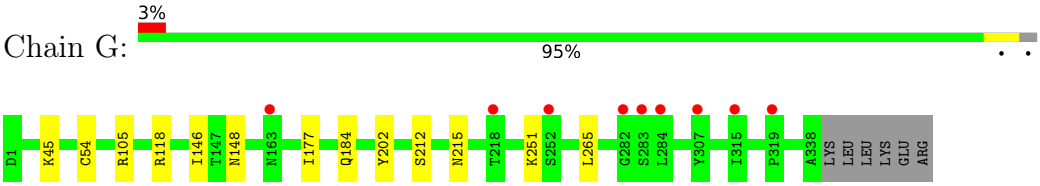
• Molecule 1: Hemagglutinin HA1

Chain E:



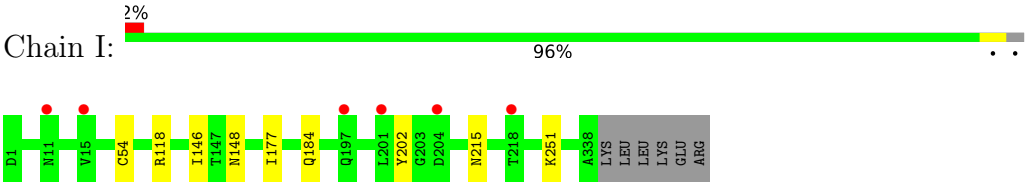
• Molecule 1: Hemagglutinin HA1

Chain G:



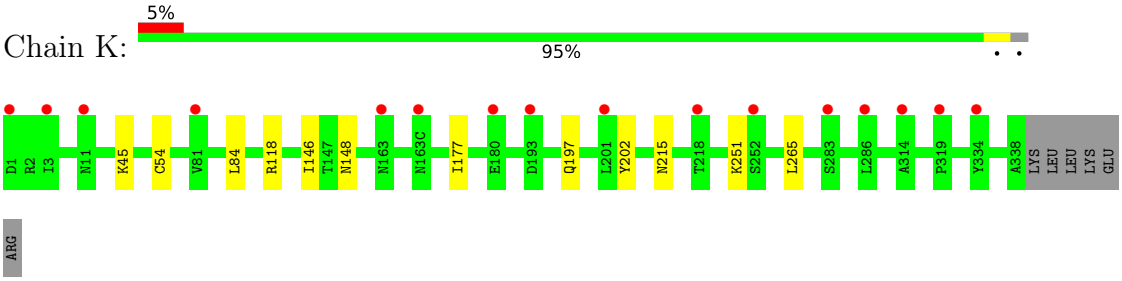
• Molecule 1: Hemagglutinin HA1

Chain I:



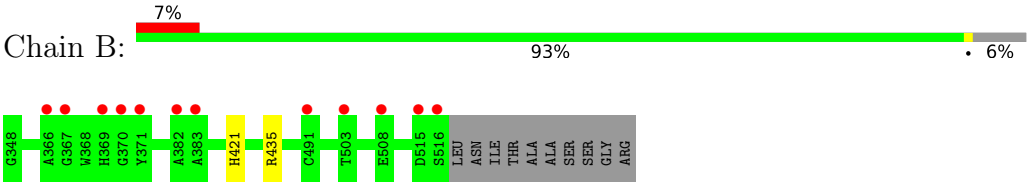
• Molecule 1: Hemagglutinin HA1

Chain K:



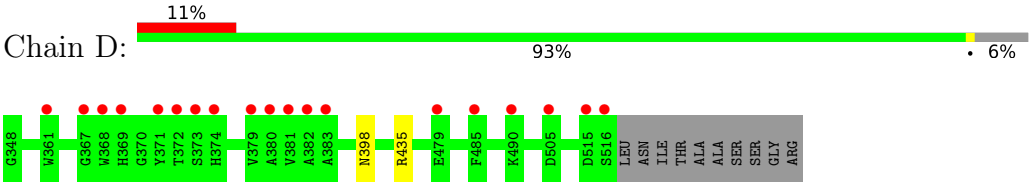
• Molecule 2: Hemagglutinin HA2

Chain B:



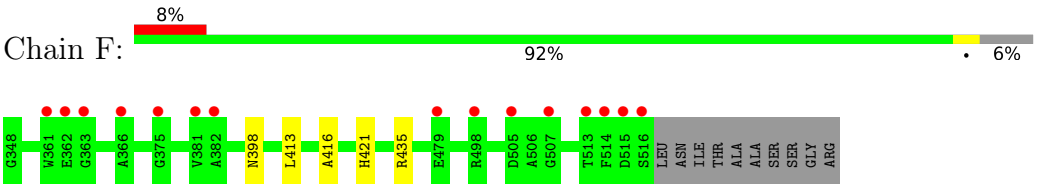
• Molecule 2: Hemagglutinin HA2

Chain D:



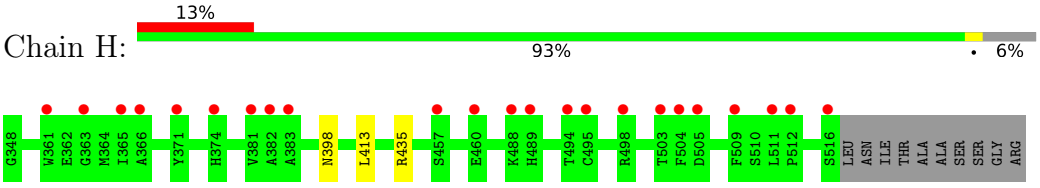
• Molecule 2: Hemagglutinin HA2

Chain F:



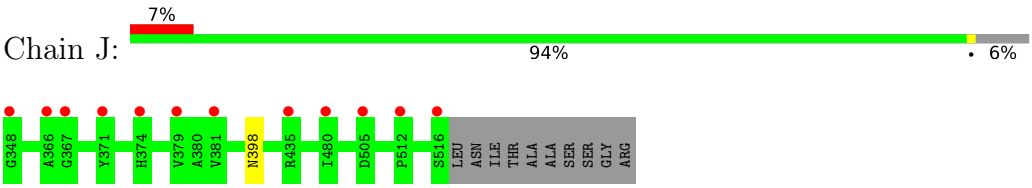
• Molecule 2: Hemagglutinin HA2

Chain H:



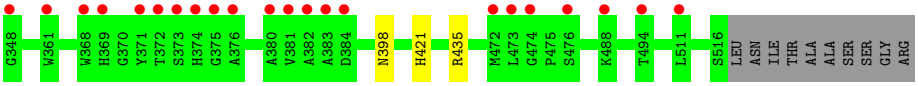
• Molecule 2: Hemagglutinin HA2

Chain J:



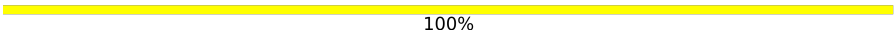
• Molecule 2: Hemagglutinin HA2

Chain L:



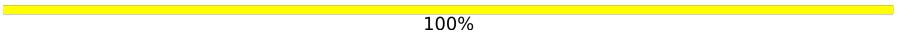
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



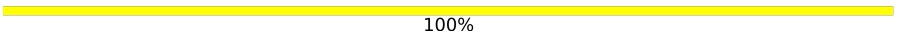
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



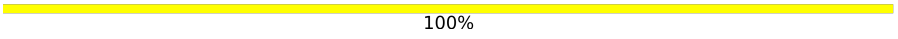
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



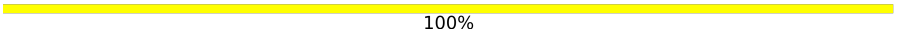
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



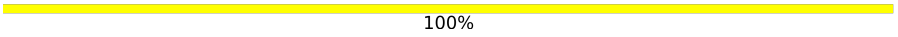
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 U:



• 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: 100%

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

Chain Y: 100%

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

Chain Z: 100%

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

Chain a: 100%

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

Chain d: 100%

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

Chain i: 100%

• 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: 100%

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

Chain k: 100%

• 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: 100%

• 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: 100%

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

Chain N: 100%

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

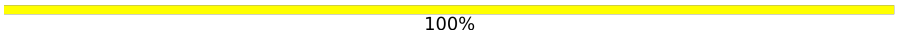
Chain O: 50% 50%

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

Chain S: 50% 50%

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

Chain W:

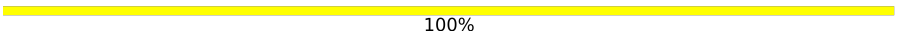


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

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

Chain b:

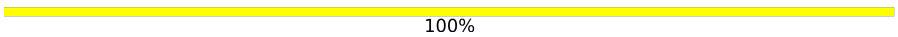


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

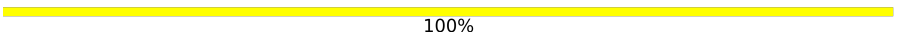
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



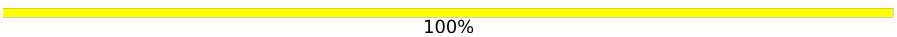
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain g:

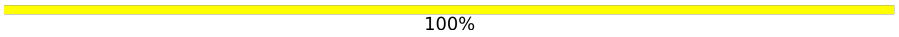


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

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

Chain l:



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

Chain m:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.69Å 242.54Å 135.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.45 49.07 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.07-3.45) 99.7 (49.07-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.257 , 0.268 0.250 , 0.261	Depositor DCC
R_{free} test set	1925 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24446	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	0/2648	0.93	2/3598 (0.1%)
1	C	0.60	0/2648	0.79	0/3598
1	E	0.58	1/2648 (0.0%)	0.77	0/3598
1	G	0.55	0/2648	0.78	0/3598
1	I	0.56	1/2648 (0.0%)	0.75	0/3598
1	K	0.53	0/2648	0.75	1/3598 (0.0%)
2	B	0.43	0/1301	0.67	0/1753
2	D	0.44	0/1301	0.69	0/1753
2	F	0.44	0/1301	0.69	1/1753 (0.1%)
2	H	0.41	0/1301	0.66	1/1753 (0.1%)
2	J	0.40	0/1301	0.66	0/1753
2	L	0.40	0/1301	0.66	0/1753
All	All	0.53	2/23694 (0.0%)	0.76	5/32106 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	184	GLN	CD-NE2	-5.86	1.18	1.32
1	E	178	CYS	CB-SG	-5.04	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	67	LEU	CB-CG-CD2	-5.74	101.25	111.00
2	H	413	LEU	CA-CB-CG	5.73	128.47	115.30
1	K	84	LEU	CA-CB-CG	5.63	128.25	115.30
2	F	413	LEU	CA-CB-CG	5.42	127.76	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	339/347 (98%)	311 (92%)	22 (6%)	6 (2%)	8 39
1	C	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	10 43
1	E	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	10 43
1	G	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	10 43
1	I	339/347 (98%)	314 (93%)	21 (6%)	4 (1%)	13 48
1	K	339/347 (98%)	316 (93%)	18 (5%)	5 (2%)	10 43
2	B	167/179 (93%)	162 (97%)	5 (3%)	0	100 100
2	D	167/179 (93%)	162 (97%)	5 (3%)	0	100 100
2	F	167/179 (93%)	162 (97%)	4 (2%)	1 (1%)	25 62
2	H	167/179 (93%)	162 (97%)	5 (3%)	0	100 100
2	J	167/179 (93%)	162 (97%)	5 (3%)	0	100 100
2	L	167/179 (93%)	162 (97%)	5 (3%)	0	100 100
All	All	3036/3156 (96%)	2855 (94%)	150 (5%)	31 (1%)	15 52

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS

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Mol	Chain	Res	Type
1	E	177	ILE

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	288/294 (98%)	283 (98%)	5 (2%)	60	82
1	C	288/294 (98%)	285 (99%)	3 (1%)	76	89
1	E	288/294 (98%)	285 (99%)	3 (1%)	76	89
1	G	288/294 (98%)	280 (97%)	8 (3%)	43	72
1	I	288/294 (98%)	284 (99%)	4 (1%)	67	85
1	K	288/294 (98%)	282 (98%)	6 (2%)	53	78
2	B	136/143 (95%)	134 (98%)	2 (2%)	65	84
2	D	136/143 (95%)	134 (98%)	2 (2%)	65	84
2	F	136/143 (95%)	133 (98%)	3 (2%)	52	77
2	H	136/143 (95%)	134 (98%)	2 (2%)	65	84
2	J	136/143 (95%)	135 (99%)	1 (1%)	84	93
2	L	136/143 (95%)	133 (98%)	3 (2%)	52	77
All	All	2544/2622 (97%)	2502 (98%)	42 (2%)	60	82

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	54	CYS
1	K	197	GLN
1	I	118	ARG
2	J	398	ASN
1	K	215	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	126	ASN
1	K	126	ASN
1	K	197	GLN
1	K	129	ASN
1	C	129	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

74 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	$\#\|Z\| > 2$
3	NAG	M	1	1,3	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
3	NAG	M	2	3	14,14,15	0.50	0	17,19,21	0.85	1 (5%)
3	BMA	M	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.40	0	17,19,21	1.81	3 (17%)
4	NAG	N	2	4	14,14,15	0.45	0	17,19,21	1.27	3 (17%)
4	NAG	O	1	1,4	14,14,15	0.39	0	17,19,21	1.93	2 (11%)
4	NAG	O	2	4	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	P	1	1,3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
3	NAG	P	2	3	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
3	BMA	P	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
3	NAG	Q	1	1,3	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
3	NAG	Q	2	3	14,14,15	0.50	0	17,19,21	1.39	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	Q	3	3	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
3	NAG	R	1	1,3	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
3	NAG	R	2	3	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
3	BMA	R	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
4	NAG	S	1	1,4	14,14,15	0.39	0	17,19,21	1.93	2 (11%)
4	NAG	S	2	4	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	T	1	1,3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
3	NAG	T	2	3	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
3	BMA	T	3	3	11,11,12	0.59	0	15,15,17	0.91	1 (6%)
3	NAG	U	1	1,3	14,14,15	0.50	0	17,19,21	2.24	3 (17%)
3	NAG	U	2	3	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
3	BMA	U	3	3	11,11,12	0.64	0	15,15,17	1.46	3 (20%)
3	NAG	V	1	1,3	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
3	NAG	V	2	3	14,14,15	0.47	0	17,19,21	0.84	1 (5%)
3	BMA	V	3	3	11,11,12	0.61	0	15,15,17	0.92	1 (6%)
4	NAG	W	1	1,4	14,14,15	0.40	0	17,19,21	1.80	3 (17%)
4	NAG	W	2	4	14,14,15	0.48	0	17,19,21	1.26	3 (17%)
4	NAG	X	1	1,4	14,14,15	0.39	0	17,19,21	1.93	2 (11%)
4	NAG	X	2	4	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	Y	1	1,3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
3	NAG	Y	2	3	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
3	BMA	Y	3	3	11,11,12	0.58	0	15,15,17	0.92	1 (6%)
3	NAG	Z	1	1,3	14,14,15	0.52	0	17,19,21	2.23	3 (17%)
3	NAG	Z	2	3	14,14,15	0.49	0	17,19,21	1.39	3 (17%)
3	BMA	Z	3	3	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
3	NAG	a	1	1,3	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
3	NAG	a	2	3	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
3	BMA	a	3	3	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
4	NAG	b	1	1,4	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
4	NAG	b	2	4	14,14,15	0.51	0	17,19,21	1.40	3 (17%)
4	NAG	c	1	1,4	14,14,15	0.38	0	17,19,21	1.92	2 (11%)
4	NAG	c	2	4	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	d	1	1,3	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
3	NAG	d	2	3	14,14,15	0.50	0	17,19,21	0.84	1 (5%)
3	BMA	d	3	3	11,11,12	0.60	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	e	1	1,4	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
4	NAG	e	2	4	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
4	NAG	f	1	1,4	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
4	NAG	f	2	4	14,14,15	0.50	0	17,19,21	0.85	1 (5%)
4	NAG	g	1	1,4	14,14,15	0.42	0	17,19,21	1.81	3 (17%)
4	NAG	g	2	4	14,14,15	0.47	0	17,19,21	1.27	3 (17%)
4	NAG	h	1	1,4	14,14,15	0.38	0	17,19,21	1.93	2 (11%)
4	NAG	h	2	4	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	i	1	1,3	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
3	NAG	i	2	3	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
3	BMA	i	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
3	NAG	j	1	1,3	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
3	NAG	j	2	3	14,14,15	0.50	0	17,19,21	1.40	3 (17%)
3	BMA	j	3	3	11,11,12	0.65	0	15,15,17	1.47	3 (20%)
3	NAG	k	1	1,3	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
3	NAG	k	2	3	14,14,15	0.50	0	17,19,21	0.86	1 (5%)
3	BMA	k	3	3	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
4	NAG	l	1	1,4	14,14,15	0.41	0	17,19,21	1.81	3 (17%)
4	NAG	l	2	4	14,14,15	0.48	0	17,19,21	1.27	3 (17%)
4	NAG	m	1	1,4	14,14,15	0.39	0	17,19,21	1.93	2 (11%)
4	NAG	m	2	4	14,14,15	0.53	0	17,19,21	0.62	0
3	NAG	n	1	1,3	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
3	NAG	n	2	3	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
3	BMA	n	3	3	11,11,12	0.58	0	15,15,17	0.92	1 (6%)
3	NAG	o	1	1,3	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
3	NAG	o	2	3	14,14,15	0.49	0	17,19,21	1.39	3 (17%)
3	BMA	o	3	3	11,11,12	0.65	0	15,15,17	1.46	3 (20%)

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
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	3/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	3/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Z	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	2/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	3/6/23/26	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	O5-C1-C2	-7.39	99.63	111.29
4	e	1	NAG	O5-C1-C2	-7.37	99.66	111.29
3	o	1	NAG	O5-C1-C2	-7.36	99.67	111.29
3	Q	1	NAG	O5-C1-C2	-7.36	99.67	111.29
3	j	1	NAG	O5-C1-C2	-7.35	99.68	111.29

There are no chirality outliers.

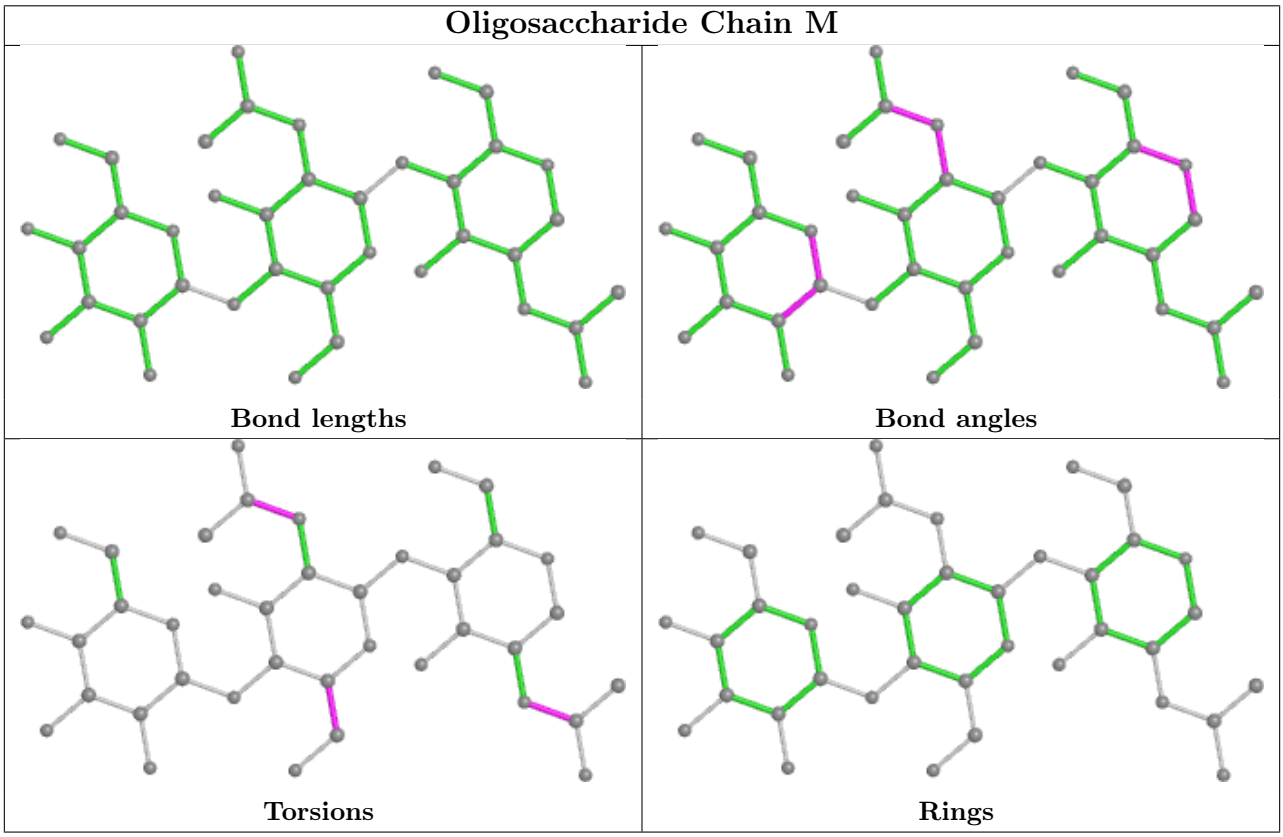
5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C8-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2

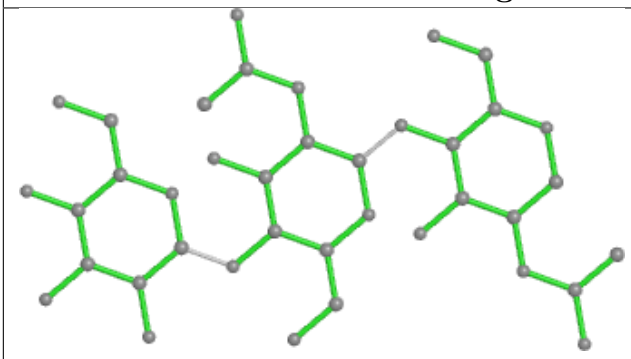
There are no ring outliers.

No monomer is involved in short contacts.

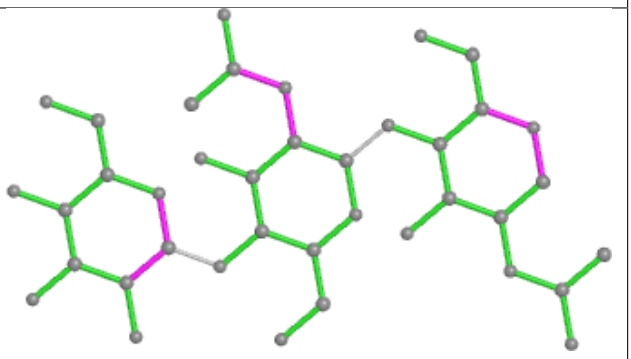
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



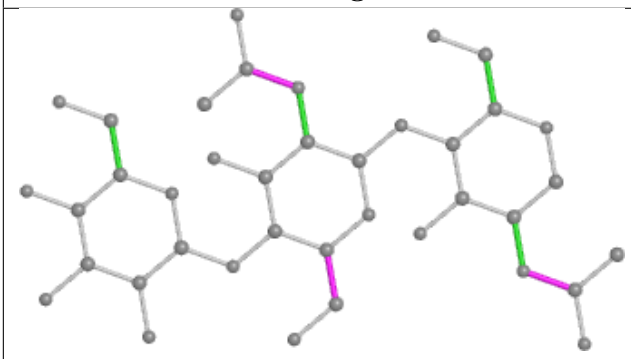
Oligosaccharide Chain P



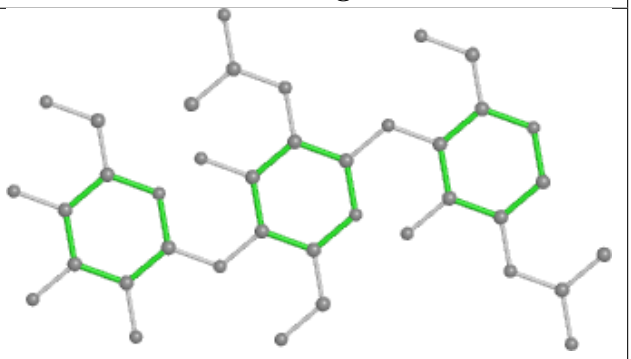
Bond lengths



Bond angles

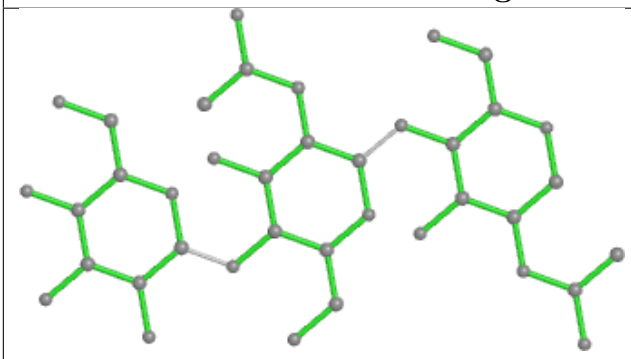


Torsions

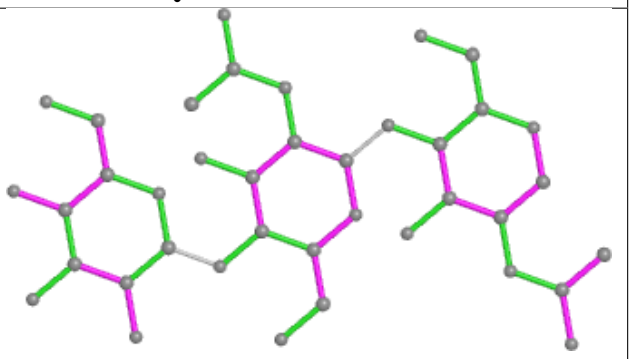


Rings

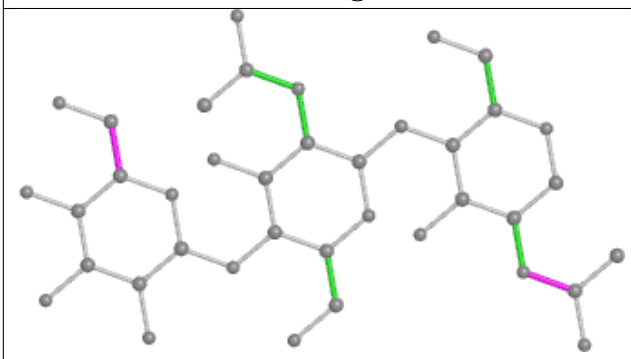
Oligosaccharide Chain Q



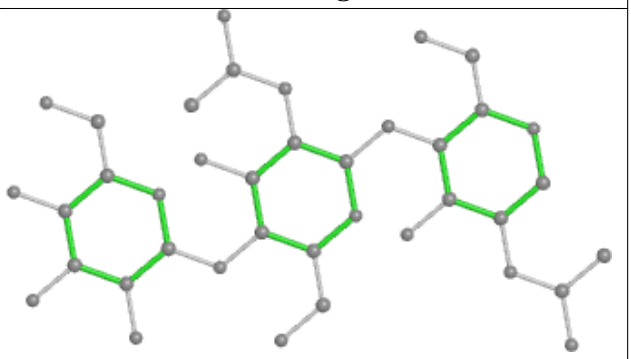
Bond lengths



Bond angles

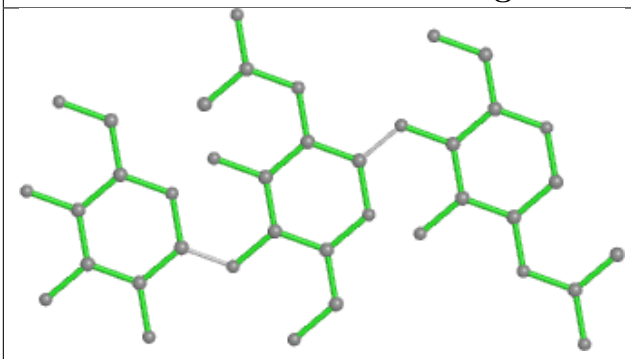


Torsions

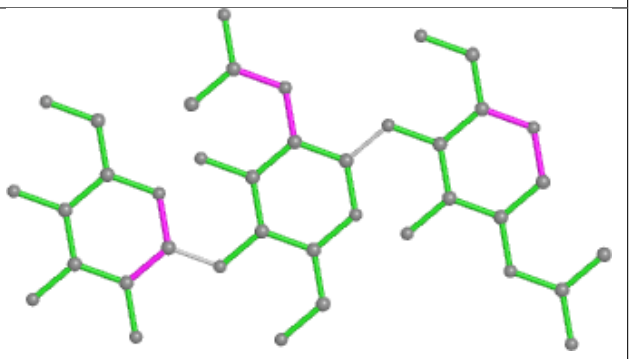


Rings

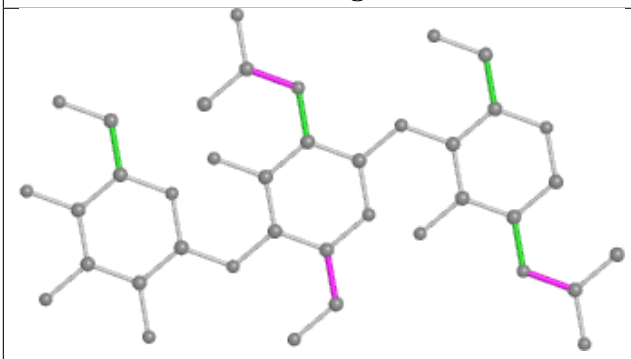
Oligosaccharide Chain R



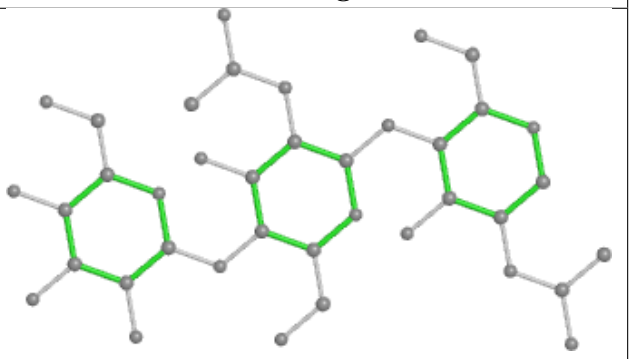
Bond lengths



Bond angles

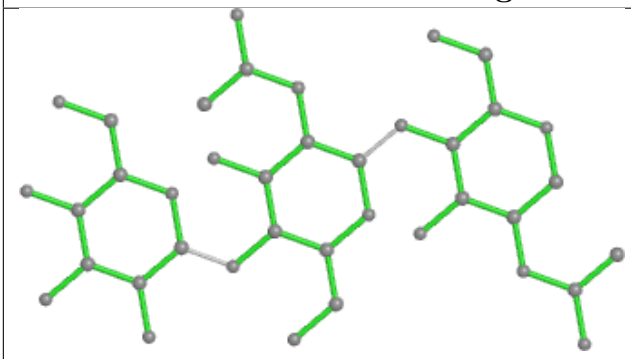


Torsions

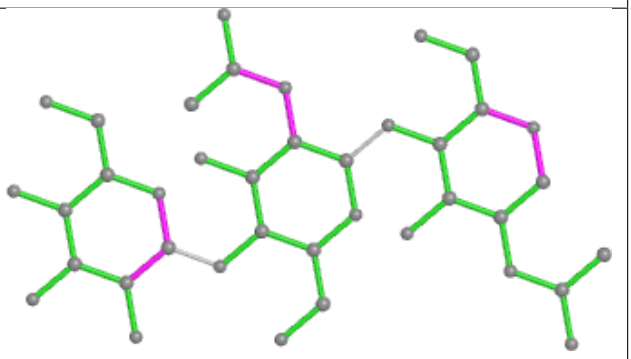


Rings

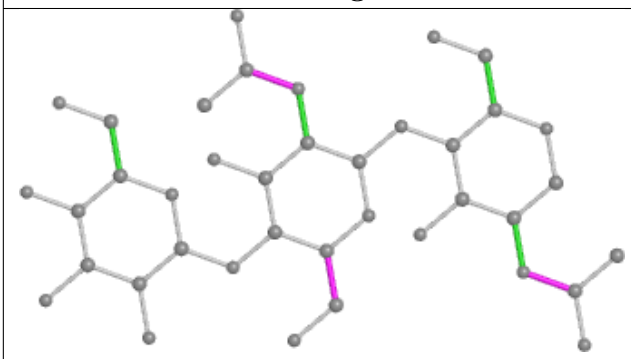
Oligosaccharide Chain T



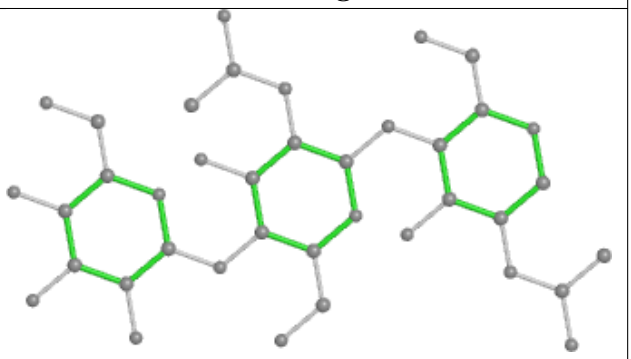
Bond lengths



Bond angles

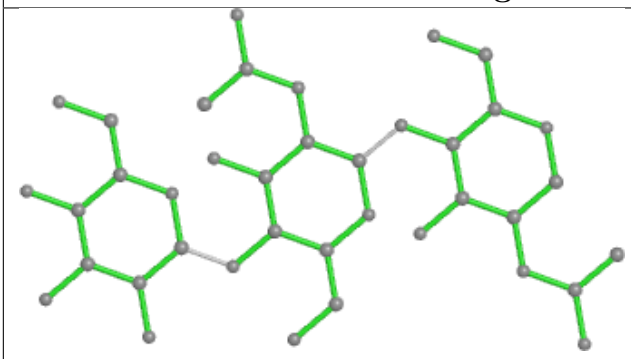


Torsions

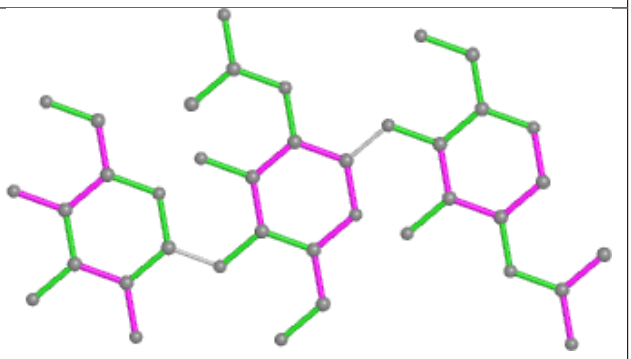


Rings

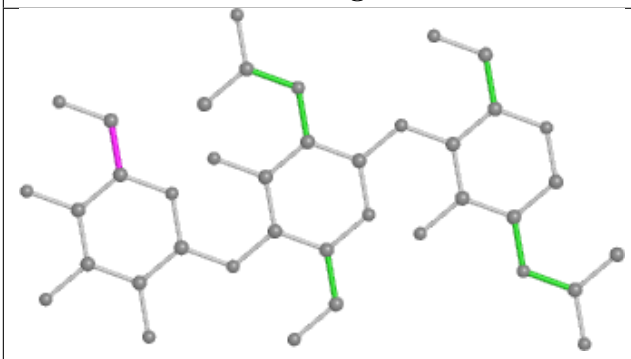
Oligosaccharide Chain U



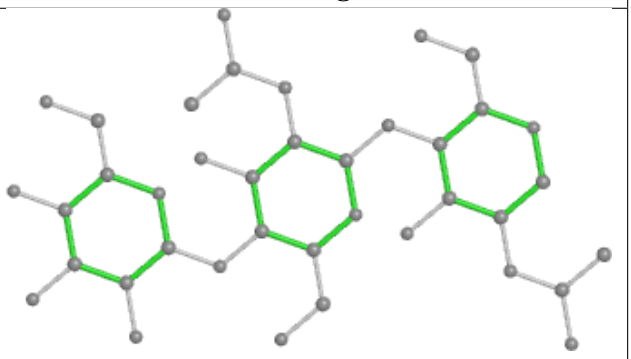
Bond lengths



Bond angles

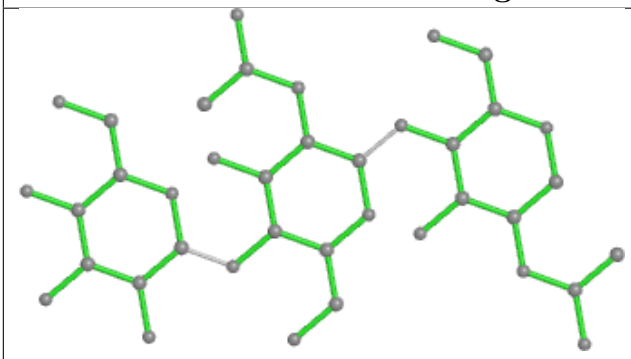


Torsions

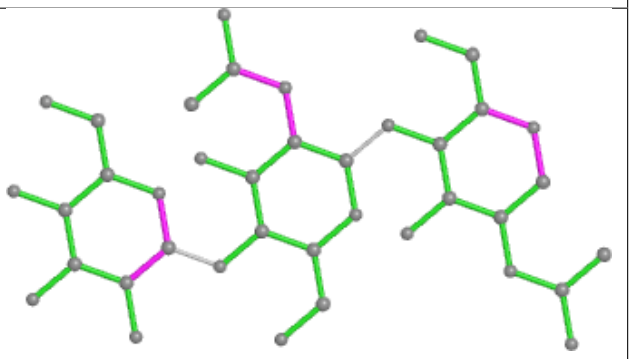


Rings

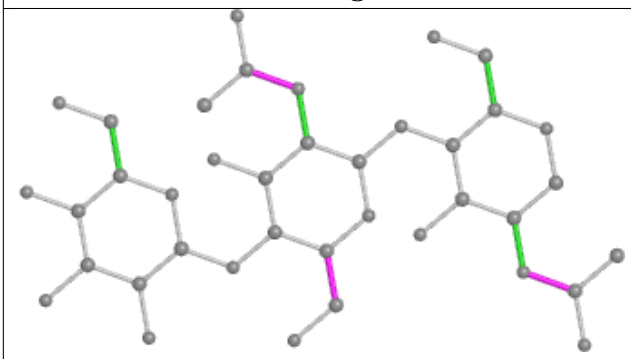
Oligosaccharide Chain V



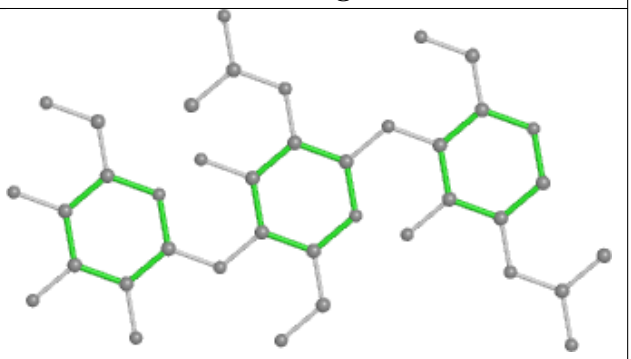
Bond lengths



Bond angles

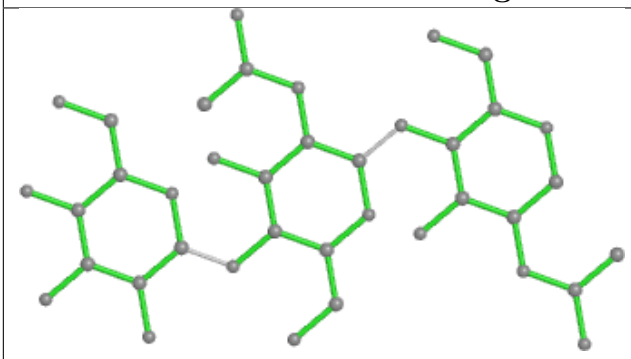


Torsions

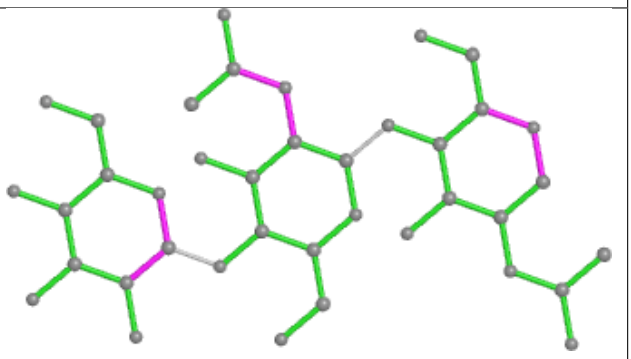


Rings

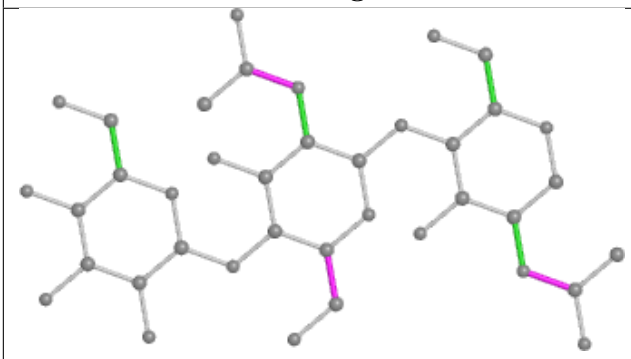
Oligosaccharide Chain Y



Bond lengths



Bond angles



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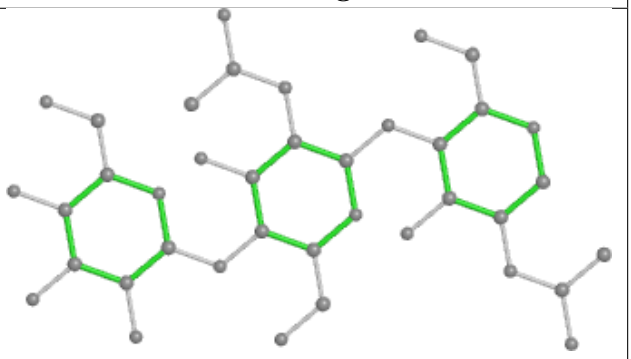
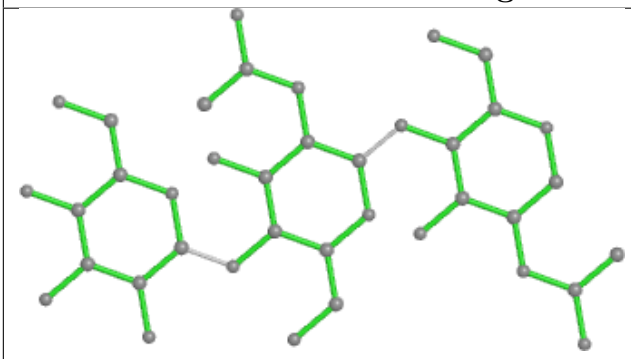
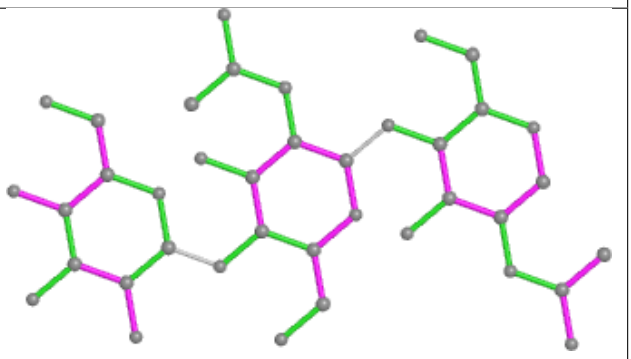


Rings

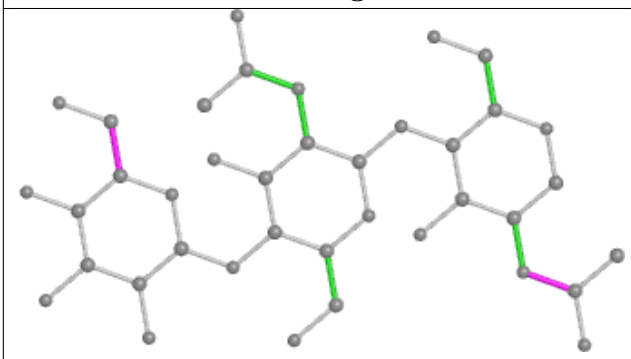
Oligosaccharide Chain Z



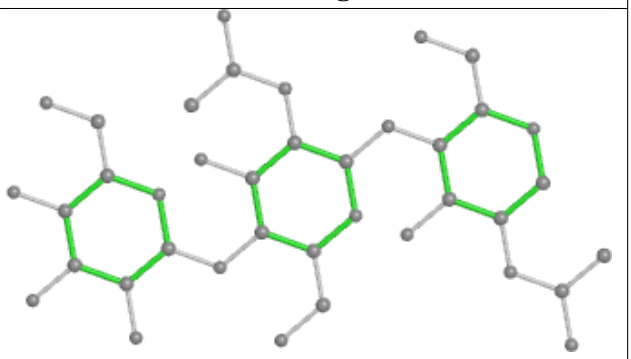
Bond lengths



Bond angles

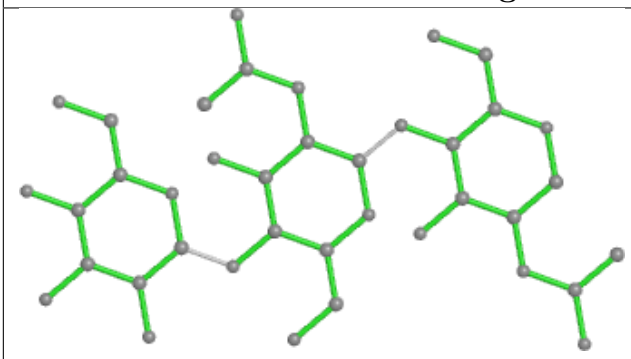


Torsions

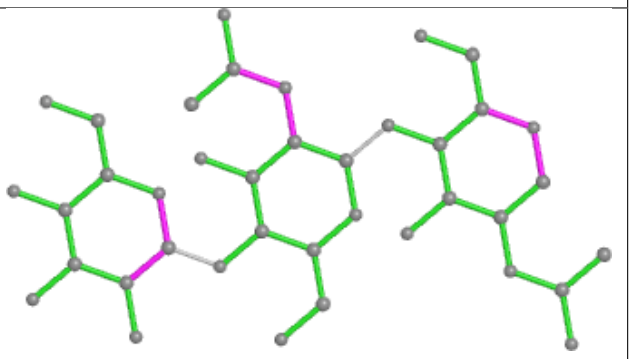


Rings

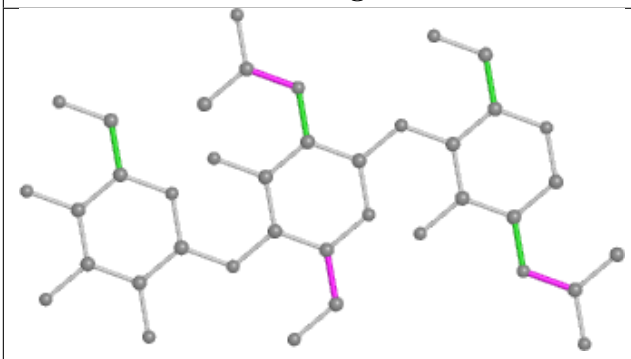
Oligosaccharide Chain a



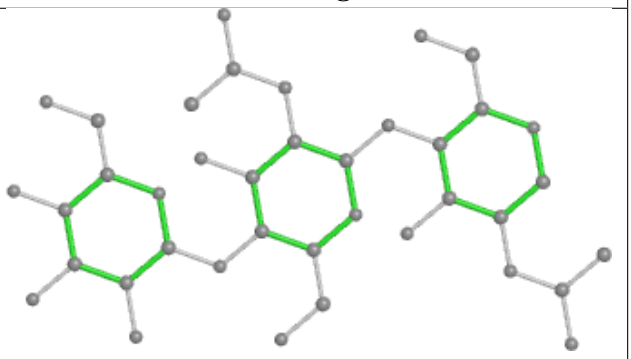
Bond lengths



Bond angles

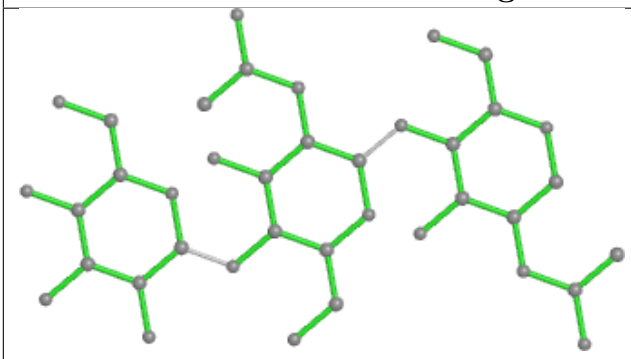


Torsions

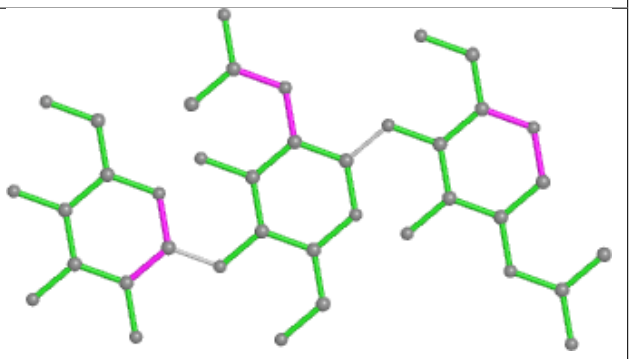


Rings

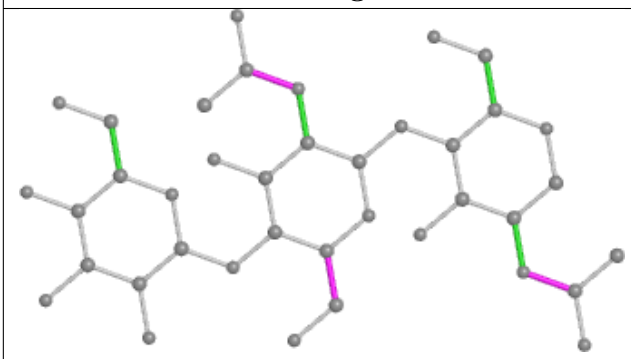
Oligosaccharide Chain d



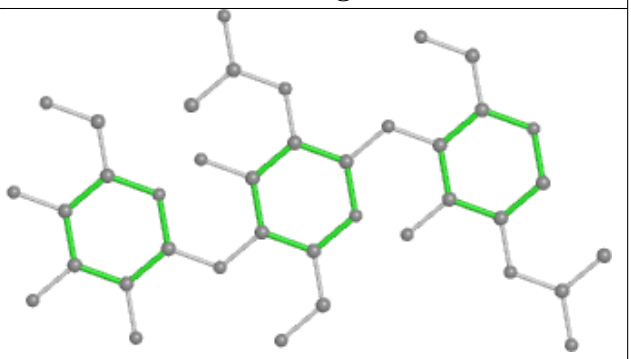
Bond lengths



Bond angles

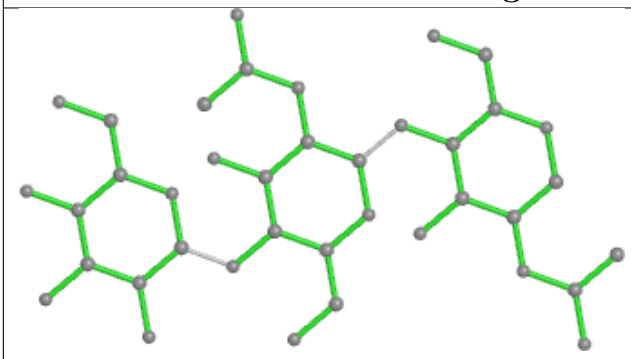


Torsions

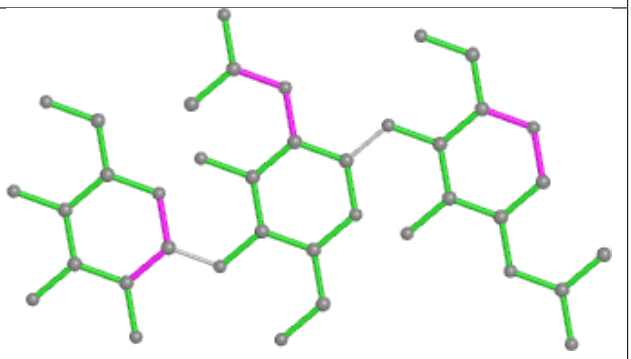


Rings

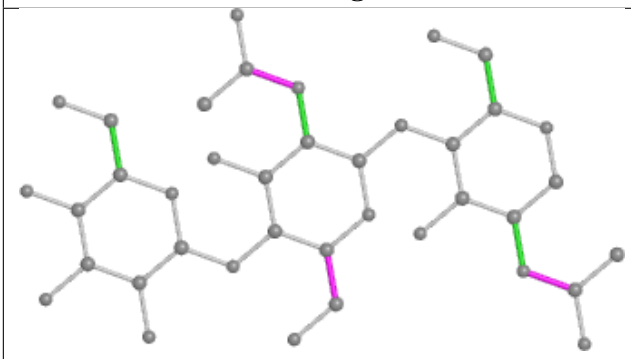
Oligosaccharide Chain i



Bond lengths



Bond angles



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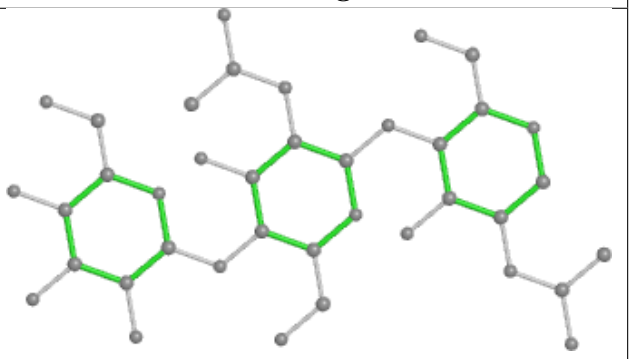
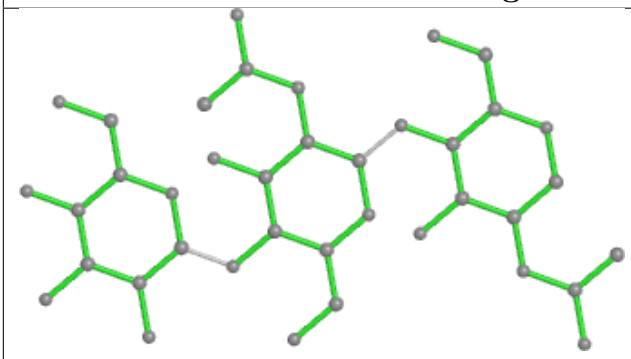


Rings

Oligosaccharide Chain j



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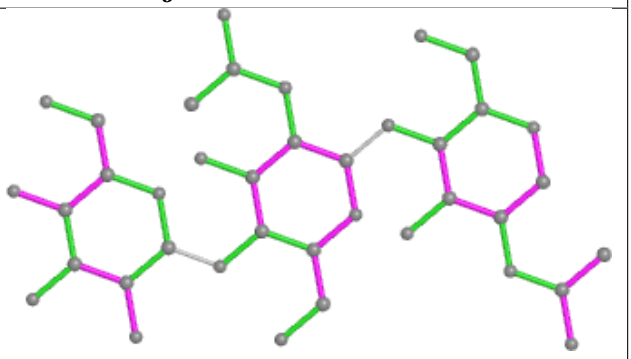
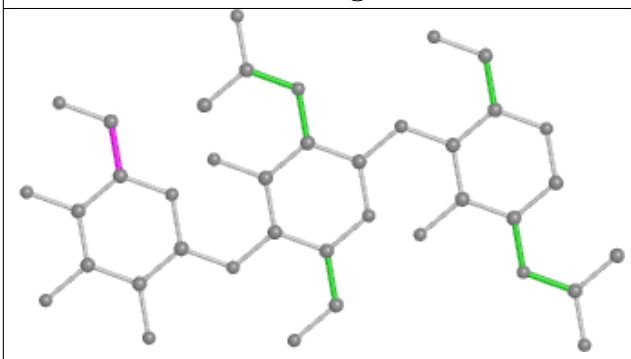
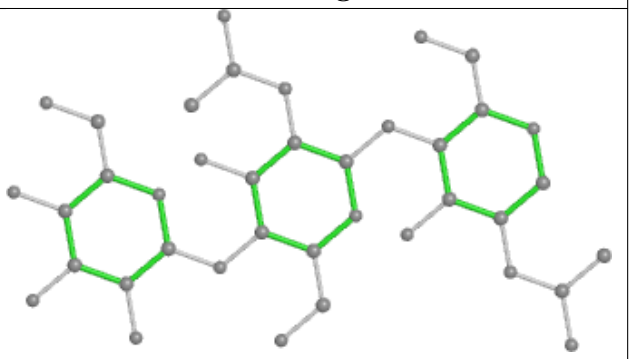


Bond angles

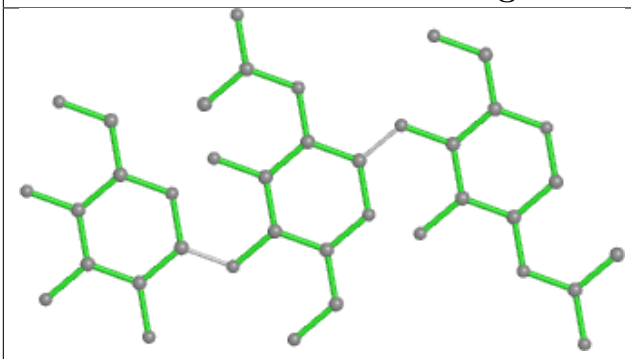


Torsions



Rings

Oligosaccharide Chain k



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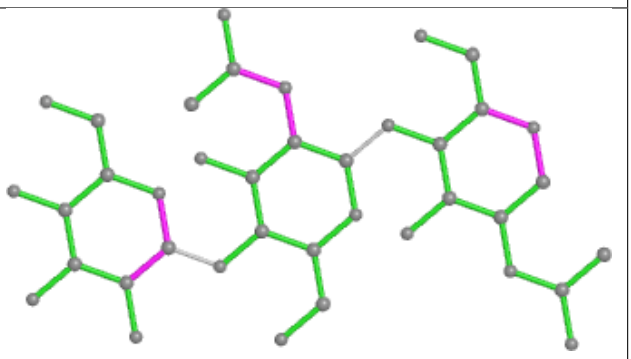
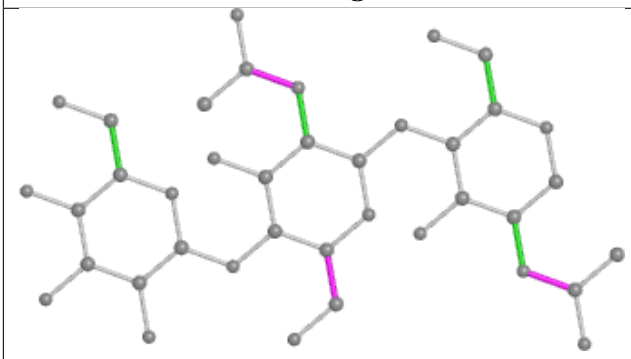


Bond angles



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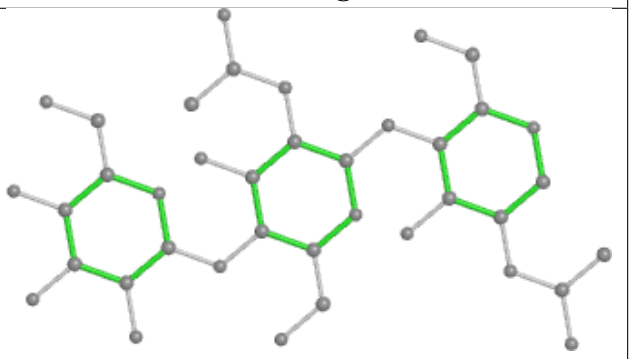
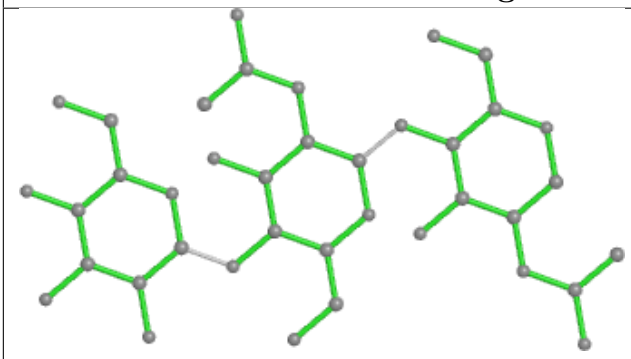


Rings

Oligosaccharide Chain n



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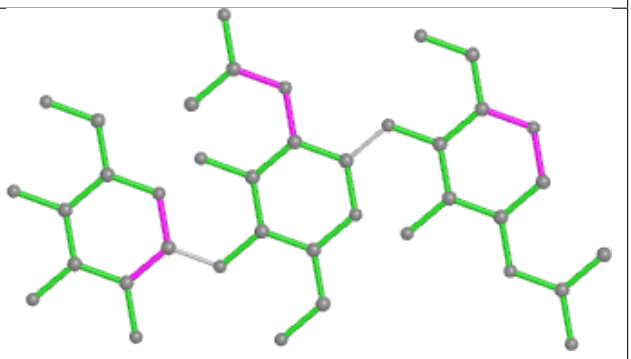
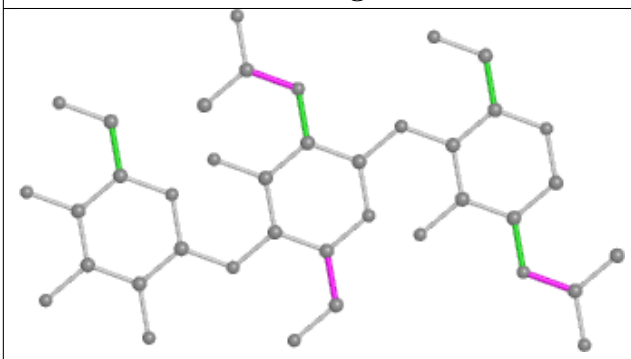


Bond angles



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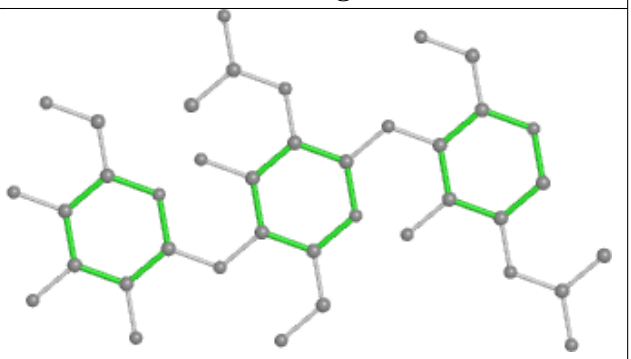
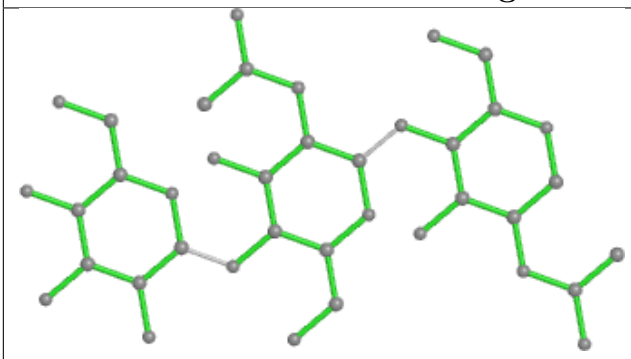


Rings

Oligosaccharide Chain o



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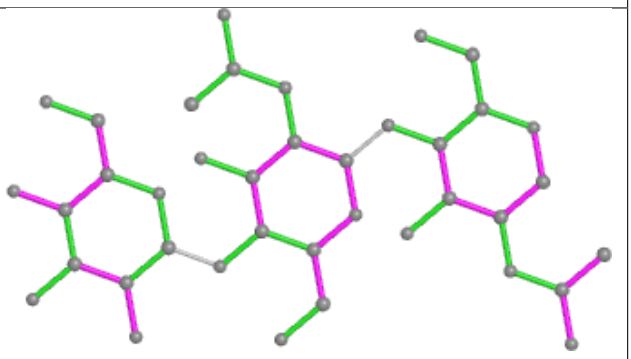
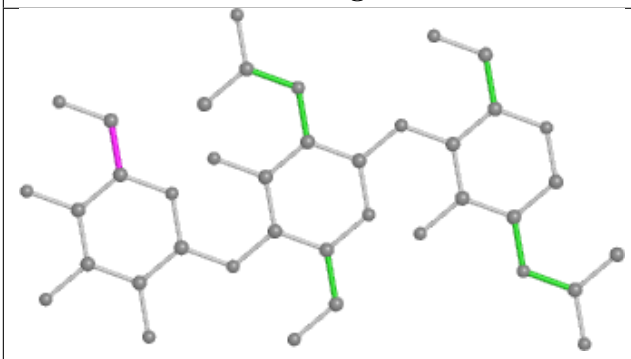


Bond angles



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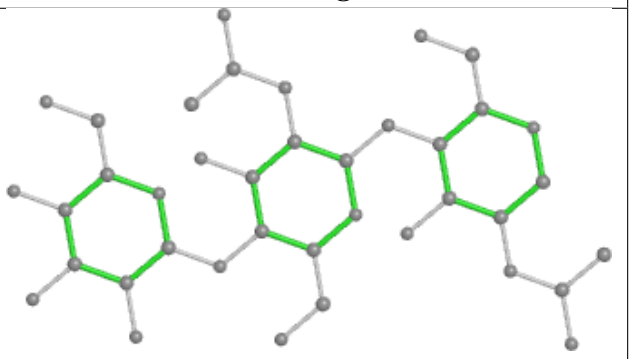
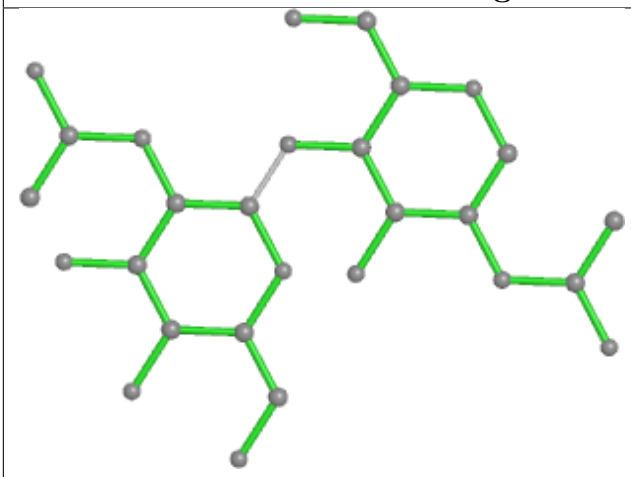


Rings

Oligosaccharide Chain N



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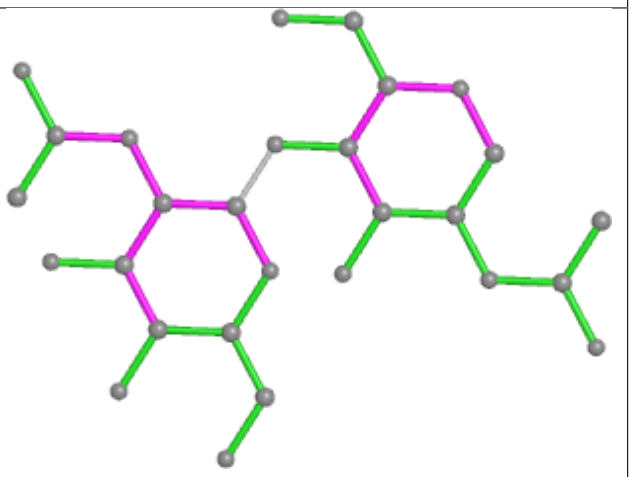
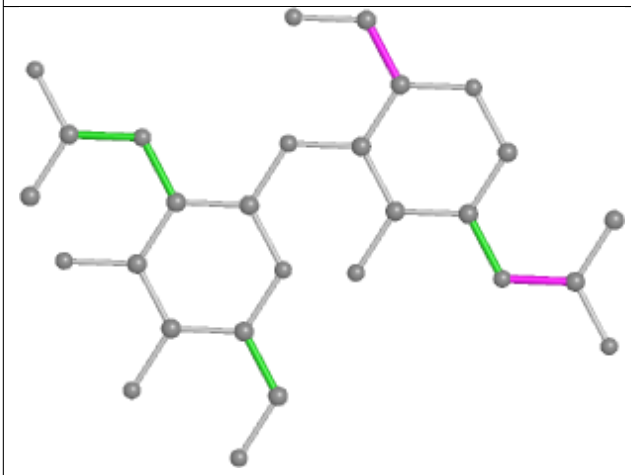


Bond angles



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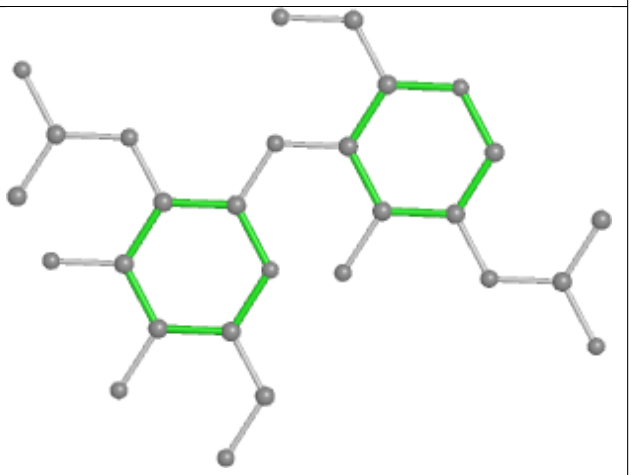
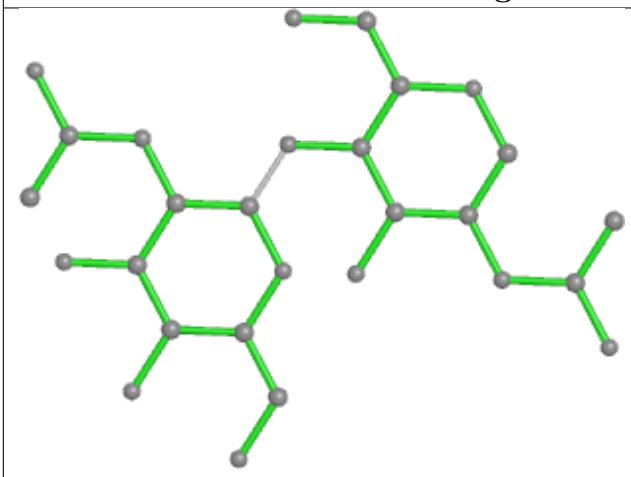


Rings

Oligosaccharide Chain O



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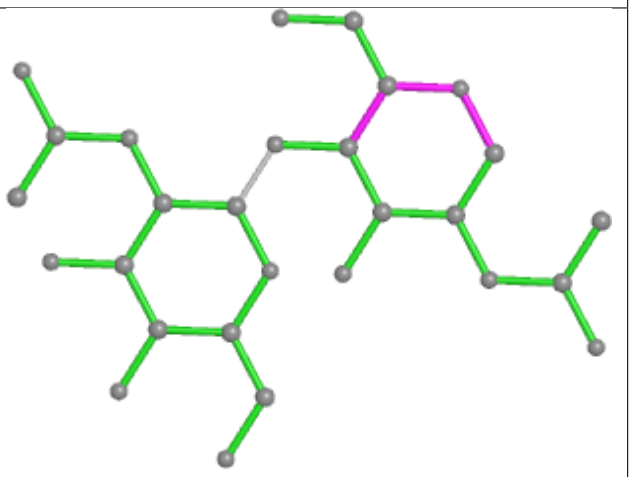
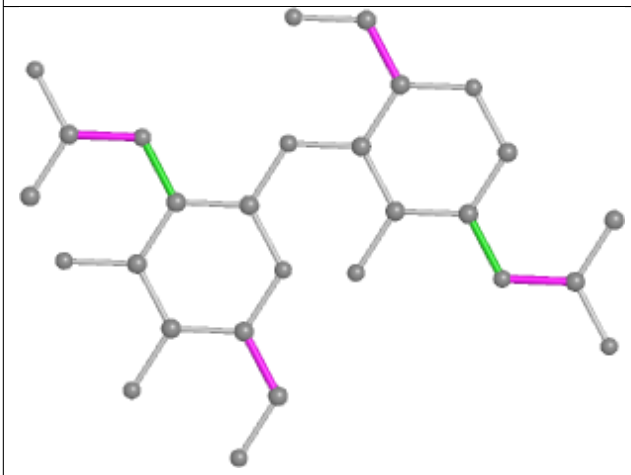


Bond angles



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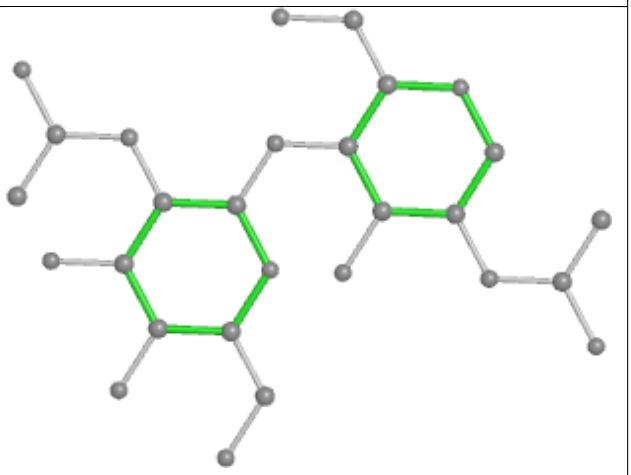
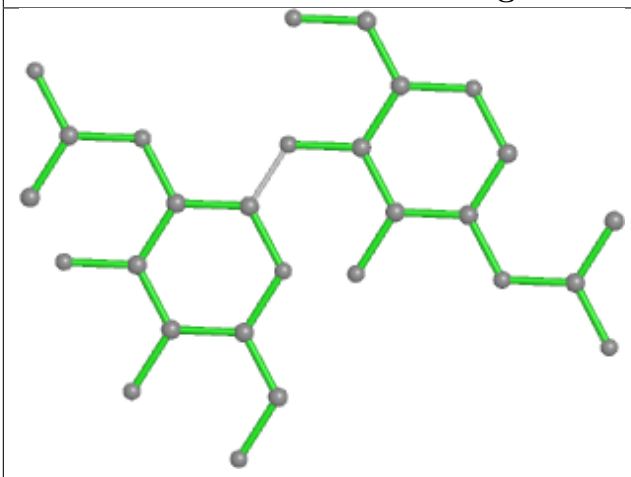


Rings

Oligosaccharide Chain S



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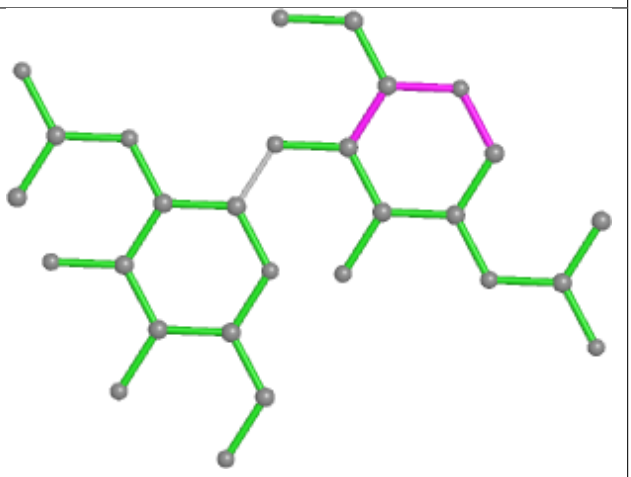
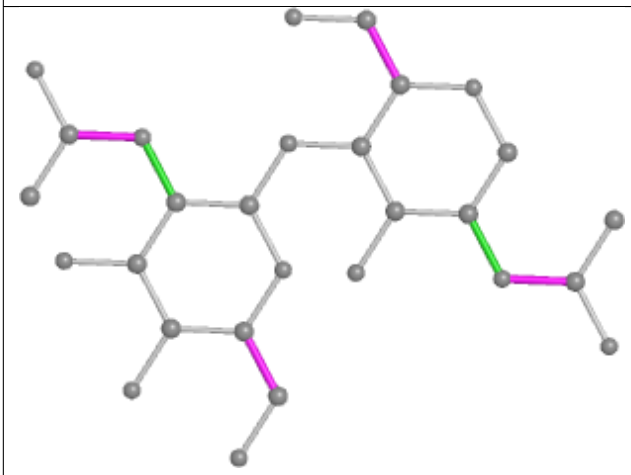


Bond angles



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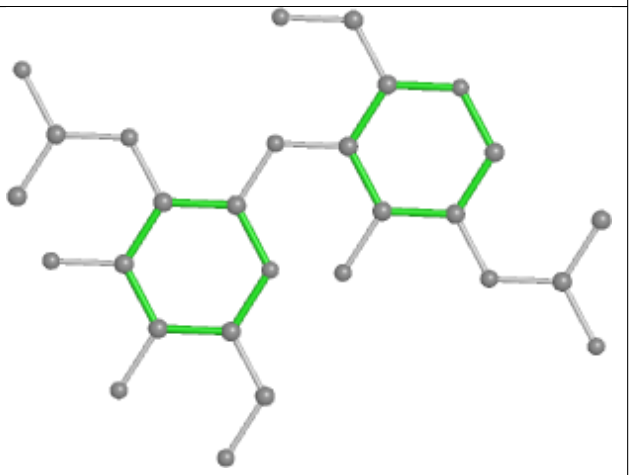
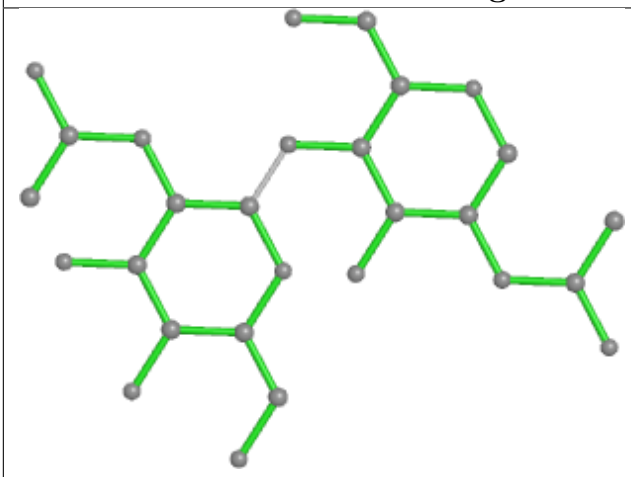


Rings

Oligosaccharide Chain W



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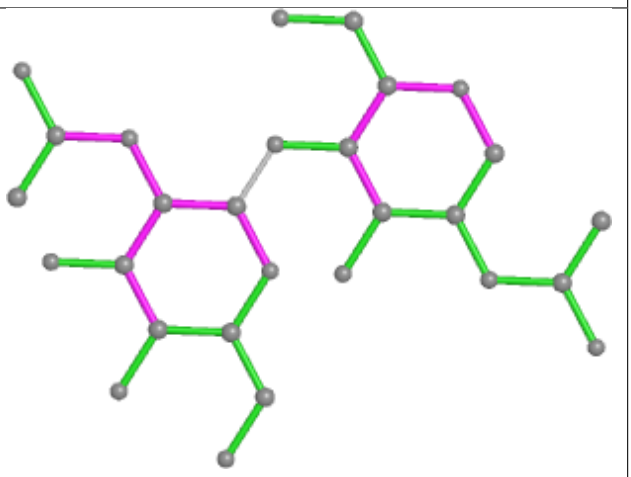
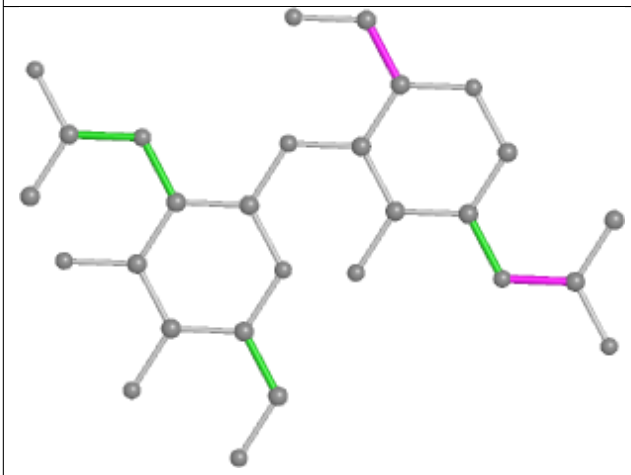


Bond angles



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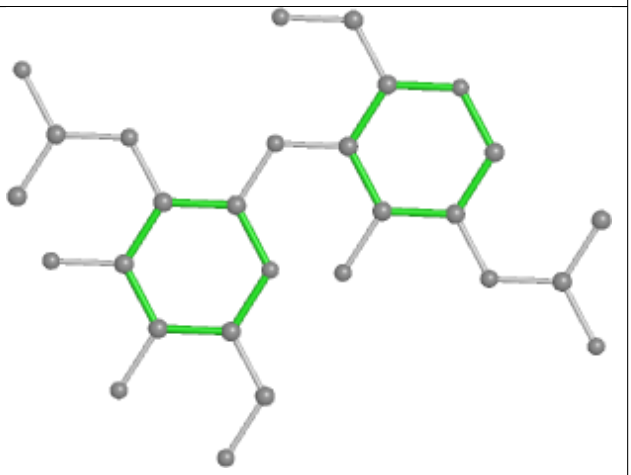
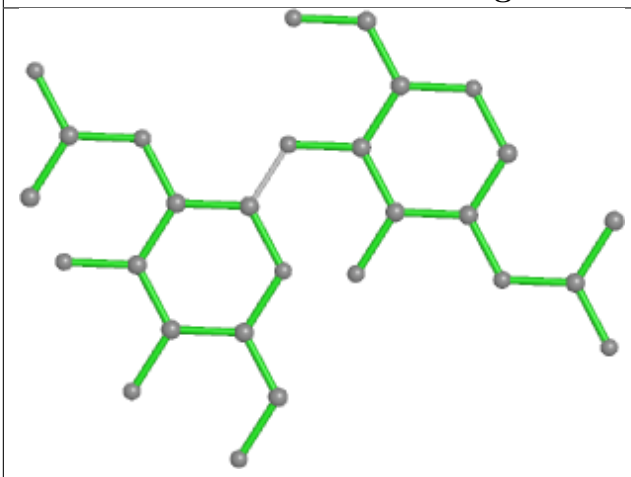


Rings

Oligosaccharide Chain X



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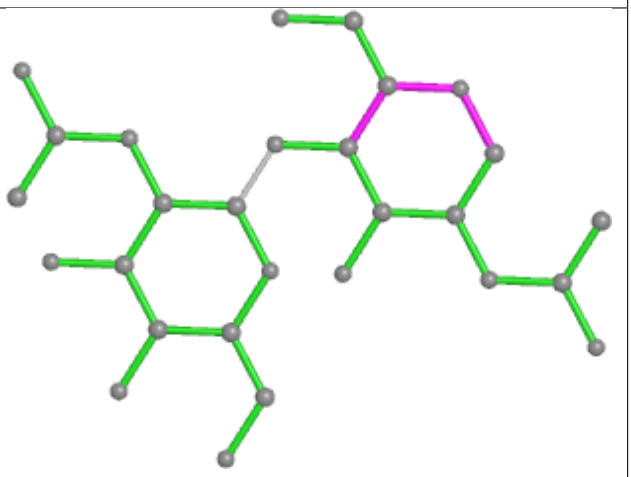
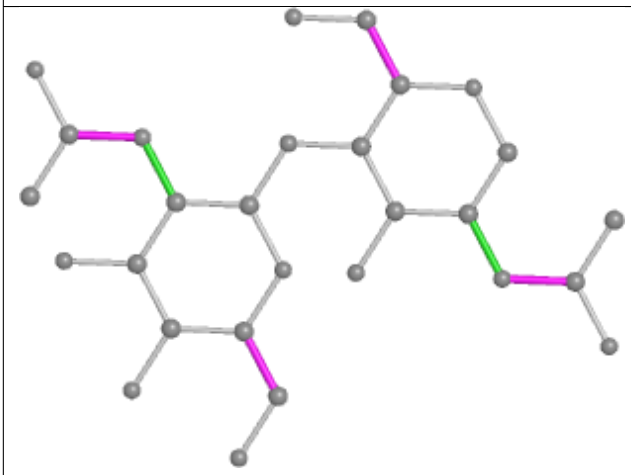


Bond angles



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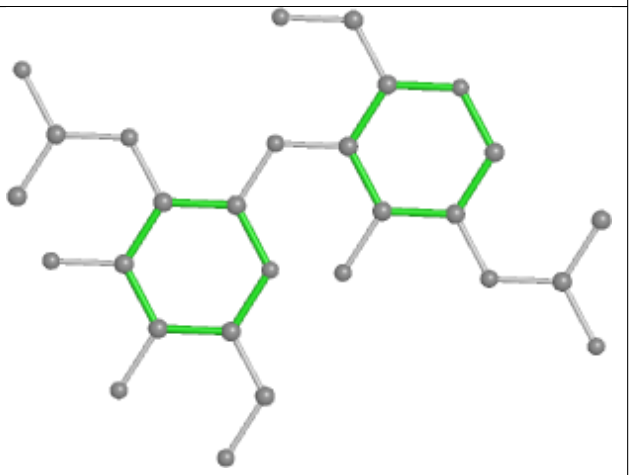
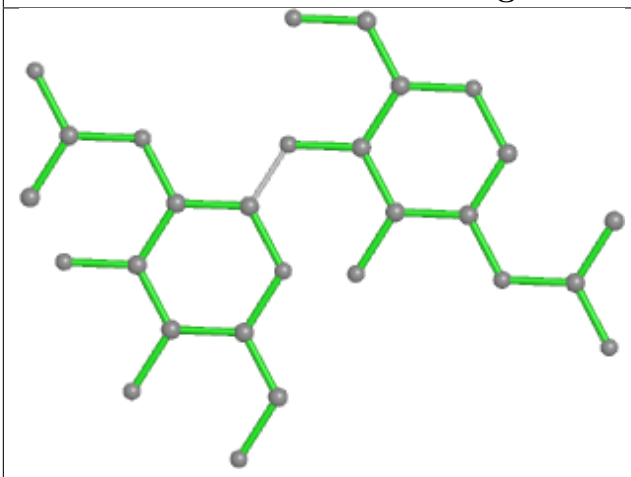


Rings

Oligosaccharide Chain b



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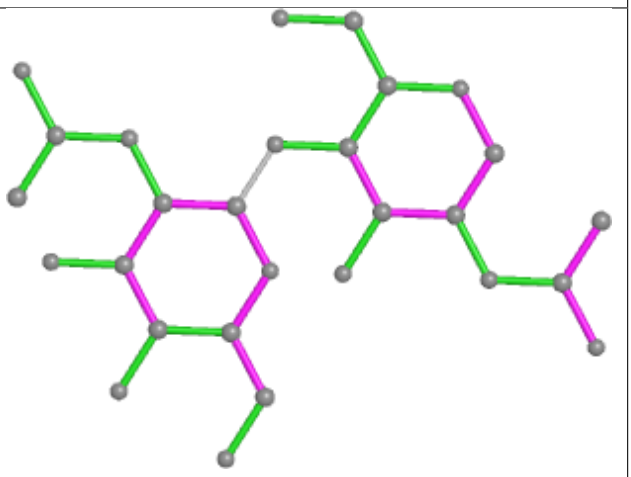

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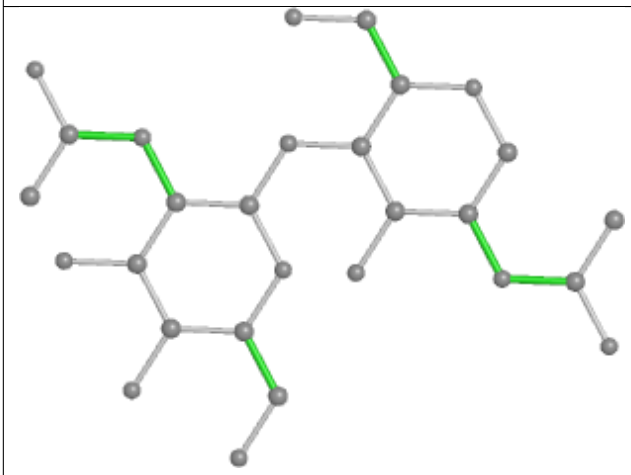

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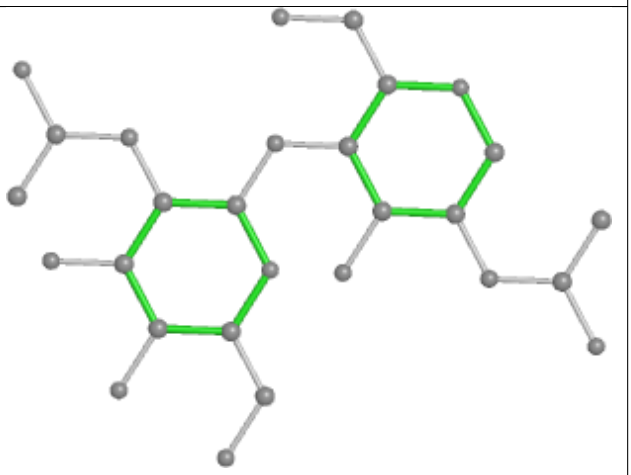
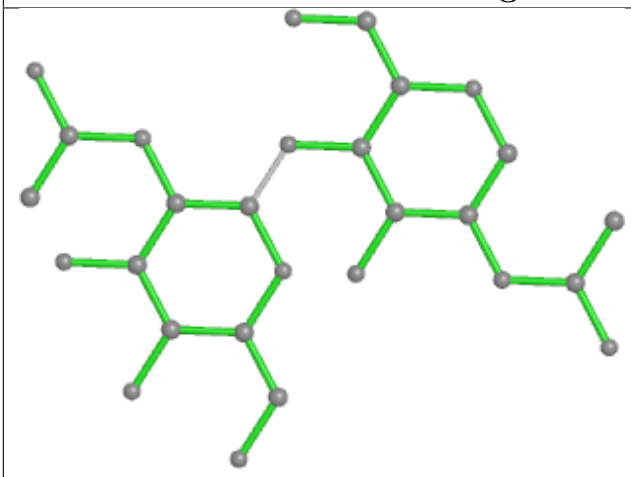


Rings

Oligosaccharide Chain c



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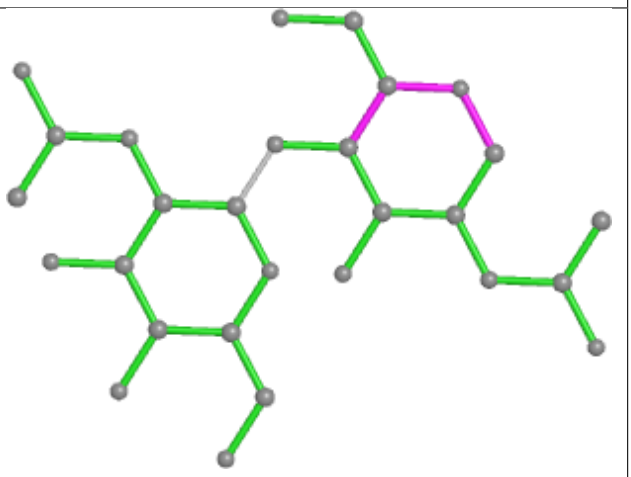
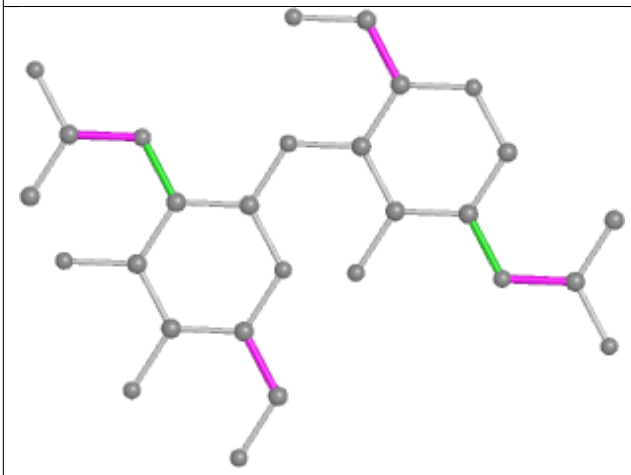


Bond angles



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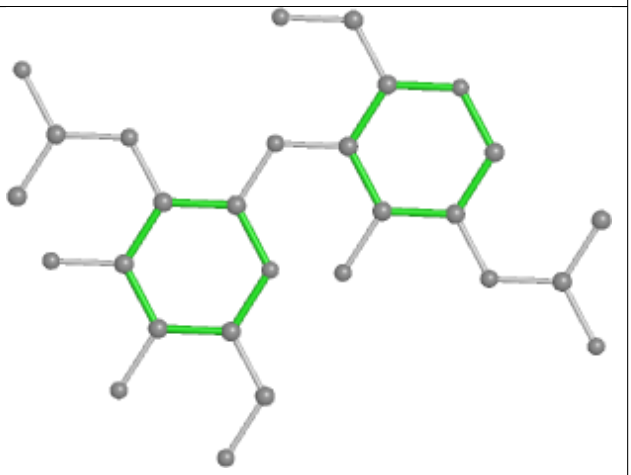
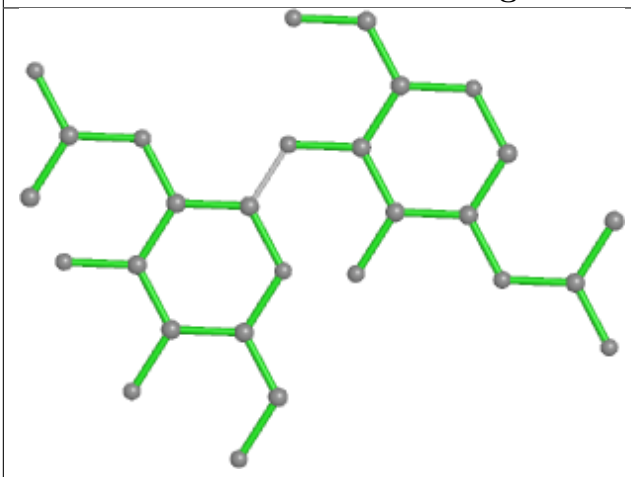


Rings

Oligosaccharide Chain e



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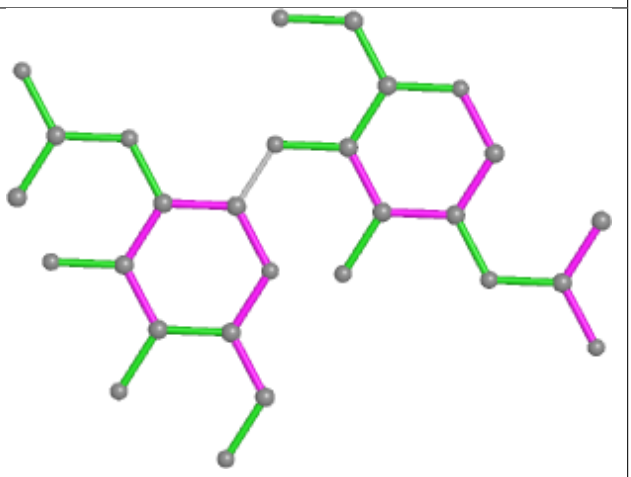
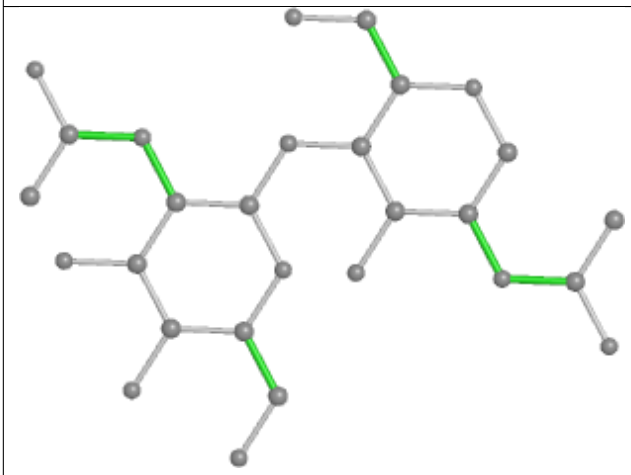
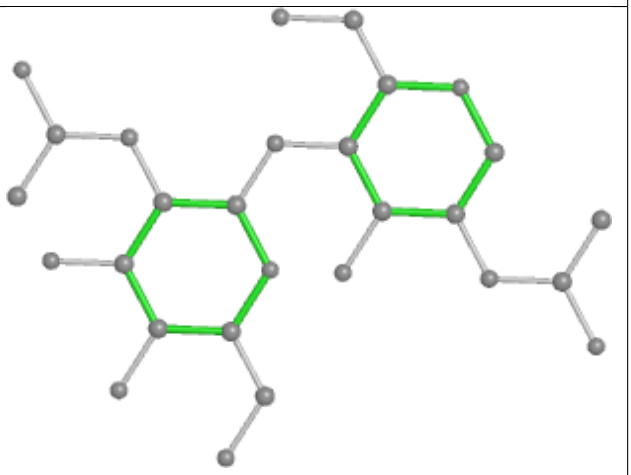


Bond angles

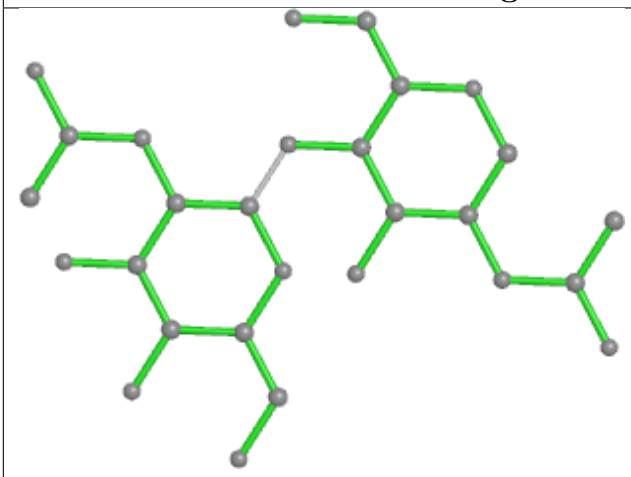


Torsions

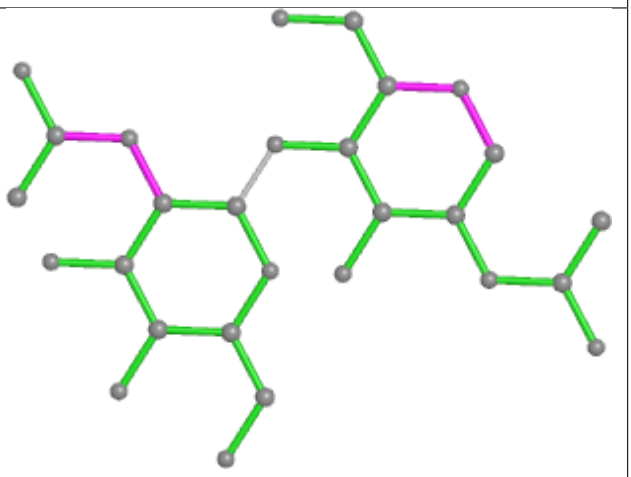


Rings

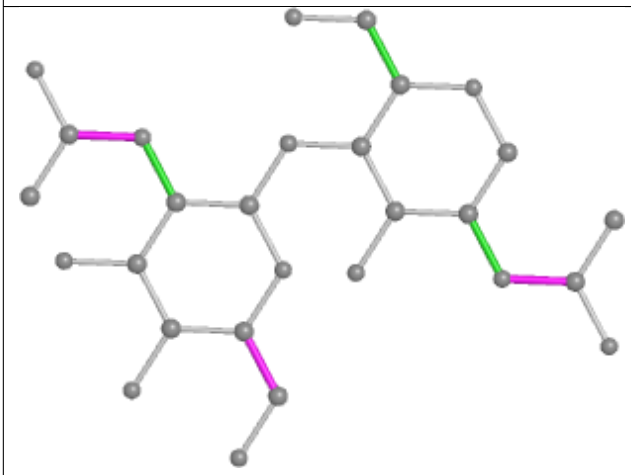
Oligosaccharide Chain f



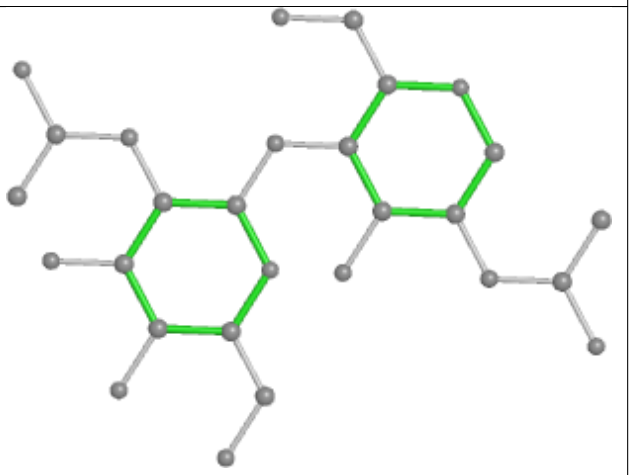
Bond lengths



Bond angles

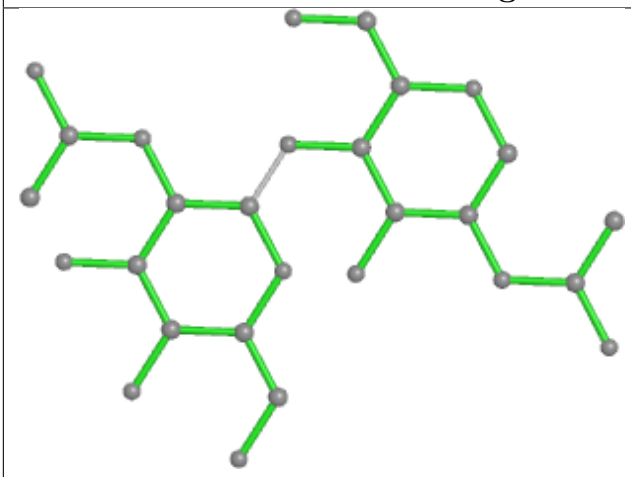


Torsions

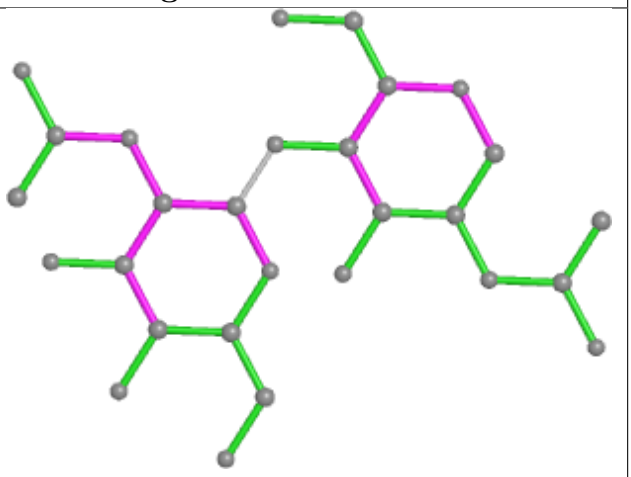


Rings

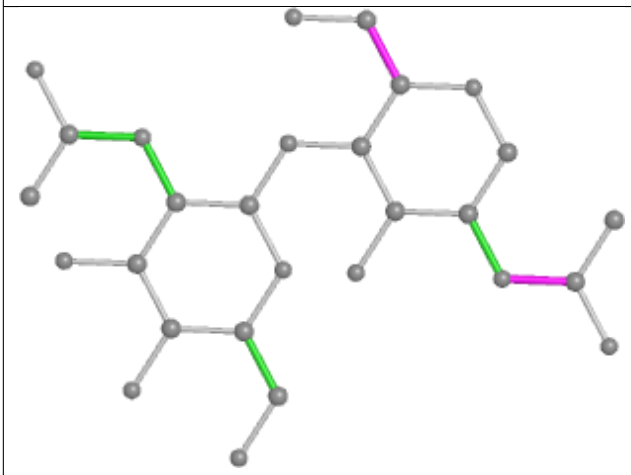
Oligosaccharide Chain g



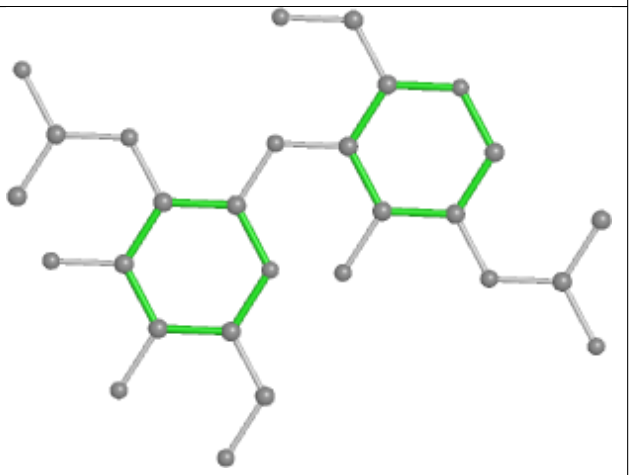
Bond lengths



Bond angles

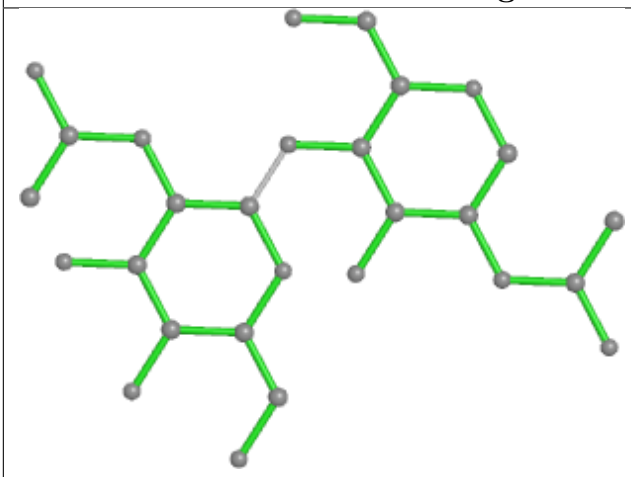


Torsions

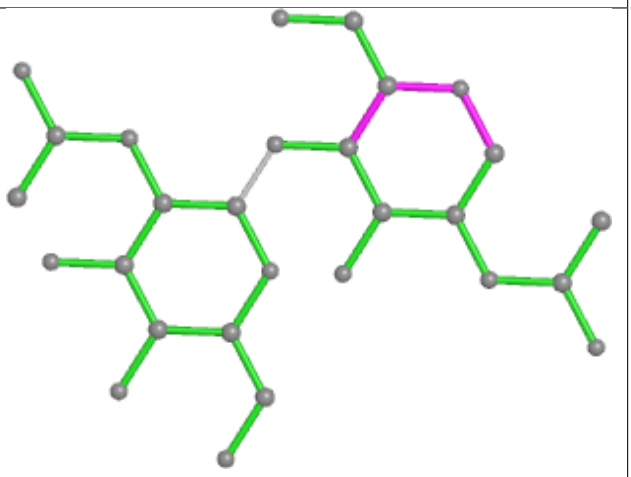


Rings

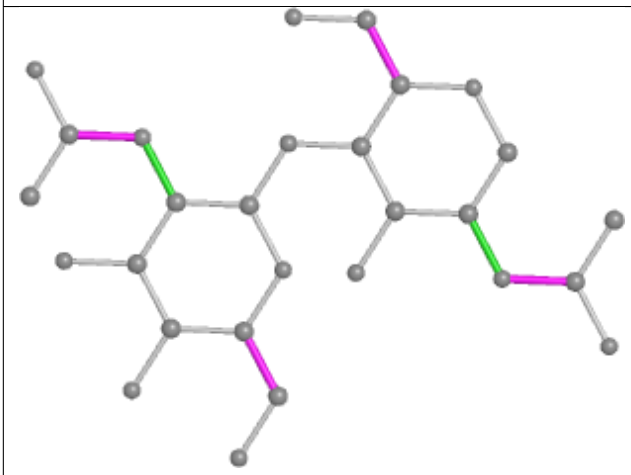
Oligosaccharide Chain h



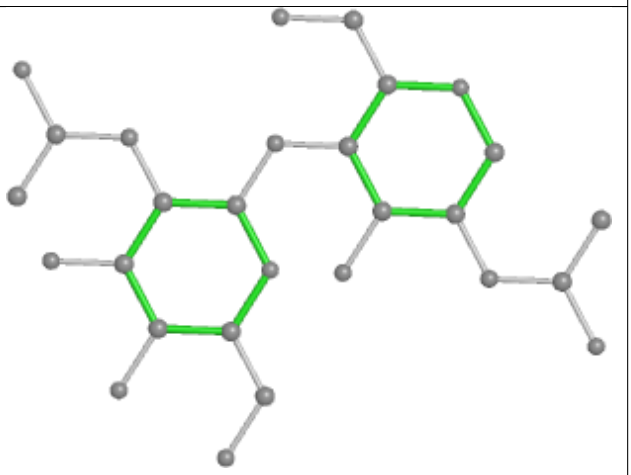
Bond lengths



Bond angles

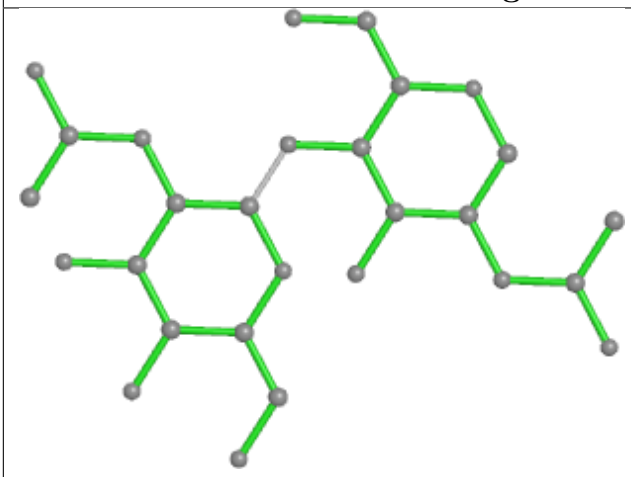


Torsions

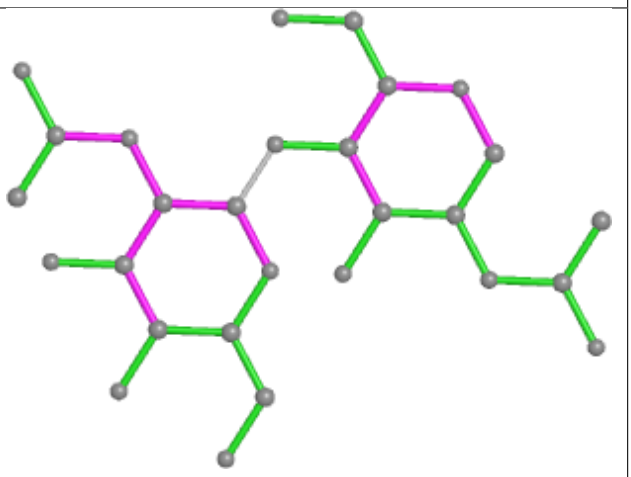


Rings

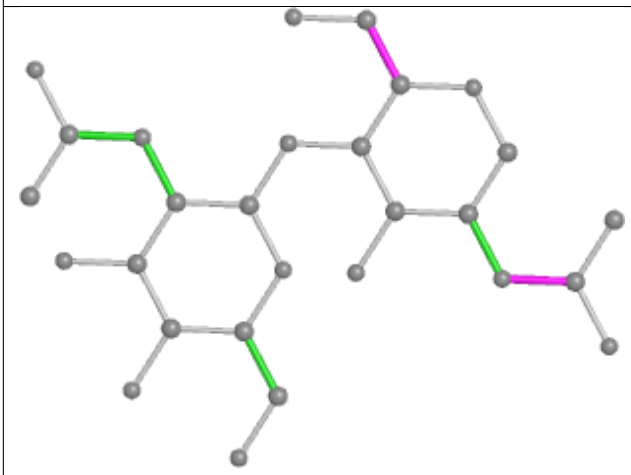
Oligosaccharide Chain l



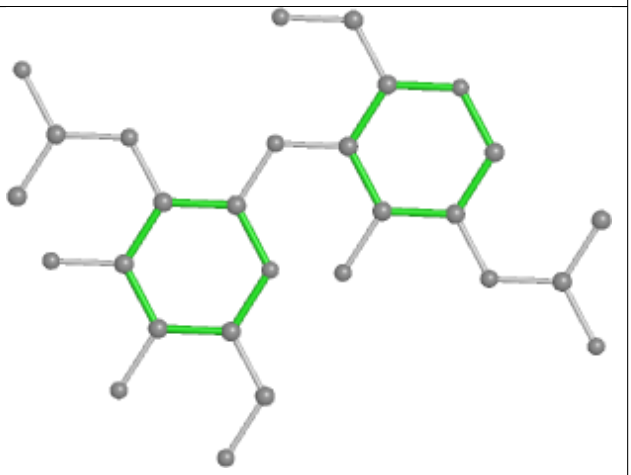
Bond lengths



Bond angles

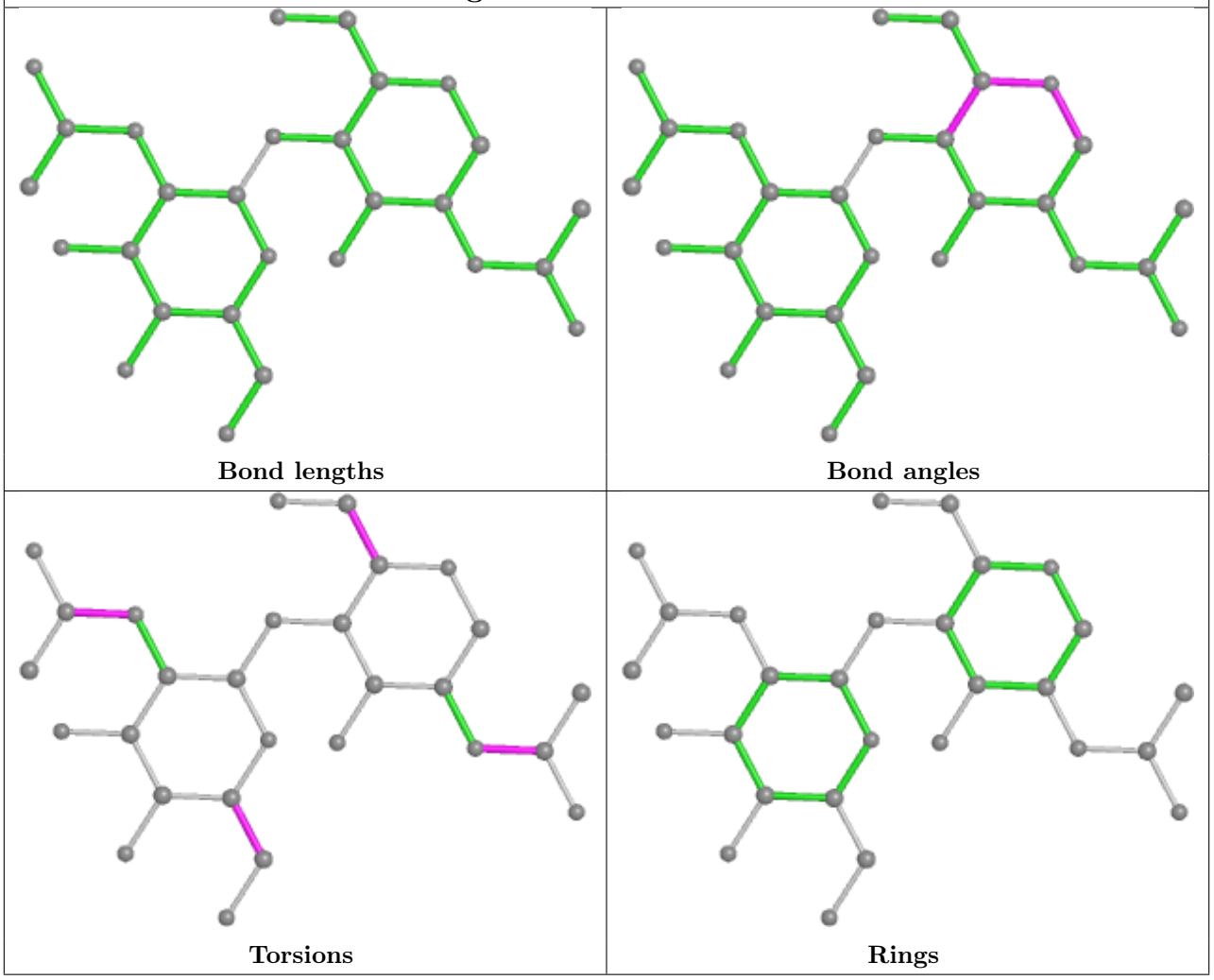


Torsions



Rings

Oligosaccharide Chain m



5.6 Ligand geometry (i)

17 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	E	415	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)
5	NAG	G	414	1	14,14,15	0.48	0	17,19,21	0.98	1 (5%)
5	NAG	A	415	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	I	414	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
5	NAG	K	414	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
5	NAG	C	404	1	14,14,15	0.41	0	17,19,21	1.80	3 (17%)
5	NAG	F	600	2	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
5	NAG	B	600	2	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
5	NAG	E	411	1	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
5	NAG	A	411	1	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
5	NAG	D	600	2	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
5	NAG	H	600	2	14,14,15	0.51	0	17,19,21	0.92	1 (5%)
5	NAG	I	410	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
5	NAG	J	600	2	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
5	NAG	G	411	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
5	NAG	C	410	1	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
5	NAG	C	414	1	14,14,15	0.50	0	17,19,21	0.98	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	E	415	1	-	2/6/23/26	0/1/1/1
5	NAG	G	414	1	-	2/6/23/26	0/1/1/1
5	NAG	A	415	1	-	2/6/23/26	0/1/1/1
5	NAG	I	414	1	-	2/6/23/26	0/1/1/1
5	NAG	K	414	1	-	2/6/23/26	0/1/1/1
5	NAG	C	404	1	-	3/6/23/26	0/1/1/1
5	NAG	F	600	2	-	2/6/23/26	0/1/1/1
5	NAG	B	600	2	-	2/6/23/26	0/1/1/1
5	NAG	E	411	1	-	0/6/23/26	0/1/1/1
5	NAG	A	411	1	-	0/6/23/26	0/1/1/1
5	NAG	D	600	2	-	2/6/23/26	0/1/1/1
5	NAG	H	600	2	-	2/6/23/26	0/1/1/1
5	NAG	I	410	1	-	0/6/23/26	0/1/1/1
5	NAG	J	600	2	-	2/6/23/26	0/1/1/1
5	NAG	G	411	1	-	0/6/23/26	0/1/1/1
5	NAG	C	410	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	414	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	410	NAG	O5-C1-C2	-7.34	99.69	111.29
5	C	404	NAG	C1-O5-C5	5.96	120.27	112.19
5	C	410	NAG	O7-C7-C8	-2.79	116.87	122.06
5	C	410	NAG	C4-C3-C2	-2.62	107.17	111.02
5	E	411	NAG	O5-C5-C6	2.60	111.28	107.20

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	NAG	C8-C7-N2-C2
5	C	404	NAG	O7-C7-N2-C2
5	C	404	NAG	O5-C5-C6-O6
5	B	600	NAG	C8-C7-N2-C2
5	D	600	NAG	C8-C7-N2-C2

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	341/347 (98%)	0.23	15 (4%) 34 33	33, 64, 133, 208	0
1	C	341/347 (98%)	0.11	10 (2%) 51 49	30, 61, 135, 195	0
1	E	341/347 (98%)	0.14	10 (2%) 51 49	26, 63, 141, 237	0
1	G	341/347 (98%)	0.20	9 (2%) 56 53	35, 73, 151, 210	0
1	I	341/347 (98%)	0.15	6 (1%) 68 65	39, 71, 141, 193	0
1	K	341/347 (98%)	0.38	16 (4%) 31 31	45, 77, 157, 209	0
2	B	169/179 (94%)	0.46	12 (7%) 16 18	30, 142, 219, 275	0
2	D	169/179 (94%)	0.52	19 (11%) 5 7	30, 132, 212, 252	0
2	F	169/179 (94%)	0.37	15 (8%) 9 12	34, 130, 207, 274	0
2	H	169/179 (94%)	0.60	23 (13%) 3 4	42, 143, 202, 255	0
2	J	169/179 (94%)	0.49	12 (7%) 16 18	40, 138, 225, 266	0
2	L	169/179 (94%)	0.68	22 (13%) 3 5	43, 149, 223, 260	0
All	All	3060/3156 (96%)	0.31	169 (5%) 25 25	26, 77, 195, 275	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	383	ALA	8.1
2	B	516	SER	7.6
2	L	382	ALA	5.5
2	D	372	THR	5.2
2	H	382	ALA	5.1

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	Q	3	11/12	0.47	0.35	161,166,172,174	0
3	BMA	Z	3	11/12	0.47	0.40	179,186,190,193	0
3	BMA	k	3	11/12	0.48	0.28	114,118,124,126	0
3	BMA	j	3	11/12	0.49	0.40	166,170,173,175	0
3	BMA	T	3	11/12	0.50	0.24	157,160,173,174	0
3	BMA	n	3	11/12	0.52	0.24	184,188,200,201	0
3	BMA	U	3	11/12	0.54	0.43	156,159,163,164	0
3	BMA	d	3	11/12	0.57	0.20	171,174,187,188	0
3	BMA	V	3	11/12	0.61	0.28	107,111,121,124	0
3	BMA	M	3	11/12	0.61	0.29	100,104,110,111	0
4	NAG	b	2	14/15	0.62	0.34	134,141,145,146	0
3	BMA	Y	3	11/12	0.64	0.22	167,171,185,186	0
3	BMA	P	3	11/12	0.64	0.20	182,186,198,199	0
3	BMA	a	3	11/12	0.64	0.36	101,105,111,113	0
3	NAG	Q	2	14/15	0.64	0.45	136,141,145,146	0
4	NAG	e	2	14/15	0.64	0.54	152,155,158,159	0
3	NAG	o	1	14/15	0.65	0.30	127,132,137,139	0
3	NAG	o	2	14/15	0.66	0.41	156,159,163,165	0
3	NAG	j	1	14/15	0.66	0.26	98,105,109,110	0
3	NAG	j	2	14/15	0.66	0.30	139,142,144,145	0
3	NAG	Z	1	14/15	0.67	0.32	99,110,115,116	0
3	BMA	o	3	11/12	0.68	0.33	136,141,144,147	0
3	BMA	R	3	11/12	0.70	0.23	100,104,110,110	0
4	NAG	W	2	14/15	0.70	0.28	98,104,113,119	0
3	BMA	i	3	11/12	0.70	0.26	157,161,173,174	0
3	NAG	Z	2	14/15	0.70	0.47	153,158,161,163	0
4	NAG	f	2	14/15	0.71	0.43	96,101,106,107	0
4	NAG	l	2	14/15	0.71	0.38	134,138,145,150	0
4	NAG	f	1	14/15	0.72	0.28	94,99,102,105	0
4	NAG	S	2	14/15	0.72	0.25	135,144,156,157	0
4	NAG	h	2	14/15	0.72	0.22	115,125,137,138	0
3	NAG	U	2	14/15	0.72	0.42	134,138,141,142	0
4	NAG	g	2	14/15	0.73	0.32	127,132,138,141	0
3	NAG	T	2	14/15	0.74	0.36	131,144,152,153	0
4	NAG	h	1	14/15	0.74	0.27	102,115,124,125	0
4	NAG	m	2	14/15	0.74	0.22	131,142,155,157	0
3	NAG	V	2	14/15	0.76	0.26	85,94,106,107	0

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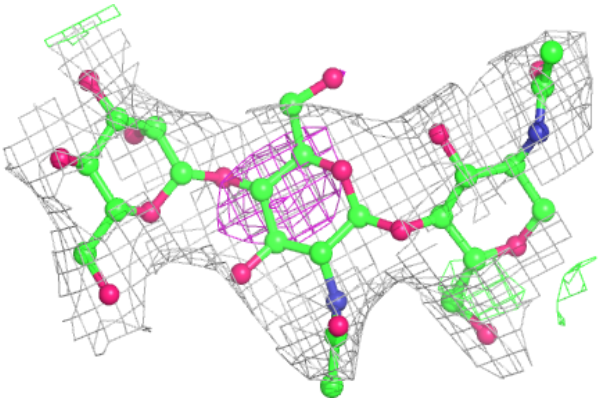
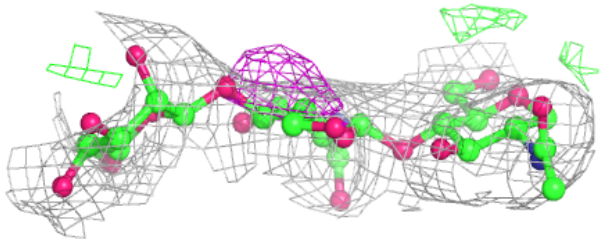
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	a	2	14/15	0.76	0.46	83,88,97,98	0
3	NAG	Y	1	14/15	0.78	0.34	112,127,138,139	0
3	NAG	V	1	14/15	0.79	0.25	84,93,101,102	0
3	NAG	Q	1	14/15	0.79	0.31	96,104,110,111	0
3	NAG	i	2	14/15	0.79	0.24	149,162,170,171	0
4	NAG	e	1	14/15	0.79	0.23	104,111,114,115	0
3	NAG	T	1	14/15	0.79	0.32	107,119,128,128	0
4	NAG	m	1	14/15	0.79	0.23	125,137,147,147	0
4	NAG	N	2	14/15	0.79	0.36	106,110,116,120	0
4	NAG	b	1	14/15	0.80	0.30	100,105,109,109	0
3	NAG	U	1	14/15	0.80	0.28	92,101,107,107	0
3	NAG	k	2	14/15	0.80	0.26	95,100,108,108	0
4	NAG	c	1	14/15	0.81	0.20	126,139,148,148	0
3	NAG	d	1	14/15	0.82	0.29	116,128,139,139	0
3	NAG	d	2	14/15	0.82	0.23	147,160,168,169	0
3	NAG	n	2	14/15	0.82	0.22	145,159,167,167	0
4	NAG	c	2	14/15	0.82	0.16	133,143,154,156	0
3	NAG	M	2	14/15	0.82	0.33	79,85,92,93	0
3	NAG	Y	2	14/15	0.82	0.37	135,150,159,160	0
4	NAG	X	1	14/15	0.82	0.23	108,122,133,133	0
4	NAG	S	1	14/15	0.83	0.17	96,109,118,118	0
3	NAG	P	2	14/15	0.84	0.19	138,151,159,160	0
3	NAG	R	1	14/15	0.85	0.23	78,83,86,88	0
4	NAG	X	2	14/15	0.85	0.27	117,129,142,144	0
3	NAG	M	1	14/15	0.86	0.20	79,85,89,90	0
3	NAG	i	1	14/15	0.86	0.25	106,118,127,127	0
4	NAG	O	2	14/15	0.87	0.14	131,141,153,155	0
3	NAG	P	1	14/15	0.88	0.23	133,145,154,154	0
4	NAG	g	1	14/15	0.88	0.21	76,87,99,101	0
3	NAG	n	1	14/15	0.88	0.26	116,128,138,138	0
3	NAG	a	1	14/15	0.88	0.24	85,91,95,95	0
3	NAG	R	2	14/15	0.89	0.19	80,84,89,90	0
3	NAG	k	1	14/15	0.89	0.18	95,101,105,106	0
4	NAG	N	1	14/15	0.90	0.44	92,101,112,113	0
4	NAG	W	1	14/15	0.90	0.27	80,91,102,105	0
4	NAG	l	1	14/15	0.91	0.26	100,110,121,123	0
4	NAG	O	1	14/15	0.93	0.11	123,135,144,144	0

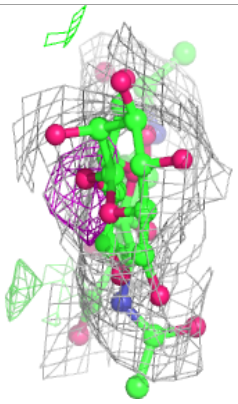
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

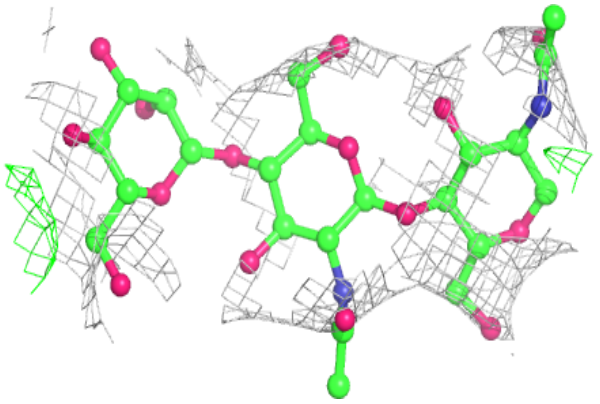


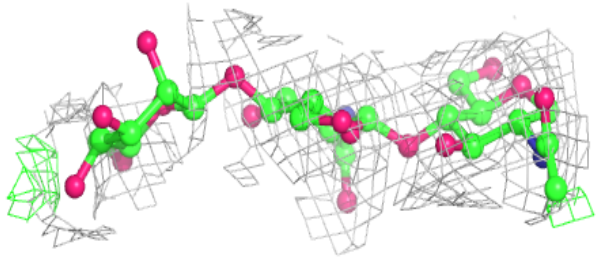


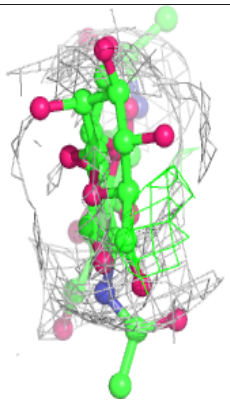


Electron density around Chain P:

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

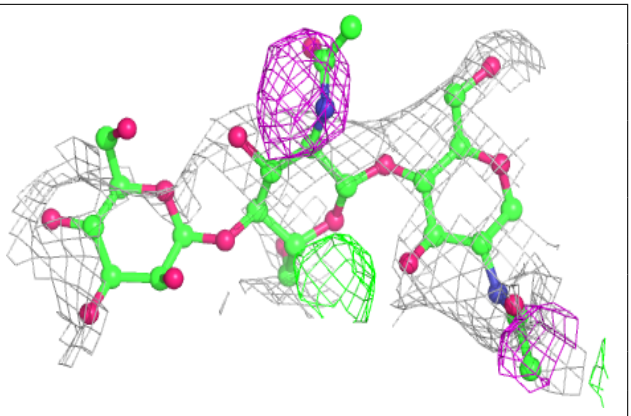


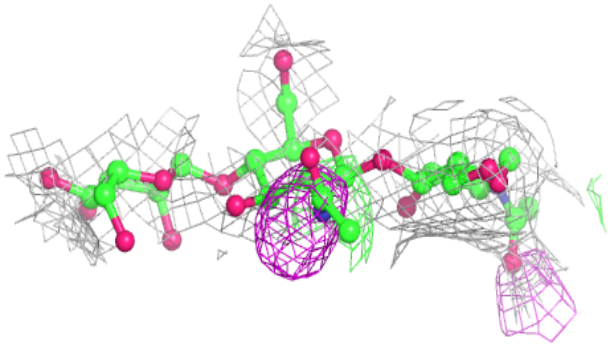




Electron density around Chain Q:

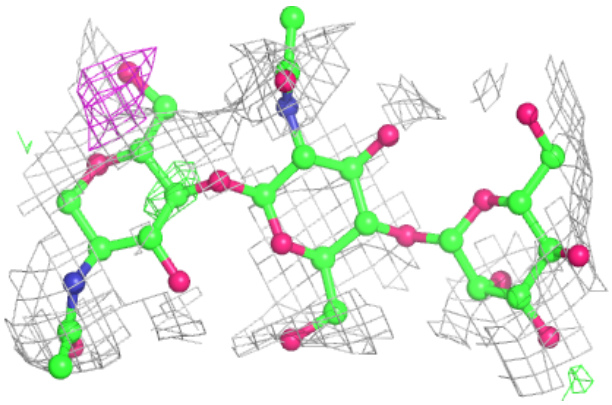
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

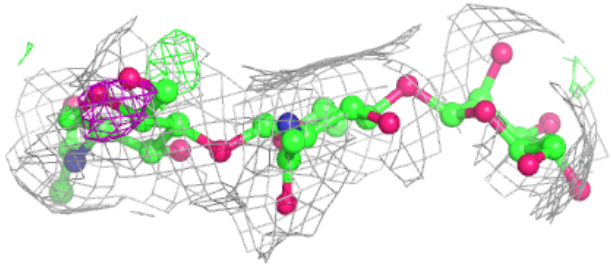


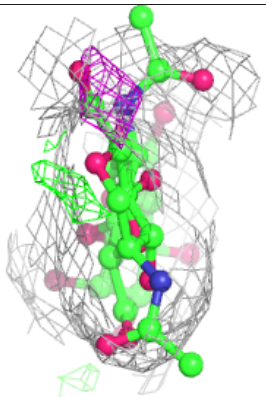


Electron density around Chain R:

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

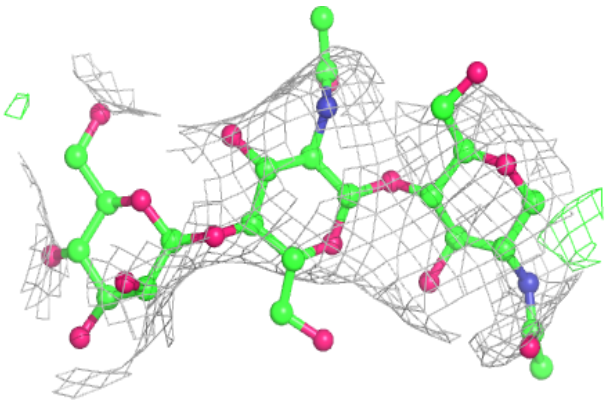


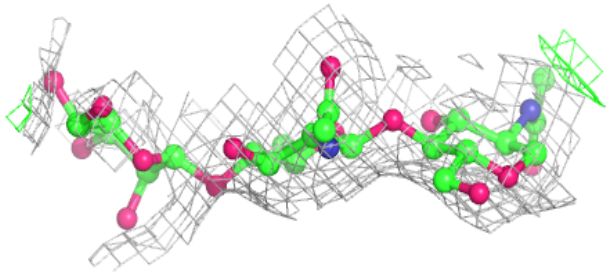


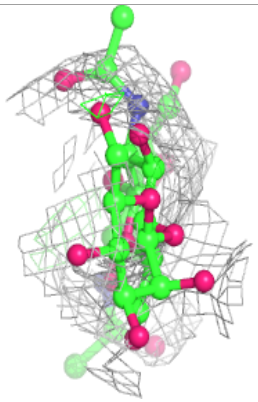


Electron density around Chain T:

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

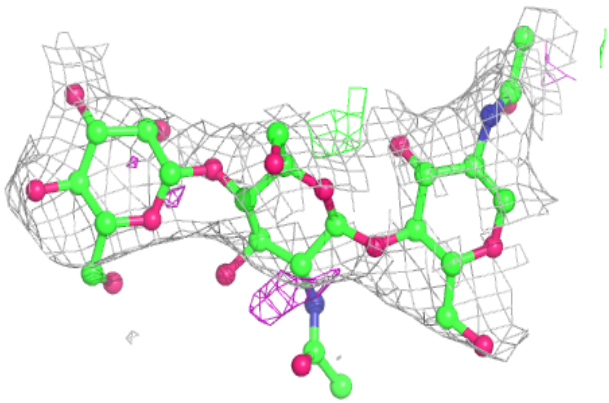


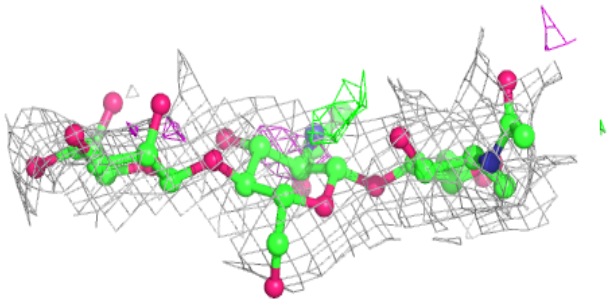


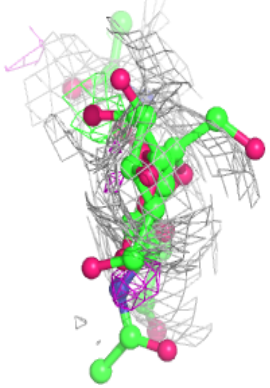


Electron density around Chain U:

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

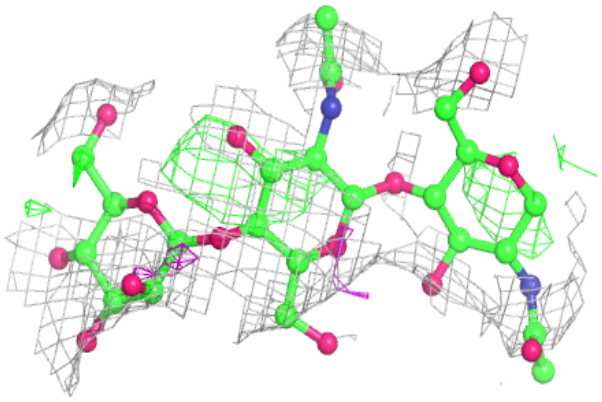


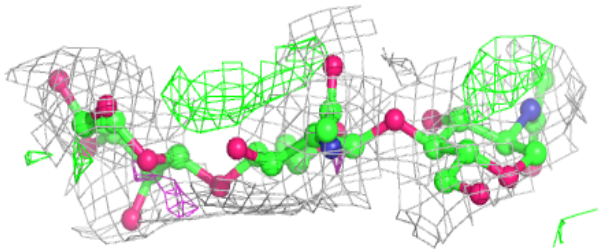


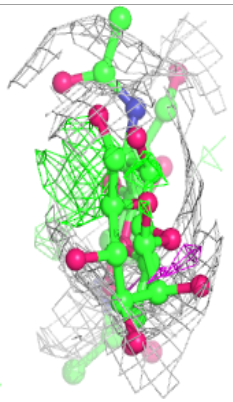


Electron density around Chain V:

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

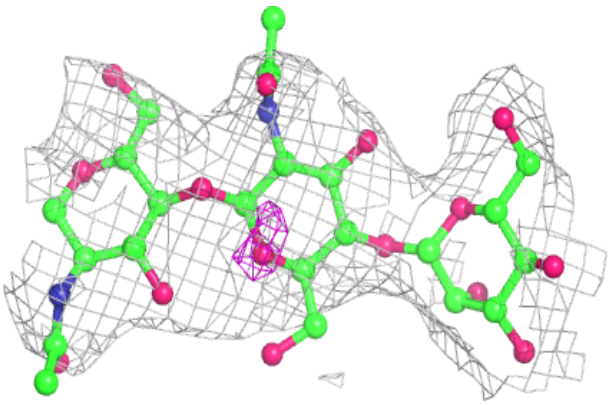


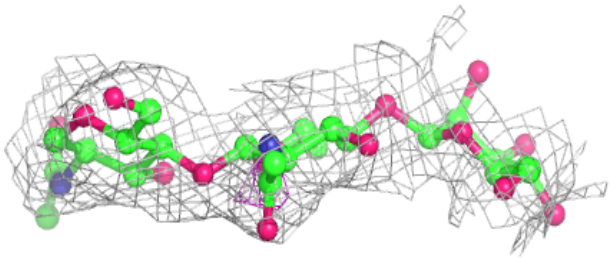


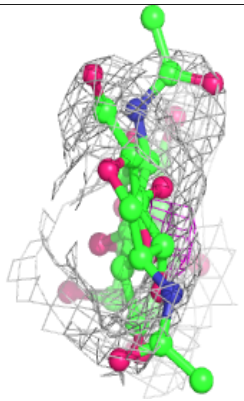


Electron density around Chain Y:

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

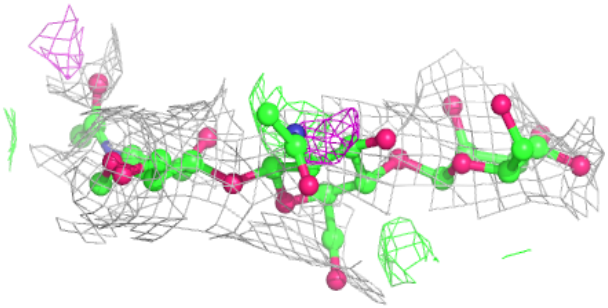


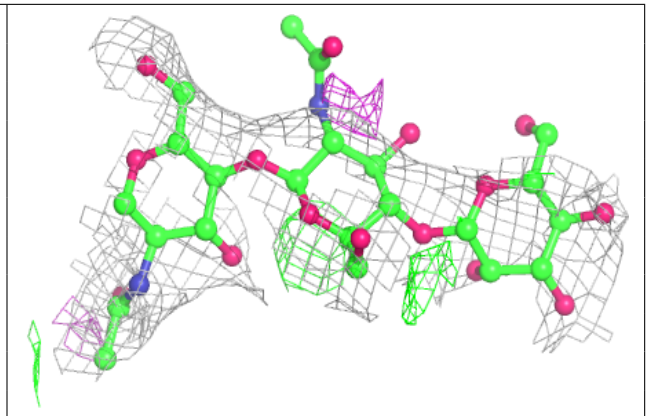


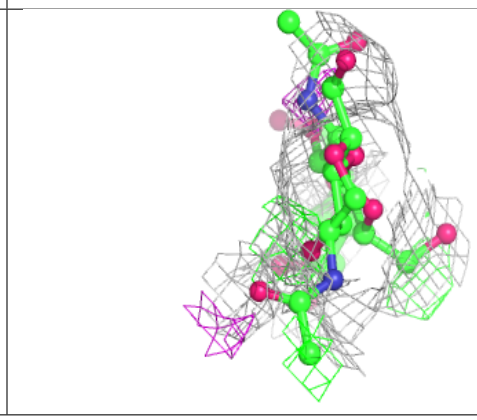


Electron density around Chain Z:

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

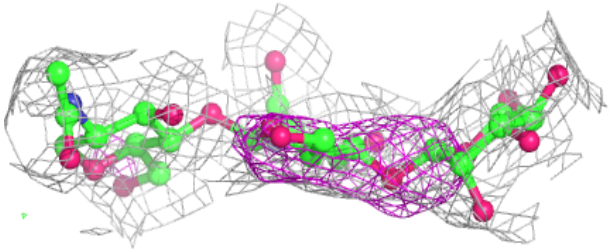


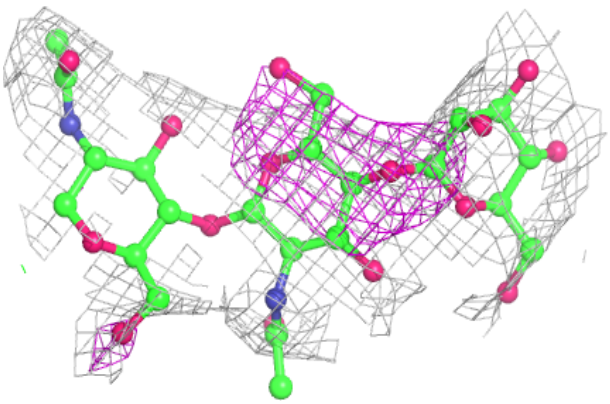


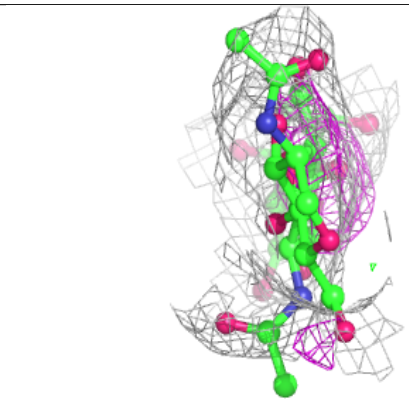


Electron density around Chain a:

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

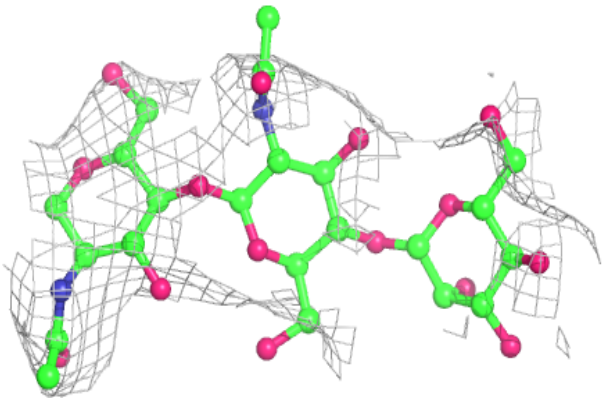


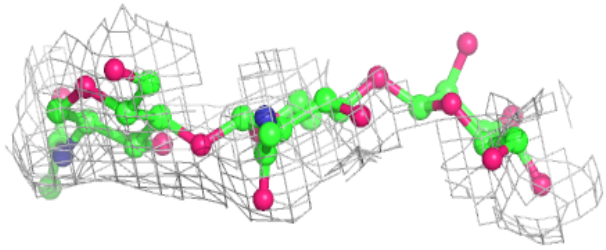


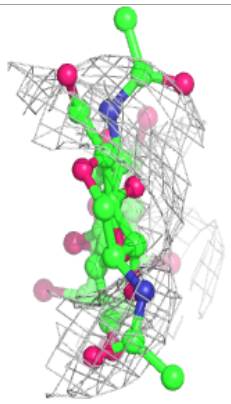


Electron density around Chain d:

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

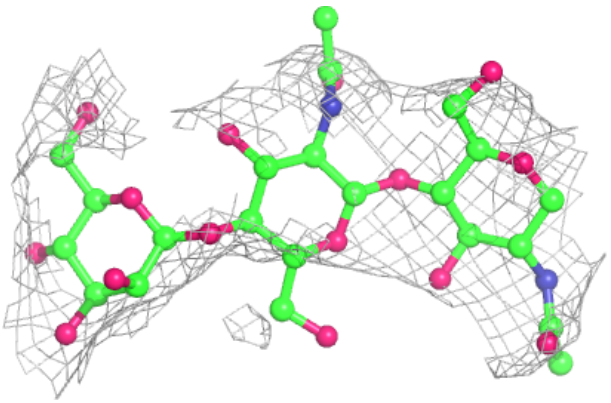


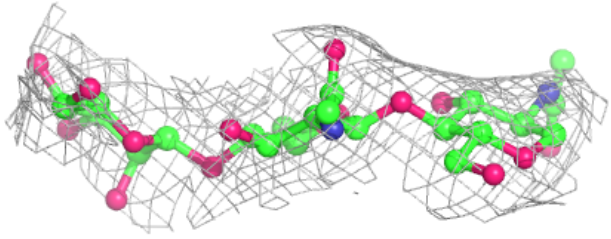


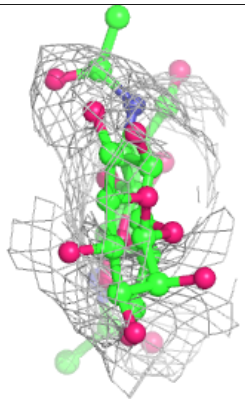


Electron density around Chain i:

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

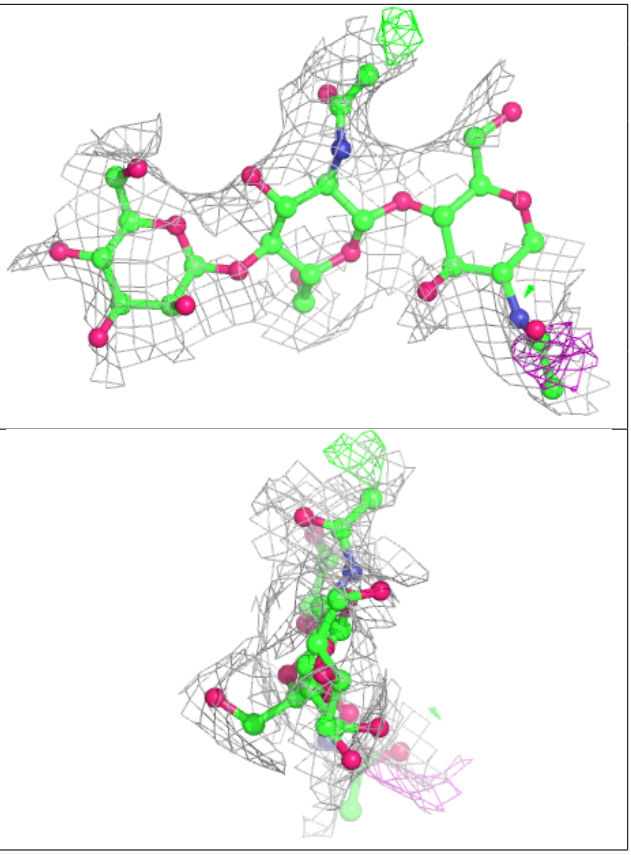






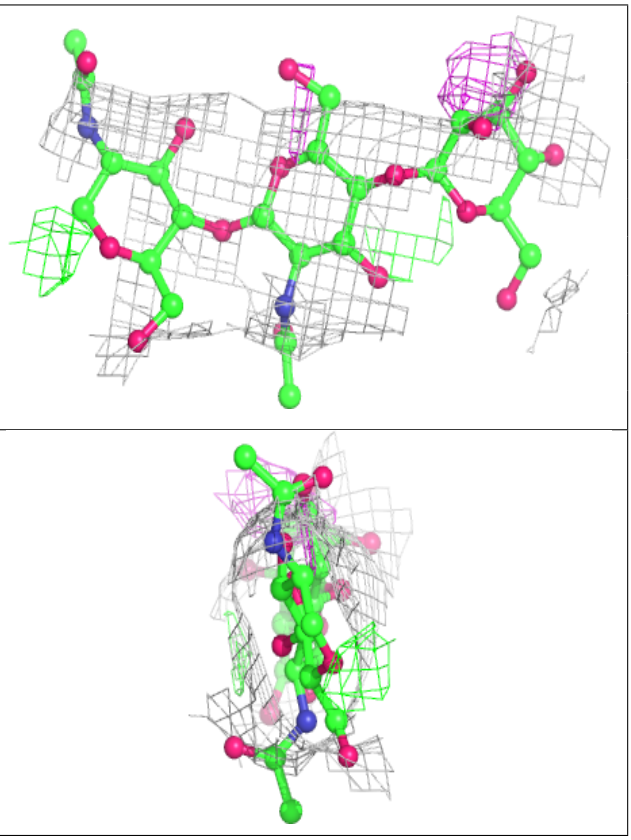
Electron density around Chain j:

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



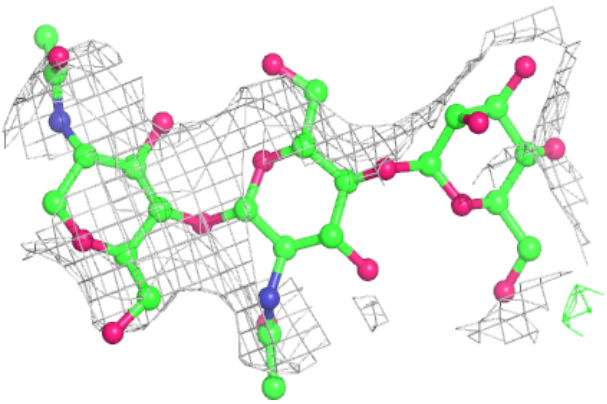
Electron density around Chain k:

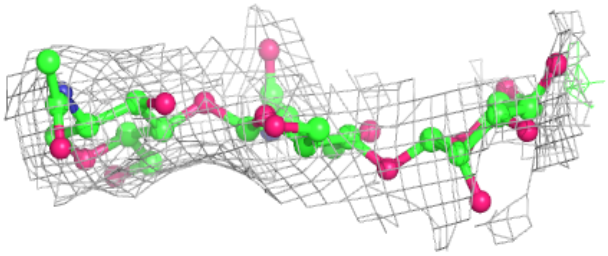
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

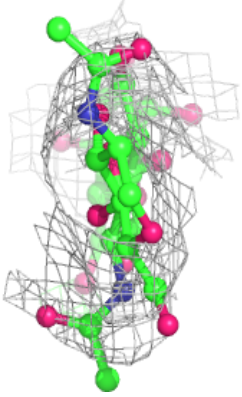


Electron density around Chain n:

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

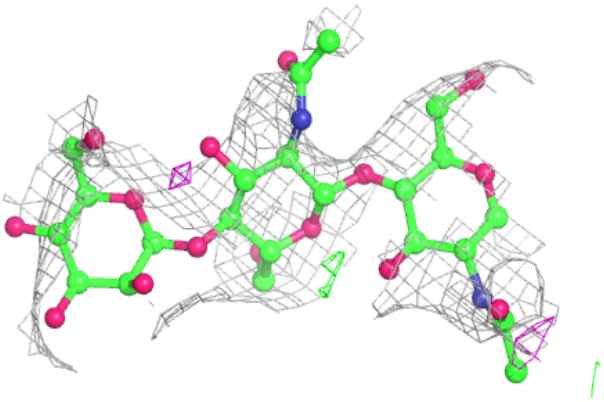


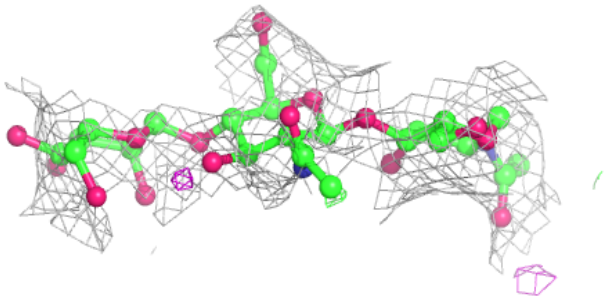


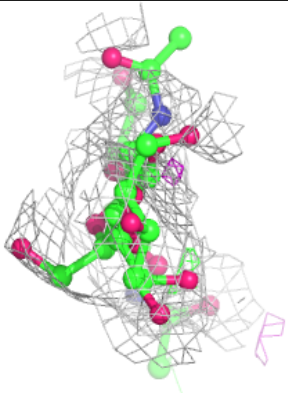


Electron density around Chain o:

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

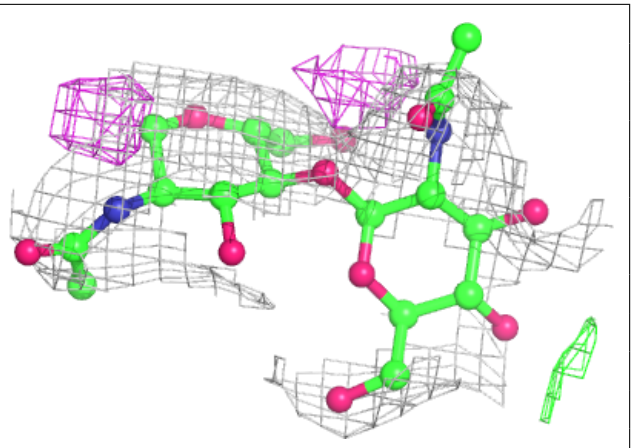


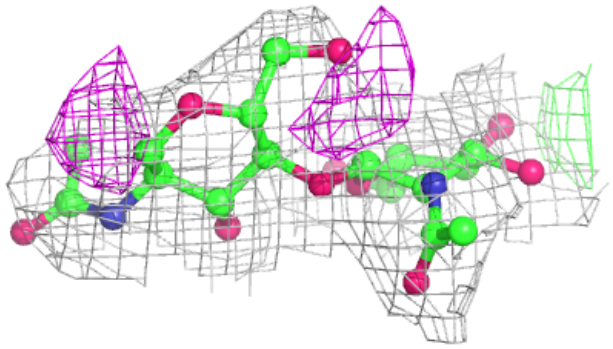


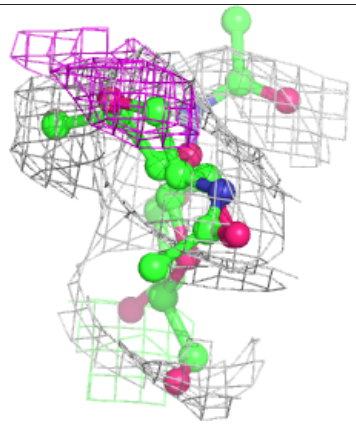


Electron density around Chain N:

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

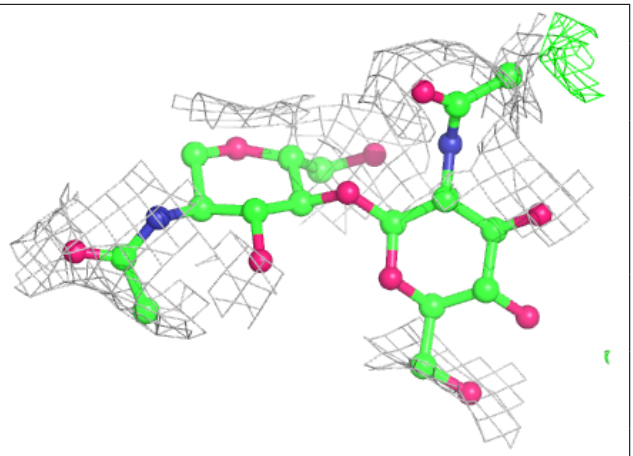


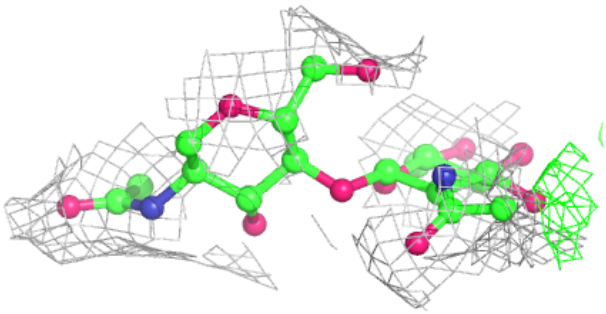


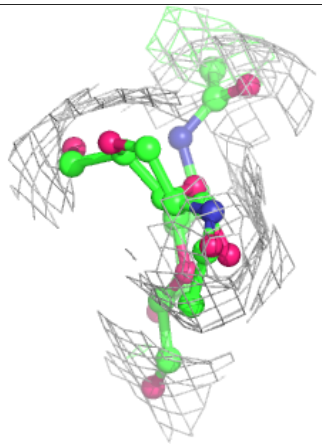


Electron density around Chain O:

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

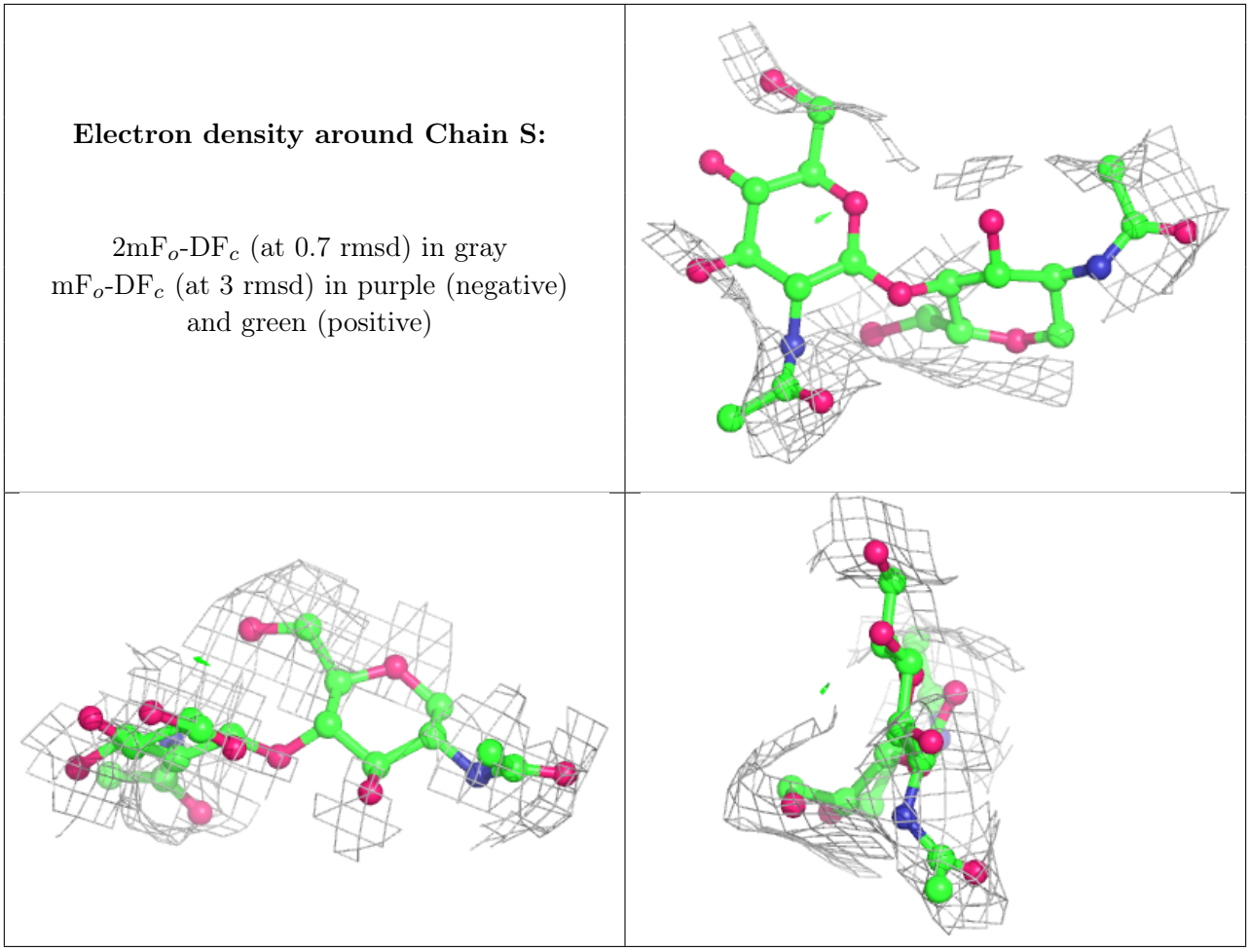






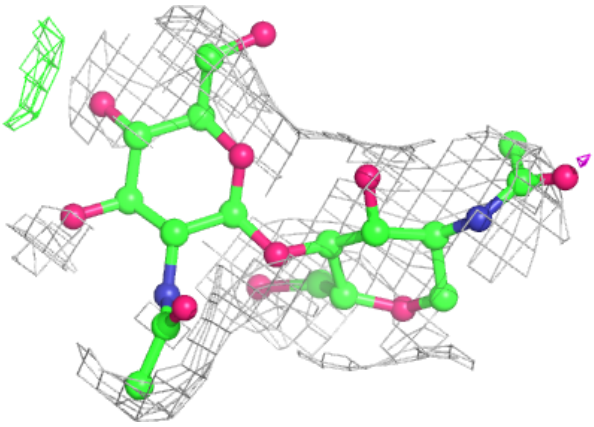
Electron density around Chain S:

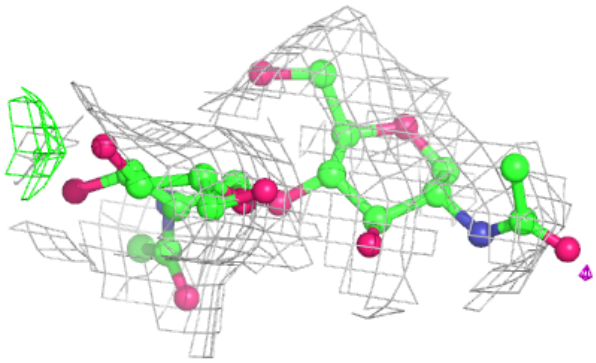
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

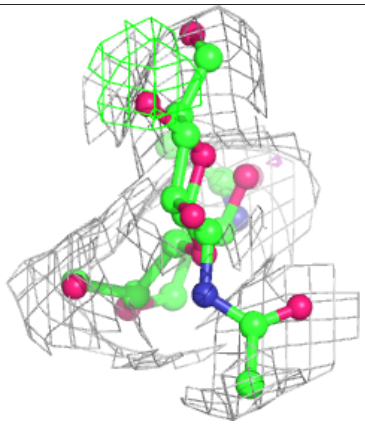


Electron density around Chain W:

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

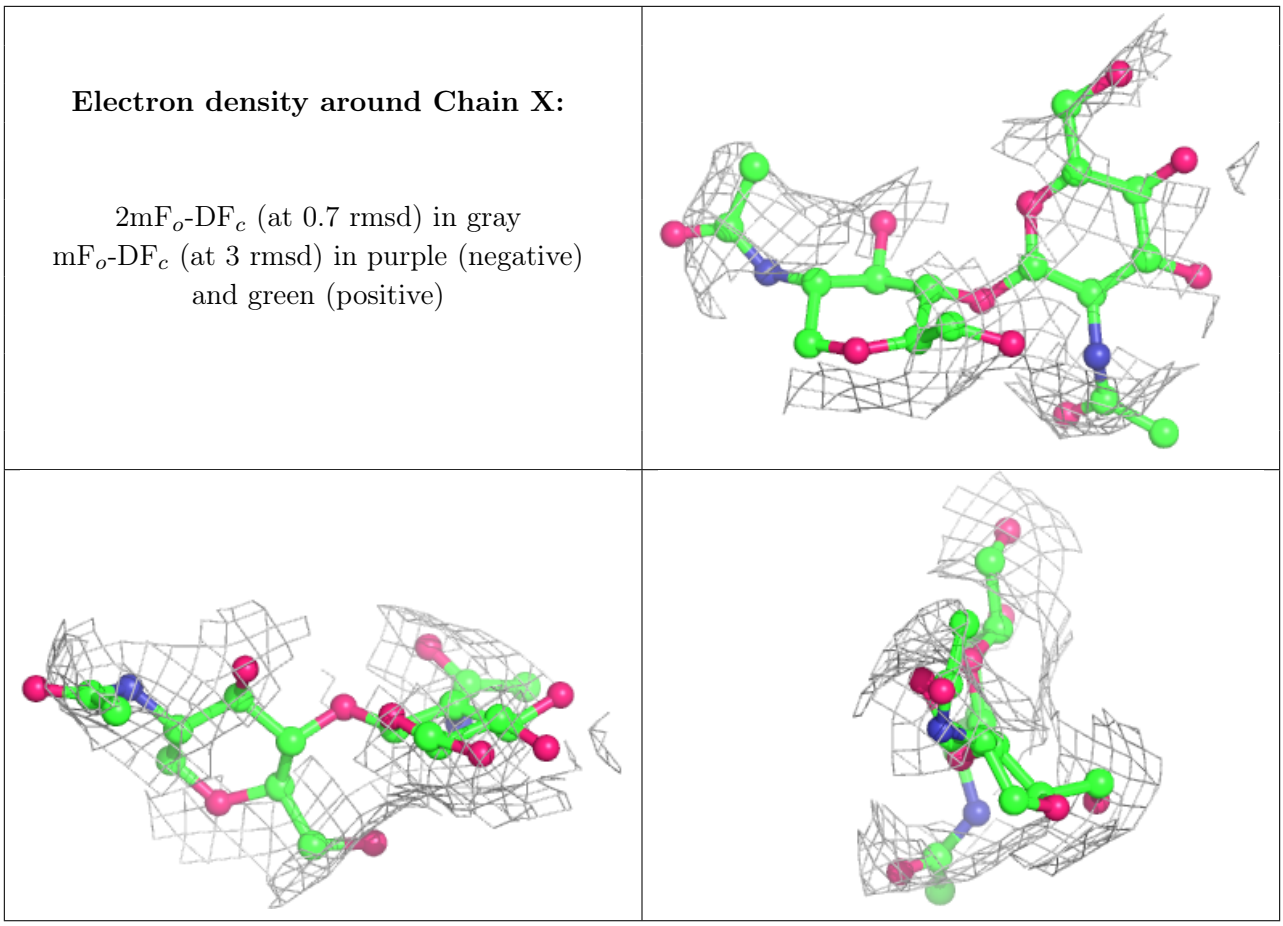






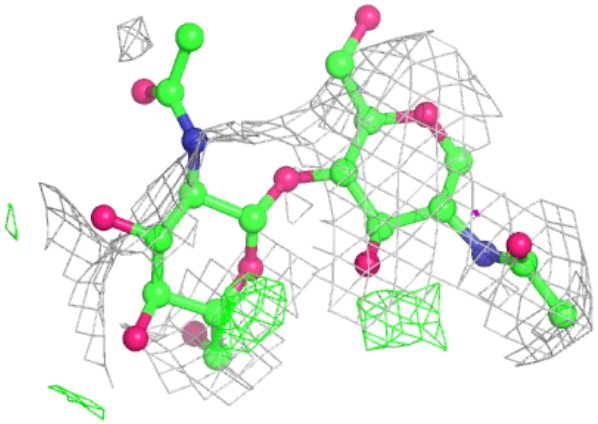
Electron density around Chain X:

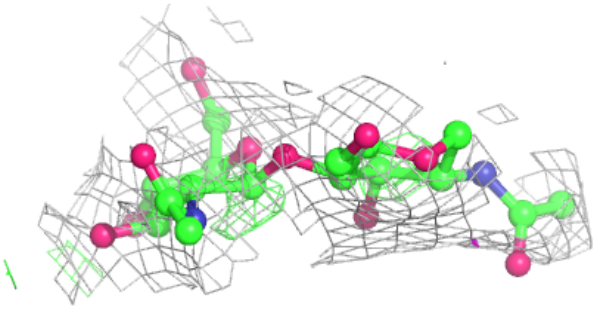
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

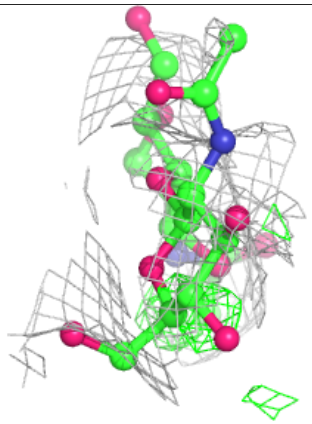


Electron density around Chain b:

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

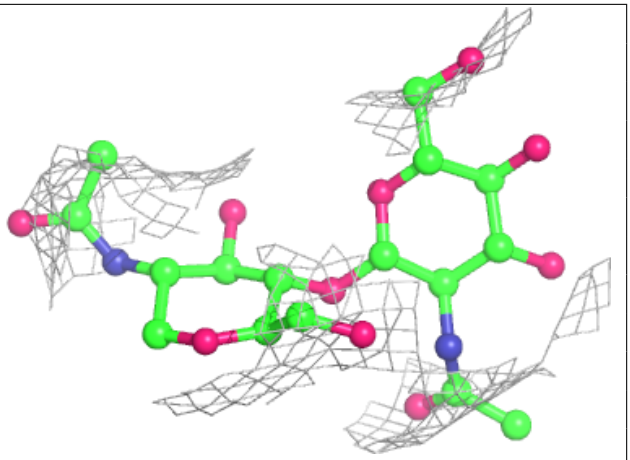


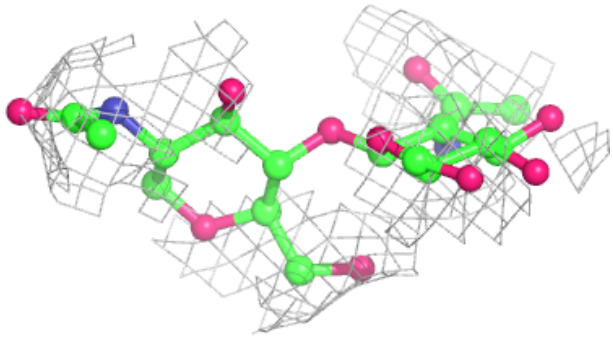


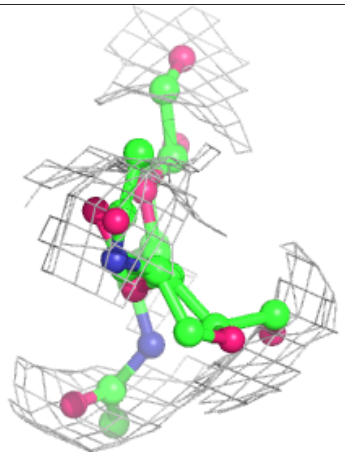


Electron density around Chain c:

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

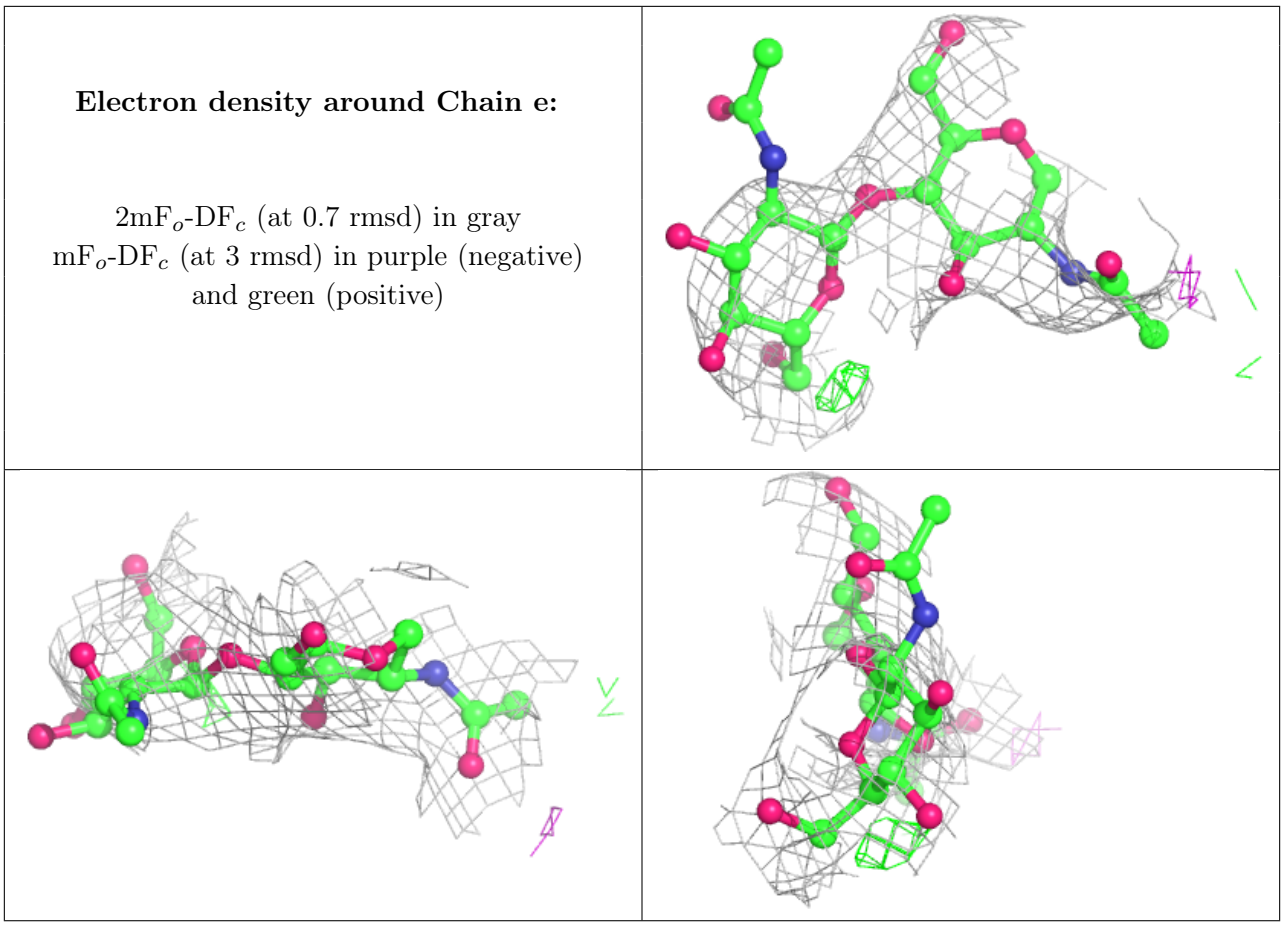






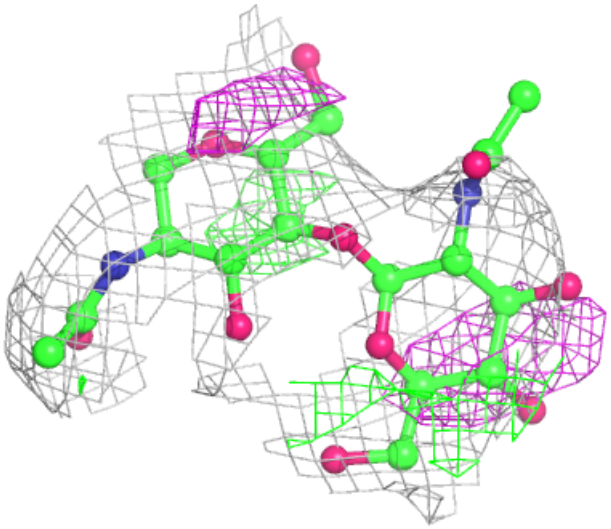
Electron density around Chain e:

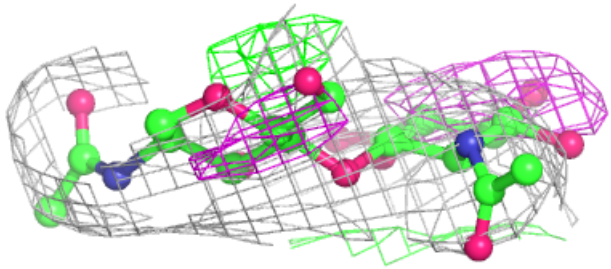
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

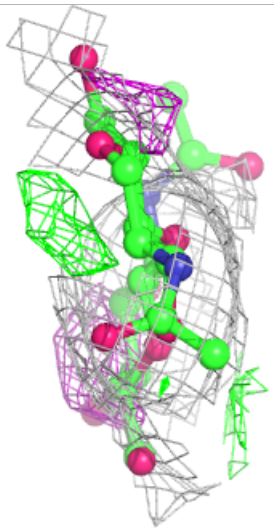


Electron density around Chain f:

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

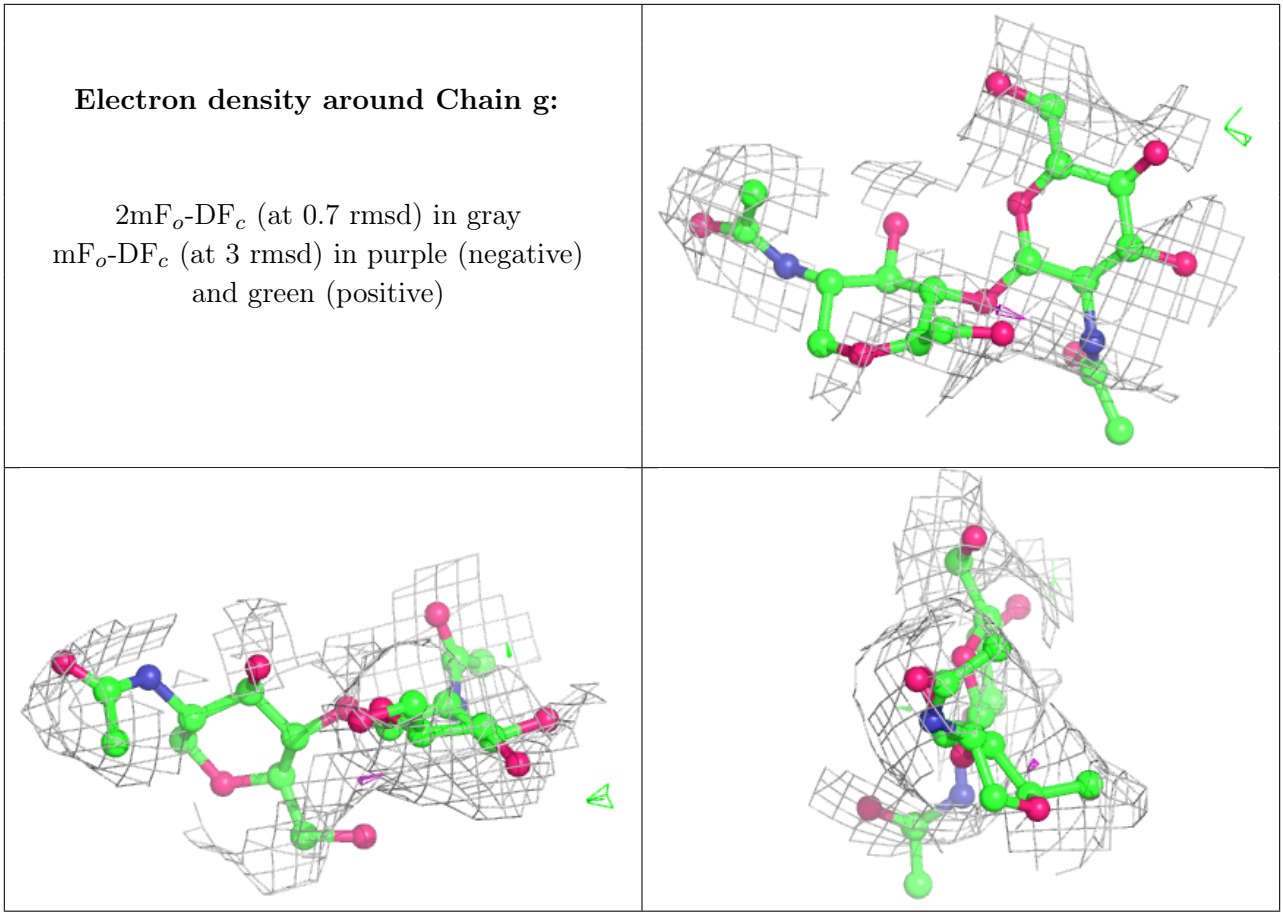






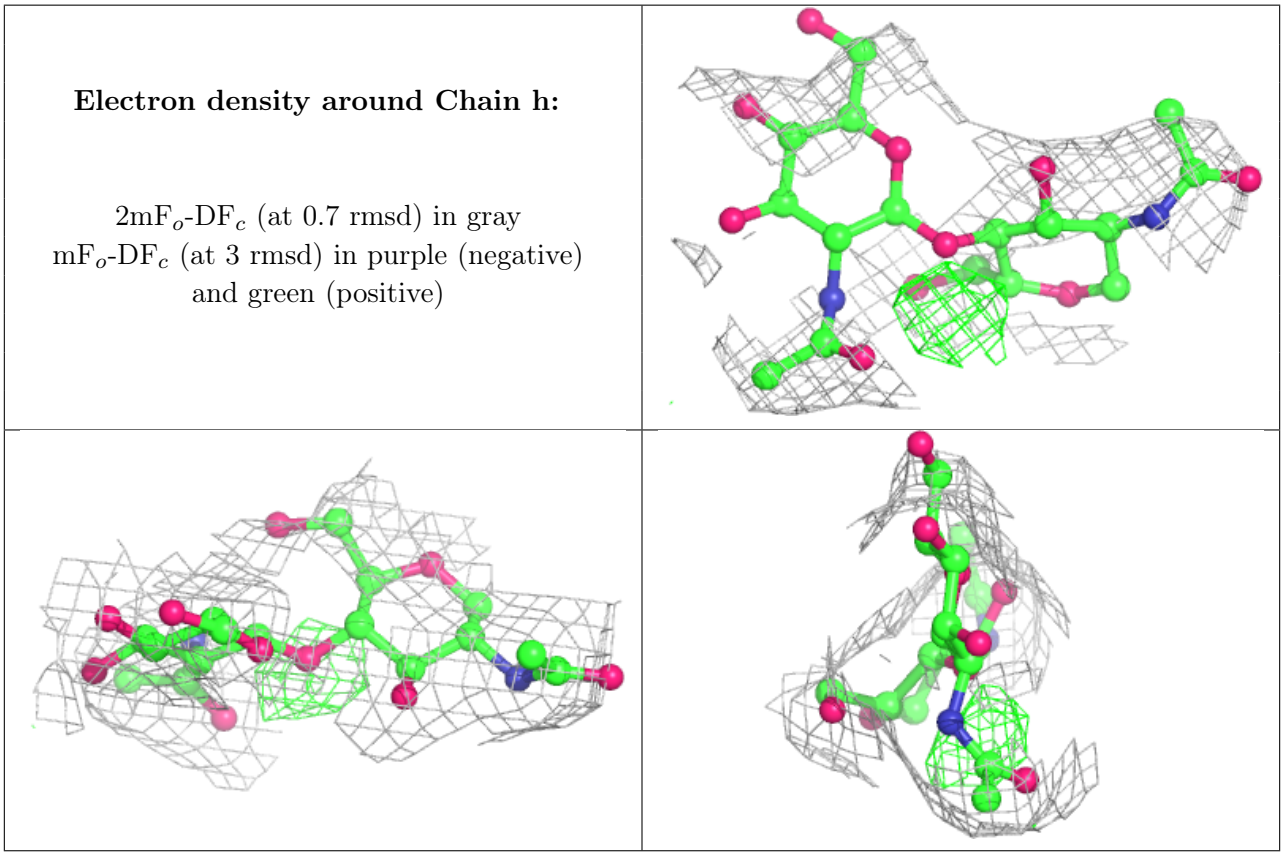
Electron density around Chain g:

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



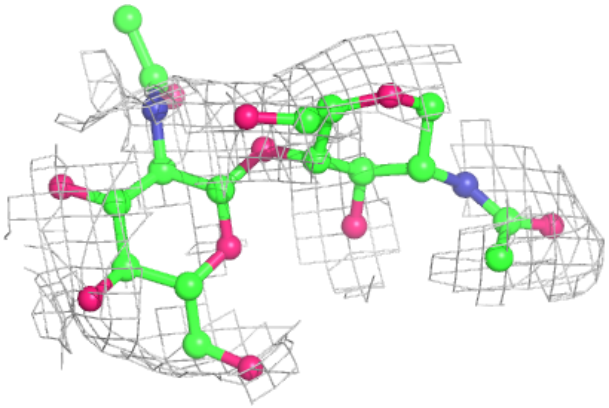
Electron density around Chain h:

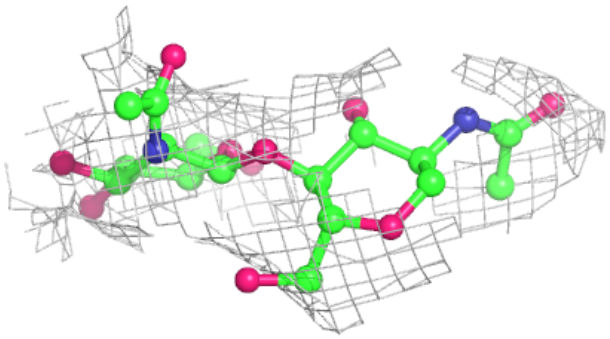
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

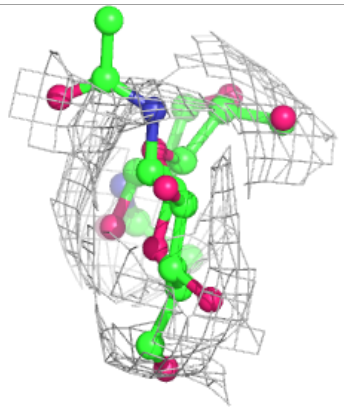


Electron density around Chain l:

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

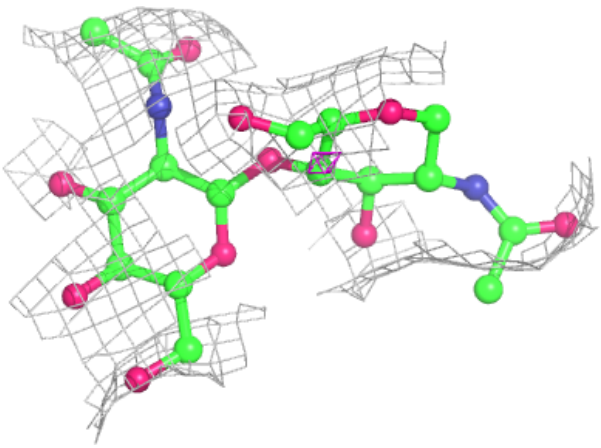


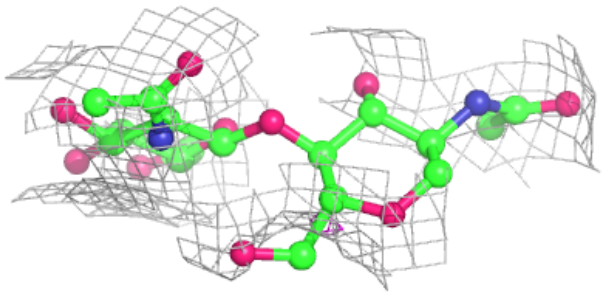


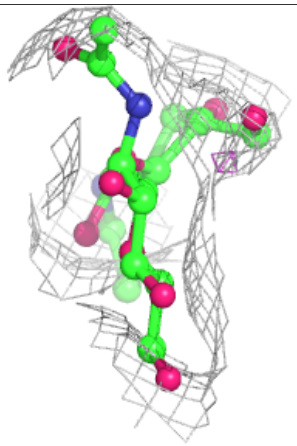


Electron density around Chain m:

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







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	600	14/15	0.41	0.44	200,206,211,213	0
5	NAG	I	414	14/15	0.46	0.54	150,161,168,169	0
5	NAG	G	414	14/15	0.55	0.37	106,119,127,128	0
5	NAG	C	414	14/15	0.56	0.51	111,122,129,129	0
5	NAG	E	411	14/15	0.56	0.56	126,134,139,142	0
5	NAG	F	600	14/15	0.58	0.27	186,193,200,200	0
5	NAG	J	600	14/15	0.58	0.38	197,206,213,214	0
5	NAG	I	410	14/15	0.64	0.42	119,125,127,129	0
5	NAG	H	600	14/15	0.65	0.26	203,207,210,211	0
5	NAG	C	404	14/15	0.74	0.29	85,96,107,109	0
5	NAG	B	600	14/15	0.74	0.26	194,202,209,210	0
5	NAG	K	414	14/15	0.74	0.23	106,117,125,126	0
5	NAG	C	410	14/15	0.77	0.27	103,107,111,111	0
5	NAG	E	415	14/15	0.80	0.23	109,119,127,129	0
5	NAG	A	411	14/15	0.81	0.35	80,87,91,93	0
5	NAG	G	411	14/15	0.84	0.36	130,138,142,145	0
5	NAG	A	415	14/15	0.91	0.16	117,130,138,139	0

6.5 Other polymers (i)

There are no such residues in this entry.