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

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

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

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

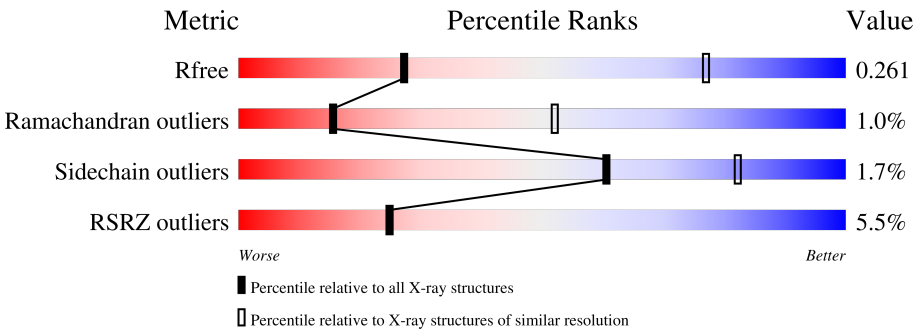
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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
			Total	C	N	O	S			
1	A	341	2588	1624	462	487	15	0	0	0
1	C	341	2588	1624	462	487	15	0	0	0
1	E	341	2588	1624	462	487	15	0	0	0
1	G	341	2588	1624	462	487	15	0	0	0
1	I	341	2588	1624	462	487	15	0	0	0
1	K	341	2588	1624	462	487	15	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2.

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

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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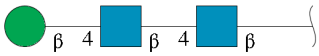
Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	linker	UNP C0LT38
B	526	ARG	-	linker	UNP C0LT38
D	524	SER	-	linker	UNP C0LT38
D	525	GLY	-	linker	UNP C0LT38
D	526	ARG	-	linker	UNP C0LT38
F	524	SER	-	linker	UNP C0LT38
F	525	GLY	-	linker	UNP C0LT38
F	526	ARG	-	linker	UNP C0LT38
H	524	SER	-	linker	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
			Total	C	N	O			
3	M	3	39	22	2	15	0	0	0
3	P	3	39	22	2	15	0	0	0
3	Q	3	39	22	2	15	0	0	0
3	R	3	39	22	2	15	0	0	0
3	T	3	39	22	2	15	0	0	0
3	U	3	39	22	2	15	0	0	0
3	V	3	39	22	2	15	0	0	0
3	Y	3	39	22	2	15	0	0	0

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	N	2	28	16	2	10	0	0	0
4	O	2	28	16	2	10	0	0	0
4	S	2	28	16	2	10	0	0	0
4	W	2	28	16	2	10	0	0	0
4	X	2	28	16	2	10	0	0	0
4	b	2	28	16	2	10	0	0	0
4	c	2	28	16	2	10	0	0	0
4	e	2	28	16	2	10	0	0	0
4	f	2	28	16	2	10	0	0	0

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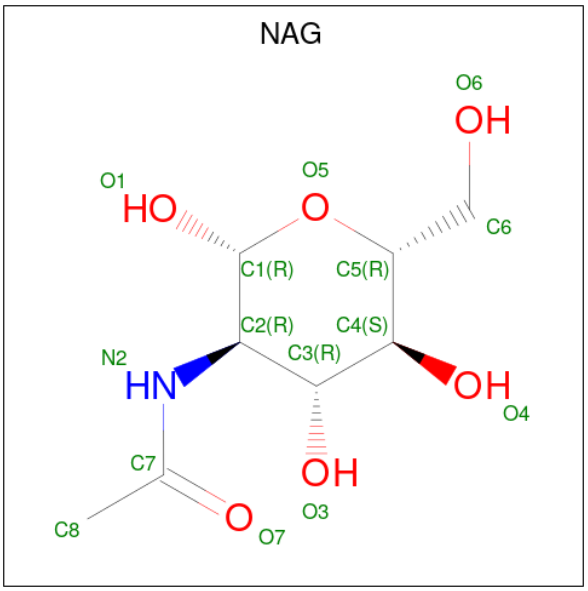
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	g	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	h	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	l	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	m	2	28	16	2	10	0	0	0

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

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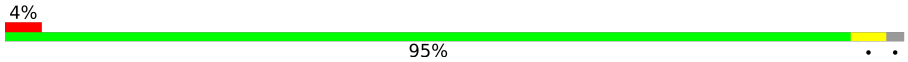
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	E	1	14	8	1	5	0	0
			Total	C	N	O		
5	E	1	14	8	1	5	0	0
			Total	C	N	O		
5	F	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	H	1	14	8	1	5	0	0
			Total	C	N	O		
5	I	1	14	8	1	5	0	0
			Total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

3 Residue-property plots (i)

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

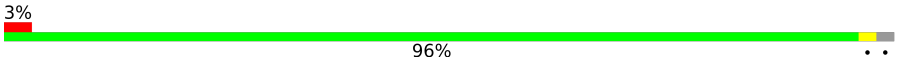
• Molecule 1: Hemagglutinin HA1

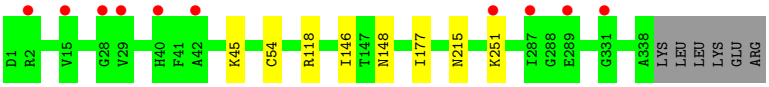
Chain A:



• Molecule 1: Hemagglutinin HA1

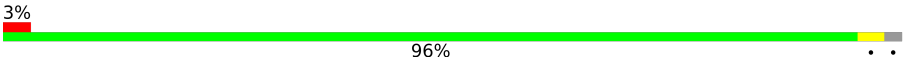
Chain C:

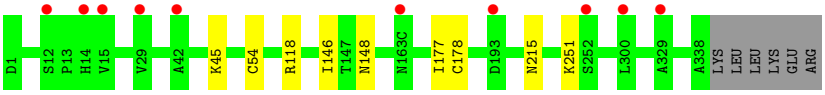




• Molecule 1: Hemagglutinin HA1

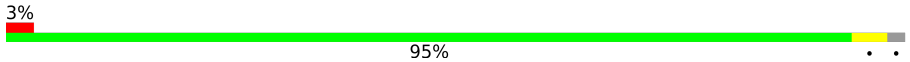
Chain E:

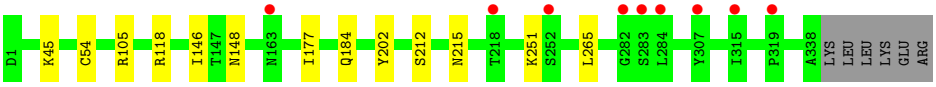




• Molecule 1: Hemagglutinin HA1

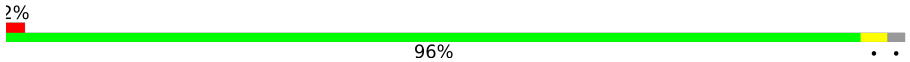
Chain G:

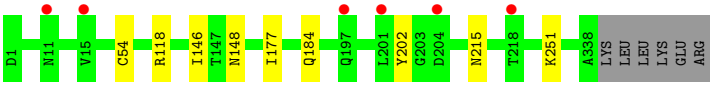




• Molecule 1: Hemagglutinin HA1

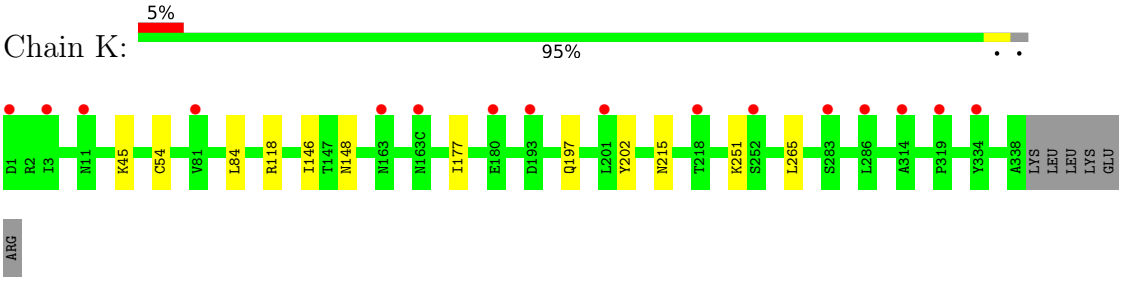
Chain I:





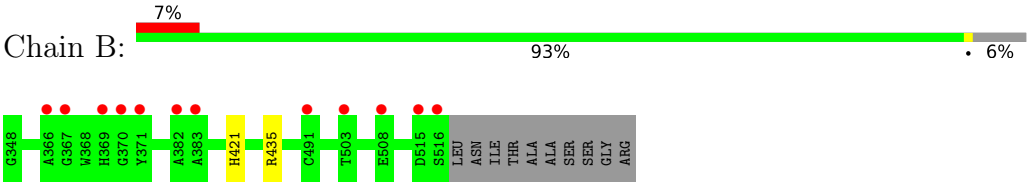
• Molecule 1: Hemagglutinin HA1

Chain K:



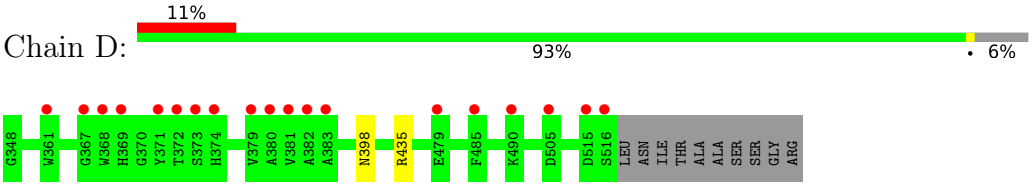
• Molecule 2: Hemagglutinin HA2

Chain B:



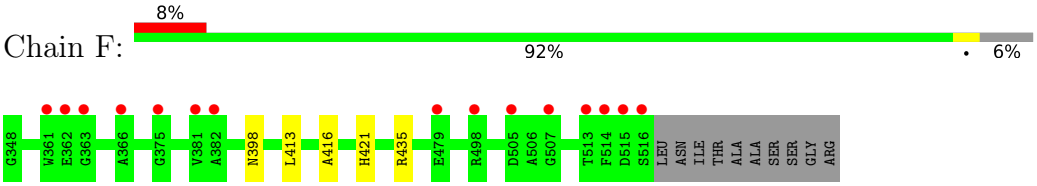
• Molecule 2: Hemagglutinin HA2

Chain D:



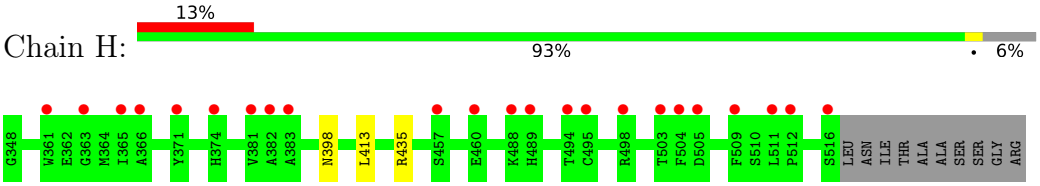
• Molecule 2: Hemagglutinin HA2

Chain F:



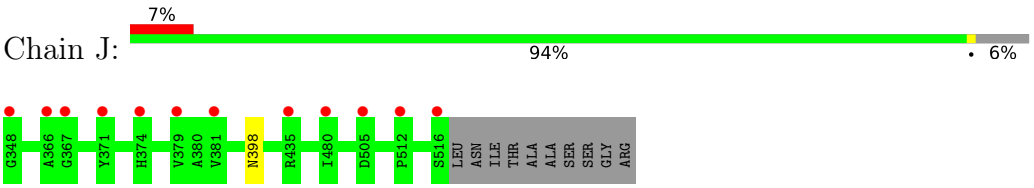
• Molecule 2: Hemagglutinin HA2

Chain H:



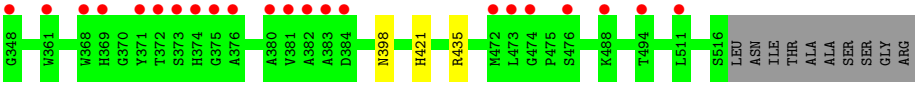
• Molecule 2: Hemagglutinin HA2

Chain J:



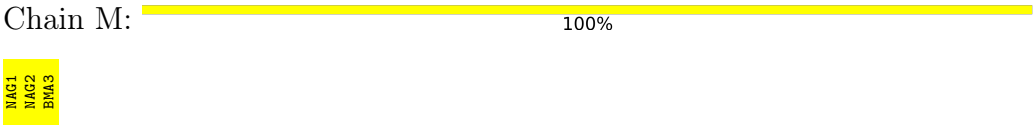
• Molecule 2: Hemagglutinin HA2

Chain L:



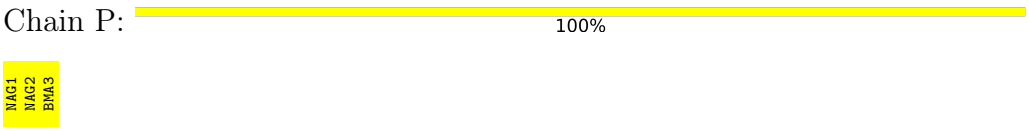
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



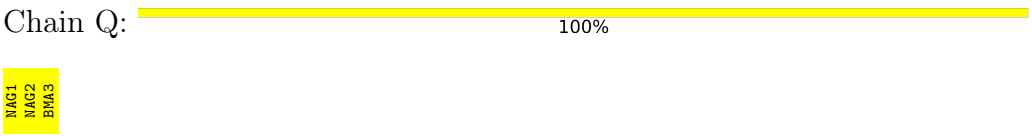
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



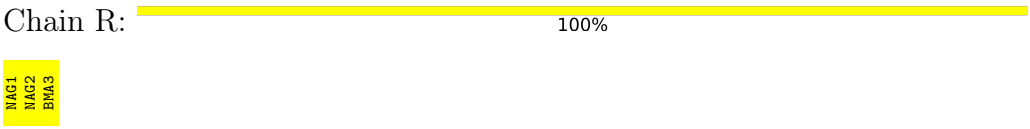
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



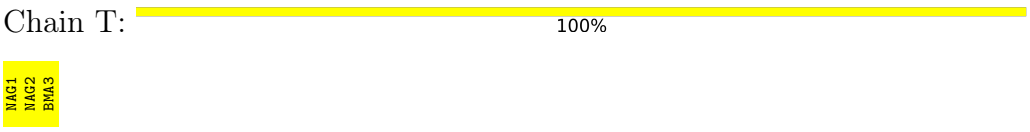
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



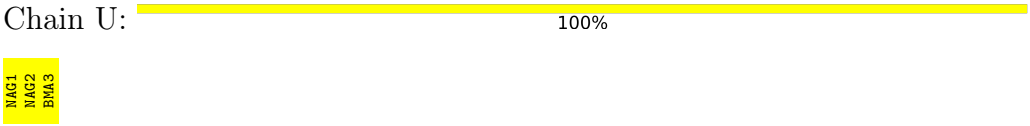
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%

NAG1
NAG2
BMA3

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

Chain Y: 100%

NAG1
NAG2
BMA3

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

Chain Z: 100%

NAG1
NAG2
BMA3

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

Chain a: 100%

NAG1
NAG2
BMA3

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

Chain d: 100%

NAG1
NAG2
BMA3

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

Chain i: 100%

NAG1
NAG2
BMA3

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

Chain j: 100%

NAG1
NAG2
BMA3

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

Chain k: 100%

NAG1
NAG2
BMA3

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

Chain n: 100%

NAG1
NAG2
BMA3

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

Chain o: 100%

NAG1
NAG2
BMA3

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

Chain N: 100%

NAG1
NAG2

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

Chain O: 50% 50%

NAG1
NAG2

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

Chain S: 50% 50%

NAG1
NAG2

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

Chain W: 100%

NAG1
NAG2

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

Chain X: 50% 50%

NAG1
NAG2

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

Chain b: 100%

NAG1
NAG2

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

Chain c: 50% 50%

NAG1
NAG2

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

Chain e: 100%

NAG1
NAG2

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

Chain f: 100%

NAG1
NAG2

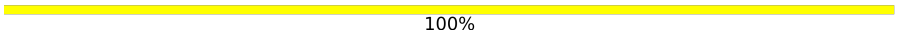
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%

• 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 (i)

5.1 Standard geometry (i)

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
1	E	251	LYS
1	G	177	ILE
1	G	251	LYS
1	I	177	ILE
1	I	251	LYS
1	K	177	ILE
1	K	251	LYS
1	A	148	ASN
1	E	146	ILE
1	I	146	ILE
1	C	146	ILE
1	G	146	ILE
1	I	148	ASN
1	K	146	ILE
1	A	45	LYS
1	A	146	ILE
1	A	147	THR
1	C	148	ASN
1	E	148	ASN
1	G	148	ASN
1	K	148	ASN
1	C	45	LYS
1	E	45	LYS
1	G	45	LYS
1	K	45	LYS
2	F	416	ALA

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	105	ARG
1	A	118	ARG
1	A	202	TYR
1	A	215	ASN
2	B	421	HIS
2	B	435	ARG
1	C	54	CYS
1	C	118	ARG
1	C	215	ASN
2	D	398	ASN
2	D	435	ARG
1	E	54	CYS
1	E	118	ARG
1	E	215	ASN
2	F	398	ASN
2	F	421	HIS
2	F	435	ARG
1	G	54	CYS
1	G	105	ARG
1	G	118	ARG
1	G	184	GLN
1	G	202	TYR
1	G	212	SER
1	G	215	ASN

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Mol	Chain	Res	Type
1	G	265	LEU
2	H	398	ASN
2	H	435	ARG
1	I	54	CYS
1	I	118	ARG
1	I	202	TYR
1	I	215	ASN
2	J	398	ASN
1	K	54	CYS
1	K	118	ARG
1	K	197	GLN
1	K	202	TYR
1	K	215	ASN
1	K	265	LEU
2	L	398	ASN
2	L	421	HIS
2	L	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	126	ASN
1	A	129	ASN
2	B	398	ASN
1	C	85	HIS
1	C	126	ASN
1	C	129	ASN
1	C	231	GLN
1	E	268	GLN
1	G	126	ASN
1	G	129	ASN
1	G	184	GLN
1	G	268	GLN
2	H	482	ASN
1	I	126	ASN
1	I	129	ASN
1	I	184	GLN
1	K	126	ASN
1	K	129	ASN
1	K	197	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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%)
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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	1	NAG	O5-C1-C2	-7.33	99.72	111.29
3	Z	1	NAG	O5-C1-C2	-7.32	99.73	111.29
4	S	1	NAG	C1-O5-C5	6.81	121.42	112.19
4	h	1	NAG	C1-O5-C5	6.81	121.42	112.19
4	X	1	NAG	C1-O5-C5	6.80	121.41	112.19
4	O	1	NAG	C1-O5-C5	6.79	121.40	112.19
4	m	1	NAG	C1-O5-C5	6.79	121.39	112.19
4	c	1	NAG	C1-O5-C5	6.76	121.35	112.19
4	l	1	NAG	C1-O5-C5	5.99	120.31	112.19
4	g	1	NAG	C1-O5-C5	5.99	120.30	112.19
4	N	1	NAG	C1-O5-C5	5.96	120.27	112.19
4	W	1	NAG	C1-O5-C5	5.94	120.24	112.19
3	o	2	NAG	O5-C5-C6	-3.58	101.59	107.20
3	U	2	NAG	O5-C5-C6	-3.57	101.61	107.20
3	Q	2	NAG	O5-C5-C6	-3.56	101.62	107.20
4	b	2	NAG	O5-C5-C6	-3.56	101.62	107.20
4	e	2	NAG	O5-C5-C6	-3.56	101.62	107.20
3	Z	2	NAG	O5-C5-C6	-3.56	101.62	107.20
3	j	2	NAG	O5-C5-C6	-3.56	101.63	107.20
3	d	1	NAG	C1-O5-C5	3.19	116.52	112.19
3	i	1	NAG	C1-O5-C5	3.18	116.50	112.19
3	n	1	NAG	C1-O5-C5	3.18	116.50	112.19
3	P	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	T	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	Y	1	NAG	C1-O5-C5	3.17	116.49	112.19
4	f	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	a	1	NAG	C1-O5-C5	3.17	116.48	112.19
3	M	1	NAG	C1-O5-C5	3.16	116.48	112.19
3	V	1	NAG	C1-O5-C5	3.16	116.47	112.19
3	R	1	NAG	C1-O5-C5	3.16	116.47	112.19
3	k	1	NAG	C1-O5-C5	3.16	116.47	112.19
3	Q	3	BMA	O2-C2-C3	2.93	116.00	110.14
3	o	3	BMA	O2-C2-C3	2.93	116.00	110.14
3	Z	3	BMA	O2-C2-C3	2.93	116.00	110.14
3	U	3	BMA	O2-C2-C3	2.92	115.98	110.14
3	j	3	BMA	O2-C2-C3	2.90	115.95	110.14
4	b	1	NAG	O7-C7-C8	-2.84	116.78	122.06
3	Z	1	NAG	O7-C7-C8	-2.81	116.83	122.06
4	e	1	NAG	O7-C7-C8	-2.80	116.86	122.06
3	j	1	NAG	O7-C7-C8	-2.79	116.87	122.06
3	Q	1	NAG	O7-C7-C8	-2.79	116.88	122.06
3	o	1	NAG	O7-C7-C8	-2.78	116.89	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	O7-C7-C8	-2.77	116.91	122.06
3	U	1	NAG	C4-C3-C2	-2.69	107.08	111.02
3	j	1	NAG	C4-C3-C2	-2.67	107.11	111.02
4	e	1	NAG	C4-C3-C2	-2.66	107.11	111.02
3	o	1	NAG	C4-C3-C2	-2.66	107.12	111.02
3	Q	1	NAG	C4-C3-C2	-2.66	107.12	111.02
3	Z	1	NAG	C4-C3-C2	-2.65	107.14	111.02
3	j	3	BMA	O4-C4-C5	-2.65	102.72	109.30
3	Z	3	BMA	O4-C4-C5	-2.65	102.73	109.30
3	Q	3	BMA	O4-C4-C5	-2.64	102.75	109.30
3	U	3	BMA	O4-C4-C5	-2.63	102.76	109.30
3	o	3	BMA	O4-C4-C5	-2.63	102.77	109.30
4	b	1	NAG	C4-C3-C2	-2.60	107.21	111.02
4	l	2	NAG	C2-N2-C7	-2.48	119.37	122.90
4	N	2	NAG	C2-N2-C7	-2.47	119.38	122.90
4	W	2	NAG	C2-N2-C7	-2.45	119.41	122.90
4	g	2	NAG	C2-N2-C7	-2.45	119.42	122.90
3	o	3	BMA	C6-C5-C4	-2.43	107.31	113.00
3	Z	3	BMA	C6-C5-C4	-2.42	107.33	113.00
4	g	1	NAG	O5-C5-C4	2.42	116.72	110.83
4	l	1	NAG	O5-C5-C4	2.42	116.71	110.83
3	Q	3	BMA	C6-C5-C4	-2.42	107.35	113.00
3	j	3	BMA	C6-C5-C4	-2.41	107.35	113.00
4	W	1	NAG	O5-C5-C4	2.41	116.70	110.83
4	N	1	NAG	O5-C5-C4	2.41	116.69	110.83
3	U	3	BMA	C6-C5-C4	-2.40	107.37	113.00
4	m	1	NAG	O5-C5-C4	2.35	116.54	110.83
4	c	1	NAG	O5-C5-C4	2.35	116.54	110.83
4	O	1	NAG	O5-C5-C4	2.33	116.50	110.83
4	S	1	NAG	O5-C5-C4	2.33	116.50	110.83
4	h	1	NAG	O5-C5-C4	2.33	116.50	110.83
4	g	2	NAG	O5-C1-C2	-2.33	107.61	111.29
4	l	2	NAG	O5-C1-C2	-2.33	107.61	111.29
4	X	1	NAG	O5-C5-C4	2.32	116.48	110.83
4	N	2	NAG	O5-C1-C2	-2.32	107.63	111.29
4	W	2	NAG	O5-C1-C2	-2.31	107.64	111.29
4	b	2	NAG	O5-C1-C2	-2.30	107.65	111.29
3	U	2	NAG	O5-C1-C2	-2.30	107.66	111.29
3	j	2	NAG	O5-C1-C2	-2.30	107.66	111.29
3	o	2	NAG	O5-C1-C2	-2.29	107.67	111.29
3	Q	2	NAG	O5-C1-C2	-2.29	107.67	111.29
3	Z	2	NAG	O5-C1-C2	-2.28	107.69	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	e	2	NAG	O5-C1-C2	-2.27	107.70	111.29
4	N	1	NAG	C3-C4-C5	2.26	114.28	110.24
4	b	2	NAG	C4-C3-C2	-2.24	107.73	111.02
3	j	2	NAG	C4-C3-C2	-2.23	107.75	111.02
4	W	1	NAG	C3-C4-C5	2.23	114.22	110.24
4	l	1	NAG	C3-C4-C5	2.21	114.18	110.24
3	Z	2	NAG	C4-C3-C2	-2.21	107.78	111.02
3	Q	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	e	2	NAG	C4-C3-C2	-2.20	107.79	111.02
3	o	2	NAG	C4-C3-C2	-2.19	107.81	111.02
4	g	1	NAG	C3-C4-C5	2.18	114.14	110.24
3	U	2	NAG	C4-C3-C2	-2.18	107.82	111.02
3	P	2	NAG	C2-N2-C7	-2.17	119.81	122.90
3	d	2	NAG	C2-N2-C7	-2.17	119.81	122.90
3	Y	2	NAG	C2-N2-C7	-2.17	119.81	122.90
3	V	2	NAG	C2-N2-C7	-2.17	119.81	122.90
3	T	2	NAG	C2-N2-C7	-2.16	119.83	122.90
3	i	2	NAG	C2-N2-C7	-2.16	119.83	122.90
3	n	2	NAG	C2-N2-C7	-2.15	119.84	122.90
3	k	2	NAG	C2-N2-C7	-2.14	119.85	122.90
3	M	2	NAG	C2-N2-C7	-2.13	119.86	122.90
3	i	3	BMA	O5-C1-C2	-2.12	107.50	110.77
3	R	2	NAG	C2-N2-C7	-2.12	119.89	122.90
3	d	3	BMA	O5-C1-C2	-2.11	107.51	110.77
3	Y	3	BMA	O5-C1-C2	-2.11	107.51	110.77
4	f	2	NAG	C2-N2-C7	-2.11	119.89	122.90
3	V	3	BMA	O5-C1-C2	-2.11	107.52	110.77
3	a	2	NAG	C2-N2-C7	-2.10	119.91	122.90
3	P	3	BMA	O5-C1-C2	-2.10	107.52	110.77
3	R	3	BMA	O5-C1-C2	-2.10	107.53	110.77
3	k	3	BMA	O5-C1-C2	-2.10	107.54	110.77
3	n	3	BMA	O5-C1-C2	-2.09	107.54	110.77
3	M	3	BMA	O5-C1-C2	-2.08	107.55	110.77
3	T	3	BMA	O5-C1-C2	-2.08	107.55	110.77
4	l	2	NAG	C4-C3-C2	-2.06	108.00	111.02
3	a	3	BMA	O5-C1-C2	-2.06	107.60	110.77
4	N	2	NAG	C4-C3-C2	-2.05	108.01	111.02
4	W	2	NAG	C4-C3-C2	-2.03	108.05	111.02
4	g	2	NAG	C4-C3-C2	-2.02	108.05	111.02

There are no chirality outliers.

All (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
4	S	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	c	1	NAG	C8-C7-N2-C2
4	c	1	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	h	1	NAG	C8-C7-N2-C2
4	h	1	NAG	O7-C7-N2-C2
4	h	2	NAG	C8-C7-N2-C2
4	h	2	NAG	O7-C7-N2-C2
4	l	1	NAG	C8-C7-N2-C2
4	m	1	NAG	C8-C7-N2-C2
4	m	1	NAG	O7-C7-N2-C2
4	m	2	NAG	C8-C7-N2-C2
4	m	2	NAG	O7-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
4	l	1	NAG	O7-C7-N2-C2
4	O	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	l	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C8-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	V	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	d	2	NAG	C8-C7-N2-C2
3	i	2	NAG	C8-C7-N2-C2
3	k	2	NAG	C8-C7-N2-C2
3	n	2	NAG	C8-C7-N2-C2
4	f	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
4	m	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O7-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	V	2	NAG	O7-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	i	2	NAG	O7-C7-N2-C2
3	k	2	NAG	O7-C7-N2-C2
3	n	2	NAG	O7-C7-N2-C2
4	f	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2

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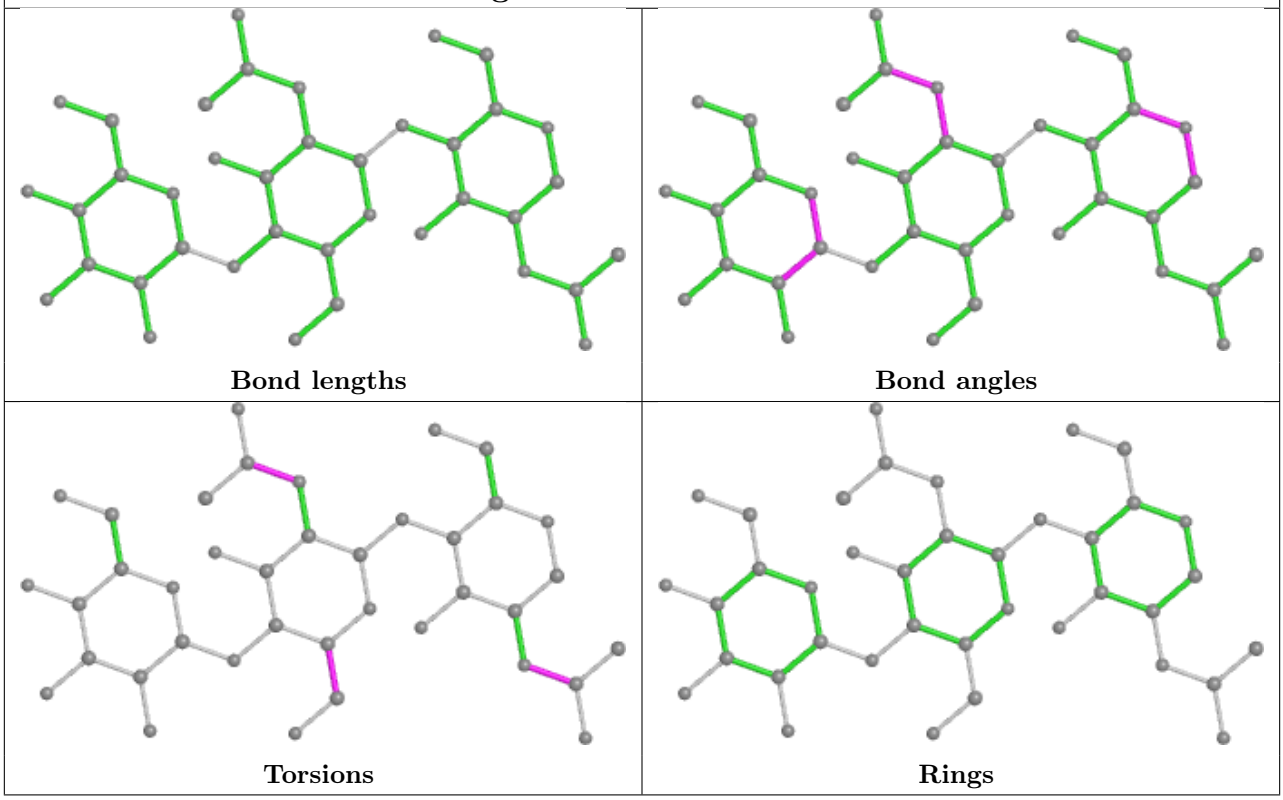
Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	i	1	NAG	C8-C7-N2-C2
3	k	1	NAG	C8-C7-N2-C2
3	n	1	NAG	C8-C7-N2-C2
4	f	1	NAG	C8-C7-N2-C2
3	o	3	BMA	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
3	Z	3	BMA	C4-C5-C6-O6
3	j	3	BMA	C4-C5-C6-O6
3	Z	3	BMA	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
3	j	3	BMA	O5-C5-C6-O6
3	V	1	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	i	1	NAG	O7-C7-N2-C2
3	k	1	NAG	O7-C7-N2-C2
3	n	1	NAG	O7-C7-N2-C2
4	f	1	NAG	O7-C7-N2-C2
3	R	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O7-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2

There are no ring outliers.

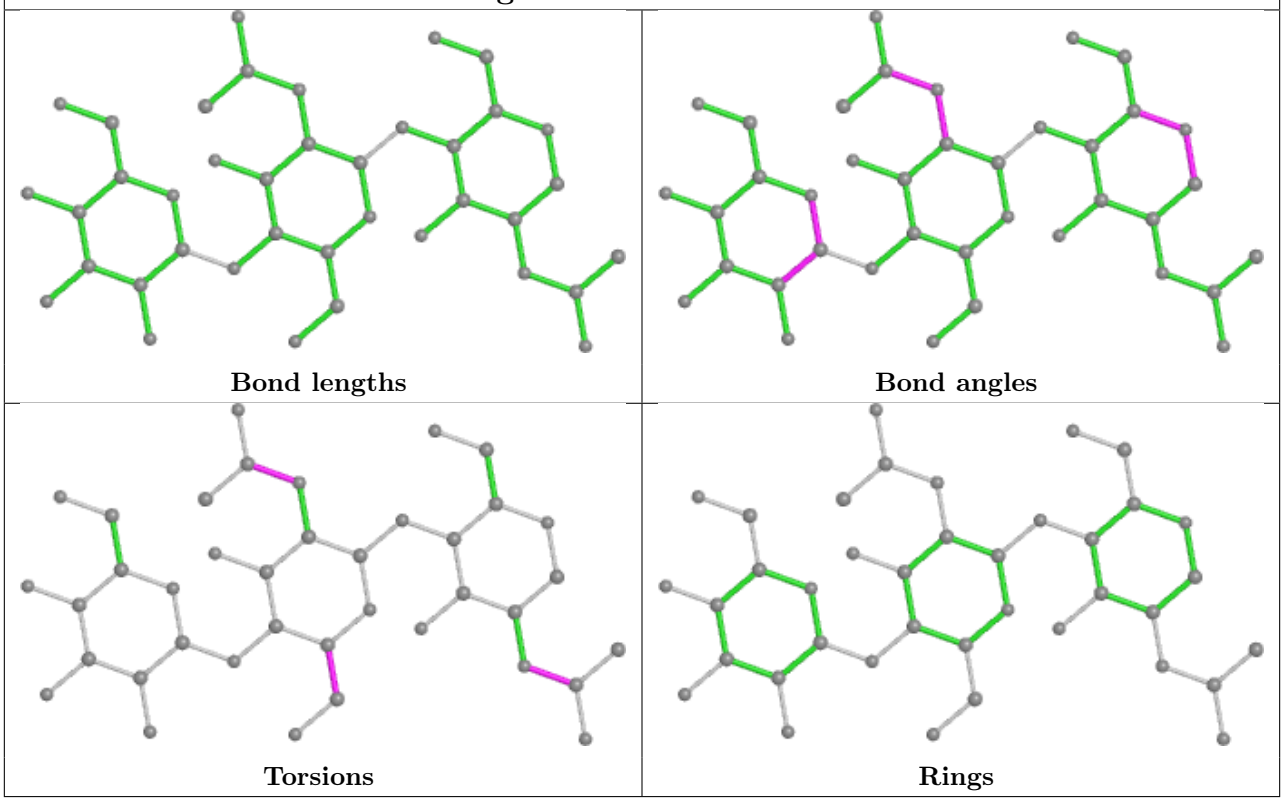
No monomer is involved in short contacts.

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

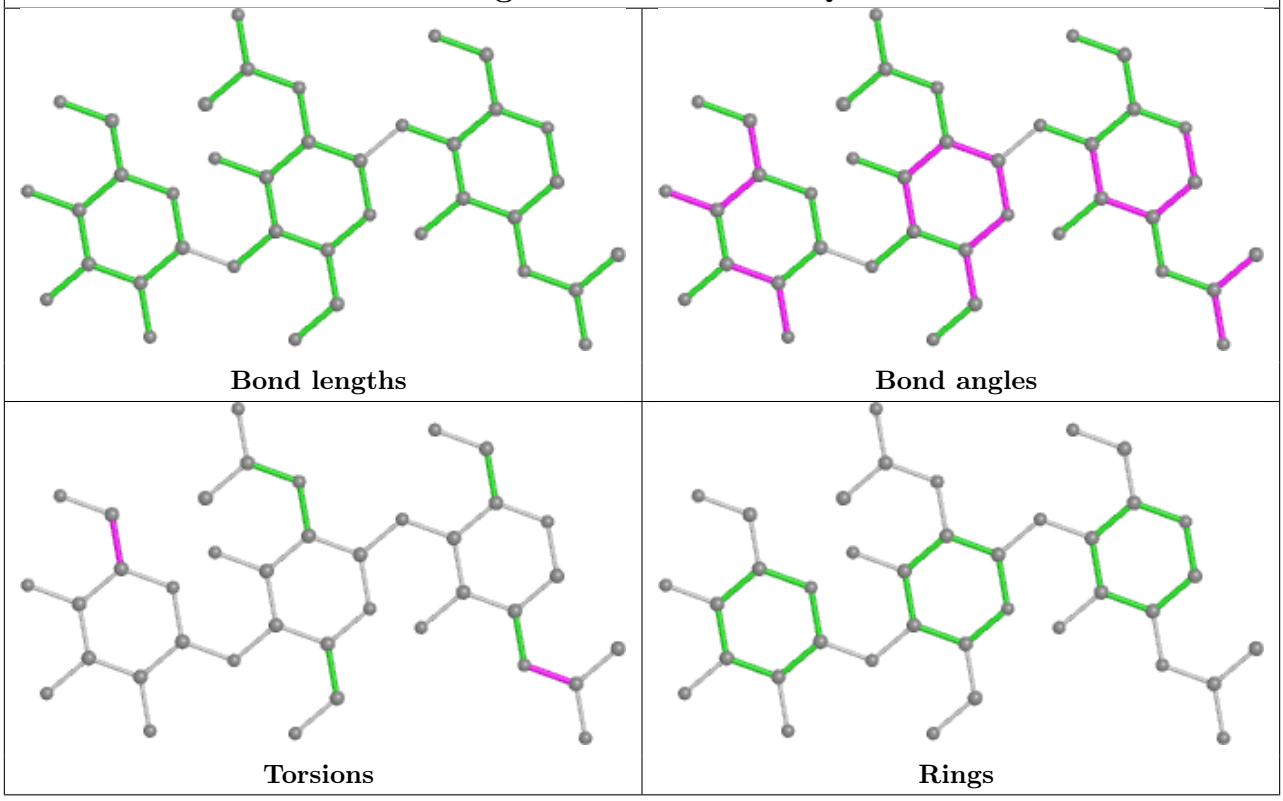
Oligosaccharide Chain M



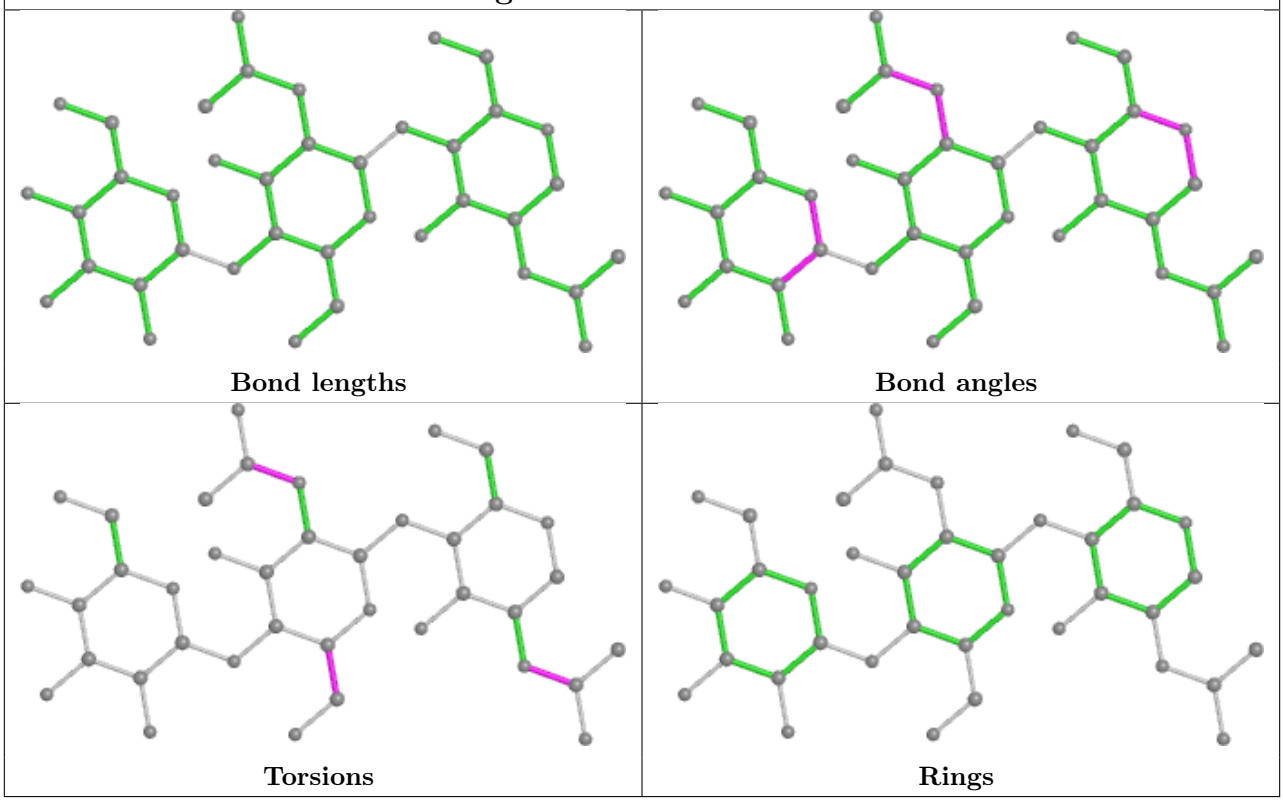
Oligosaccharide Chain P



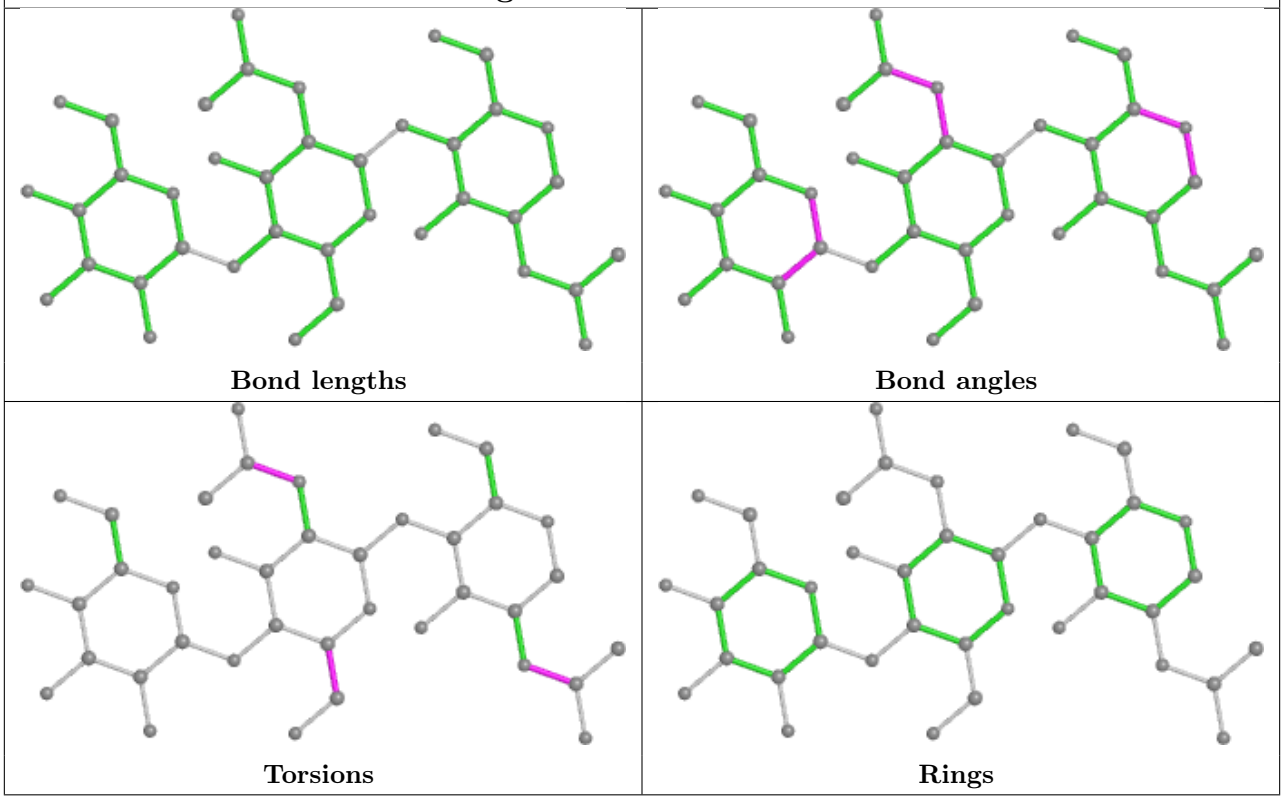
Oligosaccharide Chain Q



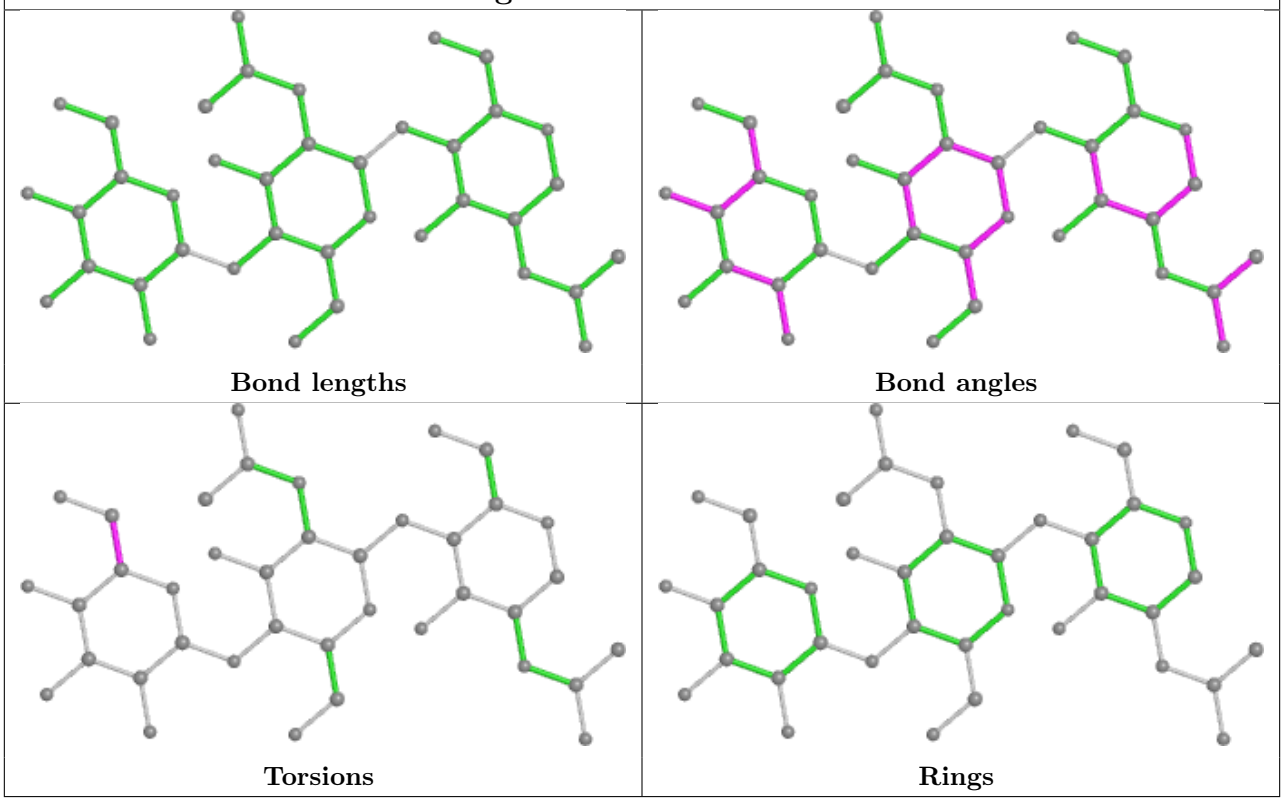
Oligosaccharide Chain R



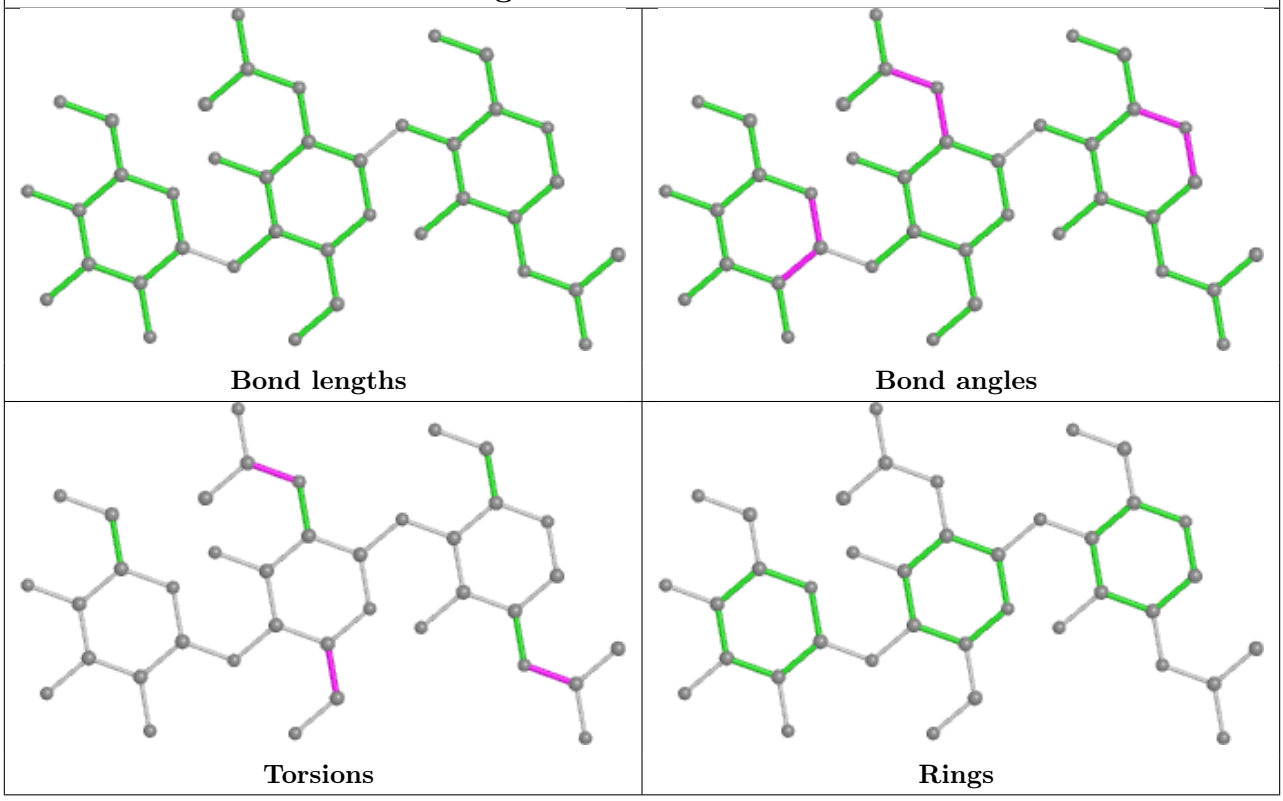
Oligosaccharide Chain T



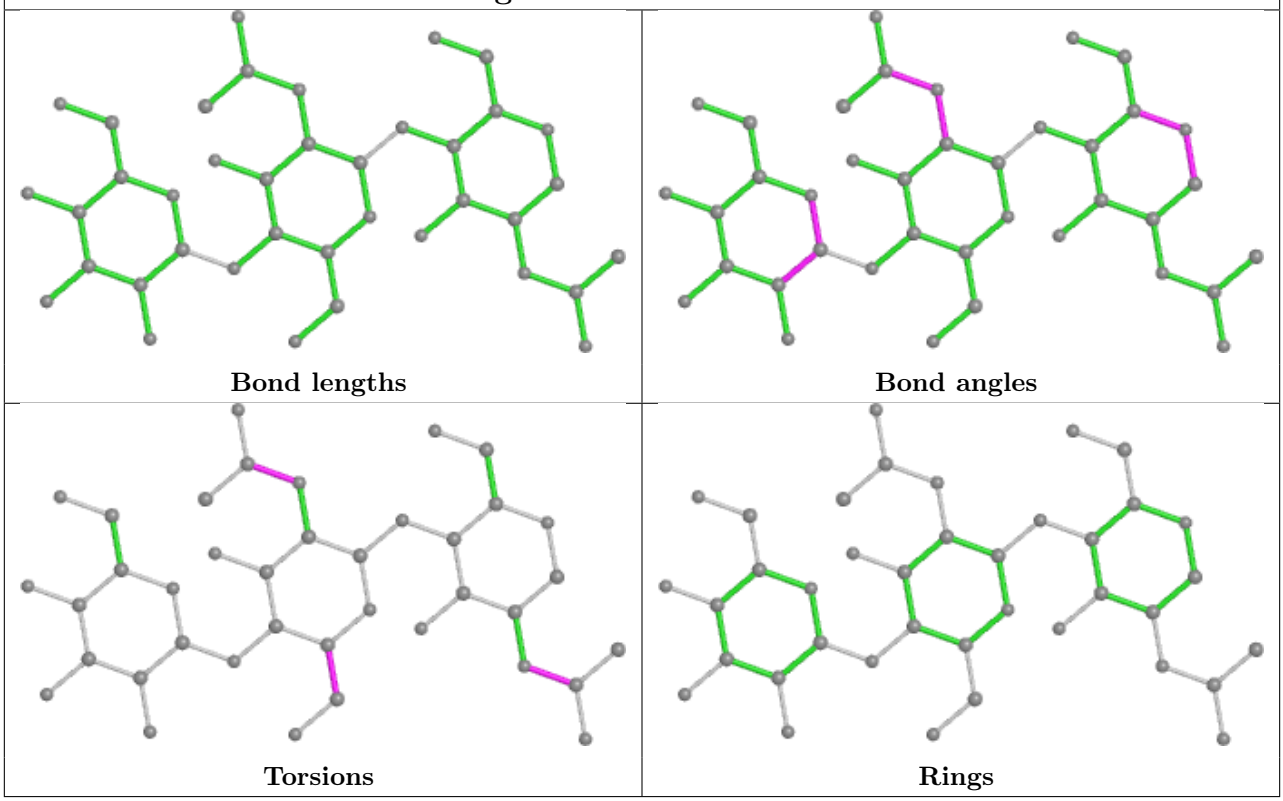
Oligosaccharide Chain U



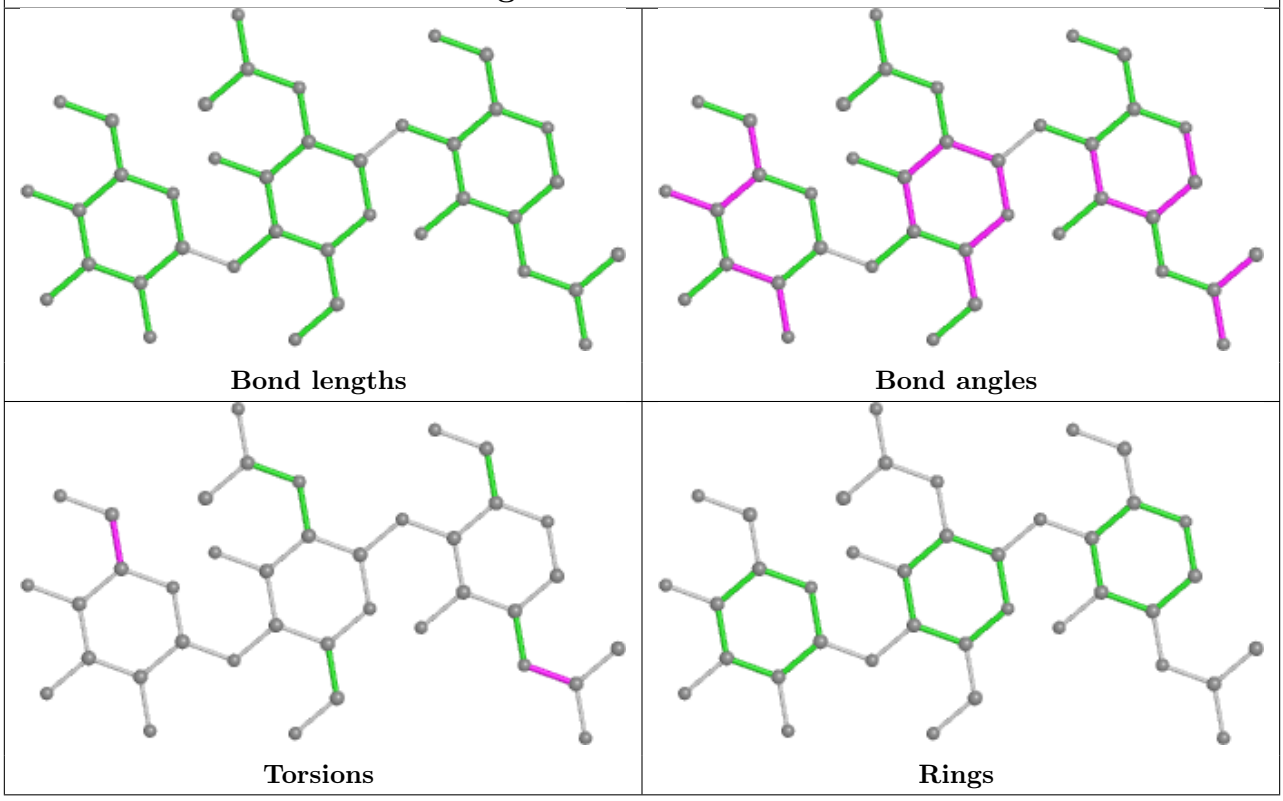
Oligosaccharide Chain V



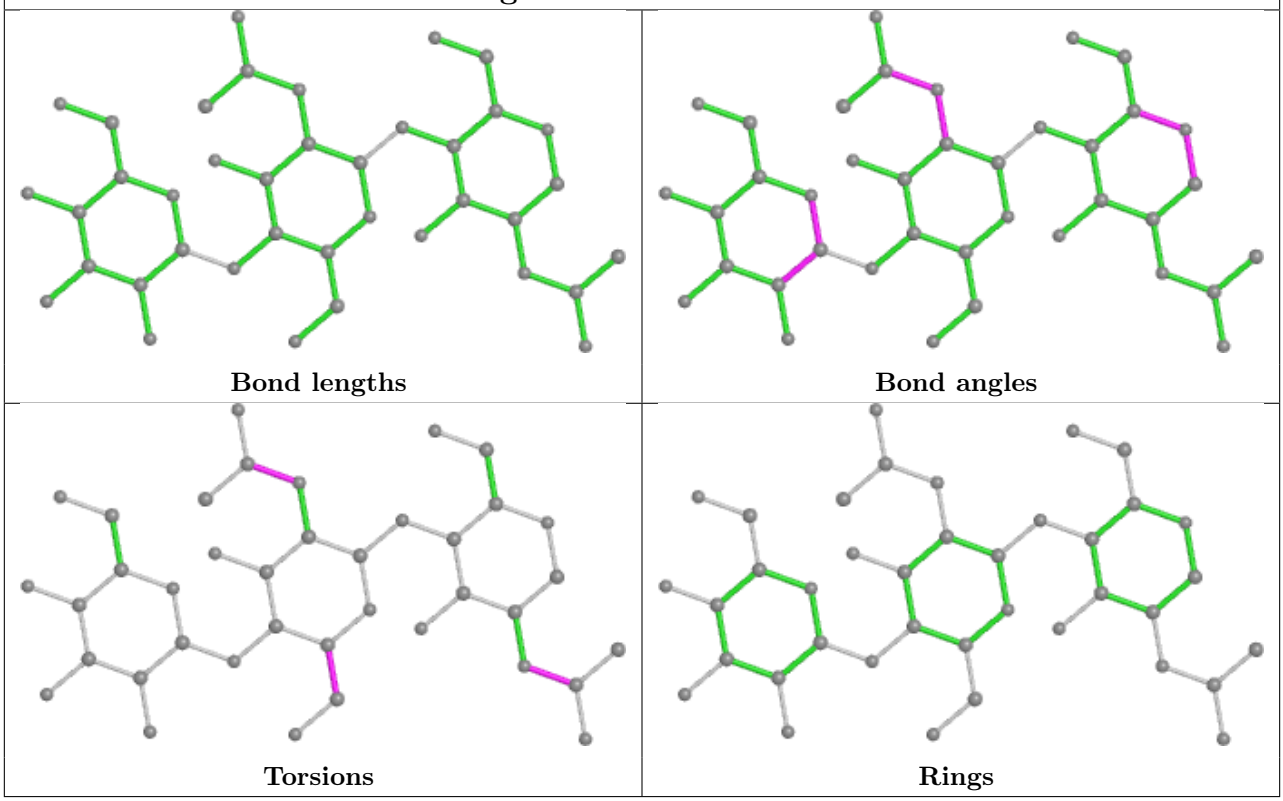
Oligosaccharide Chain Y



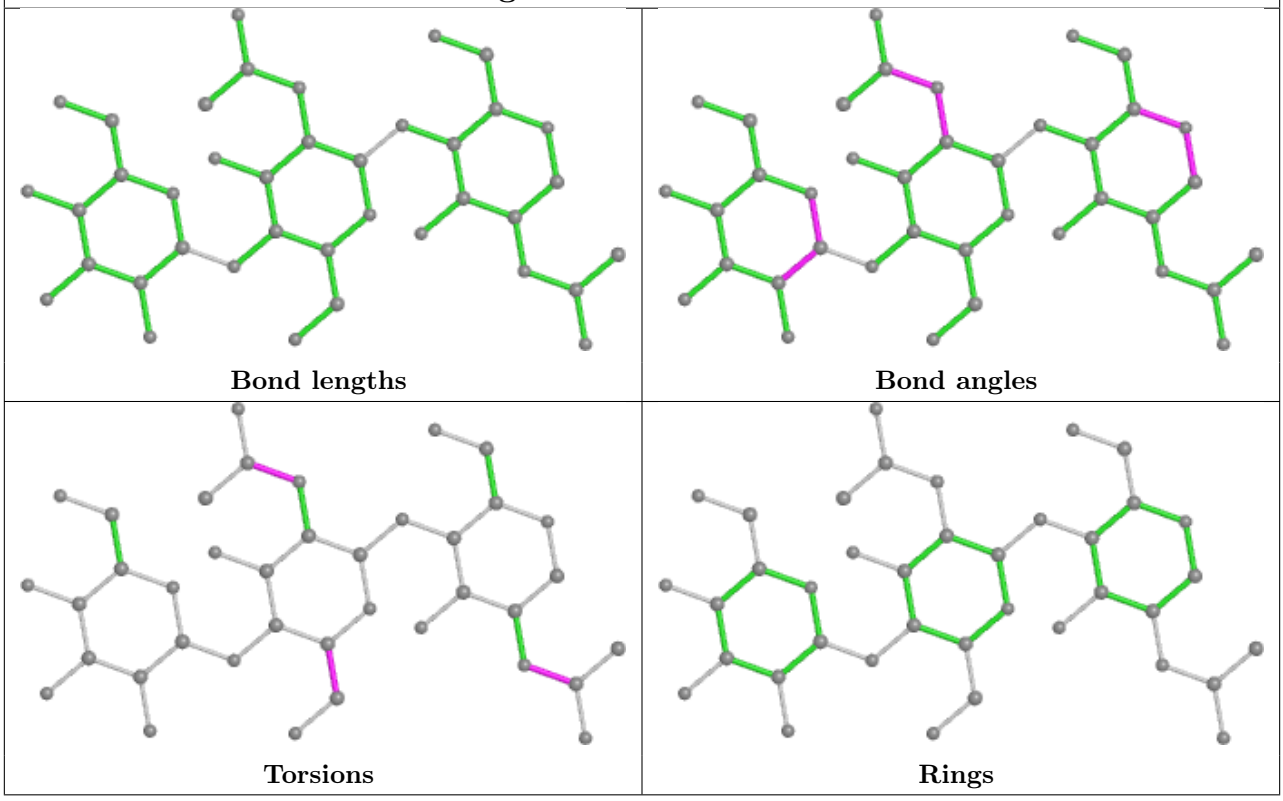
Oligosaccharide Chain Z



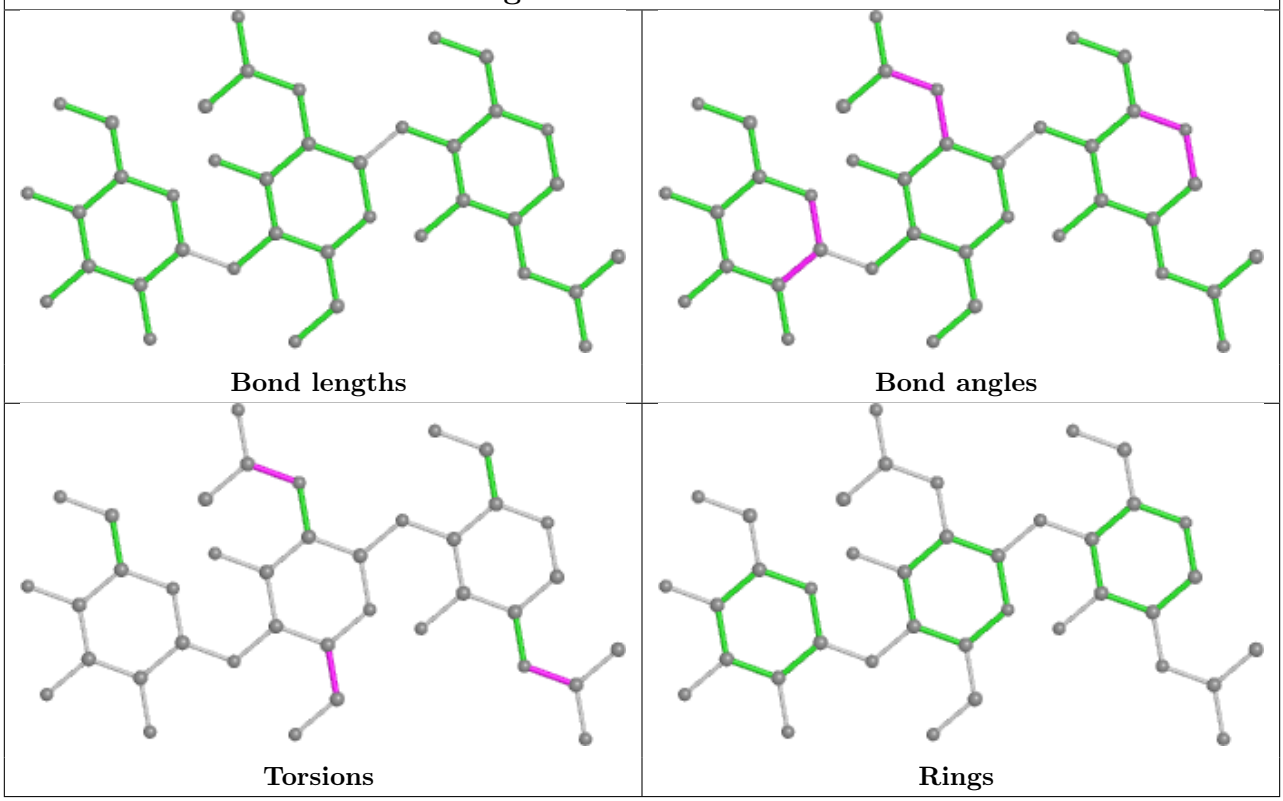
Oligosaccharide Chain a



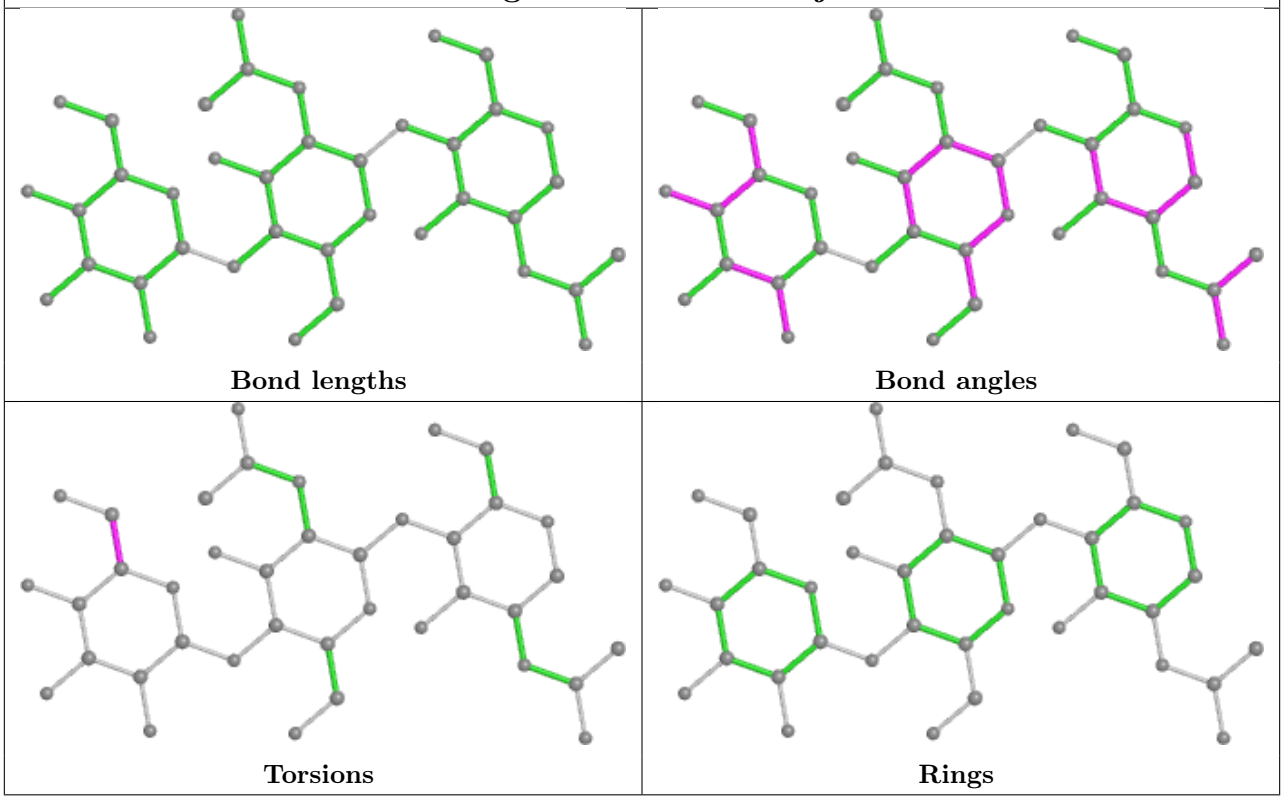
Oligosaccharide Chain d



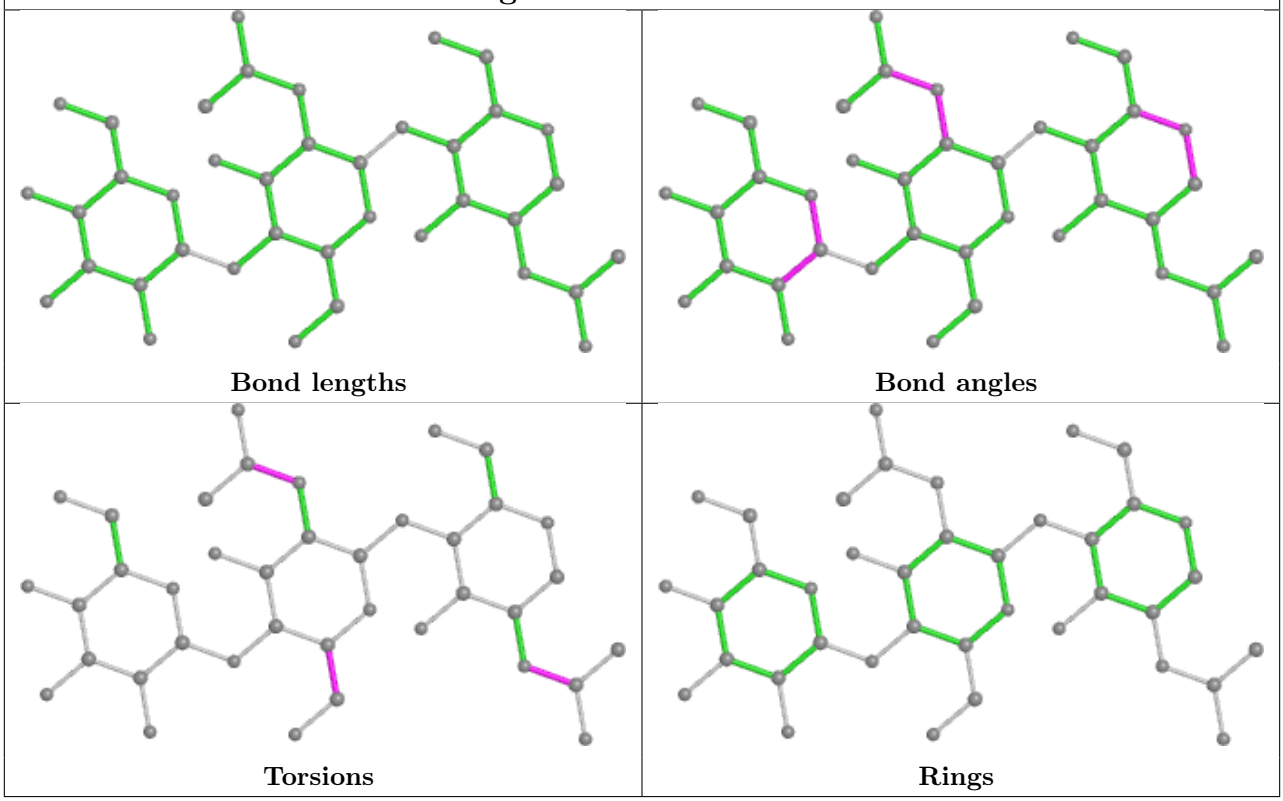
Oligosaccharide Chain i



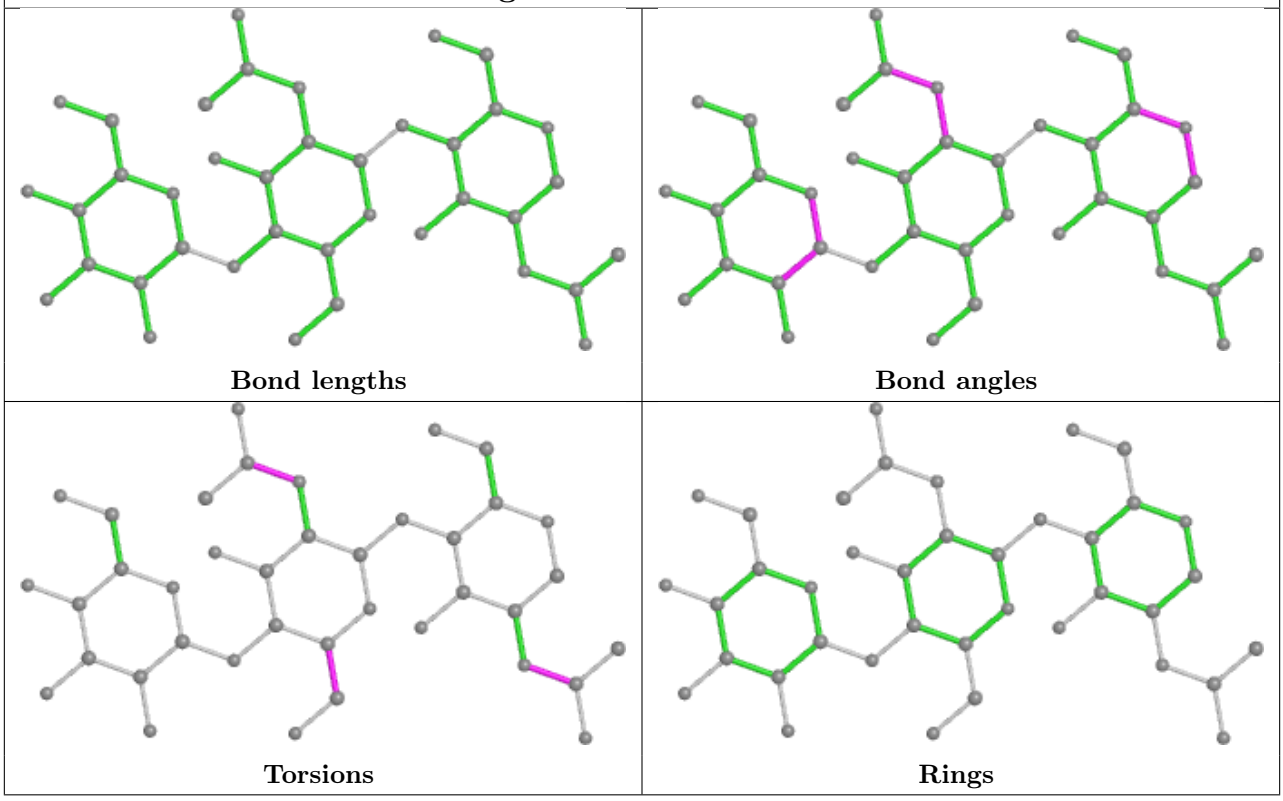
Oligosaccharide Chain j



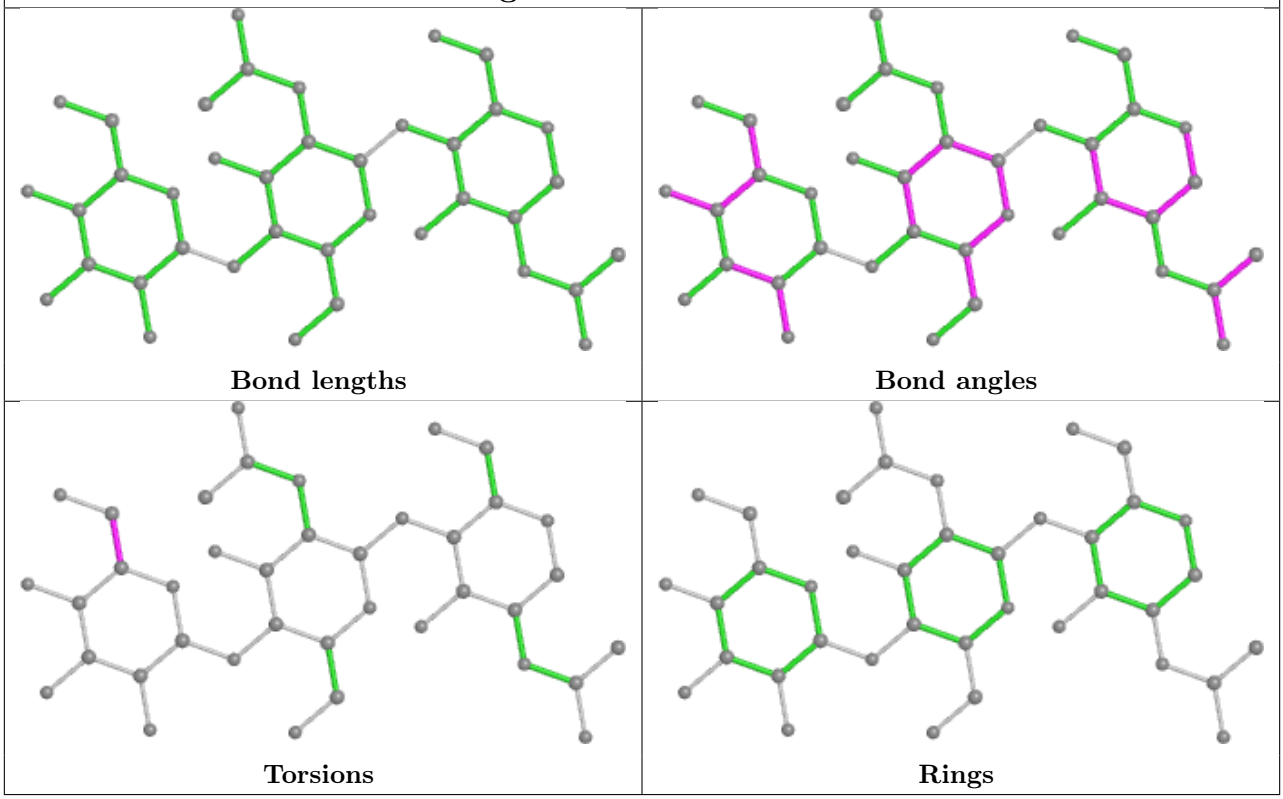
Oligosaccharide Chain k



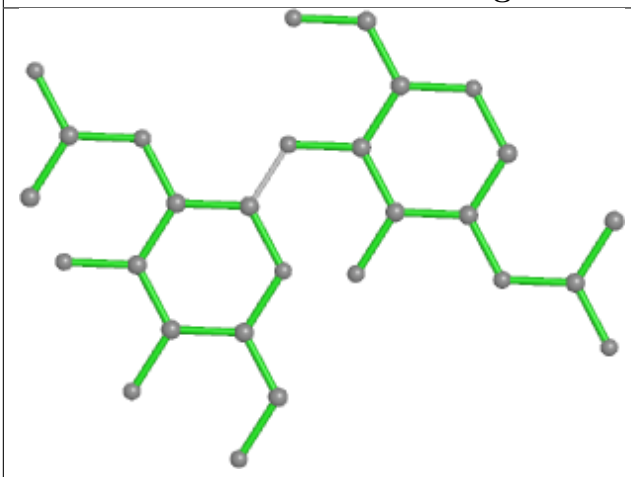
Oligosaccharide Chain n



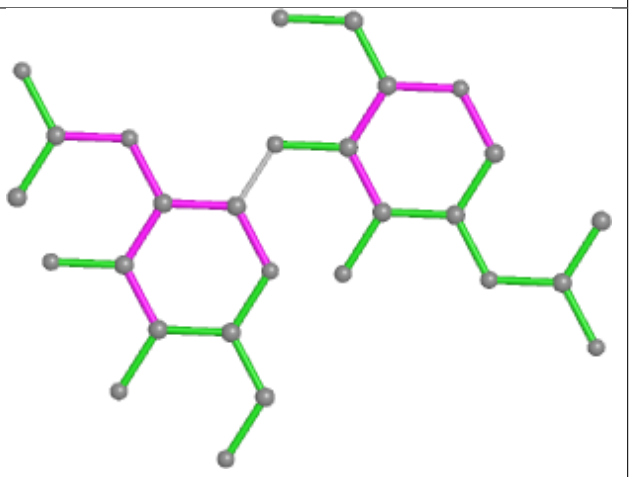
Oligosaccharide Chain o



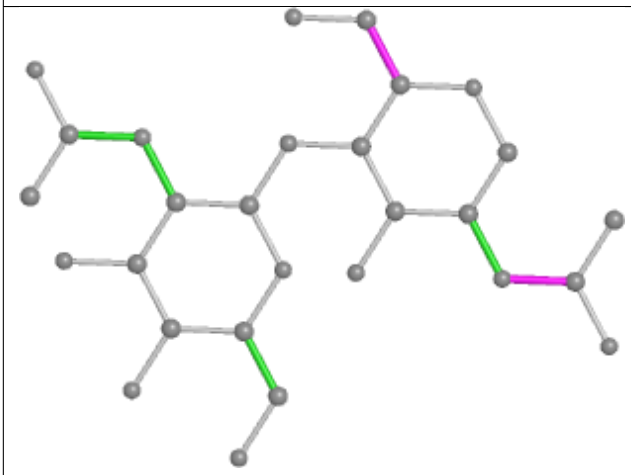
Oligosaccharide Chain N



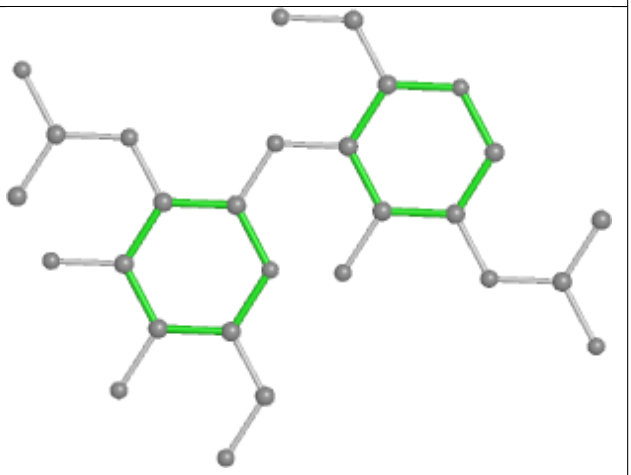
Bond lengths



Bond angles

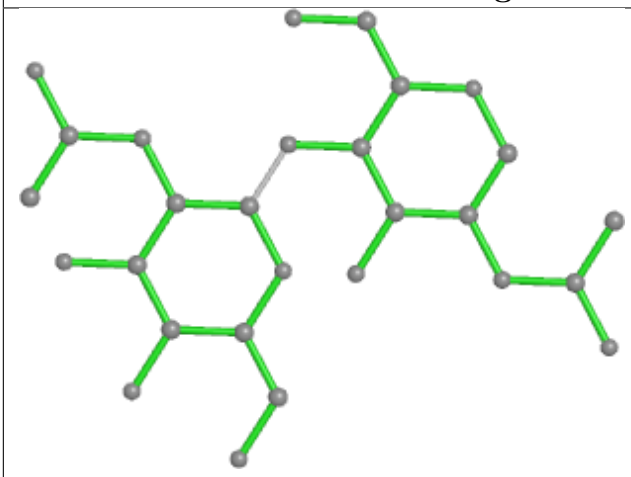


Torsions

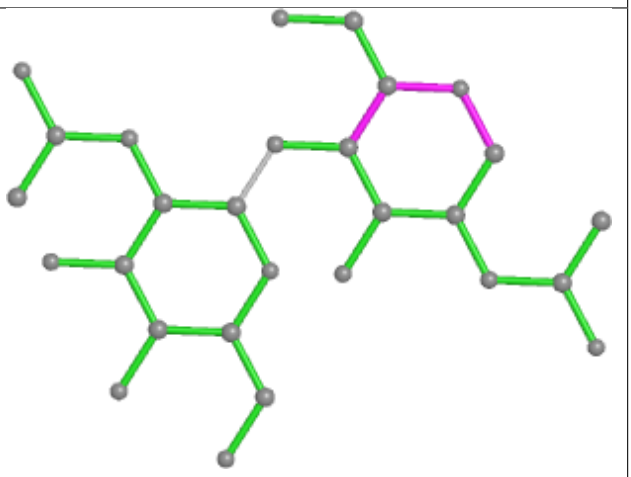


Rings

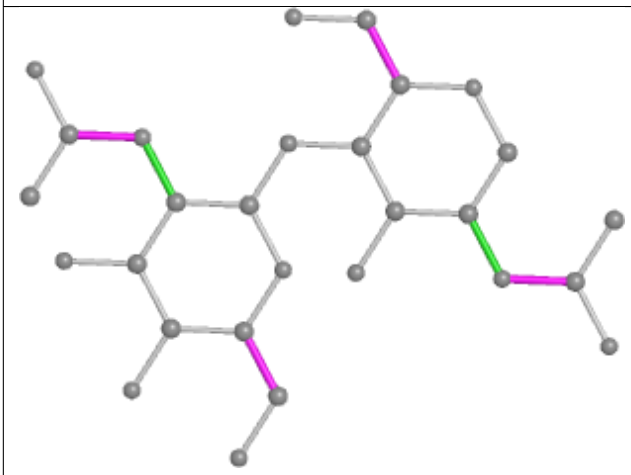
Oligosaccharide Chain O



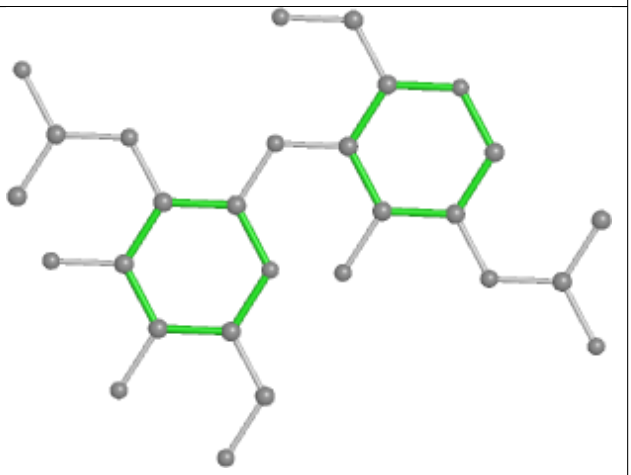
Bond lengths



Bond angles

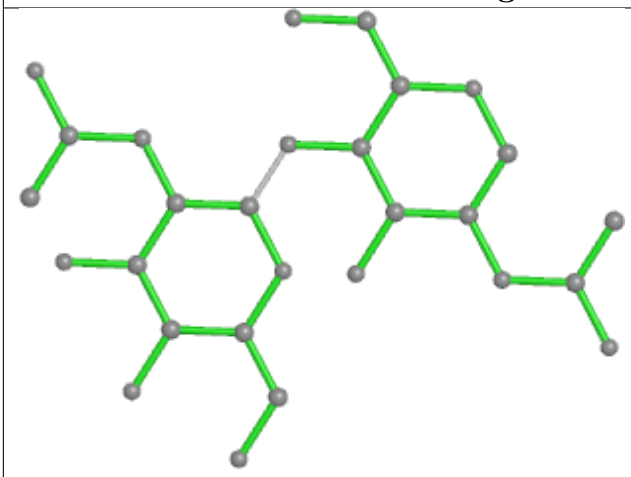


Torsions

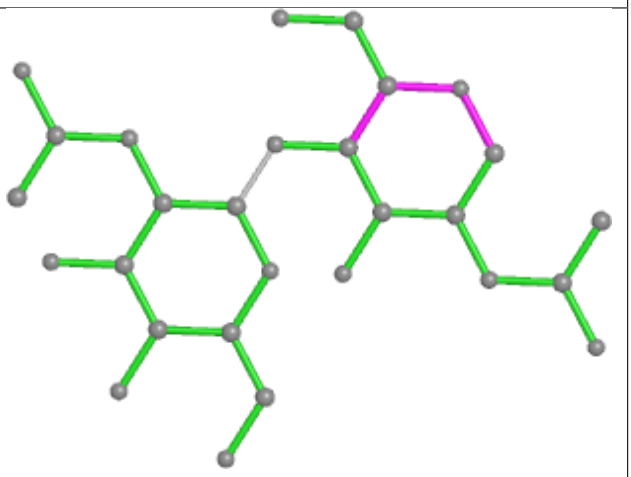


Rings

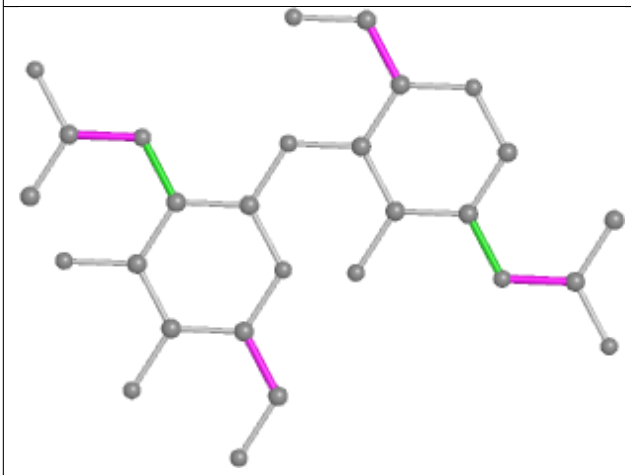
Oligosaccharide Chain S



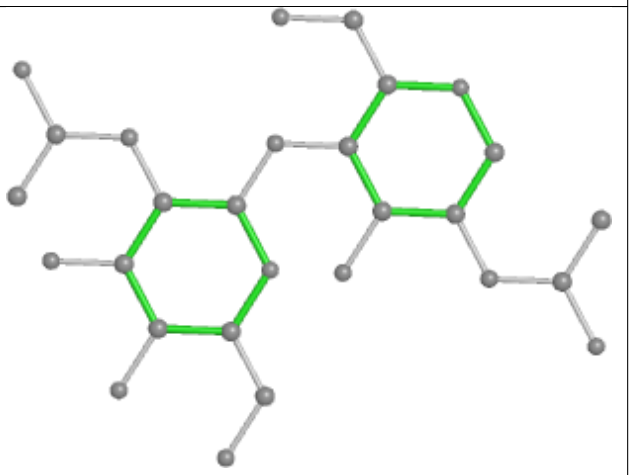
Bond lengths



Bond angles

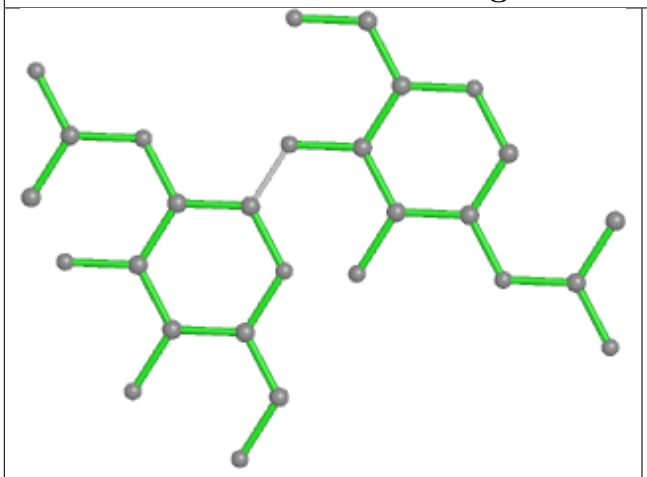


Torsions

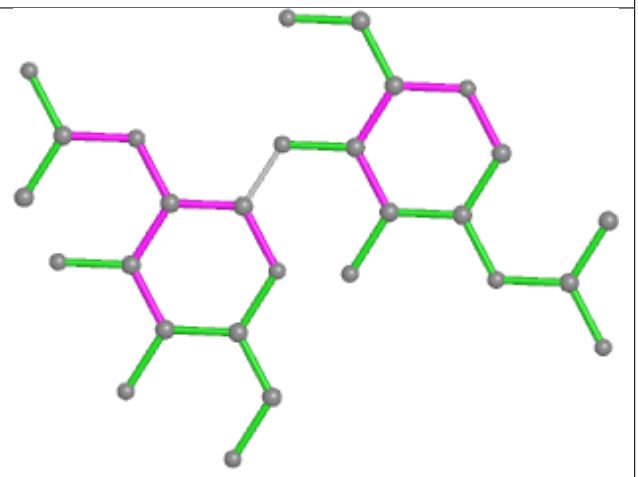


Rings

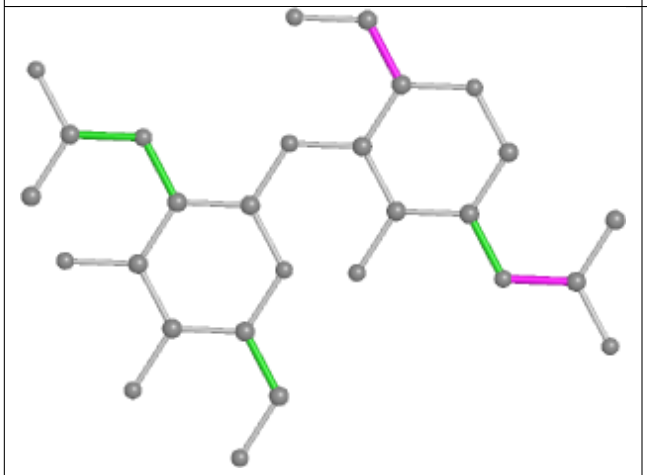
Oligosaccharide Chain W



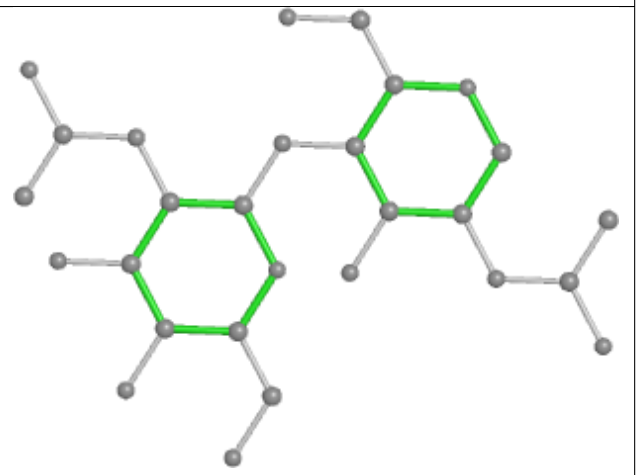
Bond lengths



Bond angles

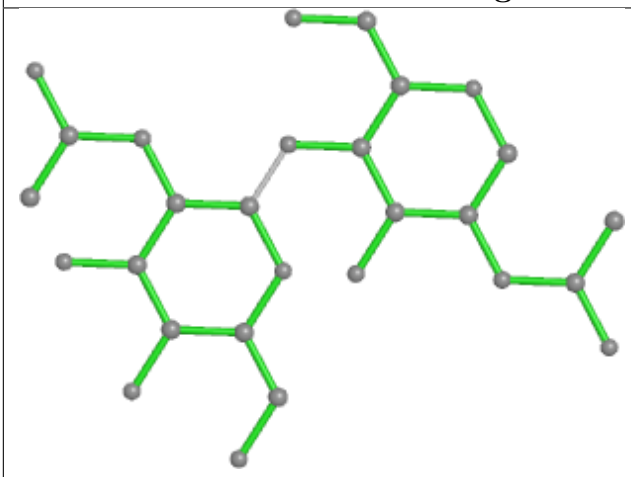


Torsions

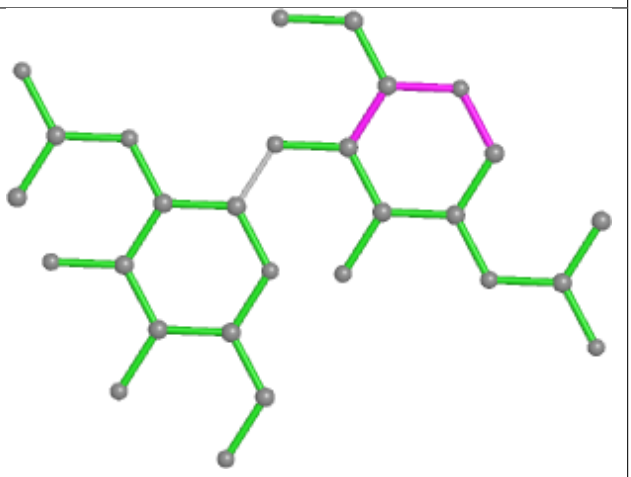


Rings

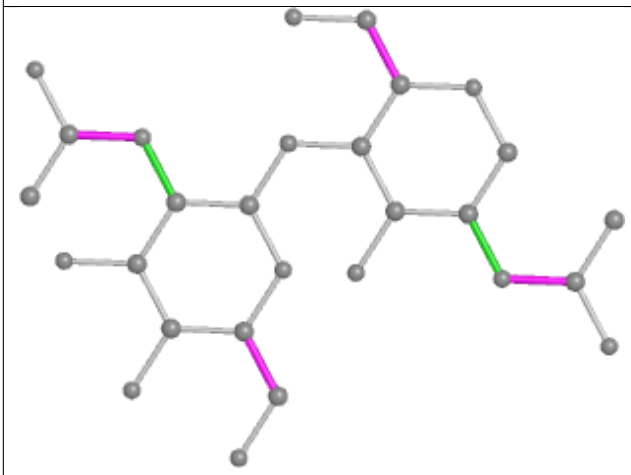
Oligosaccharide Chain X



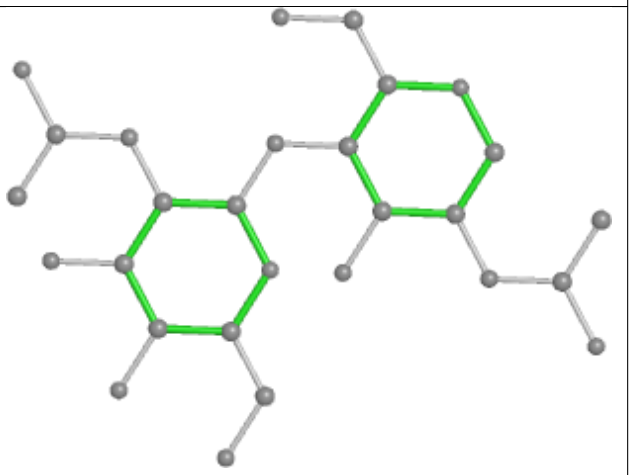
Bond lengths



Bond angles

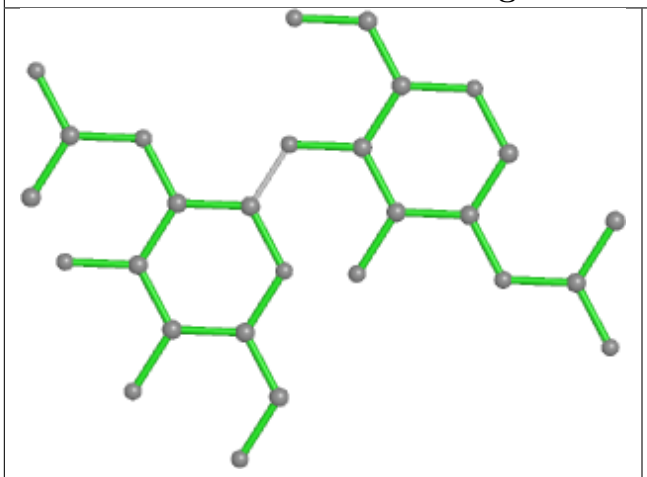


Torsions

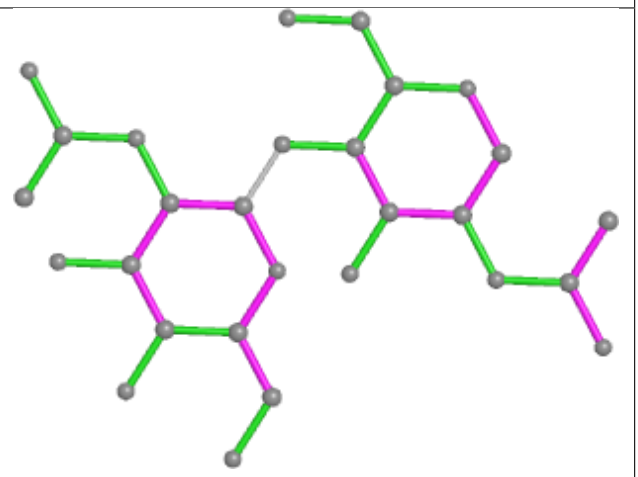


Rings

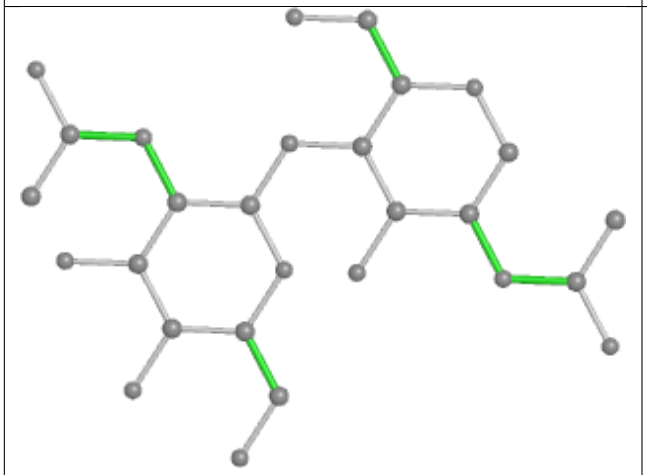
Oligosaccharide Chain b



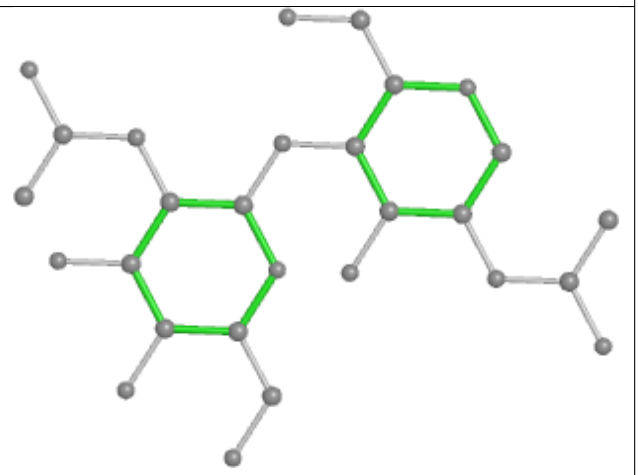
Bond lengths



Bond angles

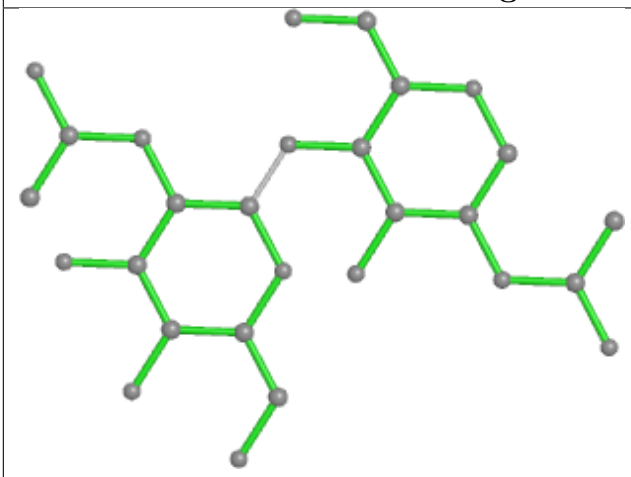


Torsions

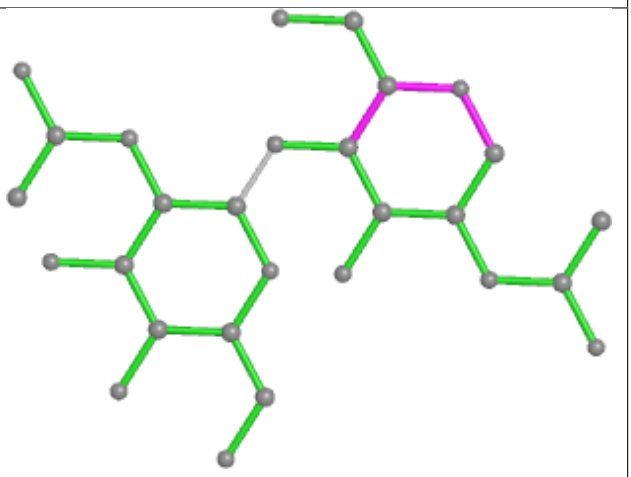


Rings

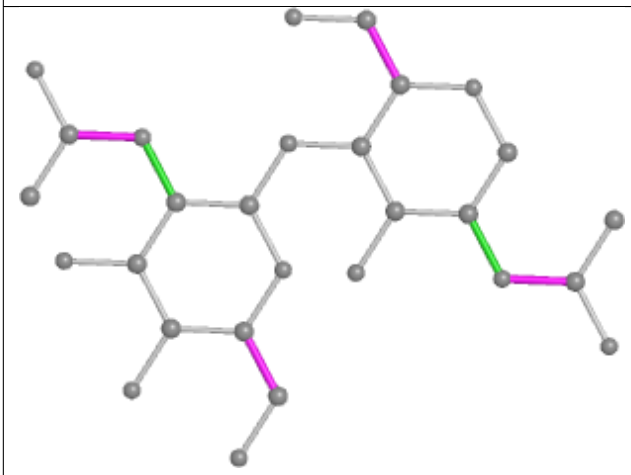
Oligosaccharide Chain c



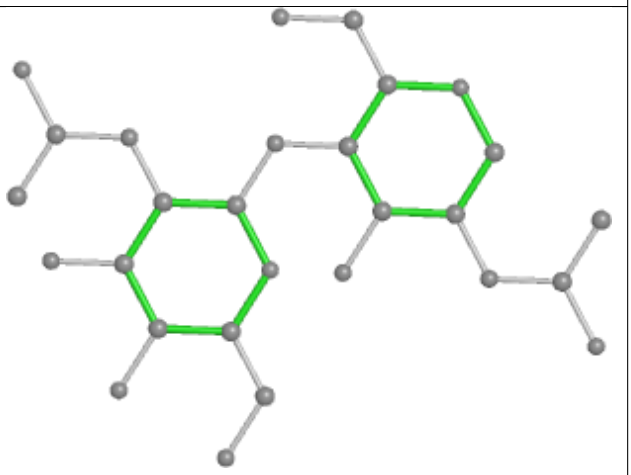
Bond lengths



Bond angles

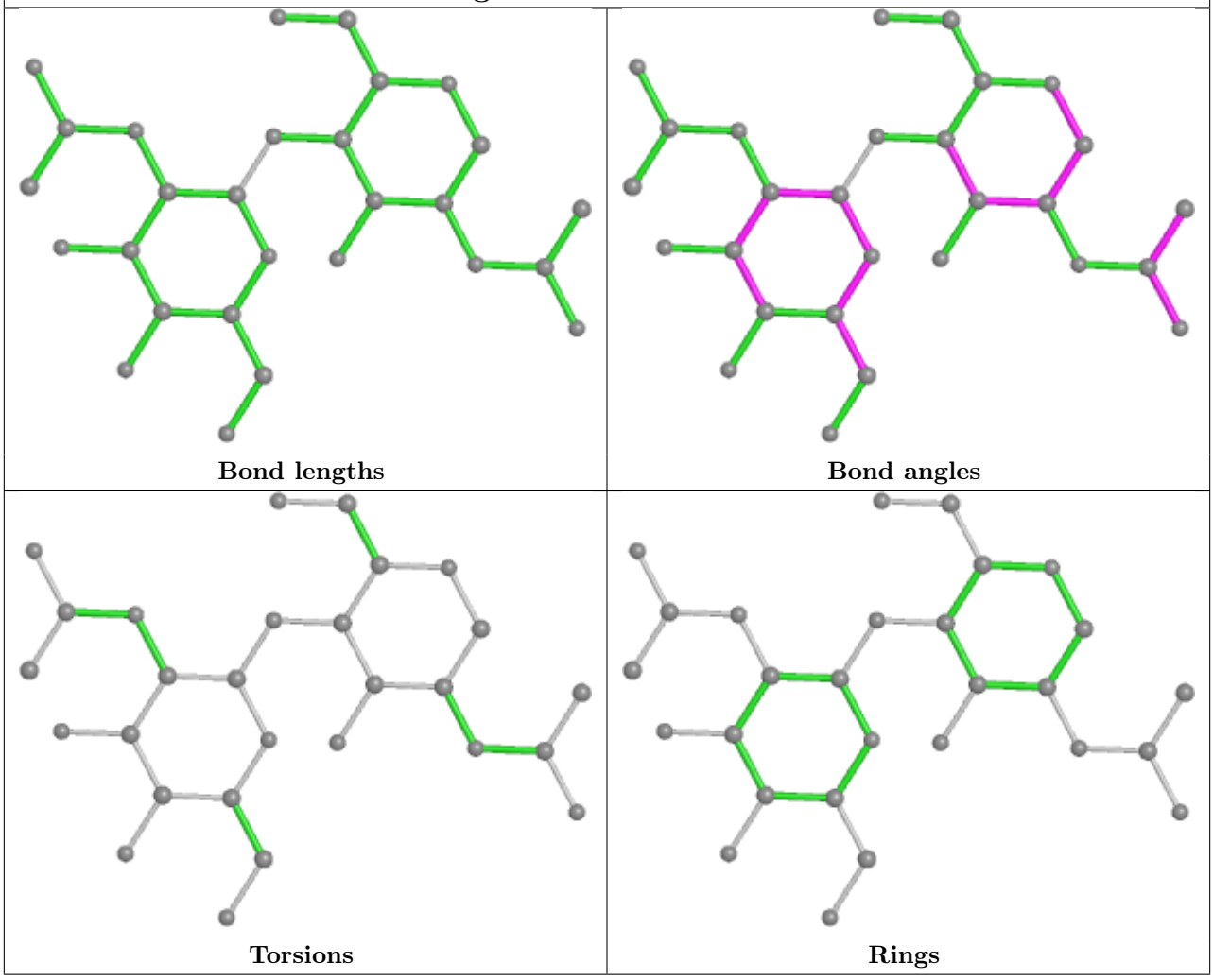


Torsions

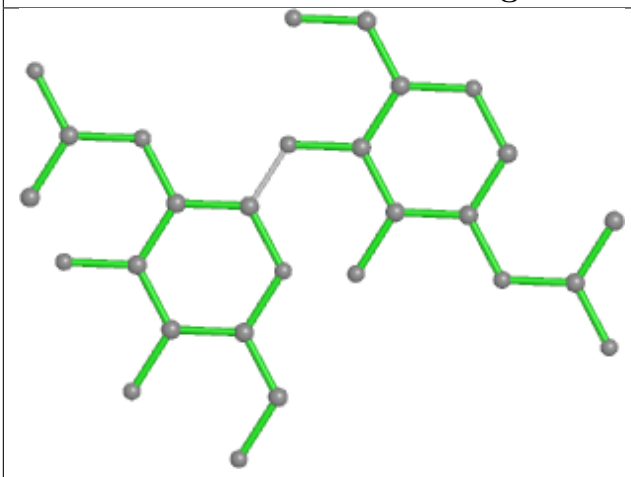


Rings

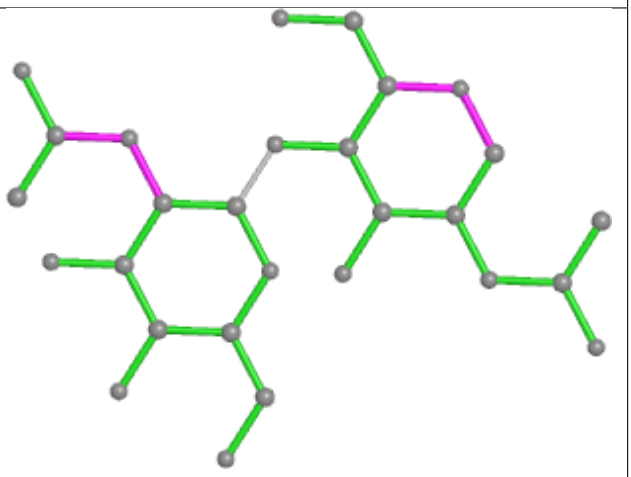
Oligosaccharide Chain e



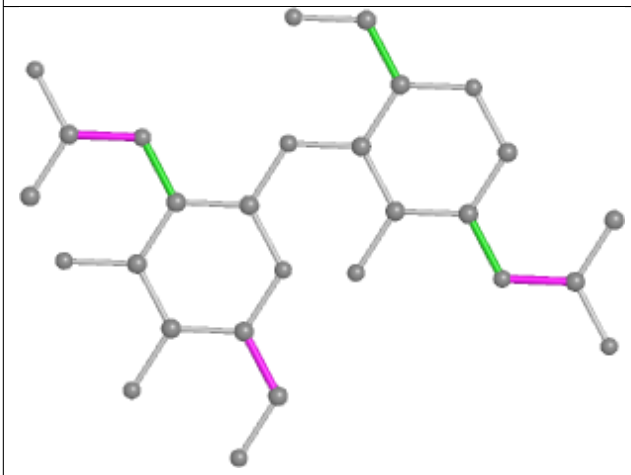
Oligosaccharide Chain f



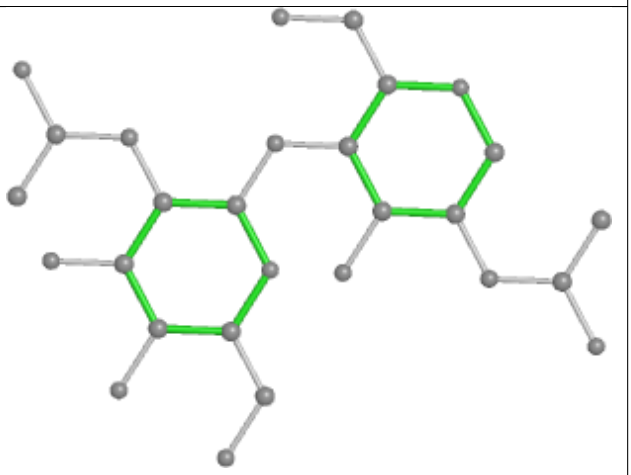
Bond lengths



Bond angles

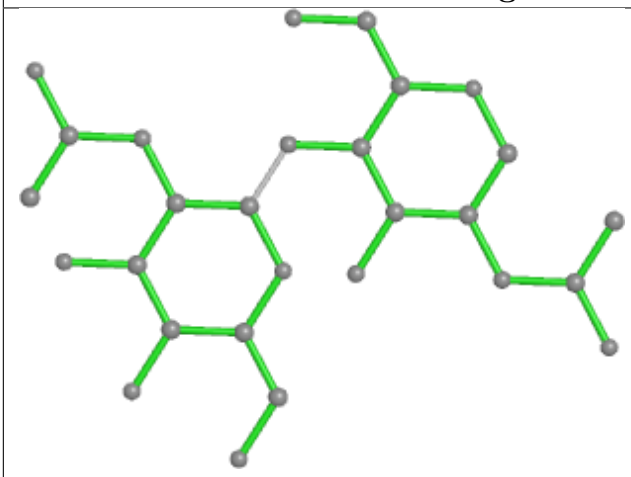


Torsions

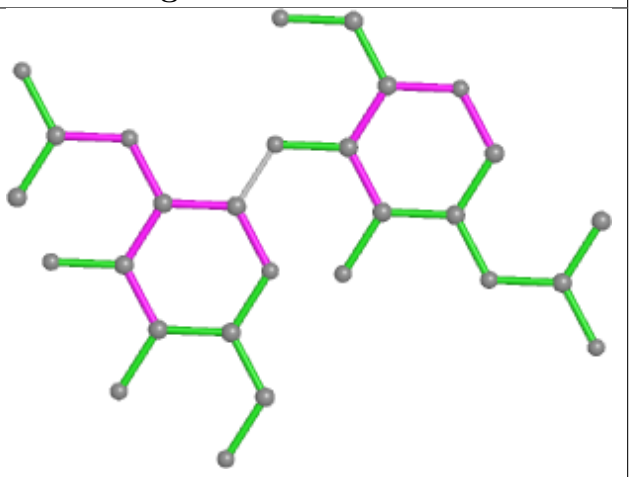


Rings

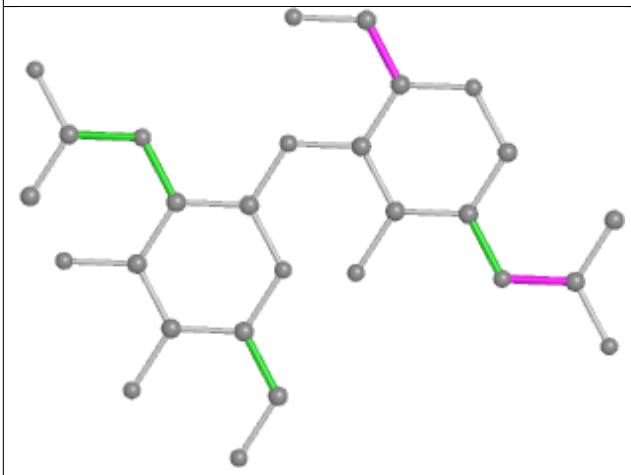
Oligosaccharide Chain g



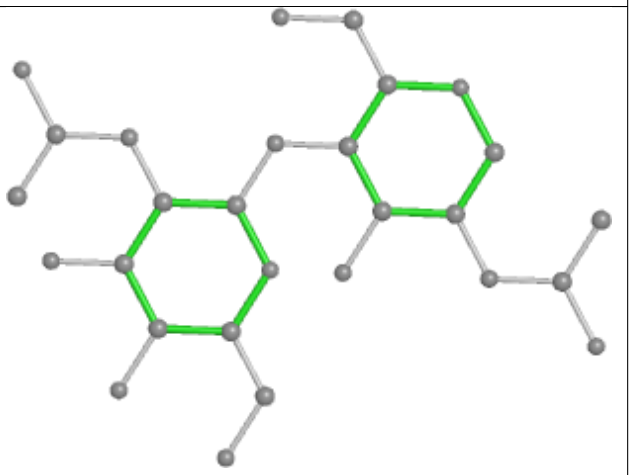
Bond lengths



Bond angles

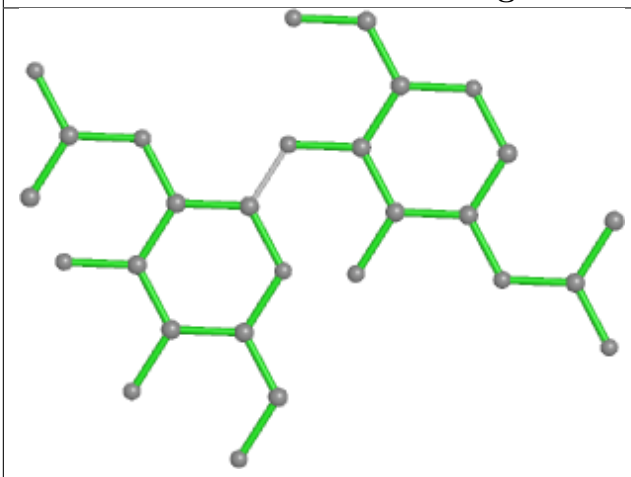


Torsions

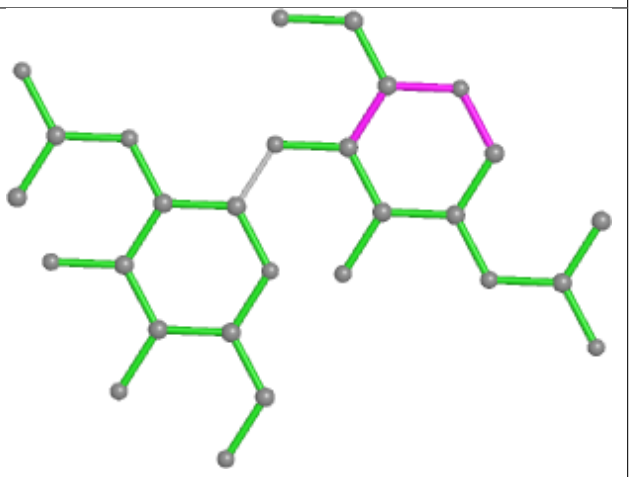


Rings

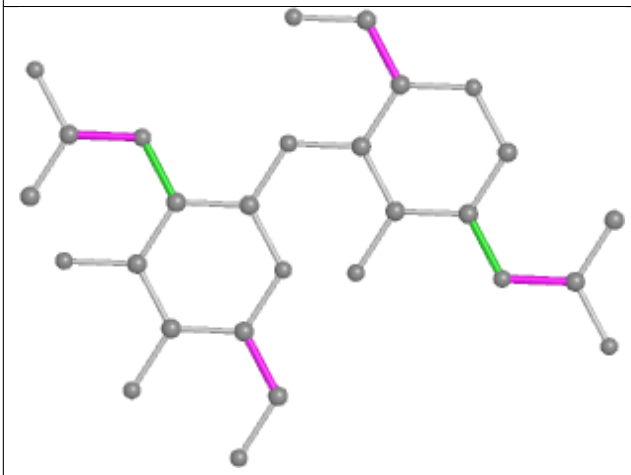
Oligosaccharide Chain h



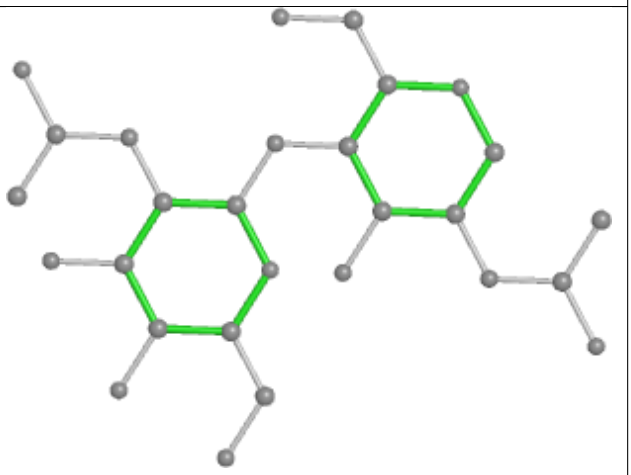
Bond lengths



Bond angles

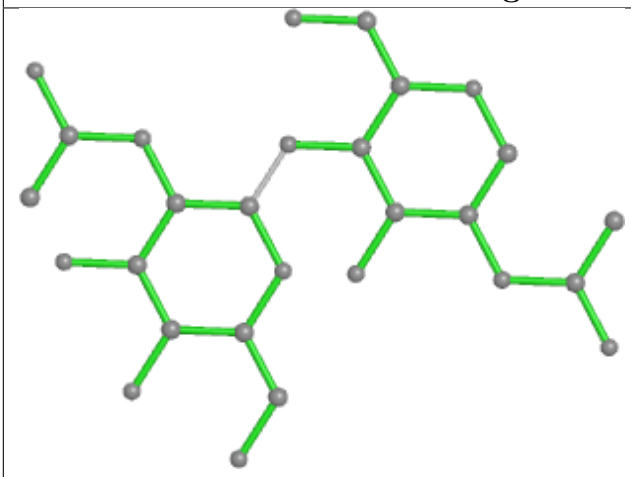


Torsions

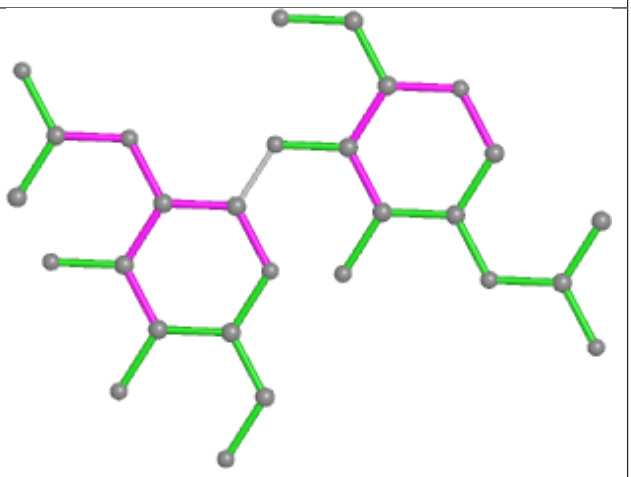


Rings

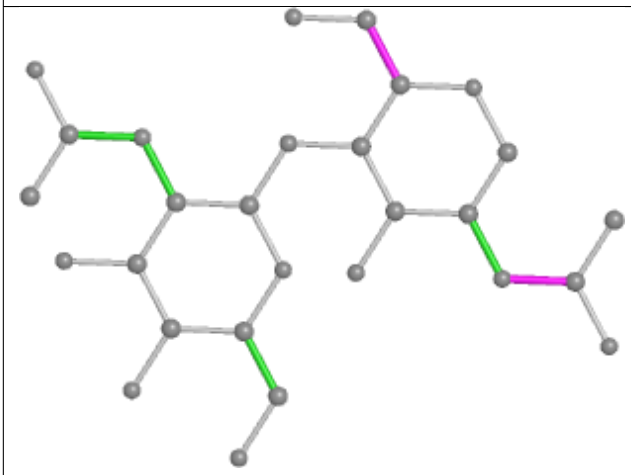
Oligosaccharide Chain l



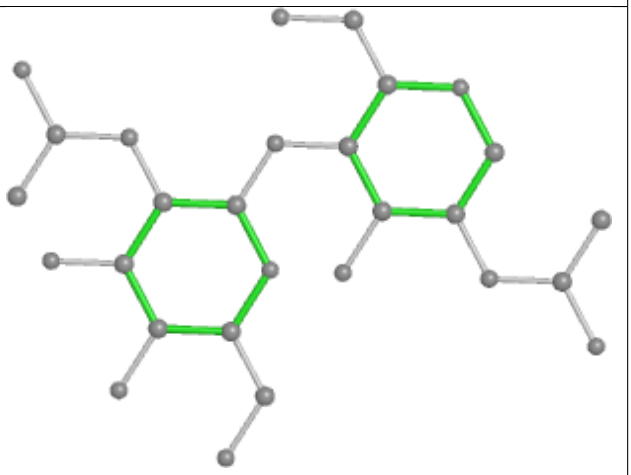
Bond lengths



Bond angles

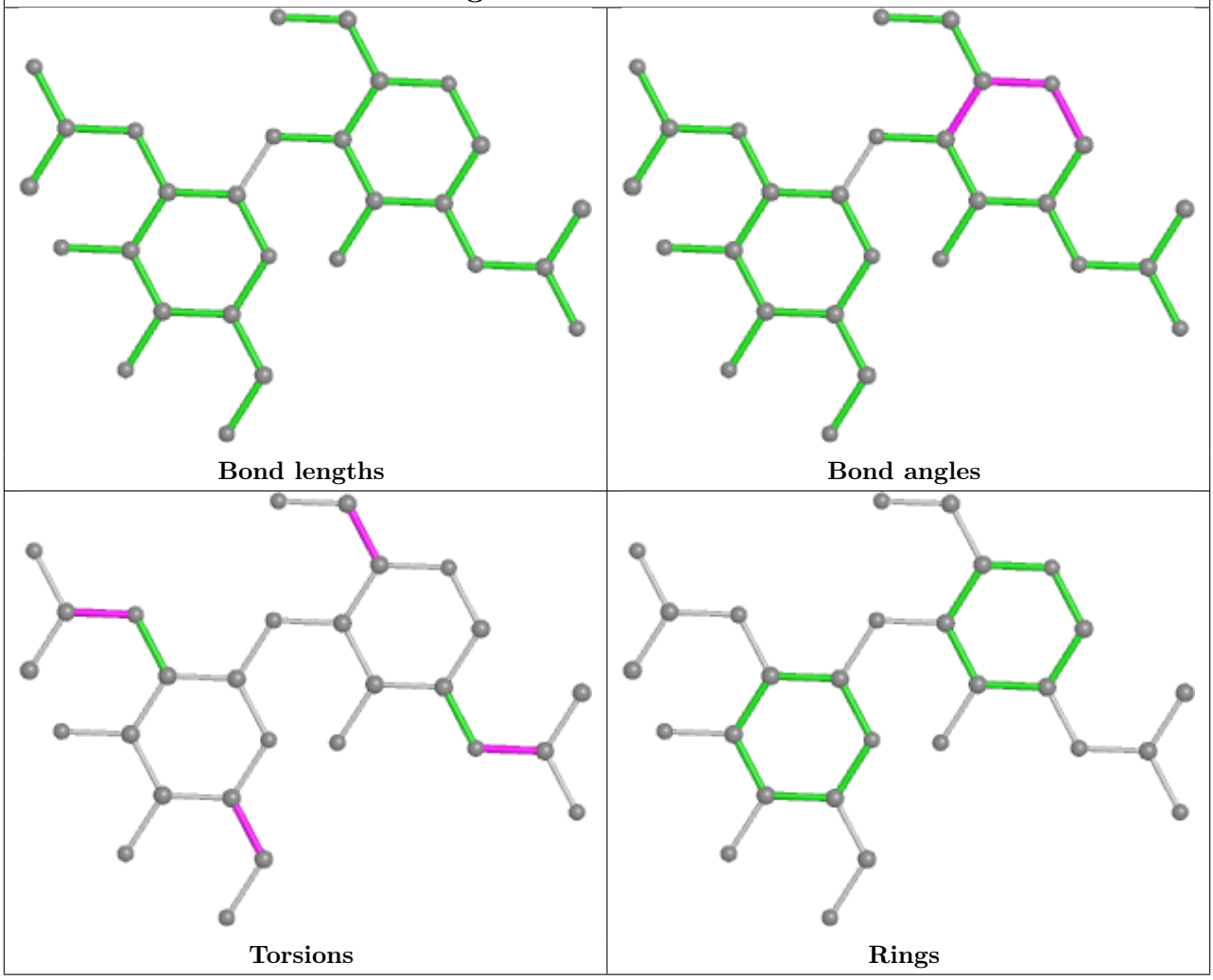


Torsions



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.

All (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
5	A	411	NAG	O5-C5-C6	2.57	111.24	107.20
5	G	411	NAG	O5-C5-C6	2.57	111.23	107.20
5	I	410	NAG	O5-C5-C6	2.56	111.22	107.20
5	C	414	NAG	C1-O5-C5	2.46	115.53	112.19
5	E	415	NAG	C1-O5-C5	2.45	115.51	112.19
5	A	415	NAG	C1-O5-C5	2.44	115.50	112.19
5	K	414	NAG	C1-O5-C5	2.44	115.50	112.19
5	G	414	NAG	C1-O5-C5	2.44	115.50	112.19
5	I	414	NAG	C1-O5-C5	2.43	115.48	112.19
5	C	404	NAG	O5-C5-C4	2.42	116.71	110.83
5	J	600	NAG	O5-C1-C2	-2.30	107.66	111.29
5	F	600	NAG	O5-C1-C2	-2.29	107.67	111.29
5	B	600	NAG	O5-C1-C2	-2.29	107.67	111.29
5	H	600	NAG	O5-C1-C2	-2.28	107.69	111.29
5	D	600	NAG	O5-C1-C2	-2.28	107.69	111.29
5	C	404	NAG	C3-C4-C5	2.23	114.22	110.24

There are no chirality outliers.

All (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
5	F	600	NAG	C8-C7-N2-C2
5	H	600	NAG	C8-C7-N2-C2
5	J	600	NAG	C8-C7-N2-C2
5	B	600	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	D	600	NAG	O7-C7-N2-C2
5	F	600	NAG	O7-C7-N2-C2
5	H	600	NAG	O7-C7-N2-C2
5	J	600	NAG	O7-C7-N2-C2
5	A	415	NAG	C8-C7-N2-C2
5	E	415	NAG	C8-C7-N2-C2
5	G	414	NAG	C8-C7-N2-C2
5	K	414	NAG	C8-C7-N2-C2
5	C	414	NAG	C8-C7-N2-C2
5	I	414	NAG	C8-C7-N2-C2
5	A	415	NAG	O7-C7-N2-C2
5	G	414	NAG	O7-C7-N2-C2
5	I	414	NAG	O7-C7-N2-C2
5	C	414	NAG	O7-C7-N2-C2
5	E	415	NAG	O7-C7-N2-C2
5	K	414	NAG	O7-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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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

All (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
2	L	361	TRP	4.8
2	F	381	VAL	4.7
2	D	361	TRP	4.7
2	H	383	ALA	4.3
2	F	516	SER	4.3
2	H	503	THR	4.3

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Mol	Chain	Res	Type	RSRZ
2	J	381	VAL	4.2
2	D	381	VAL	4.1
2	L	488	LYS	4.1
2	D	382	ALA	4.1
1	K	180	GLU	4.1
2	H	516	SER	4.1
2	F	514	PHE	4.0
2	L	374	HIS	4.0
1	C	2	ARG	4.0
2	H	366	ALA	3.9
2	L	383	ALA	3.9
2	F	479	GLU	3.8
1	C	28	GLY	3.8
2	J	516	SER	3.8
2	D	373	SER	3.7
2	J	371	TYR	3.7
2	F	507	GLY	3.6
2	H	504	PHE	3.5
2	D	374	HIS	3.5
2	H	374	HIS	3.5
2	L	511	LEU	3.4
1	K	218	THR	3.4
2	F	363	GLY	3.4
2	H	371	TYR	3.4
1	I	11	ASN	3.4
2	L	371	TYR	3.4
2	J	512	PRO	3.4
2	B	503	THR	3.4
2	D	379	VAL	3.3
2	B	367	GLY	3.3
1	K	252	SER	3.3
2	D	368	TRP	3.2
2	B	382	ALA	3.2
2	B	508	GLU	3.2
1	K	3	ILE	3.1
2	D	371	TYR	3.1
1	A	180	GLU	3.1
2	L	473	LEU	3.1
1	A	338	ALA	3.1
2	H	365	ILE	3.1
2	D	516	SER	3.1
2	B	369	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	384	ASP	3.0
2	H	494	THR	3.0
2	L	372	THR	3.0
2	L	494	THR	3.0
1	G	319	PRO	3.0
2	F	375	GLY	2.9
1	K	11	ASN	2.9
1	K	283	SER	2.8
2	J	366	ALA	2.8
1	C	289	GLU	2.8
2	F	382	ALA	2.8
2	D	515	ASP	2.8
2	J	379	VAL	2.8
2	L	368	TRP	2.8
1	K	201	LEU	2.8
1	K	193	ASP	2.8
2	J	348	GLY	2.7
2	B	371	TYR	2.7
2	L	476	SER	2.7
2	L	376	ALA	2.7
1	I	204	ASP	2.6
2	L	381	VAL	2.6
2	H	488	LYS	2.6
1	C	29	VAL	2.6
1	G	307	TYR	2.6
1	G	163	ASN	2.6
1	E	42	ALA	2.6
1	E	29	VAL	2.6
2	D	490	LYS	2.6
1	A	201	LEU	2.6
1	A	10	SER	2.6
1	G	283	SER	2.6
2	H	512	PRO	2.5
2	H	361	TRP	2.5
2	L	380	ALA	2.5
2	L	375	GLY	2.5
2	H	511	LEU	2.5
2	J	480	ILE	2.5
1	A	289	GLU	2.5
1	C	287	ILE	2.5
2	F	505	ASP	2.5
1	A	218	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	163(C)	ASN	2.4
2	J	374	HIS	2.4
2	L	472	MET	2.4
2	H	498	ARG	2.4
2	H	457	SER	2.4
1	I	197	GLN	2.4
2	F	366	ALA	2.4
2	B	370	GLY	2.4
1	A	293	LEU	2.3
1	E	12	SER	2.3
1	E	252	SER	2.3
1	K	163	ASN	2.3
2	H	509	PHE	2.3
2	B	366	ALA	2.3
2	B	491	CYS	2.3
1	C	40	HIS	2.3
1	E	193	ASP	2.3
1	K	1	ASP	2.3
2	D	367	GLY	2.3
1	E	14	HIS	2.3
2	B	383	ALA	2.3
2	H	381	VAL	2.3
1	K	319	PRO	2.2
2	L	373	SER	2.2
1	A	193	ASP	2.2
2	H	505	ASP	2.2
2	H	363	GLY	2.2
2	J	505	ASP	2.2
1	E	163(C)	ASN	2.2
2	H	460	GLU	2.2
1	G	218	THR	2.2
1	G	315	ILE	2.2
2	F	362	GLU	2.2
2	L	474	GLY	2.2
2	B	515	ASP	2.2
1	K	81	VAL	2.2
2	L	369	HIS	2.2
2	D	369	HIS	2.2
1	A	127	ALA	2.2
1	G	252	SER	2.2
1	E	15	VAL	2.2
1	C	251	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	15	VAL	2.1
1	E	329	ALA	2.1
1	E	300	LEU	2.1
1	C	15	VAL	2.1
1	G	284	LEU	2.1
1	I	201	LEU	2.1
1	A	5	THR	2.1
2	F	361	TRP	2.1
1	A	298	GLY	2.1
2	D	485	PHE	2.1
2	F	513	THR	2.1
2	J	367	GLY	2.1
1	A	252	SER	2.1
2	D	479	GLU	2.1
1	C	331	GLY	2.1
1	K	286	LEU	2.1
1	I	218	THR	2.1
1	A	290	ALA	2.1
1	K	314	ALA	2.1
2	D	380	ALA	2.1
1	G	282	GLY	2.1
1	A	6	GLY	2.0
2	D	505	ASP	2.0
2	J	435	ARG	2.0
2	F	515	ASP	2.0
1	C	42	ALA	2.0
2	H	495	CYS	2.0
1	K	334	TYR	2.0
2	H	489	HIS	2.0
2	F	498	ARG	2.0
2	L	348	GLY	2.0
1	A	41	PHE	2.0

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

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

6.3 Carbohydrates (i)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	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
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

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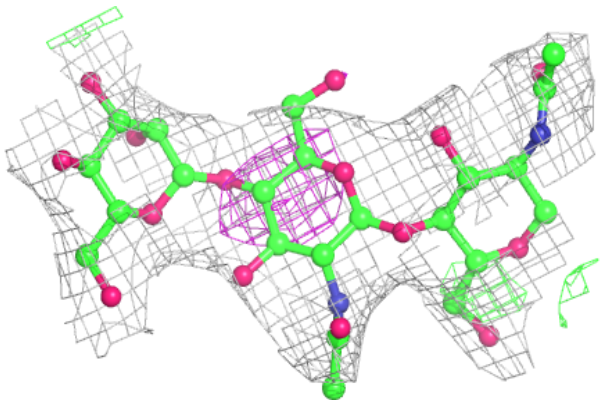
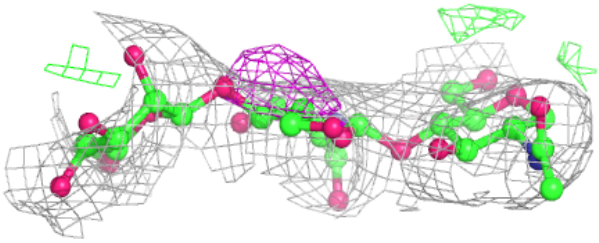
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	Q	1	14/15	0.79	0.31	96,104,110,111	0
3	NAG	i	2	14/15	0.79	0.24	149,162,170,171	0
4	NAG	e	1	14/15	0.79	0.23	104,111,114,115	0
3	NAG	T	1	14/15	0.79	0.32	107,119,128,128	0
4	NAG	m	1	14/15	0.79	0.23	125,137,147,147	0
4	NAG	N	2	14/15	0.79	0.36	106,110,116,120	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

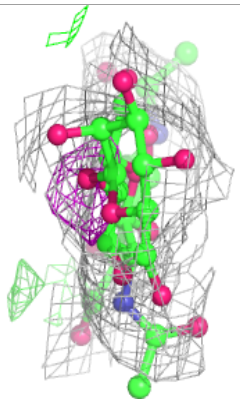
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

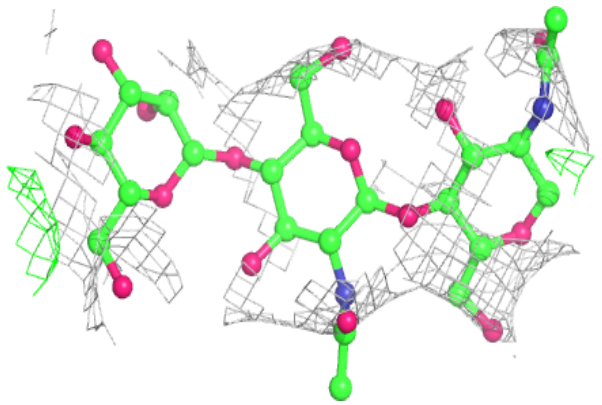


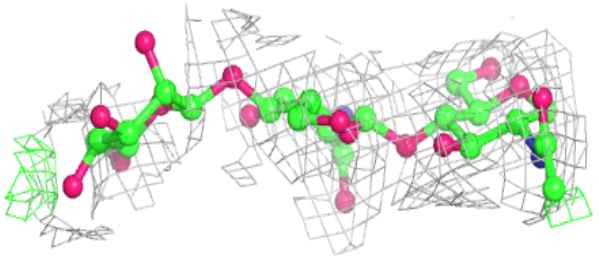


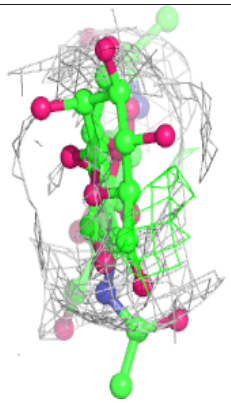


Electron density around Chain P:

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

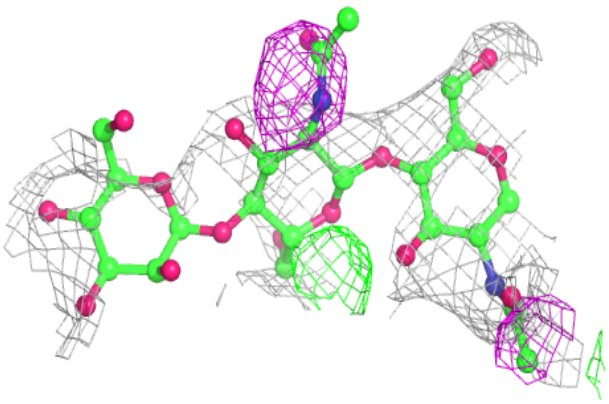


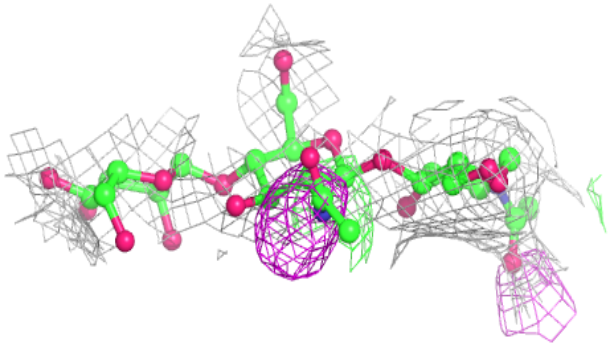




Electron density around Chain Q:

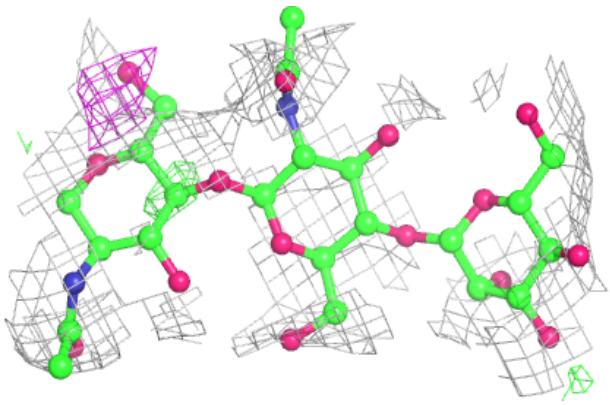
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

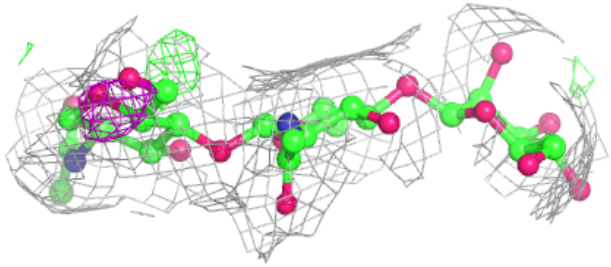


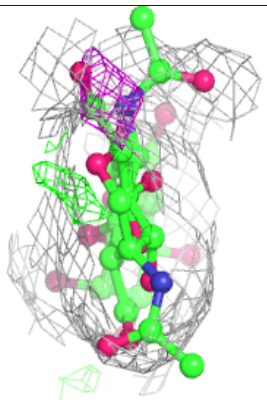


Electron density around Chain R:

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

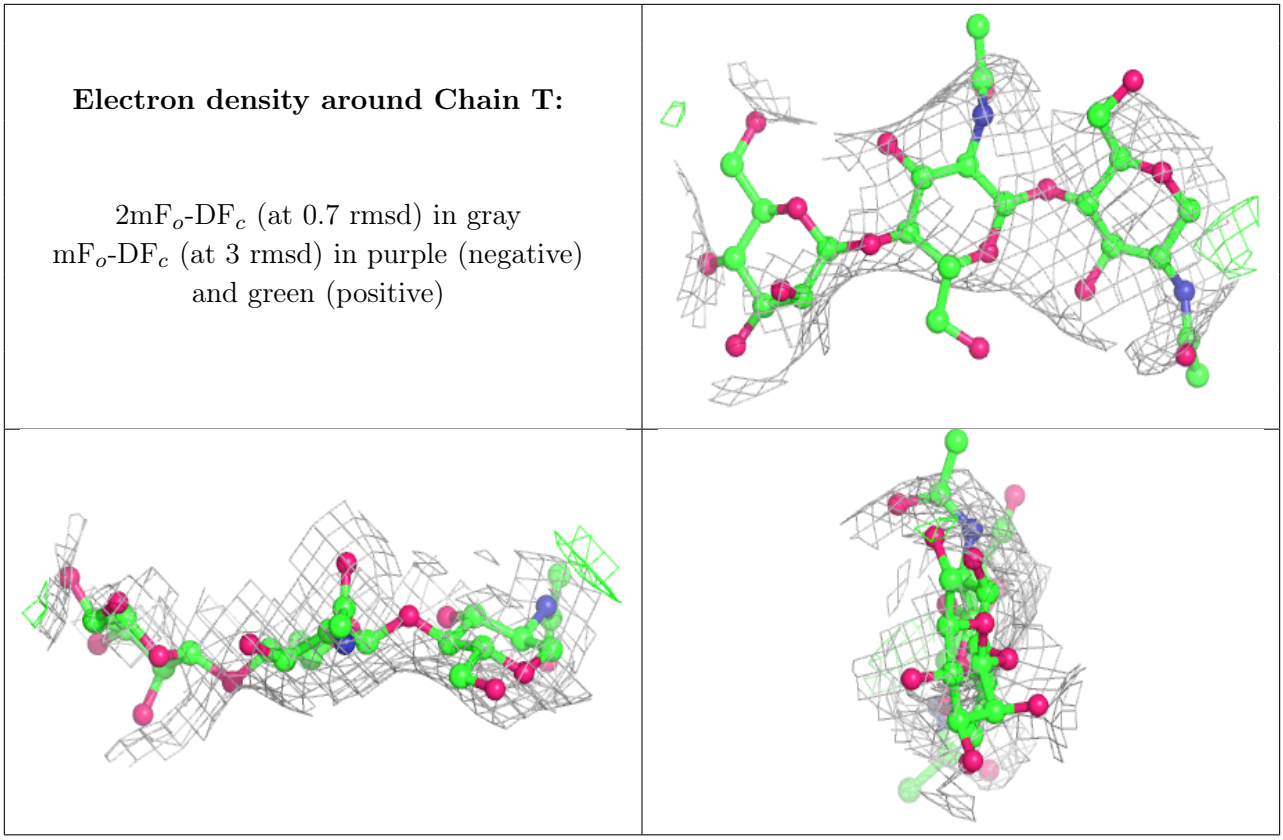






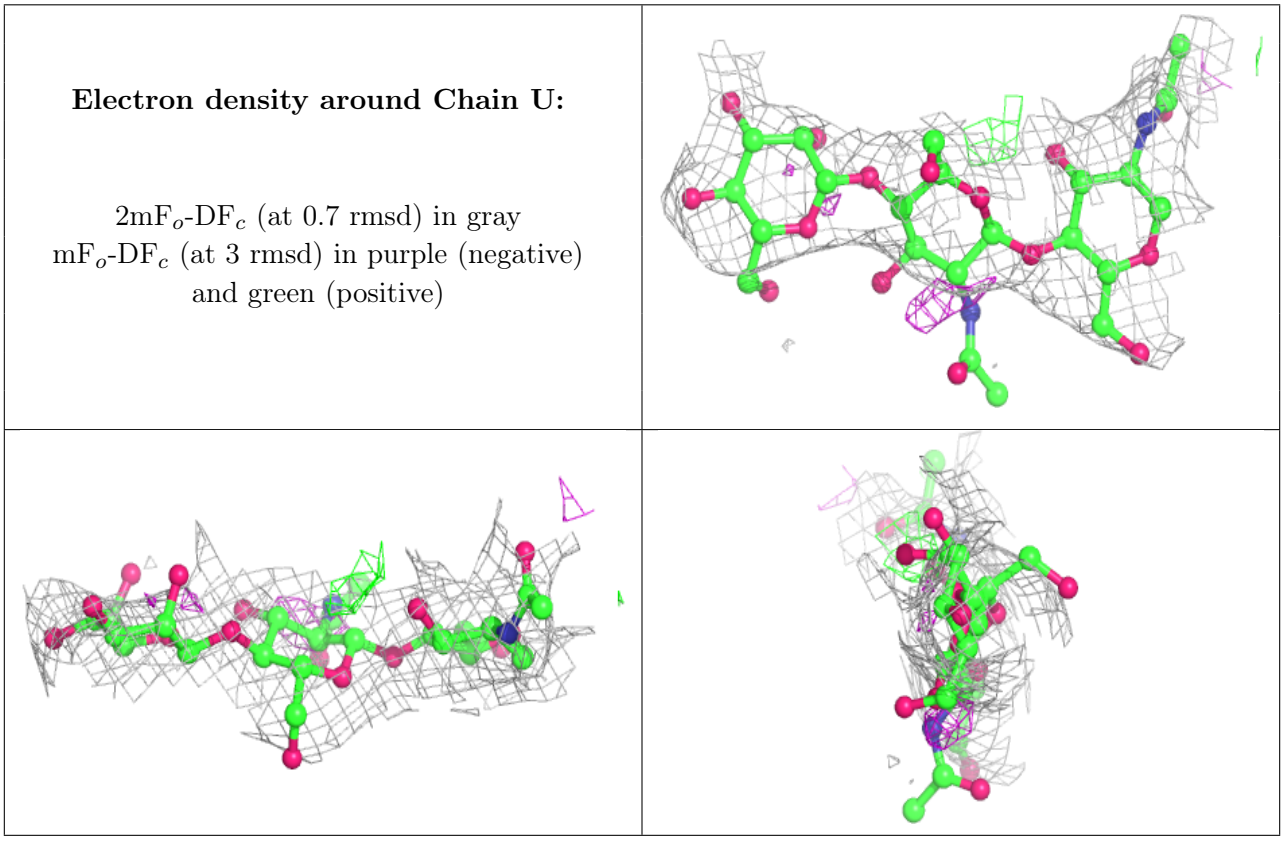
Electron density around Chain T:

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



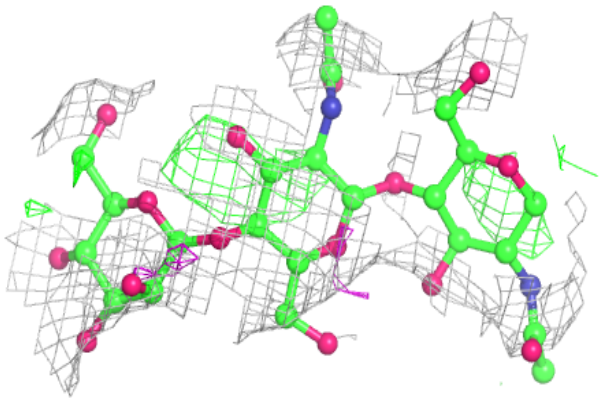
Electron density around Chain U:

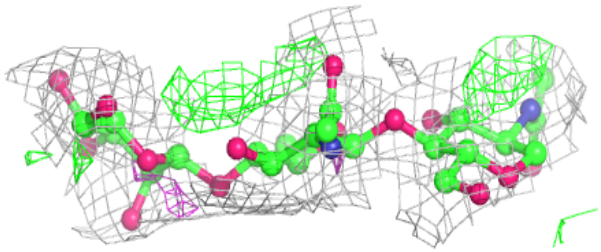
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain V:

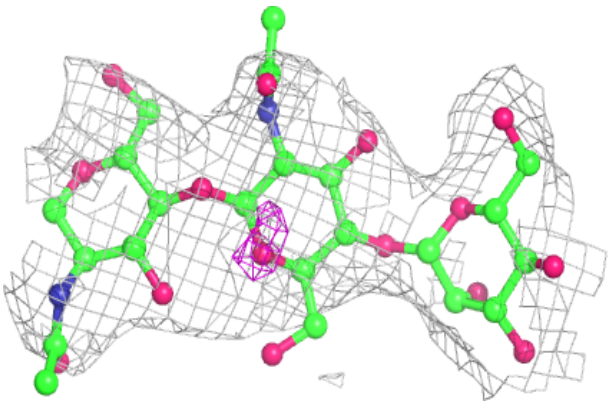
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

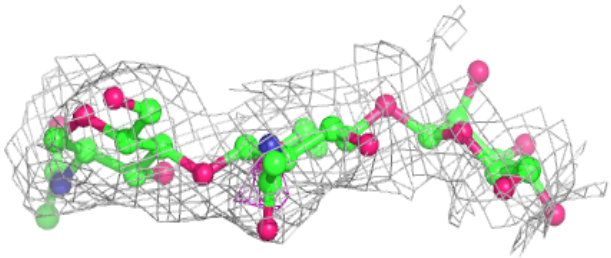


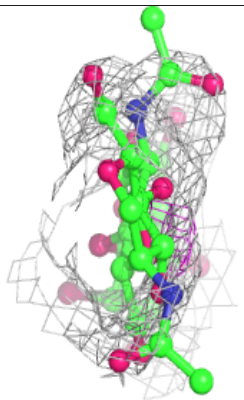


Electron density around Chain Y:

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

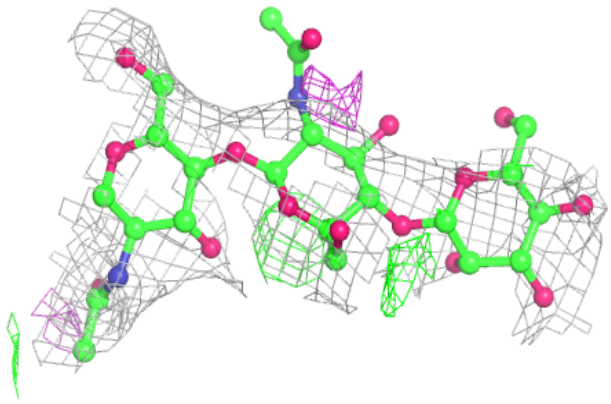


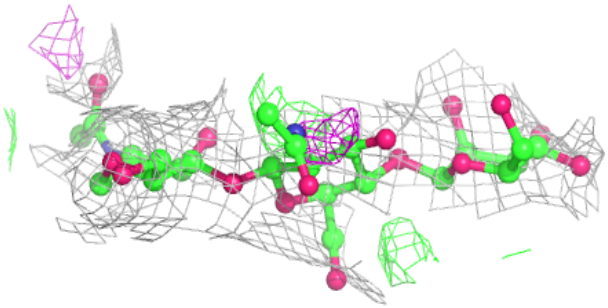


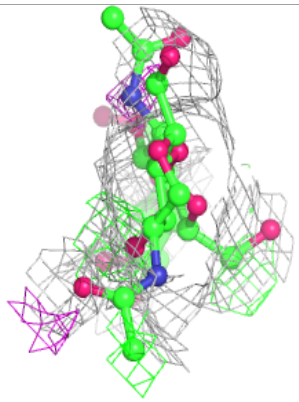


Electron density around Chain Z:

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

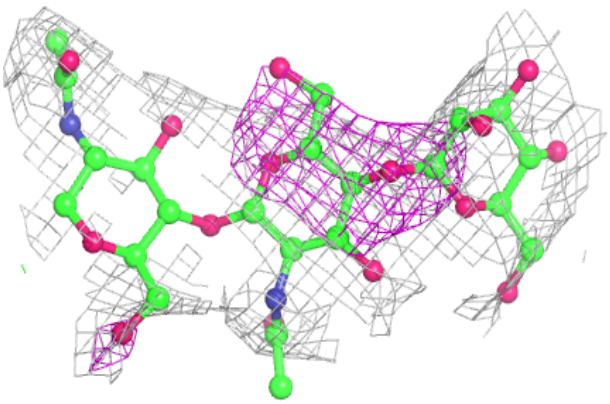


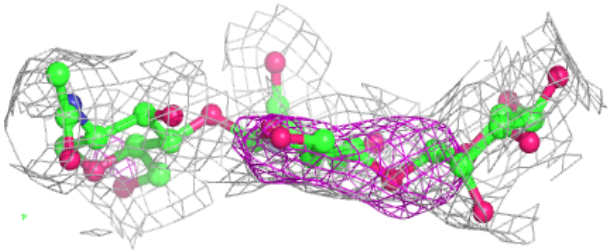


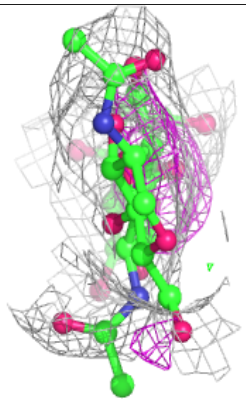


Electron density around Chain a:

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

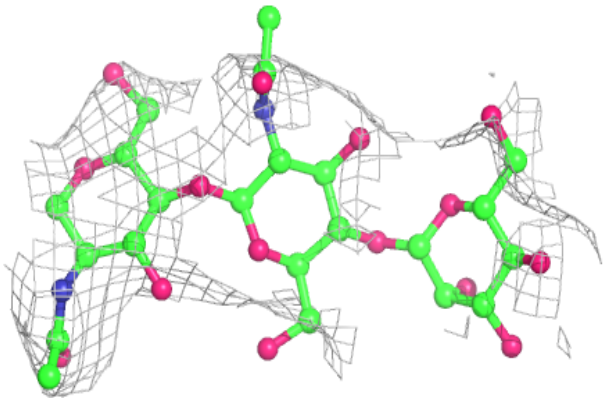


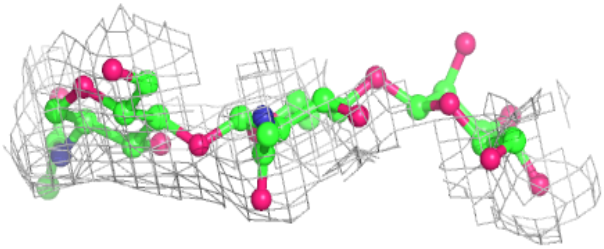


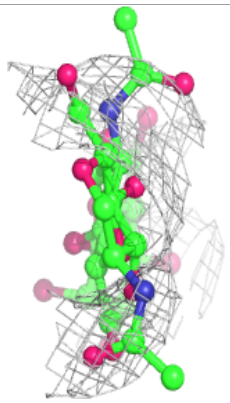


Electron density around Chain d:

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

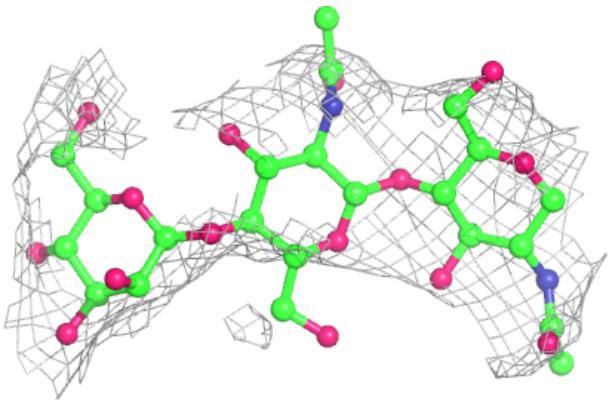


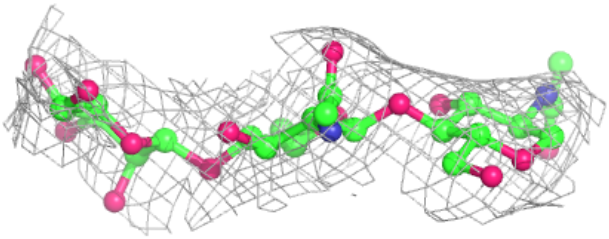


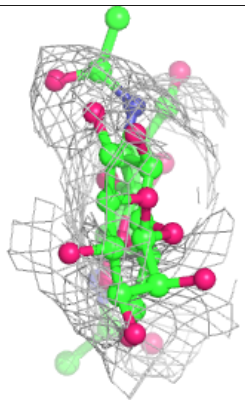


Electron density around Chain i:

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

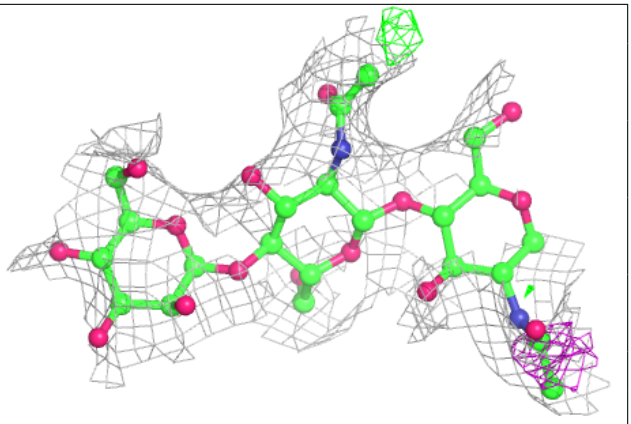


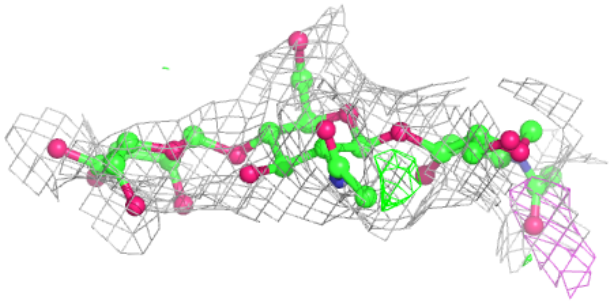


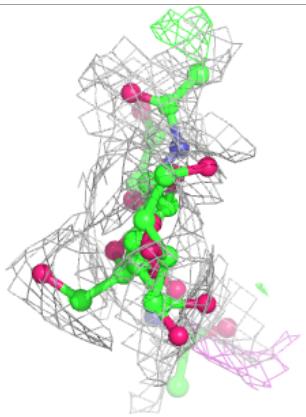


Electron density around Chain j:

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

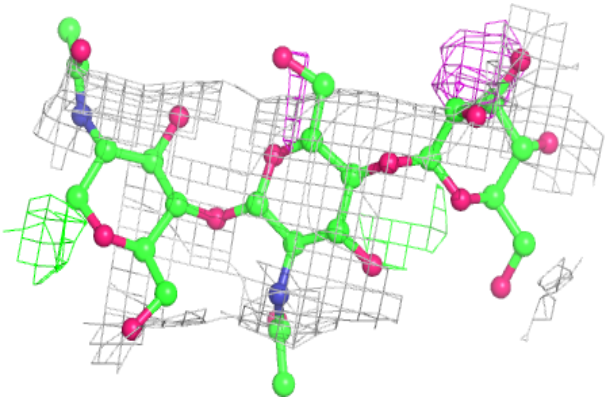


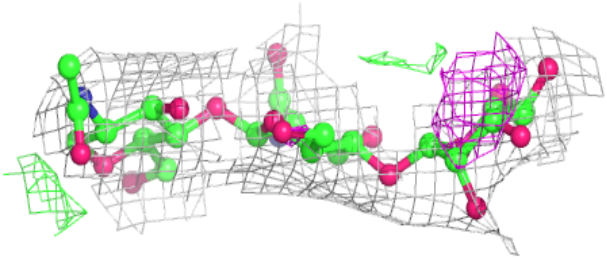


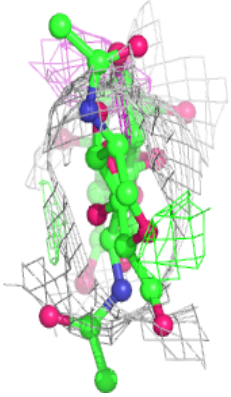


Electron density around Chain k:

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

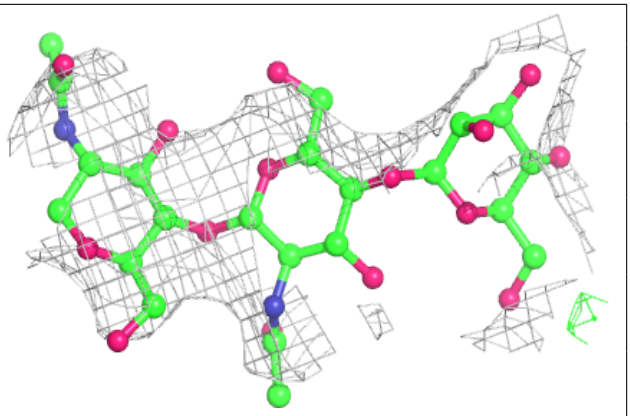


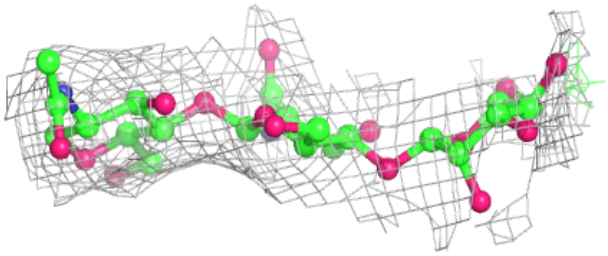


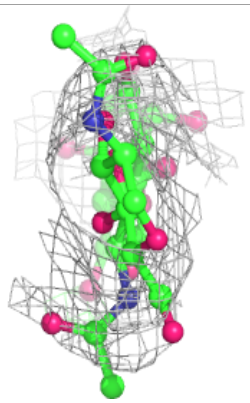


Electron density around Chain n:

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

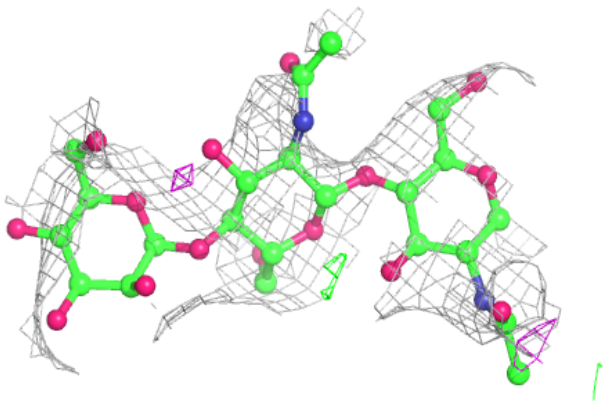


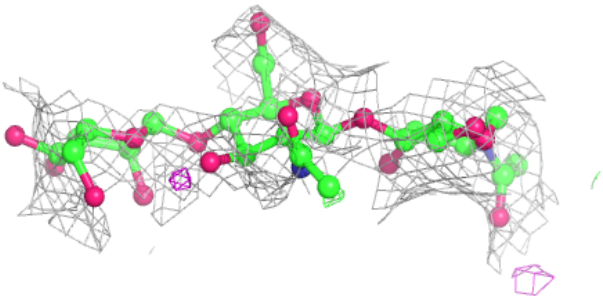


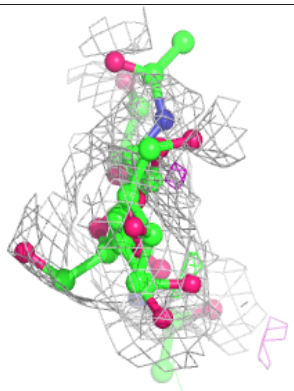


Electron density around Chain o:

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

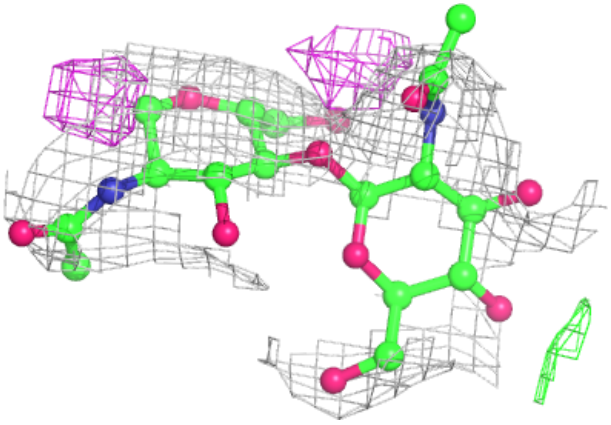


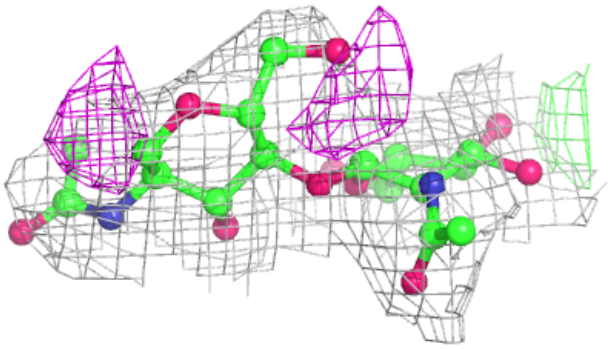


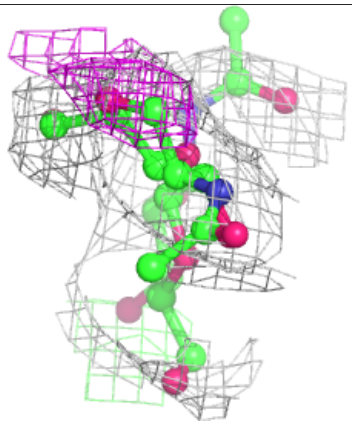


Electron density around Chain N:

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

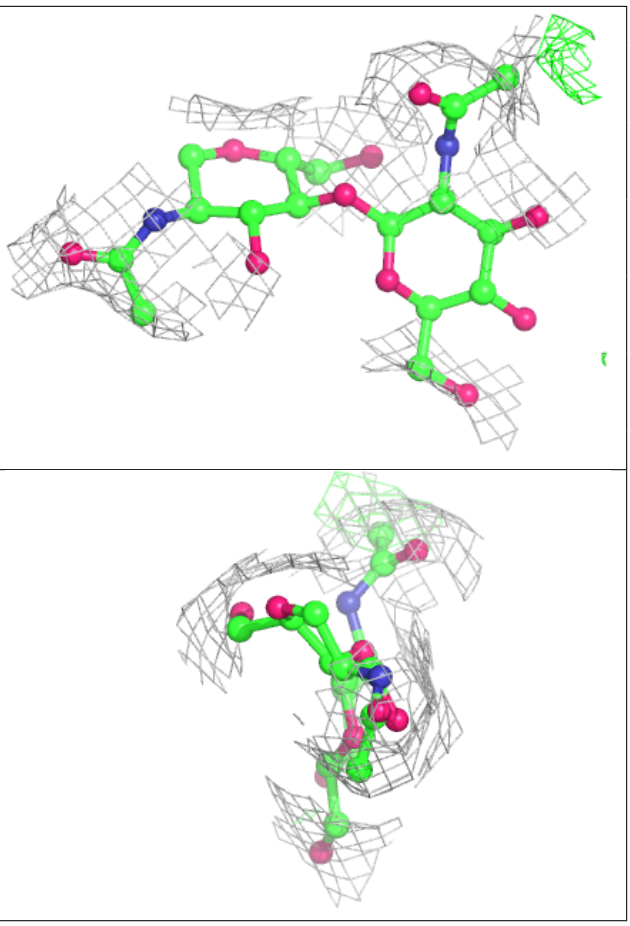






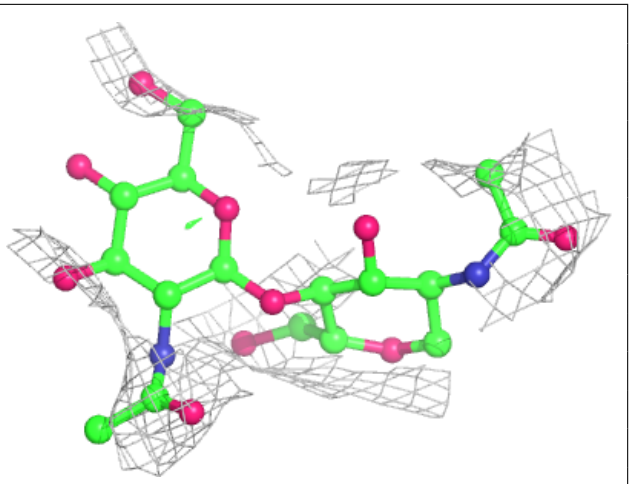
Electron density around Chain O:

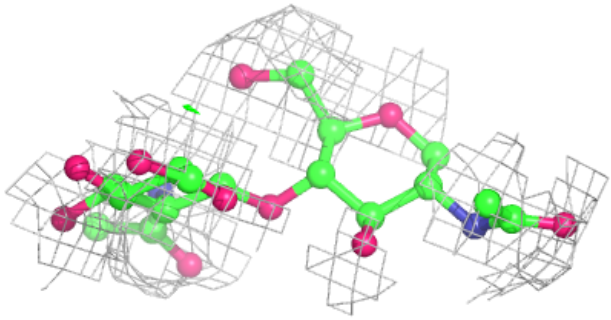
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

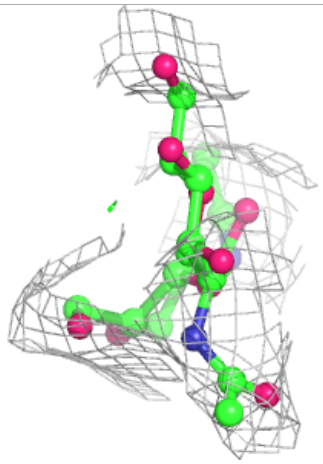


Electron density around Chain S:

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

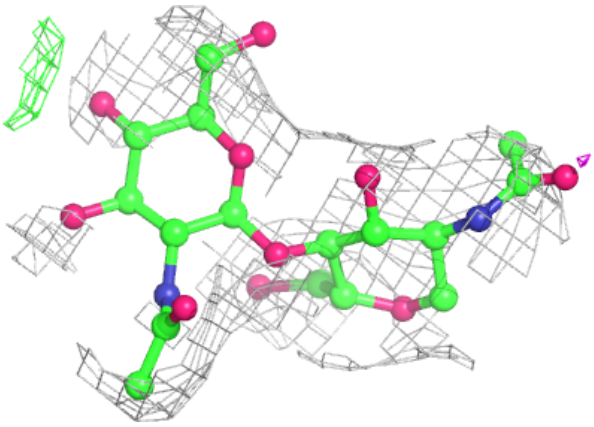


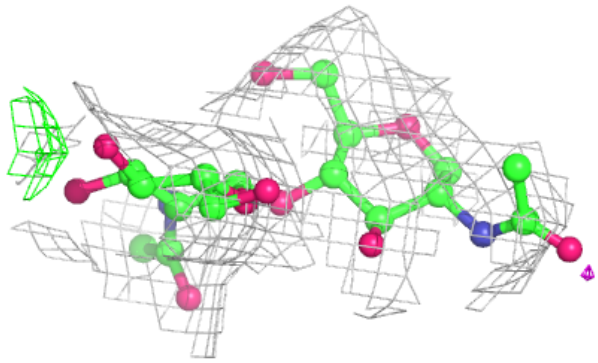


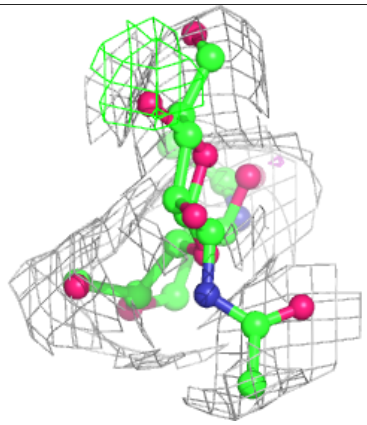


Electron density around Chain W:

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

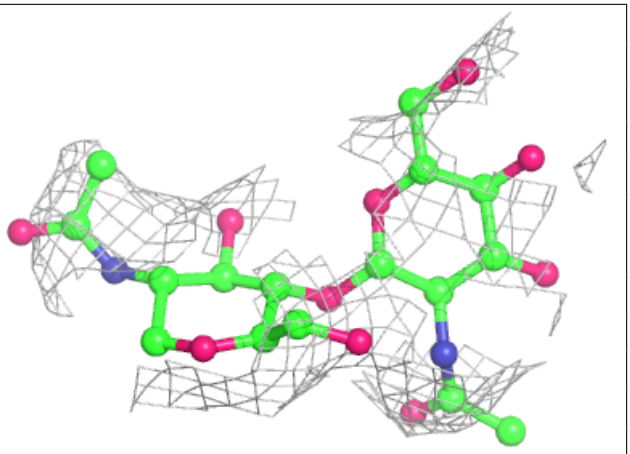


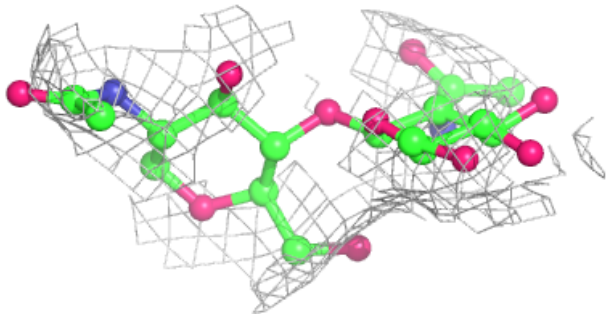


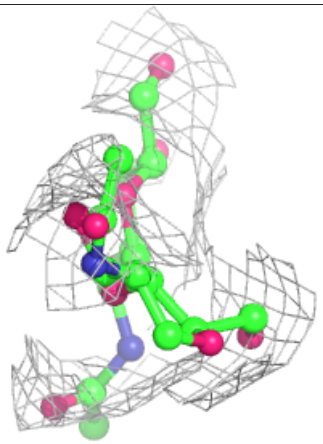


Electron density around Chain X:

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

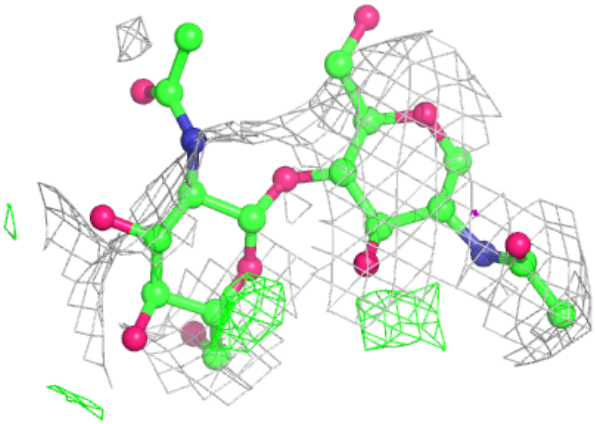


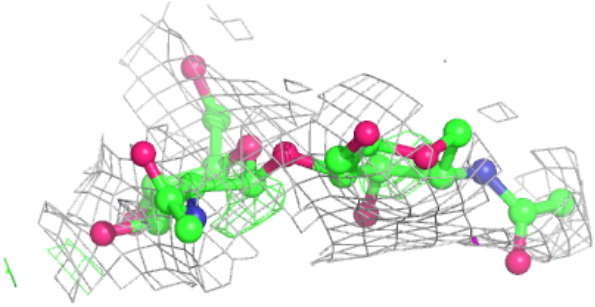


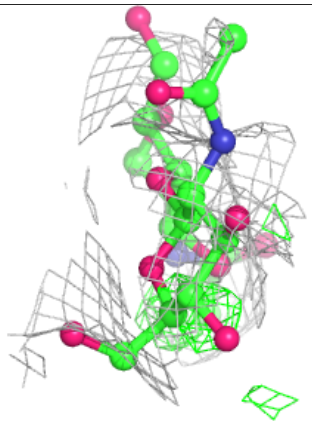


Electron density around Chain b:

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

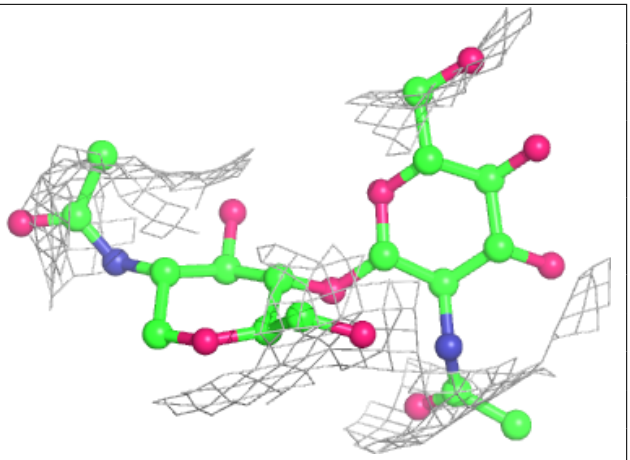


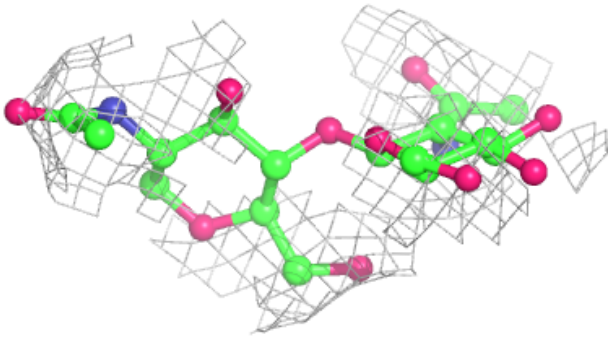


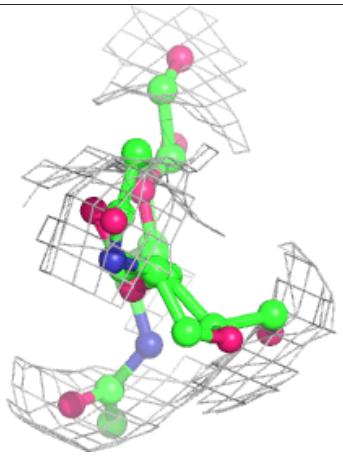


Electron density around Chain c:

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

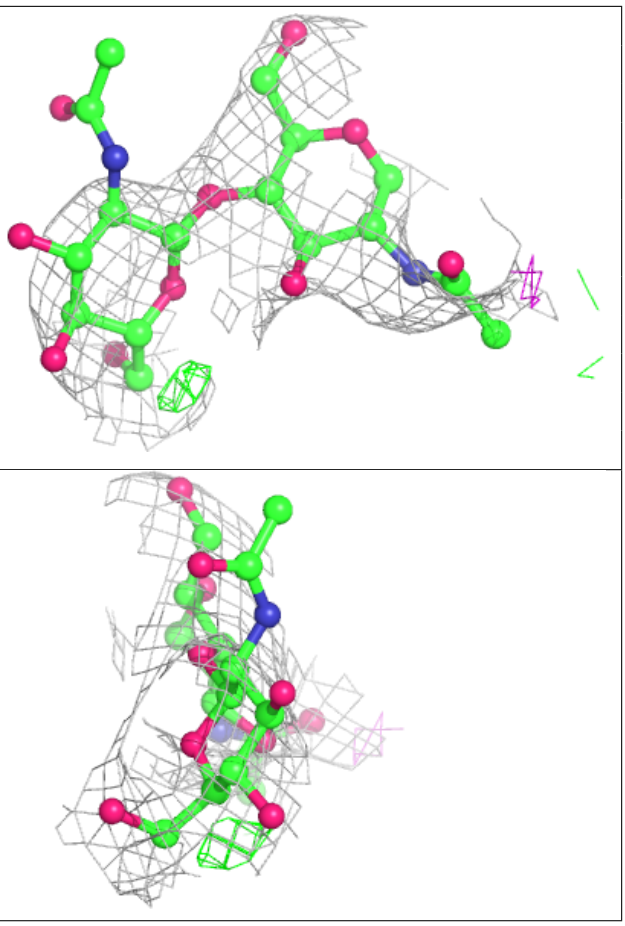






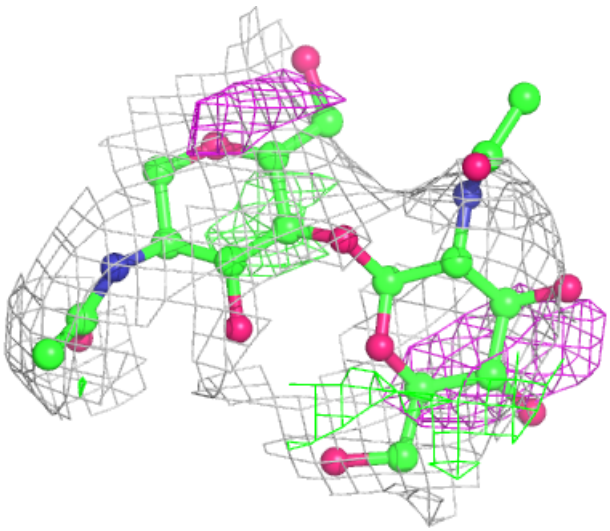
Electron density around Chain e:

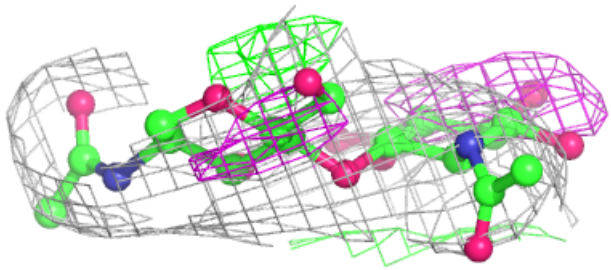
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

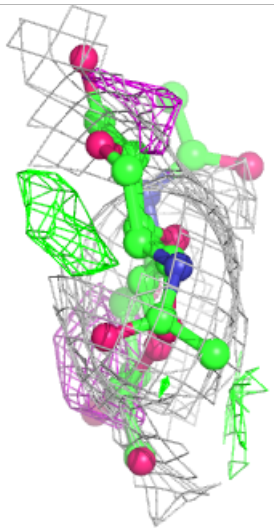


Electron density around Chain f:

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

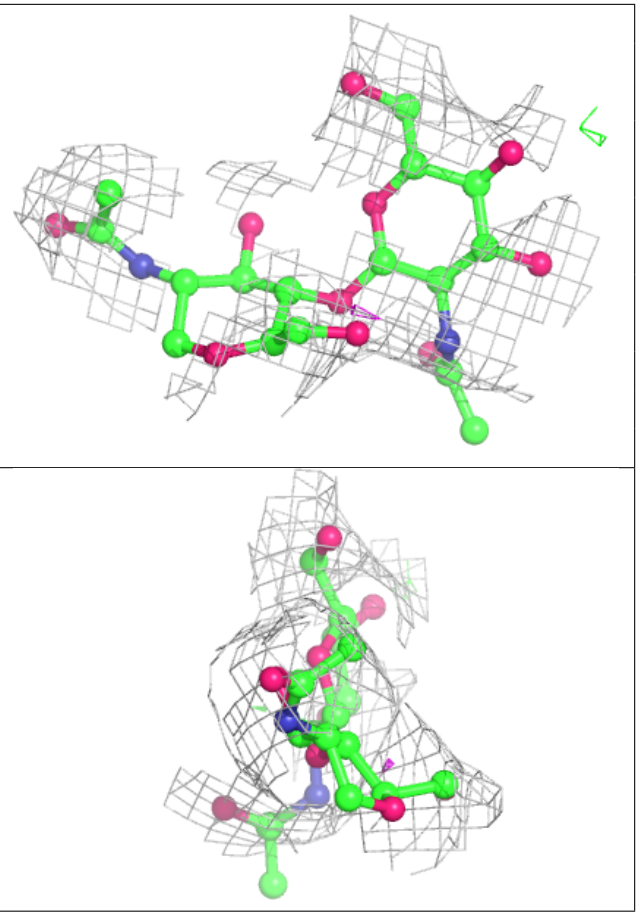






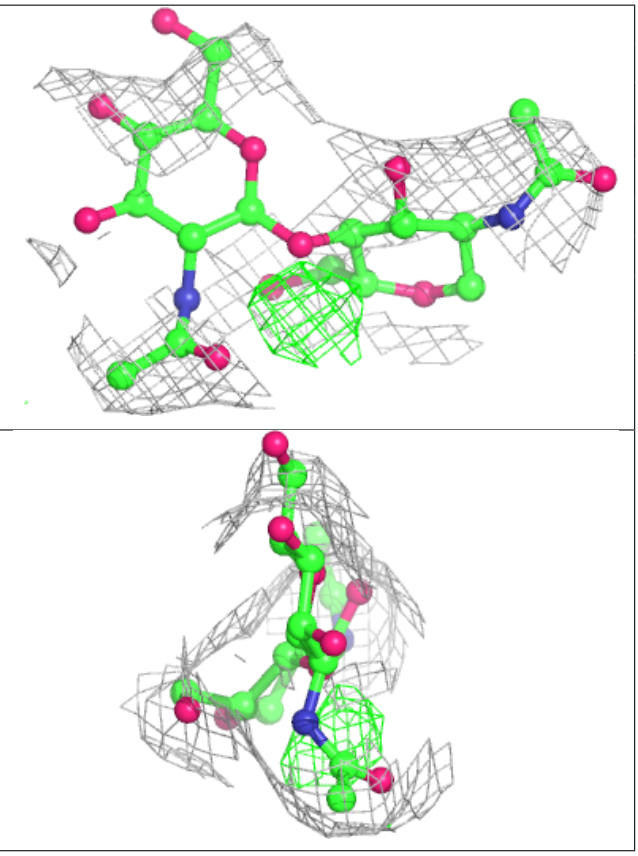
Electron density around Chain g:

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



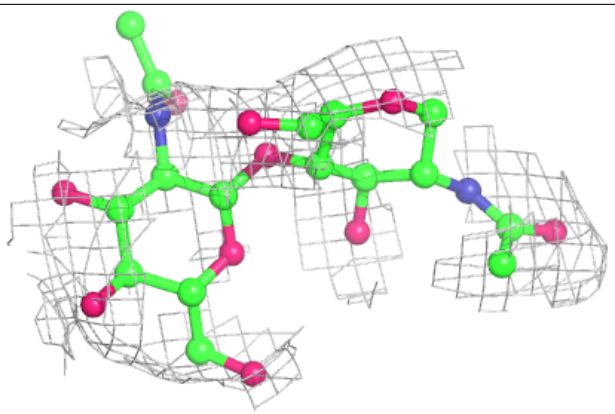
Electron density around Chain h:

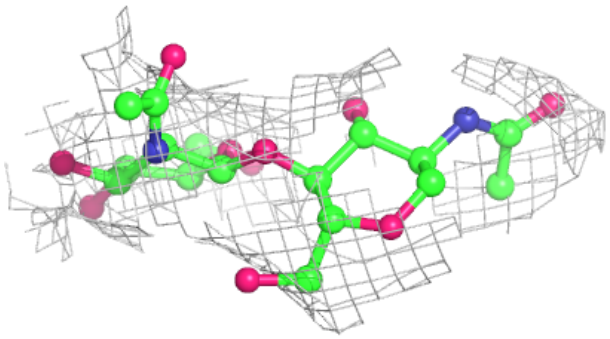
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

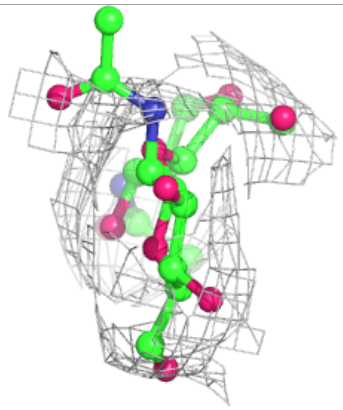


Electron density around Chain l:

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

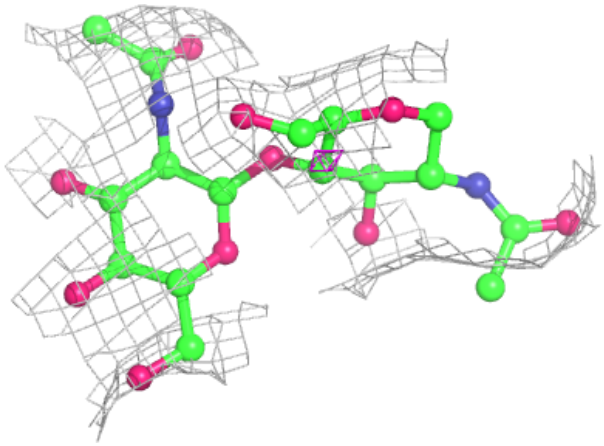


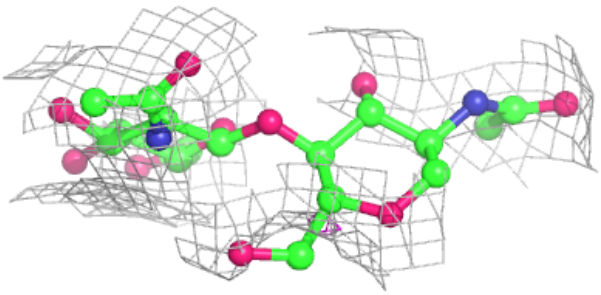


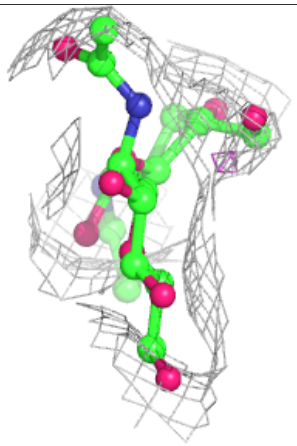


Electron density around Chain m:

$2mF_o$-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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.