Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 12:35 AM EDT

PDB ID	:	5D9Q
Title	:	Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122 and scFv NIH45-46
Authors	:	Julien, J.-P.; Stanfield, R.L.; Ward, A.B.; Wilson, I.A.
Deposited on	:	2015-08-18
Resolution	:	4.40 Å(reported)

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

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

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

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

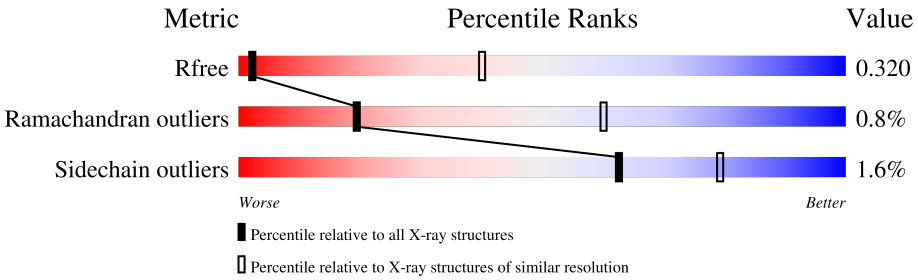
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	1043 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	472	93% · 5%
1	G	472	93% · 5%
1	J	472	93% · 5%
2	B	152	76% · 20%
2	C	152	76% · 20%
2	K	152	76% · 20%
3	E	211	97% ··
3	L	211	97% ··

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Mol	Chain	Length	Quality of chain
3	M	211	97%
4	F	235	96%
4	H	235	96%
4	N	235	96%
5	D	241	89% 8%
5	I	241	89% 8%
5	O	241	88% 8%
6	P	5	20% 80%
6	R	5	60% 40%
6	V	5	20% 80%
6	d	5	60% 40%
6	f	5	60% 40%
6	j	5	20% 80%
6	r	5	20% 80%
6	t	5	60% 40%
6	x	5	20% 80%
7	Q	4	75% 25%
7	e	4	75% 25%
7	s	4	75% 25%
8	1	2	100%
8	2	2	100%
8	3	2	100%
8	4	2	50% 50%
8	S	2	50% 50%
8	W	2	100%

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Mol	Chain	Length	Quality of chain
8	Z	2	100%
8	a	2	100%
8	b	2	100%
8	c	2	50% 50%
8	g	2	50% 50%
8	k	2	100%
8	n	2	100%
8	o	2	100%
8	p	2	100%
8	q	2	50% 50%
8	u	2	50% 50%
8	y	2	100%
9	T	7	29% 71%
9	X	7	29% 71%
9	h	7	29% 71%
9	l	7	29% 71%
9	v	7	29% 71%
9	z	7	29% 71%
10	U	11	9% 91%
10	i	11	9% 91%
10	w	11	9% 91%
11	0	10	20% 80%
11	Y	10	20% 80%
11	m	10	20% 80%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 31374 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	A	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	J	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	460	ALA	SER	conflict	UNP Q2N0S6
G	461	ASN	THR	conflict	UNP Q2N0S6
G	463	THR	SER	conflict	UNP Q2N0S6
G	464	SER	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	460	ALA	SER	conflict	UNP Q2N0S6
A	461	ASN	THR	conflict	UNP Q2N0S6
A	463	THR	SER	conflict	UNP Q2N0S6
A	464	SER	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
J	332	ASN	THR	conflict	UNP Q2N0S6
J	460	ALA	SER	conflict	UNP Q2N0S6
J	461	ASN	THR	conflict	UNP Q2N0S6
J	463	THR	SER	conflict	UNP Q2N0S6
J	464	SER	THR	conflict	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	C	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	K	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
C	559	PRO	ILE	conflict	UNP Q2N0S9
C	605	CYS	THR	conflict	UNP Q2N0S9
K	559	PRO	ILE	conflict	UNP Q2N0S9
K	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called PGT122 light chain,Ig lambda-3 chain C regions.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	E	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	M	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	156	VAL	ALA	conflict	UNP P0CG06
E	156	VAL	ALA	conflict	UNP P0CG06
M	156	VAL	ALA	conflict	UNP P0CG06

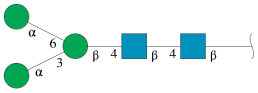
- Molecule 4 is a protein called PGT122 heavy chain,IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	F	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	N	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			

- Molecule 5 is a protein called NIH45-46 single chain Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	I	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	O	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
6	P	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	R	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	V	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	j	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	r	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	t	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	x	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 8 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
8	S	2	Total C N O 28 16 2 10	0	0	0
8	W	2	Total C N O 28 16 2 10	0	0	0
8	Z	2	Total C N O 28 16 2 10	0	0	0
8	a	2	Total C N O 28 16 2 10	0	0	0
8	b	2	Total C N O 28 16 2 10	0	0	0
8	c	2	Total C N O 28 16 2 10	0	0	0
8	g	2	Total C N O 28 16 2 10	0	0	0
8	k	2	Total C N O 28 16 2 10	0	0	0
8	n	2	Total C N O 28 16 2 10	0	0	0
8	o	2	Total C N O 28 16 2 10	0	0	0
8	p	2	Total C N O 28 16 2 10	0	0	0
8	q	2	Total C N O 28 16 2 10	0	0	0

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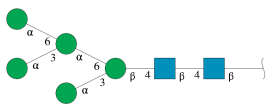
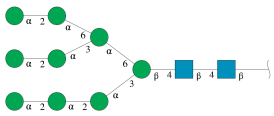
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	u	2	Total C N O 28 16 2 10	0	0	0
8	y	2	Total C N O 28 16 2 10	0	0	0
8	1	2	Total C N O 28 16 2 10	0	0	0
8	2	2	Total C N O 28 16 2 10	0	0	0
8	3	2	Total C N O 28 16 2 10	0	0	0
8	4	2	Total C N O 28 16 2 10	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



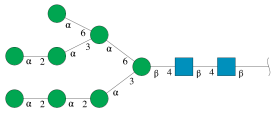
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	T	7	Total C N O 83 46 2 35	0	0	0
9	X	7	Total C N O 83 46 2 35	0	0	0
9	h	7	Total C N O 83 46 2 35	0	0	0
9	l	7	Total C N O 83 46 2 35	0	0	0
9	v	7	Total C N O 83 46 2 35	0	0	0
9	z	7	Total C N O 83 46 2 35	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



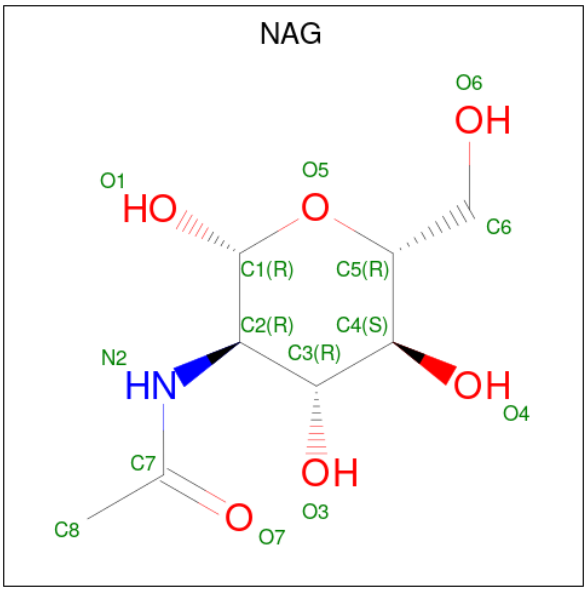
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	U	11	Total	C	N	O	0	0	0
			127	70	2	55			
10	i	11	Total	C	N	O	0	0	0
			127	70	2	55			
10	w	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]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
11	Y	10	Total	C	N	O	0	0	0
			116	64	2	50			
11	m	10	Total	C	N	O	0	0	0
			116	64	2	50			
11	0	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	G	1	Total C N O 14 8 1 5	0	0
12	G	1	Total C N O 14 8 1 5	0	0
12	G	1	Total C N O 14 8 1 5	0	0
12	G	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	B	1	Total C N O 14 8 1 5	0	0
12	A	1	Total C N O 14 8 1 5	0	0
12	A	1	Total C N O 14 8 1 5	0	0
12	A	1	Total C N O 14 8 1 5	0	0
12	A	1	Total C N O 14 8 1 5	0	0
12	C	1	Total C N O 14 8 1 5	0	0
12	C	1	Total C N O 14 8 1 5	0	0
12	J	1	Total C N O 14 8 1 5	0	0
12	J	1	Total C N O 14 8 1 5	0	0

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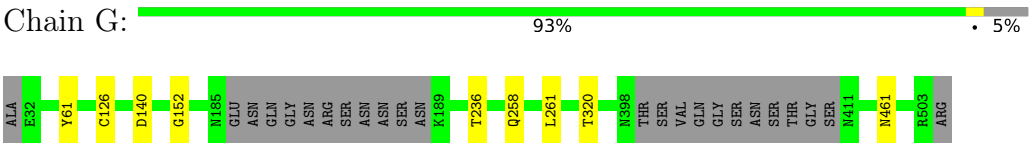
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	J	1	Total	C	N	O	0	0
			14	8	1	5		
12	J	1	Total	C	N	O	0	0
			14	8	1	5		
12	K	1	Total	C	N	O	0	0
			14	8	1	5		
12	K	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

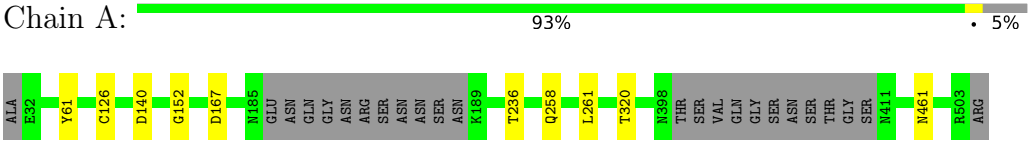
• Molecule 1: Envelope glycoprotein gp120

Chain G:



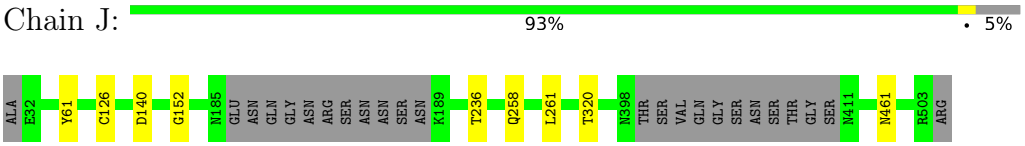
• Molecule 1: Envelope glycoprotein gp120

Chain A:



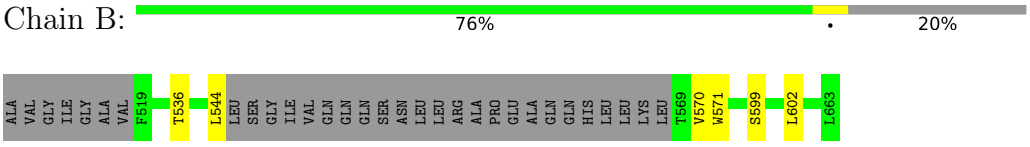
• Molecule 1: Envelope glycoprotein gp120

Chain J:



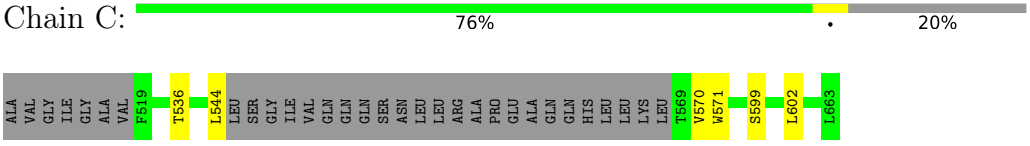
• Molecule 2: Envelope glycoprotein gp41

Chain B:



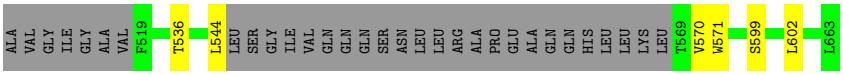
• Molecule 2: Envelope glycoprotein gp41

Chain C:



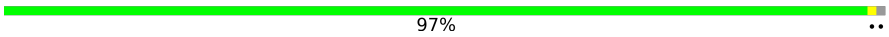
• Molecule 2: Envelope glycoprotein gp41

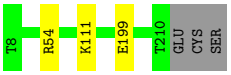
Chain K:



• Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions

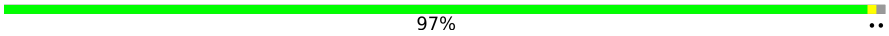
Chain L:





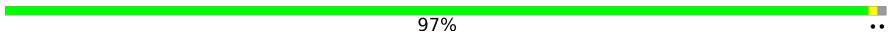
• Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions

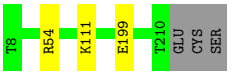
Chain E:



• Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions

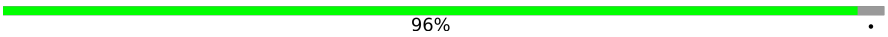
Chain M:





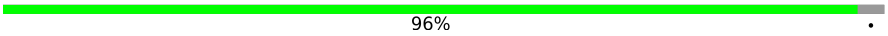
• Molecule 4: PGT122 heavy chain,IgG H chain

Chain H:



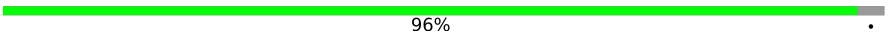
• Molecule 4: PGT122 heavy chain,IgG H chain

Chain F:



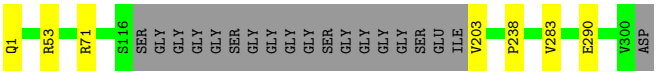
• Molecule 4: PGT122 heavy chain,IgG H chain

Chain N:



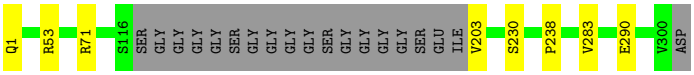
• Molecule 5: NIH45-46 single chain Fv

Chain D:



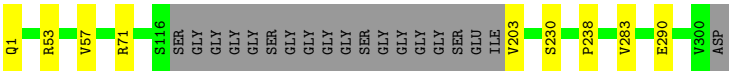
• Molecule 5: NIH45-46 single chain Fv

Chain I:



• Molecule 5: NIH45-46 single chain Fv

Chain O:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

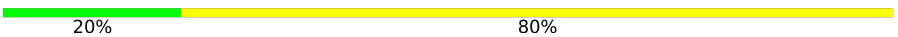
Chain P:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

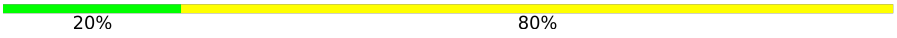
Chain d:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

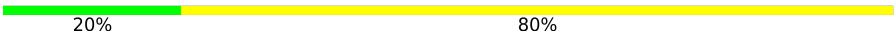
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

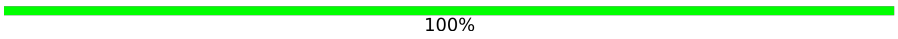
Chain s:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

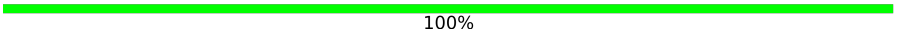
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



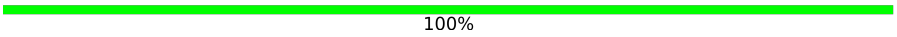
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



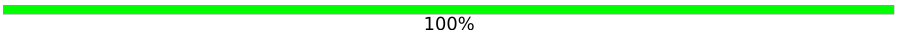
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

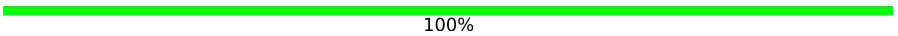
Chain c:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

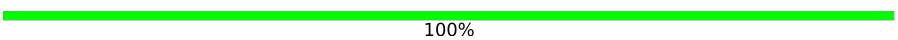
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



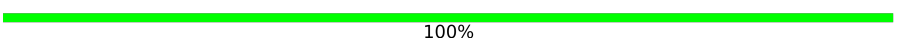
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



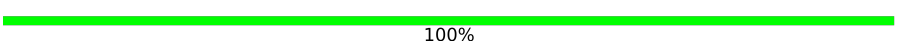
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

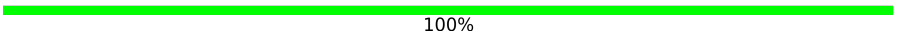
Chain q:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

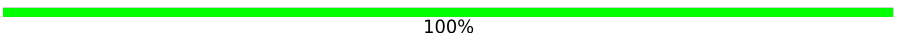
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



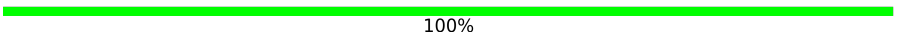
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:



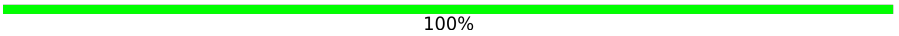
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

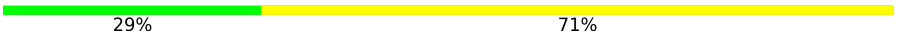
Chain 4:

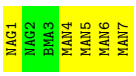
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



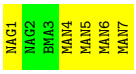


• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

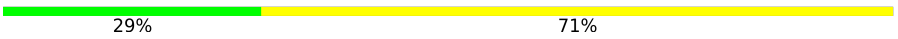
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



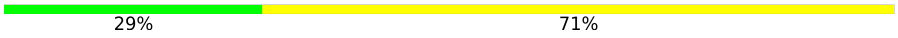
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

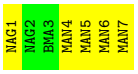
Chain v:



• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



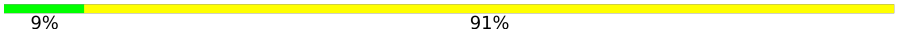


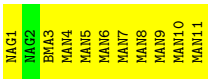
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

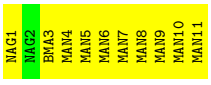
Chain i:





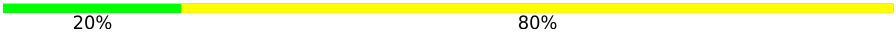
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

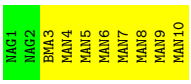


• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.76Å 254.35Å 283.55Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	39.89 – 4.40 39.89 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.89-4.40) 100.0 (39.89-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.290 , 0.320 0.298 , 0.320	Depositor DCC
R_{free} test set	1008 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	144.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 99.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	31374	wwPDB-VP
Average B, all atoms (Å^2)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, PCA, 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	0.28	0/3602	0.48	0/4891
1	G	0.27	0/3602	0.47	0/4891
1	J	0.27	0/3602	0.48	0/4891
2	B	0.26	0/986	0.44	0/1337
2	C	0.26	0/986	0.45	0/1337
2	K	0.27	0/986	0.44	0/1337
3	E	0.24	0/1619	0.42	0/2217
3	L	0.24	0/1619	0.41	0/2217
3	M	0.25	0/1619	0.42	0/2217
4	F	0.26	0/1785	0.45	0/2437
4	H	0.26	0/1785	0.44	0/2437
4	N	0.25	0/1785	0.44	0/2437
5	D	0.24	0/1792	0.41	0/2428
5	I	0.25	0/1792	0.41	0/2428
5	O	0.24	0/1792	0.41	0/2428
All	All	0.26	0/29352	0.45	0/39930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles (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	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	17	56
1	G	442/472 (94%)	410 (93%)	28 (6%)	4 (1%)	17	56
1	J	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	17	56
2	B	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	9	43
2	C	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	9	43
2	K	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	9	43
3	E	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	29	68
3	L	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	29	68
3	M	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	29	68
4	F	223/235 (95%)	214 (96%)	9 (4%)	0	100	100
4	H	223/235 (95%)	213 (96%)	10 (4%)	0	100	100
4	N	223/235 (95%)	212 (95%)	11 (5%)	0	100	100
5	D	218/241 (90%)	205 (94%)	11 (5%)	2 (1%)	17	56
5	I	218/241 (90%)	206 (94%)	9 (4%)	3 (1%)	11	47
5	O	218/241 (90%)	205 (94%)	10 (5%)	3 (1%)	11	47
All	All	3618/3933 (92%)	3371 (93%)	218 (6%)	29 (1%)	19	60

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	140	ASP
5	D	53	ARG
1	A	140	ASP
5	I	53	ARG
1	J	140	ASP
5	O	53	ARG
2	B	599	SER
2	B	602	LEU

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Mol	Chain	Res	Type
1	A	258	GLN
1	A	461	ASN
2	C	602	LEU
1	J	461	ASN
2	K	599	SER
2	K	602	LEU
1	G	258	GLN
1	G	461	ASN
3	L	199	GLU
2	C	599	SER
3	E	199	GLU
1	J	258	GLN
3	M	199	GLU
1	J	152	GLY
5	O	230	SER
5	I	230	SER
1	G	152	GLY
1	A	152	GLY
5	D	238	PRO
5	O	238	PRO
5	I	238	PRO

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	399/419 (95%)	393 (98%)	6 (2%)	65	80
1	G	399/419 (95%)	394 (99%)	5 (1%)	69	82
1	J	399/419 (95%)	394 (99%)	5 (1%)	69	82
2	B	104/128 (81%)	100 (96%)	4 (4%)	33	58
2	C	104/128 (81%)	100 (96%)	4 (4%)	33	58
2	K	104/128 (81%)	100 (96%)	4 (4%)	33	58
3	E	177/180 (98%)	175 (99%)	2 (1%)	73	85
3	L	177/180 (98%)	175 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	177/180 (98%)	175 (99%)	2 (1%)	73 85
4	F	197/205 (96%)	196 (100%)	1 (0%)	88 93
4	H	197/205 (96%)	196 (100%)	1 (0%)	88 93
4	N	197/205 (96%)	196 (100%)	1 (0%)	88 93
5	D	183/190 (96%)	179 (98%)	4 (2%)	52 71
5	I	183/190 (96%)	179 (98%)	4 (2%)	52 71
5	O	183/190 (96%)	178 (97%)	5 (3%)	44 66
All	All	3180/3366 (94%)	3130 (98%)	50 (2%)	62 79

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	61	TYR
1	G	126	CYS
1	G	236	THR
1	G	261	LEU
1	G	320	THR
2	B	536	THR
2	B	544	LEU
2	B	570	VAL
2	B	571	TRP
3	L	54	ARG
3	L	111	LYS
4	H	108	THR
5	D	71	ARG
5	D	203	VAL
5	D	283	VAL
5	D	290	GLU
1	A	61	TYR
1	A	126	CYS
1	A	167	ASP
1	A	236	THR
1	A	261	LEU
1	A	320	THR
2	C	536	THR
2	C	544	LEU
2	C	570	VAL
2	C	571	TRP
3	E	54	ARG
3	E	111	LYS

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Mol	Chain	Res	Type
4	F	108	THR
5	I	71	ARG
5	I	203	VAL
5	I	283	VAL
5	I	290	GLU
1	J	61	TYR
1	J	126	CYS
1	J	236	THR
1	J	261	LEU
1	J	320	THR
2	K	536	THR
2	K	544	LEU
2	K	570	VAL
2	K	571	TRP
3	M	54	ARG
3	M	111	LYS
4	N	108	THR
5	O	57	VAL
5	O	71	ARG
5	O	203	VAL
5	O	283	VAL
5	O	290	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	85	HIS
1	G	136	ASN
1	G	170	GLN
1	G	283	ASN
1	G	352	HIS
1	G	422	GLN
1	G	428	GLN
1	G	461	ASN
4	H	76	ASN
4	H	153	ASN
4	H	197	ASN
5	D	106	HIS
5	D	288	GLN
1	A	85	HIS
1	A	136	ASN
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	280	ASN
1	A	283	ASN
1	A	352	HIS
1	A	422	GLN
1	A	428	GLN
1	A	461	ASN
4	F	76	ASN
4	F	153	ASN
4	F	197	ASN
5	I	106	HIS
5	I	288	GLN
1	J	85	HIS
1	J	99	ASN
1	J	170	GLN
1	J	283	ASN
1	J	352	HIS
1	J	422	GLN
1	J	461	ASN
3	M	51	ASN
4	N	76	ASN
4	N	153	ASN
4	N	197	ASN
5	O	106	HIS
5	O	288	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PCA	D	1	5	7,8,9	1.79	1 (14%)	9,10,12	2.19	5 (55%)
5	PCA	I	1	5	7,8,9	1.81	1 (14%)	9,10,12	2.24	5 (55%)
5	PCA	O	1	5	7,8,9	1.81	1 (14%)	9,10,12	2.22	5 (55%)

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	PCA	D	1	5	-	0/0/11/13	0/1/1/1
5	PCA	I	1	5	-	0/0/11/13	0/1/1/1
5	PCA	O	1	5	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	PCA	CD-N	4.70	1.47	1.34
5	O	1	PCA	CD-N	4.66	1.46	1.34
5	D	1	PCA	CD-N	4.64	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	PCA	CB-CA-C	-3.20	108.30	112.70
5	O	1	PCA	OE-CD-CG	-3.13	121.29	126.76
5	O	1	PCA	CB-CA-C	-3.11	108.42	112.70
5	I	1	PCA	OE-CD-CG	-3.10	121.36	126.76
5	D	1	PCA	OE-CD-CG	-3.08	121.40	126.76
5	D	1	PCA	CB-CA-C	-2.86	108.77	112.70
5	O	1	PCA	CA-N-CD	-2.86	103.79	113.58
5	I	1	PCA	CA-N-CD	-2.85	103.81	113.58
5	D	1	PCA	CA-N-CD	-2.85	103.82	113.58
5	D	1	PCA	CB-CA-N	2.60	110.77	103.30
5	O	1	PCA	CB-CA-N	2.55	110.61	103.30
5	I	1	PCA	CB-CA-N	2.54	110.59	103.30
5	D	1	PCA	CG-CD-N	2.42	114.66	108.39
5	O	1	PCA	CG-CD-N	2.40	114.61	108.39
5	I	1	PCA	CG-CD-N	2.40	114.61	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

198 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	$\#\|Z\| > 2$
11	NAG	0	1	11,1	14,14,15	0.24	0	17,19,21	0.40	0
11	MAN	0	10	11	11,11,12	0.77	1 (9%)	15,15,17	1.05	1 (6%)
11	NAG	0	2	11	14,14,15	0.32	0	17,19,21	0.53	0
11	BMA	0	3	11	11,11,12	0.74	0	15,15,17	1.22	1 (6%)
11	MAN	0	4	11	11,11,12	0.73	0	15,15,17	1.34	3 (20%)
11	MAN	0	5	11	11,11,12	0.74	1 (9%)	15,15,17	0.91	1 (6%)
11	MAN	0	6	11	11,11,12	0.57	0	15,15,17	1.26	3 (20%)
11	MAN	0	7	11	11,11,12	0.87	1 (9%)	15,15,17	1.03	2 (13%)
11	MAN	0	8	11	11,11,12	0.74	0	15,15,17	1.02	1 (6%)
11	MAN	0	9	11	11,11,12	0.80	0	15,15,17	1.17	2 (13%)
8	NAG	1	1	8,1	14,14,15	0.25	0	17,19,21	0.60	0
8	NAG	1	2	8	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	2	1	8,1	14,14,15	0.25	0	17,19,21	0.41	0
8	NAG	2	2	8	14,14,15	0.39	0	17,19,21	0.48	0
8	NAG	3	1	8,1	14,14,15	0.21	0	17,19,21	0.56	0
8	NAG	3	2	8	14,14,15	0.27	0	17,19,21	0.40	0
8	NAG	4	1	8,1	14,14,15	0.70	1 (7%)	17,19,21	0.65	0
8	NAG	4	2	8	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	P	1	6,1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	P	2	6	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
6	BMA	P	3	6	11,11,12	0.62	0	15,15,17	0.79	1 (6%)
6	MAN	P	4	6	11,11,12	0.82	0	15,15,17	1.31	3 (20%)
6	MAN	P	5	6	11,11,12	0.93	0	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	Q	1	7,1	14,14,15	0.54	0	17,19,21	0.41	0
7	NAG	Q	2	7	14,14,15	0.29	0	17,19,21	0.36	0
7	BMA	Q	3	7	11,11,12	0.63	0	15,15,17	0.71	0
7	MAN	Q	4	7	11,11,12	0.92	1 (9%)	15,15,17	0.94	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.23	0	17,19,21	0.49	0
6	NAG	R	2	6	14,14,15	0.24	0	17,19,21	0.35	0
6	BMA	R	3	6	11,11,12	0.63	0	15,15,17	0.58	0
6	MAN	R	4	6	11,11,12	0.74	0	15,15,17	1.10	2 (13%)
6	MAN	R	5	6	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
8	NAG	S	1	8,1	14,14,15	0.25	0	17,19,21	0.49	0
8	NAG	S	2	8	14,14,15	0.50	0	17,19,21	1.23	1 (5%)
9	NAG	T	1	9,1	14,14,15	0.49	0	17,19,21	0.64	0
9	NAG	T	2	9	14,14,15	0.36	0	17,19,21	0.41	0
9	BMA	T	3	9	11,11,12	0.66	0	15,15,17	1.45	2 (13%)
9	MAN	T	4	9	11,11,12	1.23	2 (18%)	15,15,17	1.34	3 (20%)
9	MAN	T	5	9	11,11,12	0.79	0	15,15,17	1.36	2 (13%)
9	MAN	T	6	9	11,11,12	0.69	0	15,15,17	1.36	3 (20%)
9	MAN	T	7	9	11,11,12	0.70	0	15,15,17	1.32	3 (20%)
10	NAG	U	1	10,1	14,14,15	0.64	1 (7%)	17,19,21	0.67	0
10	MAN	U	10	10	11,11,12	0.65	0	15,15,17	1.42	2 (13%)
10	MAN	U	11	10	11,11,12	0.77	0	15,15,17	1.25	2 (13%)
10	NAG	U	2	10	14,14,15	0.39	0	17,19,21	0.40	0
10	BMA	U	3	10	11,11,12	0.70	0	15,15,17	1.25	2 (13%)
10	MAN	U	4	10	11,11,12	0.67	0	15,15,17	1.33	2 (13%)
10	MAN	U	5	10	11,11,12	0.91	1 (9%)	15,15,17	1.09	2 (13%)
10	MAN	U	6	10	11,11,12	0.91	0	15,15,17	1.13	1 (6%)
10	MAN	U	7	10	11,11,12	1.20	2 (18%)	15,15,17	1.39	3 (20%)
10	MAN	U	8	10	11,11,12	1.04	0	15,15,17	1.21	1 (6%)
10	MAN	U	9	10	11,11,12	0.80	0	15,15,17	1.20	1 (6%)
6	NAG	V	1	6,1	14,14,15	0.79	1 (7%)	17,19,21	0.65	0
6	NAG	V	2	6	14,14,15	0.33	0	17,19,21	0.47	0
6	BMA	V	3	6	11,11,12	0.66	0	15,15,17	1.03	1 (6%)
6	MAN	V	4	6	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
6	MAN	V	5	6	11,11,12	0.89	0	15,15,17	1.05	1 (6%)
8	NAG	W	1	8,1	14,14,15	0.39	0	17,19,21	0.48	0
8	NAG	W	2	8	14,14,15	0.21	0	17,19,21	0.38	0
9	NAG	X	1	9,1	14,14,15	0.68	1 (7%)	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	X	2	9	14,14,15	0.44	0	17,19,21	0.34	0
9	BMA	X	3	9	11,11,12	0.65	0	15,15,17	0.80	0
9	MAN	X	4	9	11,11,12	1.05	0	15,15,17	1.22	1 (6%)
9	MAN	X	5	9	11,11,12	0.69	0	15,15,17	1.17	2 (13%)
9	MAN	X	6	9	11,11,12	0.72	0	15,15,17	1.40	2 (13%)
9	MAN	X	7	9	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
11	NAG	Y	1	11,1	14,14,15	0.31	0	17,19,21	0.41	0
11	MAN	Y	10	11	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
11	NAG	Y	2	11	14,14,15	0.28	0	17,19,21	0.53	0
11	BMA	Y	3	11	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
11	MAN	Y	4	11	11,11,12	0.69	0	15,15,17	1.34	3 (20%)
11	MAN	Y	5	11	11,11,12	0.72	1 (9%)	15,15,17	0.91	1 (6%)
11	MAN	Y	6	11	11,11,12	0.56	0	15,15,17	1.30	3 (20%)
11	MAN	Y	7	11	11,11,12	0.86	1 (9%)	15,15,17	1.11	2 (13%)
11	MAN	Y	8	11	11,11,12	0.72	0	15,15,17	1.06	2 (13%)
11	MAN	Y	9	11	11,11,12	0.75	0	15,15,17	1.17	2 (13%)
8	NAG	Z	1	8,1	14,14,15	0.25	0	17,19,21	0.64	0
8	NAG	Z	2	8	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	a	1	8,1	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	a	2	8	14,14,15	0.44	0	17,19,21	0.47	0
8	NAG	b	1	8,1	14,14,15	0.17	0	17,19,21	0.52	0
8	NAG	b	2	8	14,14,15	0.27	0	17,19,21	0.36	0
8	NAG	c	1	8,1	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
8	NAG	c	2	8	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	d	1	6,1	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	d	2	6	14,14,15	0.53	0	17,19,21	1.27	1 (5%)
6	BMA	d	3	6	11,11,12	0.66	0	15,15,17	0.77	0
6	MAN	d	4	6	11,11,12	0.92	1 (9%)	15,15,17	1.39	3 (20%)
6	MAN	d	5	6	11,11,12	0.92	0	15,15,17	1.00	0
7	NAG	e	1	7,1	14,14,15	0.47	0	17,19,21	0.45	0
7	NAG	e	2	7	14,14,15	0.28	0	17,19,21	0.35	0
7	BMA	e	3	7	11,11,12	0.66	0	15,15,17	0.71	0
7	MAN	e	4	7	11,11,12	0.77	1 (9%)	15,15,17	0.98	1 (6%)
6	NAG	f	1	6,1	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	f	2	6	14,14,15	0.25	0	17,19,21	0.34	0
6	BMA	f	3	6	11,11,12	0.63	0	15,15,17	0.54	0
6	MAN	f	4	6	11,11,12	0.82	0	15,15,17	1.01	1 (6%)
6	MAN	f	5	6	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
8	NAG	g	1	8,1	14,14,15	0.26	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	g	2	8	14,14,15	0.46	0	17,19,21	1.23	1 (5%)
9	NAG	h	1	9,1	14,14,15	0.54	0	17,19,21	0.61	0
9	NAG	h	2	9	14,14,15	0.29	0	17,19,21	0.42	0
9	BMA	h	3	9	11,11,12	0.68	0	15,15,17	1.61	2 (13%)
9	MAN	h	4	9	11,11,12	1.17	2 (18%)	15,15,17	1.38	3 (20%)
9	MAN	h	5	9	11,11,12	0.84	0	15,15,17	1.35	2 (13%)
9	MAN	h	6	9	11,11,12	0.74	0	15,15,17	1.49	3 (20%)
9	MAN	h	7	9	11,11,12	0.72	0	15,15,17	1.39	3 (20%)
10	NAG	i	1	10,1	14,14,15	0.80	1 (7%)	17,19,21	0.70	0
10	MAN	i	10	10	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
10	MAN	i	11	10	11,11,12	0.70	0	15,15,17	1.19	2 (13%)
10	NAG	i	2	10	14,14,15	0.44	0	17,19,21	0.42	0
10	BMA	i	3	10	11,11,12	0.68	0	15,15,17	1.17	2 (13%)
10	MAN	i	4	10	11,11,12	0.67	0	15,15,17	1.38	2 (13%)
10	MAN	i	5	10	11,11,12	0.88	0	15,15,17	1.15	1 (6%)
10	MAN	i	6	10	11,11,12	0.94	0	15,15,17	1.08	1 (6%)
10	MAN	i	7	10	11,11,12	1.13	2 (18%)	15,15,17	1.32	2 (13%)
10	MAN	i	8	10	11,11,12	0.97	0	15,15,17	1.27	1 (6%)
10	MAN	i	9	10	11,11,12	0.84	0	15,15,17	1.18	2 (13%)
6	NAG	j	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0
6	NAG	j	2	6	14,14,15	0.30	0	17,19,21	0.43	0
6	BMA	j	3	6	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
6	MAN	j	4	6	11,11,12	0.74	0	15,15,17	1.33	2 (13%)
6	MAN	j	5	6	11,11,12	0.81	0	15,15,17	1.08	2 (13%)
8	NAG	k	1	8,1	14,14,15	0.31	0	17,19,21	0.51	0
8	NAG	k	2	8	14,14,15	0.25	0	17,19,21	0.39	0
9	NAG	l	1	9,1	14,14,15	0.61	1 (7%)	17,19,21	0.78	0
9	NAG	l	2	9	14,14,15	0.48	0	17,19,21	0.35	0
9	BMA	l	3	9	11,11,12	0.64	0	15,15,17	0.85	0
9	MAN	l	4	9	11,11,12	1.00	0	15,15,17	1.30	2 (13%)
9	MAN	l	5	9	11,11,12	0.67	0	15,15,17	1.23	1 (6%)
9	MAN	l	6	9	11,11,12	0.75	0	15,15,17	1.39	2 (13%)
9	MAN	l	7	9	11,11,12	0.71	0	15,15,17	1.23	1 (6%)
11	NAG	m	1	11,1	14,14,15	0.40	0	17,19,21	0.38	0
11	MAN	m	10	11	11,11,12	0.73	0	15,15,17	1.06	2 (13%)
11	NAG	m	2	11	14,14,15	0.35	0	17,19,21	0.50	0
11	BMA	m	3	11	11,11,12	0.77	0	15,15,17	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	m	4	11	11,11,12	0.78	0	15,15,17	1.37	3 (20%)
11	MAN	m	5	11	11,11,12	0.85	1 (9%)	15,15,17	0.87	1 (6%)
11	MAN	m	6	11	11,11,12	0.63	0	15,15,17	1.21	2 (13%)
11	MAN	m	7	11	11,11,12	0.82	1 (9%)	15,15,17	1.01	2 (13%)
11	MAN	m	8	11	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
11	MAN	m	9	11	11,11,12	0.77	0	15,15,17	1.16	2 (13%)
8	NAG	n	1	8,1	14,14,15	0.27	0	17,19,21	0.65	0
8	NAG	n	2	8	14,14,15	0.23	0	17,19,21	0.40	0
8	NAG	o	1	8,1	14,14,15	0.26	0	17,19,21	0.38	0
8	NAG	o	2	8	14,14,15	0.36	0	17,19,21	0.46	0
8	NAG	p	1	8,1	14,14,15	0.21	0	17,19,21	0.54	0
8	NAG	p	2	8	14,14,15	0.28	0	17,19,21	0.39	0
8	NAG	q	1	8,1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0
8	NAG	q	2	8	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	r	1	6,1	14,14,15	0.34	0	17,19,21	0.47	0
6	NAG	r	2	6	14,14,15	0.55	0	17,19,21	1.29	1 (5%)
6	BMA	r	3	6	11,11,12	0.60	0	15,15,17	0.71	1 (6%)
6	MAN	r	4	6	11,11,12	0.87	0	15,15,17	1.28	3 (20%)
6	MAN	r	5	6	11,11,12	0.93	1 (9%)	15,15,17	0.98	1 (6%)
7	NAG	s	1	7,1	14,14,15	0.47	0	17,19,21	0.49	0
7	NAG	s	2	7	14,14,15	0.28	0	17,19,21	0.36	0
7	BMA	s	3	7	11,11,12	0.67	0	15,15,17	0.68	0
7	MAN	s	4	7	11,11,12	0.79	1 (9%)	15,15,17	0.97	1 (6%)
6	NAG	t	1	6,1	14,14,15	0.15	0	17,19,21	0.49	0
6	NAG	t	2	6	14,14,15	0.20	0	17,19,21	0.39	0
6	BMA	t	3	6	11,11,12	0.63	0	15,15,17	0.57	0
6	MAN	t	4	6	11,11,12	0.81	0	15,15,17	1.06	2 (13%)
6	MAN	t	5	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
8	NAG	u	1	8,1	14,14,15	0.26	0	17,19,21	0.49	0
8	NAG	u	2	8	14,14,15	0.52	0	17,19,21	1.26	2 (11%)
9	NAG	v	1	9,1	14,14,15	0.51	0	17,19,21	0.61	0
9	NAG	v	2	9	14,14,15	0.37	0	17,19,21	0.40	0
9	BMA	v	3	9	11,11,12	0.65	0	15,15,17	1.35	1 (6%)
9	MAN	v	4	9	11,11,12	1.26	1 (9%)	15,15,17	1.29	1 (6%)
9	MAN	v	5	9	11,11,12	0.82	0	15,15,17	1.26	2 (13%)
9	MAN	v	6	9	11,11,12	0.65	0	15,15,17	1.40	3 (20%)
9	MAN	v	7	9	11,11,12	0.69	0	15,15,17	1.32	3 (20%)
10	NAG	w	1	10,1	14,14,15	0.68	1 (7%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	w	10	10	11,11,12	0.63	0	15,15,17	1.44	2 (13%)
10	MAN	w	11	10	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
10	NAG	w	2	10	14,14,15	0.39	0	17,19,21	0.38	0
10	BMA	w	3	10	11,11,12	0.70	0	15,15,17	1.30	3 (20%)
10	MAN	w	4	10	11,11,12	0.69	0	15,15,17	1.33	2 (13%)
10	MAN	w	5	10	11,11,12	0.92	0	15,15,17	1.16	1 (6%)
10	MAN	w	6	10	11,11,12	0.94	0	15,15,17	1.11	1 (6%)
10	MAN	w	7	10	11,11,12	1.14	2 (18%)	15,15,17	1.28	2 (13%)
10	MAN	w	8	10	11,11,12	0.92	0	15,15,17	1.27	1 (6%)
10	MAN	w	9	10	11,11,12	0.77	0	15,15,17	1.13	1 (6%)
6	NAG	x	1	6,1	14,14,15	0.86	1 (7%)	17,19,21	0.64	0
6	NAG	x	2	6	14,14,15	0.36	0	17,19,21	0.47	0
6	BMA	x	3	6	11,11,12	0.66	0	15,15,17	1.05	1 (6%)
6	MAN	x	4	6	11,11,12	0.80	0	15,15,17	1.25	2 (13%)
6	MAN	x	5	6	11,11,12	0.85	0	15,15,17	1.03	1 (6%)
8	NAG	y	1	8,1	14,14,15	0.35	0	17,19,21	0.50	0
8	NAG	y	2	8	14,14,15	0.24	0	17,19,21	0.36	0
9	NAG	z	1	9,1	14,14,15	0.69	1 (7%)	17,19,21	0.81	1 (5%)
9	NAG	z	2	9	14,14,15	0.43	0	17,19,21	0.37	0
9	BMA	z	3	9	11,11,12	0.65	0	15,15,17	0.88	0
9	MAN	z	4	9	11,11,12	1.06	0	15,15,17	1.26	2 (13%)
9	MAN	z	5	9	11,11,12	0.71	0	15,15,17	1.19	2 (13%)
9	MAN	z	6	9	11,11,12	0.72	0	15,15,17	1.41	3 (20%)
9	MAN	z	7	9	11,11,12	0.69	0	15,15,17	1.24	1 (6%)

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
11	NAG	0	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	0	10	11	-	0/2/19/22	0/1/1/1
11	NAG	0	2	11	-	3/6/23/26	0/1/1/1
11	BMA	0	3	11	-	0/2/19/22	0/1/1/1
11	MAN	0	4	11	-	0/2/19/22	0/1/1/1
11	MAN	0	5	11	-	0/2/19/22	0/1/1/1
11	MAN	0	6	11	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	0	7	11	-	2/2/19/22	0/1/1/1
11	MAN	0	8	11	-	0/2/19/22	0/1/1/1
11	MAN	0	9	11	-	0/2/19/22	1/1/1/1
8	NAG	1	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	NAG	2	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	2	2	8	-	2/6/23/26	0/1/1/1
8	NAG	3	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	3	2	8	-	0/6/23/26	0/1/1/1
8	NAG	4	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	4	2	8	-	2/6/23/26	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	4/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	0/2/19/22	0/1/1/1
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1
8	NAG	S	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	S	2	8	-	3/6/23/26	0/1/1/1
9	NAG	T	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	2/2/19/22	0/1/1/1
9	MAN	T	5	9	-	0/2/19/22	0/1/1/1
9	MAN	T	6	9	-	0/2/19/22	0/1/1/1
9	MAN	T	7	9	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	U	10	10	-	1/2/19/22	0/1/1/1
10	MAN	U	11	10	-	0/2/19/22	0/1/1/1
10	NAG	U	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	U	3	10	-	2/2/19/22	0/1/1/1
10	MAN	U	4	10	-	0/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
10	MAN	U	6	10	-	0/2/19/22	0/1/1/1
10	MAN	U	7	10	-	0/2/19/22	0/1/1/1
10	MAN	U	8	10	-	0/2/19/22	0/1/1/1
10	MAN	U	9	10	-	0/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
8	NAG	W	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
9	NAG	X	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	0/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	0/2/19/22	0/1/1/1
11	NAG	Y	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	Y	10	11	-	0/2/19/22	0/1/1/1
11	NAG	Y	2	11	-	3/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	6	11	-	1/2/19/22	0/1/1/1
11	MAN	Y	7	11	-	2/2/19/22	0/1/1/1
11	MAN	Y	8	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	9	11	-	0/2/19/22	1/1/1/1
8	NAG	Z	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	d	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	3/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
6	MAN	d	4	6	-	0/2/19/22	0/1/1/1
6	MAN	d	5	6	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	BMA	e	3	7	-	0/2/19/22	0/1/1/1
7	MAN	e	4	7	-	2/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
6	MAN	f	4	6	-	1/2/19/22	0/1/1/1
6	MAN	f	5	6	-	0/2/19/22	0/1/1/1
8	NAG	g	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	g	2	8	-	4/6/23/26	0/1/1/1
9	NAG	h	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
9	MAN	h	4	9	-	2/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	0/2/19/22	0/1/1/1
9	MAN	h	7	9	-	0/2/19/22	0/1/1/1
10	NAG	i	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	i	10	10	-	1/2/19/22	0/1/1/1
10	MAN	i	11	10	-	0/2/19/22	0/1/1/1
10	NAG	i	2	10	-	1/6/23/26	0/1/1/1
10	BMA	i	3	10	-	2/2/19/22	0/1/1/1
10	MAN	i	4	10	-	0/2/19/22	0/1/1/1
10	MAN	i	5	10	-	0/2/19/22	0/1/1/1
10	MAN	i	6	10	-	0/2/19/22	0/1/1/1
10	MAN	i	7	10	-	0/2/19/22	0/1/1/1
10	MAN	i	8	10	-	0/2/19/22	0/1/1/1
10	MAN	i	9	10	-	0/2/19/22	0/1/1/1
6	NAG	j	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	BMA	j	3	6	-	0/2/19/22	0/1/1/1
6	MAN	j	4	6	-	0/2/19/22	0/1/1/1
6	MAN	j	5	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	k	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
9	NAG	l	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	2/2/19/22	0/1/1/1
9	MAN	l	4	9	-	0/2/19/22	0/1/1/1
9	MAN	l	5	9	-	0/2/19/22	0/1/1/1
9	MAN	l	6	9	-	0/2/19/22	0/1/1/1
9	MAN	l	7	9	-	0/2/19/22	0/1/1/1
11	NAG	m	1	11,1	-	0/6/23/26	0/1/1/1
11	MAN	m	10	11	-	0/2/19/22	0/1/1/1
11	NAG	m	2	11	-	4/6/23/26	0/1/1/1
11	BMA	m	3	11	-	0/2/19/22	0/1/1/1
11	MAN	m	4	11	-	0/2/19/22	0/1/1/1
11	MAN	m	5	11	-	0/2/19/22	0/1/1/1
11	MAN	m	6	11	-	1/2/19/22	0/1/1/1
11	MAN	m	7	11	-	2/2/19/22	0/1/1/1
11	MAN	m	8	11	-	0/2/19/22	0/1/1/1
11	MAN	m	9	11	-	0/2/19/22	1/1/1/1
8	NAG	n	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	n	2	8	-	0/6/23/26	0/1/1/1
8	NAG	o	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
8	NAG	p	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	p	2	8	-	0/6/23/26	0/1/1/1
8	NAG	q	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
6	NAG	r	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	r	2	6	-	3/6/23/26	0/1/1/1
6	BMA	r	3	6	-	0/2/19/22	0/1/1/1
6	MAN	r	4	6	-	0/2/19/22	0/1/1/1
6	MAN	r	5	6	-	0/2/19/22	0/1/1/1
7	NAG	s	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	s	2	7	-	0/6/23/26	0/1/1/1
7	BMA	s	3	7	-	0/2/19/22	0/1/1/1
7	MAN	s	4	7	-	2/2/19/22	0/1/1/1
6	NAG	t	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	t	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	t	3	6	-	2/2/19/22	0/1/1/1
6	MAN	t	4	6	-	1/2/19/22	0/1/1/1
6	MAN	t	5	6	-	0/2/19/22	0/1/1/1
8	NAG	u	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	u	2	8	-	4/6/23/26	0/1/1/1
9	NAG	v	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
9	BMA	v	3	9	-	2/2/19/22	0/1/1/1
9	MAN	v	4	9	-	2/2/19/22	0/1/1/1
9	MAN	v	5	9	-	0/2/19/22	0/1/1/1
9	MAN	v	6	9	-	0/2/19/22	0/1/1/1
9	MAN	v	7	9	-	0/2/19/22	0/1/1/1
10	NAG	w	1	10,1	-	2/6/23/26	0/1/1/1
10	MAN	w	10	10	-	1/2/19/22	0/1/1/1
10	MAN	w	11	10	-	0/2/19/22	0/1/1/1
10	NAG	w	2	10	-	2/6/23/26	0/1/1/1
10	BMA	w	3	10	-	2/2/19/22	0/1/1/1
10	MAN	w	4	10	-	0/2/19/22	0/1/1/1
10	MAN	w	5	10	-	0/2/19/22	0/1/1/1
10	MAN	w	6	10	-	0/2/19/22	0/1/1/1
10	MAN	w	7	10	-	0/2/19/22	0/1/1/1
10	MAN	w	8	10	-	0/2/19/22	0/1/1/1
10	MAN	w	9	10	-	0/2/19/22	0/1/1/1
6	NAG	x	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	x	2	6	-	0/6/23/26	0/1/1/1
6	BMA	x	3	6	-	0/2/19/22	0/1/1/1
6	MAN	x	4	6	-	0/2/19/22	0/1/1/1
6	MAN	x	5	6	-	0/2/19/22	0/1/1/1
8	NAG	y	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
9	NAG	z	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	z	5	9	-	0/2/19/22	0/1/1/1
9	MAN	z	6	9	-	0/2/19/22	0/1/1/1
9	MAN	z	7	9	-	0/2/19/22	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	x	1	NAG	O5-C1	-3.03	1.38	1.43
8	c	1	NAG	O5-C1	-2.92	1.39	1.43
6	V	1	NAG	O5-C1	-2.80	1.39	1.43
10	i	1	NAG	O5-C1	-2.70	1.39	1.43
9	v	4	MAN	C2-C3	2.66	1.56	1.52
10	U	7	MAN	C1-C2	2.65	1.58	1.52
11	m	5	MAN	O5-C1	-2.62	1.39	1.43
6	j	1	NAG	O5-C1	-2.52	1.39	1.43
9	z	1	NAG	O5-C1	-2.48	1.39	1.43
7	Q	4	MAN	O5-C1	-2.48	1.39	1.43
8	q	1	NAG	O5-C1	-2.47	1.39	1.43
9	X	1	NAG	O5-C1	-2.46	1.39	1.43
8	4	1	NAG	O5-C1	-2.44	1.39	1.43
6	d	4	MAN	C1-C2	2.42	1.57	1.52
10	i	7	MAN	C1-C2	2.35	1.57	1.52
9	h	4	MAN	C2-C3	2.28	1.55	1.52
11	0	7	MAN	O5-C1	-2.28	1.40	1.43
9	T	4	MAN	C2-C3	2.27	1.55	1.52
7	s	4	MAN	O5-C1	-2.27	1.40	1.43
11	Y	7	MAN	O5-C1	-2.27	1.40	1.43
10	w	7	MAN	C1-C2	2.24	1.57	1.52
11	0	5	MAN	O5-C1	-2.24	1.40	1.43
10	w	7	MAN	C2-C3	2.21	1.55	1.52
9	T	4	MAN	C1-C2	2.20	1.57	1.52
9	l	1	NAG	O5-C1	-2.18	1.40	1.43
10	U	7	MAN	C2-C3	2.17	1.55	1.52
11	Y	5	MAN	O5-C1	-2.14	1.40	1.43
10	i	7	MAN	C2-C3	2.14	1.55	1.52
10	w	1	NAG	O5-C1	-2.11	1.40	1.43
10	U	5	MAN	O5-C1	-2.11	1.40	1.43
6	r	5	MAN	O5-C1	-2.09	1.40	1.43
11	0	10	MAN	O5-C1	-2.08	1.40	1.43
9	h	4	MAN	C1-C2	2.07	1.56	1.52
7	e	4	MAN	O5-C1	-2.06	1.40	1.43
10	U	1	NAG	O5-C1	-2.04	1.40	1.43
11	m	7	MAN	O5-C1	-2.03	1.40	1.43

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	r	2	NAG	C2-N2-C7	4.34	129.08	122.90
6	P	2	NAG	C2-N2-C7	4.33	129.07	122.90
6	d	2	NAG	C2-N2-C7	4.33	129.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	u	2	NAG	C2-N2-C7	4.31	129.04	122.90
9	X	6	MAN	C1-O5-C5	4.28	117.99	112.19
8	g	2	NAG	C2-N2-C7	4.26	128.98	122.90
9	h	3	BMA	C1-C2-C3	4.26	114.90	109.67
8	S	2	NAG	C2-N2-C7	4.23	128.92	122.90
10	w	10	MAN	C1-O5-C5	4.20	117.89	112.19
10	U	10	MAN	C1-O5-C5	4.16	117.83	112.19
9	l	6	MAN	C1-O5-C5	4.14	117.81	112.19
9	z	6	MAN	C1-O5-C5	4.11	117.77	112.19
9	v	6	MAN	C1-O5-C5	4.04	117.67	112.19
10	i	10	MAN	C1-O5-C5	4.02	117.64	112.19
9	T	6	MAN	C1-O5-C5	3.98	117.58	112.19
9	h	6	MAN	C1-O5-C5	3.89	117.46	112.19
10	i	4	MAN	C1-O5-C5	3.88	117.45	112.19
9	T	5	MAN	C1-O5-C5	3.88	117.44	112.19
9	h	5	MAN	C1-O5-C5	3.85	117.41	112.19
10	w	8	MAN	C1-O5-C5	3.77	117.29	112.19
6	j	4	MAN	C1-O5-C5	3.71	117.22	112.19
10	i	8	MAN	C1-O5-C5	3.66	117.15	112.19
9	X	7	MAN	C1-O5-C5	3.65	117.13	112.19
9	T	3	BMA	C1-C2-C3	3.61	114.11	109.67
9	v	5	MAN	C1-O5-C5	3.58	117.04	112.19
9	v	3	BMA	C1-C2-C3	3.57	114.06	109.67
9	l	7	MAN	C1-O5-C5	3.55	117.00	112.19
9	l	5	MAN	C1-O5-C5	3.54	116.99	112.19
10	U	11	MAN	C1-O5-C5	3.51	116.95	112.19
10	U	8	MAN	C1-O5-C5	3.51	116.94	112.19
11	0	3	BMA	C1-C2-C3	3.48	113.94	109.67
11	Y	6	MAN	C1-O5-C5	3.46	116.88	112.19
10	w	4	MAN	C1-O5-C5	3.45	116.86	112.19
10	U	4	MAN	C1-O5-C5	3.44	116.86	112.19
9	z	7	MAN	C1-O5-C5	3.44	116.86	112.19
9	h	7	MAN	C1-O5-C5	3.44	116.85	112.19
6	V	4	MAN	C1-O5-C5	3.38	116.78	112.19
9	v	7	MAN	C1-O5-C5	3.38	116.78	112.19
6	x	4	MAN	C1-O5-C5	3.31	116.68	112.19
11	0	6	MAN	C1-O5-C5	3.26	116.61	112.19
9	z	5	MAN	C1-O5-C5	3.26	116.60	112.19
11	Y	3	BMA	C1-C2-C3	3.25	113.66	109.67
6	d	4	MAN	C1-O5-C5	3.24	116.58	112.19
11	m	4	MAN	O2-C2-C3	-3.21	103.71	110.14
9	h	4	MAN	C1-O5-C5	3.18	116.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	m	9	MAN	C1-O5-C5	3.18	116.50	112.19
10	i	11	MAN	C1-O5-C5	3.18	116.50	112.19
10	U	9	MAN	C1-O5-C5	3.16	116.47	112.19
6	P	4	MAN	C1-O5-C5	3.15	116.46	112.19
11	0	9	MAN	C1-O5-C5	3.13	116.44	112.19
11	Y	9	MAN	C1-O5-C5	3.13	116.44	112.19
11	m	3	BMA	C1-C2-C3	3.12	113.50	109.67
9	X	5	MAN	C1-O5-C5	3.11	116.41	112.19
9	T	7	MAN	C1-O5-C5	3.11	116.41	112.19
10	w	3	BMA	C1-C2-C3	3.08	113.46	109.67
6	r	4	MAN	C1-O5-C5	3.05	116.32	112.19
10	U	3	BMA	C1-C2-C3	3.05	113.41	109.67
11	m	6	MAN	C1-O5-C5	3.03	116.29	112.19
9	v	4	MAN	C1-O5-C5	3.01	116.28	112.19
10	w	9	MAN	C1-O5-C5	3.01	116.28	112.19
10	w	5	MAN	C1-O5-C5	3.01	116.27	112.19
10	i	5	MAN	C1-O5-C5	2.98	116.23	112.19
9	h	6	MAN	O2-C2-C3	-2.97	104.18	110.14
10	w	11	MAN	C1-O5-C5	2.94	116.17	112.19
11	Y	4	MAN	C1-O5-C5	2.92	116.15	112.19
9	T	4	MAN	C1-O5-C5	2.90	116.12	112.19
11	0	4	MAN	O2-C2-C3	-2.90	104.33	110.14
10	w	4	MAN	O2-C2-C3	-2.88	104.38	110.14
10	i	9	MAN	C1-O5-C5	2.87	116.08	112.19
10	i	3	BMA	C1-C2-C3	2.83	113.15	109.67
10	U	4	MAN	O2-C2-C3	-2.83	104.47	110.14
11	0	4	MAN	C1-O5-C5	2.82	116.02	112.19
10	i	11	MAN	O2-C2-C3	-2.80	104.53	110.14
10	i	4	MAN	O2-C2-C3	-2.77	104.59	110.14
10	w	6	MAN	C1-O5-C5	2.76	115.93	112.19
10	U	6	MAN	C1-O5-C5	2.73	115.90	112.19
10	U	11	MAN	O2-C2-C3	-2.73	104.67	110.14
6	x	3	BMA	C1-C2-C3	2.66	112.93	109.67
7	s	4	MAN	O2-C2-C3	-2.62	104.89	110.14
9	l	4	MAN	C1-O5-C5	2.62	115.74	112.19
11	m	4	MAN	C1-O5-C5	2.62	115.74	112.19
10	U	10	MAN	O2-C2-C3	-2.58	104.96	110.14
10	w	10	MAN	O2-C2-C3	-2.58	104.98	110.14
11	Y	4	MAN	O2-C2-C3	-2.57	104.99	110.14
10	i	6	MAN	C1-O5-C5	2.55	115.65	112.19
9	h	3	BMA	O3-C3-C2	-2.54	105.13	109.99
7	e	4	MAN	O2-C2-C3	-2.51	105.10	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	z	4	MAN	C1-O5-C5	2.51	115.59	112.19
6	j	5	MAN	C1-O5-C5	2.51	115.59	112.19
10	i	10	MAN	O2-C2-C3	-2.47	105.18	110.14
6	V	3	BMA	C1-C2-C3	2.47	112.70	109.67
6	x	4	MAN	O2-C2-C3	-2.46	105.20	110.14
11	0	10	MAN	O2-C2-C3	-2.46	105.21	110.14
9	T	7	MAN	O5-C1-C2	2.46	114.57	110.77
11	m	6	MAN	O2-C2-C3	-2.46	105.21	110.14
11	Y	10	MAN	O2-C2-C3	-2.46	105.22	110.14
11	m	10	MAN	O2-C2-C3	-2.46	105.22	110.14
10	U	7	MAN	C1-O5-C5	2.44	115.50	112.19
11	Y	8	MAN	C1-O5-C5	2.43	115.49	112.19
10	U	5	MAN	C1-O5-C5	2.42	115.48	112.19
6	f	5	MAN	O2-C2-C3	-2.42	105.30	110.14
7	Q	4	MAN	O2-C2-C3	-2.42	105.30	110.14
11	0	8	MAN	C1-O5-C5	2.40	115.44	112.19
9	h	7	MAN	O5-C1-C2	2.37	114.43	110.77
11	0	6	MAN	O2-C2-C3	-2.37	105.39	110.14
6	t	5	MAN	O2-C2-C3	-2.37	105.39	110.14
11	Y	6	MAN	O2-C2-C3	-2.37	105.39	110.14
9	h	5	MAN	O2-C2-C3	-2.37	105.40	110.14
10	i	7	MAN	C1-O5-C5	2.36	115.39	112.19
9	z	1	NAG	O4-C4-C5	-2.34	103.48	109.30
6	V	4	MAN	O2-C2-C3	-2.34	105.44	110.14
6	d	4	MAN	O2-C2-C3	-2.33	105.47	110.14
10	w	11	MAN	O2-C2-C3	-2.33	105.47	110.14
9	v	6	MAN	O2-C2-C3	-2.31	105.51	110.14
11	Y	7	MAN	O2-C2-C3	-2.31	105.52	110.14
9	T	5	MAN	O2-C2-C3	-2.30	105.53	110.14
11	m	8	MAN	C1-O5-C5	2.30	115.31	112.19
10	i	9	MAN	O2-C2-C3	-2.30	105.53	110.14
6	V	5	MAN	C1-O5-C5	2.29	115.30	112.19
6	j	3	BMA	C1-C2-C3	2.29	112.48	109.67
11	Y	9	MAN	O2-C2-C3	-2.29	105.56	110.14
10	U	3	BMA	C1-O5-C5	2.28	115.28	112.19
11	0	7	MAN	O2-C2-C3	-2.28	105.57	110.14
6	x	5	MAN	C1-O5-C5	2.26	115.26	112.19
11	0	9	MAN	O2-C2-C3	-2.26	105.61	110.14
6	P	4	MAN	O2-C2-C3	-2.26	105.61	110.14
9	v	5	MAN	O2-C2-C3	-2.26	105.62	110.14
9	h	6	MAN	O5-C1-C2	2.25	114.25	110.77
9	X	4	MAN	C1-O5-C5	2.25	115.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	4	MAN	C1-C2-C3	2.24	112.42	109.67
6	d	4	MAN	O5-C1-C2	2.24	114.22	110.77
9	v	7	MAN	O5-C1-C2	2.23	114.22	110.77
10	w	7	MAN	C1-O5-C5	2.22	115.20	112.19
9	z	5	MAN	O2-C2-C3	-2.22	105.70	110.14
6	t	4	MAN	C1-O5-C5	2.21	115.19	112.19
9	z	6	MAN	O5-C1-C2	2.21	114.19	110.77
11	Y	7	MAN	C1-O5-C5	2.21	115.18	112.19
11	m	9	MAN	O2-C2-C3	-2.21	105.72	110.14
6	R	5	MAN	O2-C2-C3	-2.20	105.73	110.14
10	U	5	MAN	O2-C2-C3	-2.20	105.74	110.14
9	v	6	MAN	O5-C1-C2	2.20	114.16	110.77
11	m	10	MAN	C1-O5-C5	2.19	115.16	112.19
6	R	4	MAN	O2-C2-C3	-2.19	105.75	110.14
6	j	4	MAN	O2-C2-C3	-2.19	105.75	110.14
9	T	6	MAN	O2-C2-C3	-2.18	105.76	110.14
9	l	6	MAN	O5-C1-C2	2.18	114.14	110.77
11	Y	4	MAN	O5-C1-C2	2.18	114.14	110.77
11	m	3	BMA	C1-O5-C5	2.18	115.15	112.19
6	t	5	MAN	C1-O5-C5	2.18	115.14	112.19
6	R	5	MAN	C1-O5-C5	2.18	115.14	112.19
6	r	5	MAN	O2-C2-C3	-2.17	105.79	110.14
9	X	5	MAN	O2-C2-C3	-2.17	105.79	110.14
10	U	7	MAN	O2-C2-C3	-2.17	105.79	110.14
11	Y	8	MAN	O2-C2-C3	-2.16	105.80	110.14
10	i	7	MAN	O2-C2-C3	-2.16	105.81	110.14
6	r	3	BMA	O5-C5-C6	2.15	110.58	107.20
11	m	7	MAN	C1-O5-C5	2.15	115.10	112.19
9	h	4	MAN	O5-C1-C2	2.14	114.08	110.77
10	U	7	MAN	C1-C2-C3	2.14	112.30	109.67
11	0	4	MAN	O5-C1-C2	2.14	114.08	110.77
9	h	4	MAN	C1-C2-C3	2.13	112.28	109.67
9	h	7	MAN	O2-C2-C3	-2.13	105.88	110.14
9	l	4	MAN	O2-C2-C3	-2.12	105.89	110.14
11	Y	3	BMA	C1-O5-C5	2.12	115.06	112.19
11	0	7	MAN	C1-O5-C5	2.11	115.06	112.19
10	w	3	BMA	C1-O5-C5	2.11	115.06	112.19
11	m	7	MAN	O2-C2-C3	-2.11	105.91	110.14
6	P	5	MAN	O2-C2-C3	-2.11	105.91	110.14
9	X	1	NAG	O4-C4-C5	-2.11	104.06	109.30
11	Y	6	MAN	O5-C1-C2	2.10	114.02	110.77
6	P	3	BMA	O5-C5-C6	2.10	110.50	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	4	MAN	O5-C1-C2	2.09	114.00	110.77
9	T	6	MAN	O5-C1-C2	2.09	113.99	110.77
6	r	4	MAN	O5-C1-C2	2.08	113.99	110.77
9	X	6	MAN	O5-C1-C2	2.08	113.98	110.77
11	m	8	MAN	O2-C2-C3	-2.08	105.97	110.14
6	R	4	MAN	C1-O5-C5	2.08	115.01	112.19
11	m	4	MAN	O5-C1-C2	2.08	113.97	110.77
11	0	5	MAN	O2-C2-C3	-2.07	105.98	110.14
6	r	4	MAN	O2-C2-C3	-2.06	106.01	110.14
11	Y	5	MAN	O2-C2-C3	-2.06	106.01	110.14
10	w	7	MAN	O2-C2-C3	-2.06	106.01	110.14
8	u	2	NAG	C1-C2-N2	2.06	114.00	110.49
6	P	4	MAN	O5-C1-C2	2.06	113.95	110.77
6	f	4	MAN	O2-C2-C3	-2.06	106.02	110.14
9	z	6	MAN	O2-C2-C3	-2.06	106.02	110.14
11	0	6	MAN	O5-C1-C2	2.05	113.94	110.77
9	v	7	MAN	O2-C2-C3	-2.04	106.04	110.14
6	f	5	MAN	C1-O5-C5	2.04	114.95	112.19
6	P	2	NAG	C1-C2-N2	2.03	113.96	110.49
9	T	7	MAN	O2-C2-C3	-2.03	106.06	110.14
9	X	7	MAN	O2-C2-C3	-2.03	106.07	110.14
10	w	3	BMA	C3-C4-C5	2.03	113.86	110.24
6	j	5	MAN	O2-C2-C3	-2.03	106.07	110.14
9	T	3	BMA	C1-O5-C5	2.03	114.94	112.19
6	t	4	MAN	O2-C2-C3	-2.02	106.09	110.14
10	i	3	BMA	C3-C4-C5	2.02	113.83	110.24
11	m	5	MAN	O2-C2-C3	-2.02	106.10	110.14
9	z	4	MAN	O2-C2-C3	-2.00	106.12	110.14

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	e	4	MAN	C4-C5-C6-O6
11	0	2	NAG	O5-C5-C6-O6
10	U	1	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
11	m	2	NAG	O5-C5-C6-O6
6	t	2	NAG	O5-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	f	3	BMA	C4-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	w	1	NAG	O5-C5-C6-O6
6	t	3	BMA	C4-C5-C6-O6
7	s	4	MAN	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
7	Q	4	MAN	C4-C5-C6-O6
10	i	1	NAG	O5-C5-C6-O6
8	b	1	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	t	2	NAG	C4-C5-C6-O6
10	w	1	NAG	C4-C5-C6-O6
7	e	4	MAN	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
8	y	1	NAG	O5-C5-C6-O6
10	U	1	NAG	C4-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	t	3	BMA	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
8	o	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	2	2	NAG	O5-C5-C6-O6
8	4	2	NAG	O5-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
7	s	4	MAN	O5-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
11	m	2	NAG	C4-C5-C6-O6
11	0	2	NAG	C4-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
8	y	1	NAG	C4-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
8	3	1	NAG	C4-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
8	o	2	NAG	C4-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	4	2	NAG	C4-C5-C6-O6
6	P	2	NAG	C8-C7-N2-C2
6	P	2	NAG	O7-C7-N2-C2
6	d	2	NAG	C8-C7-N2-C2
6	d	2	NAG	O7-C7-N2-C2
6	r	2	NAG	C8-C7-N2-C2
6	r	2	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
8	S	2	NAG	C8-C7-N2-C2
8	S	2	NAG	O7-C7-N2-C2
8	b	1	NAG	C8-C7-N2-C2
8	b	1	NAG	O7-C7-N2-C2
8	g	1	NAG	C8-C7-N2-C2
8	g	1	NAG	O7-C7-N2-C2
8	g	2	NAG	C8-C7-N2-C2
8	g	2	NAG	O7-C7-N2-C2
8	p	1	NAG	C8-C7-N2-C2
8	p	1	NAG	O7-C7-N2-C2
8	u	1	NAG	C8-C7-N2-C2
8	u	1	NAG	O7-C7-N2-C2
8	u	2	NAG	C8-C7-N2-C2
8	u	2	NAG	O7-C7-N2-C2
8	3	1	NAG	C8-C7-N2-C2
8	3	1	NAG	O7-C7-N2-C2
7	Q	4	MAN	O5-C5-C6-O6
6	d	1	NAG	C4-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
8	c	2	NAG	C4-C5-C6-O6
8	2	2	NAG	C4-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
8	4	1	NAG	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
8	3	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	c	1	NAG	O5-C5-C6-O6
9	T	4	MAN	O5-C5-C6-O6
9	v	4	MAN	O5-C5-C6-O6
11	0	7	MAN	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
11	m	7	MAN	O5-C5-C6-O6
6	r	1	NAG	C4-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
8	k	2	NAG	C4-C5-C6-O6
11	Y	7	MAN	O5-C5-C6-O6
8	u	1	NAG	C4-C5-C6-O6
11	0	7	MAN	C4-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
11	m	7	MAN	C4-C5-C6-O6
9	h	4	MAN	O5-C5-C6-O6
11	Y	6	MAN	O5-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6
11	Y	7	MAN	C4-C5-C6-O6
11	0	6	MAN	O5-C5-C6-O6
8	y	2	NAG	C4-C5-C6-O6
11	m	6	MAN	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
10	i	10	MAN	O5-C5-C6-O6
8	W	2	NAG	C4-C5-C6-O6
8	k	2	NAG	O5-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
8	u	1	NAG	O5-C5-C6-O6
6	f	4	MAN	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
6	t	4	MAN	O5-C5-C6-O6
6	t	1	NAG	C4-C5-C6-O6
8	4	1	NAG	C4-C5-C6-O6
9	l	3	BMA	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
9	l	3	BMA	C4-C5-C6-O6
8	y	2	NAG	O5-C5-C6-O6
8	q	1	NAG	C4-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
10	w	2	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
9	T	4	MAN	C4-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	X	3	BMA	C4-C5-C6-O6
10	U	10	MAN	O5-C5-C6-O6
10	w	10	MAN	O5-C5-C6-O6
8	n	1	NAG	C4-C5-C6-O6
9	v	4	MAN	C4-C5-C6-O6
9	X	1	NAG	O5-C5-C6-O6
10	w	2	NAG	O5-C5-C6-O6
8	n	1	NAG	O5-C5-C6-O6
9	l	1	NAG	O5-C5-C6-O6
10	i	3	BMA	C4-C5-C6-O6
10	U	3	BMA	O5-C5-C6-O6
6	V	1	NAG	C3-C2-N2-C7
6	j	1	NAG	C3-C2-N2-C7
6	x	1	NAG	C3-C2-N2-C7
8	Z	1	NAG	C3-C2-N2-C7
8	n	1	NAG	C3-C2-N2-C7
8	1	1	NAG	C3-C2-N2-C7
11	Y	2	NAG	C3-C2-N2-C7
8	c	1	NAG	C4-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
10	i	3	BMA	O5-C5-C6-O6
6	t	1	NAG	O5-C5-C6-O6
10	U	3	BMA	C4-C5-C6-O6
9	z	3	BMA	O5-C5-C6-O6
9	z	3	BMA	C4-C5-C6-O6
8	u	2	NAG	O5-C5-C6-O6
9	h	4	MAN	C4-C5-C6-O6
10	w	3	BMA	C4-C5-C6-O6
9	z	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
10	w	3	BMA	O5-C5-C6-O6
9	v	3	BMA	O5-C5-C6-O6
8	1	1	NAG	C4-C5-C6-O6
6	P	2	NAG	C3-C2-N2-C7
6	d	2	NAG	C3-C2-N2-C7
6	r	2	NAG	C3-C2-N2-C7
8	S	2	NAG	C3-C2-N2-C7
8	g	2	NAG	C3-C2-N2-C7
8	u	2	NAG	C3-C2-N2-C7
11	m	2	NAG	C3-C2-N2-C7
11	0	2	NAG	C3-C2-N2-C7
8	g	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	i	2	NAG	C4-C5-C6-O6
8	1	1	NAG	O5-C5-C6-O6
11	m	2	NAG	C1-C2-N2-C7
9	v	3	BMA	C4-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6

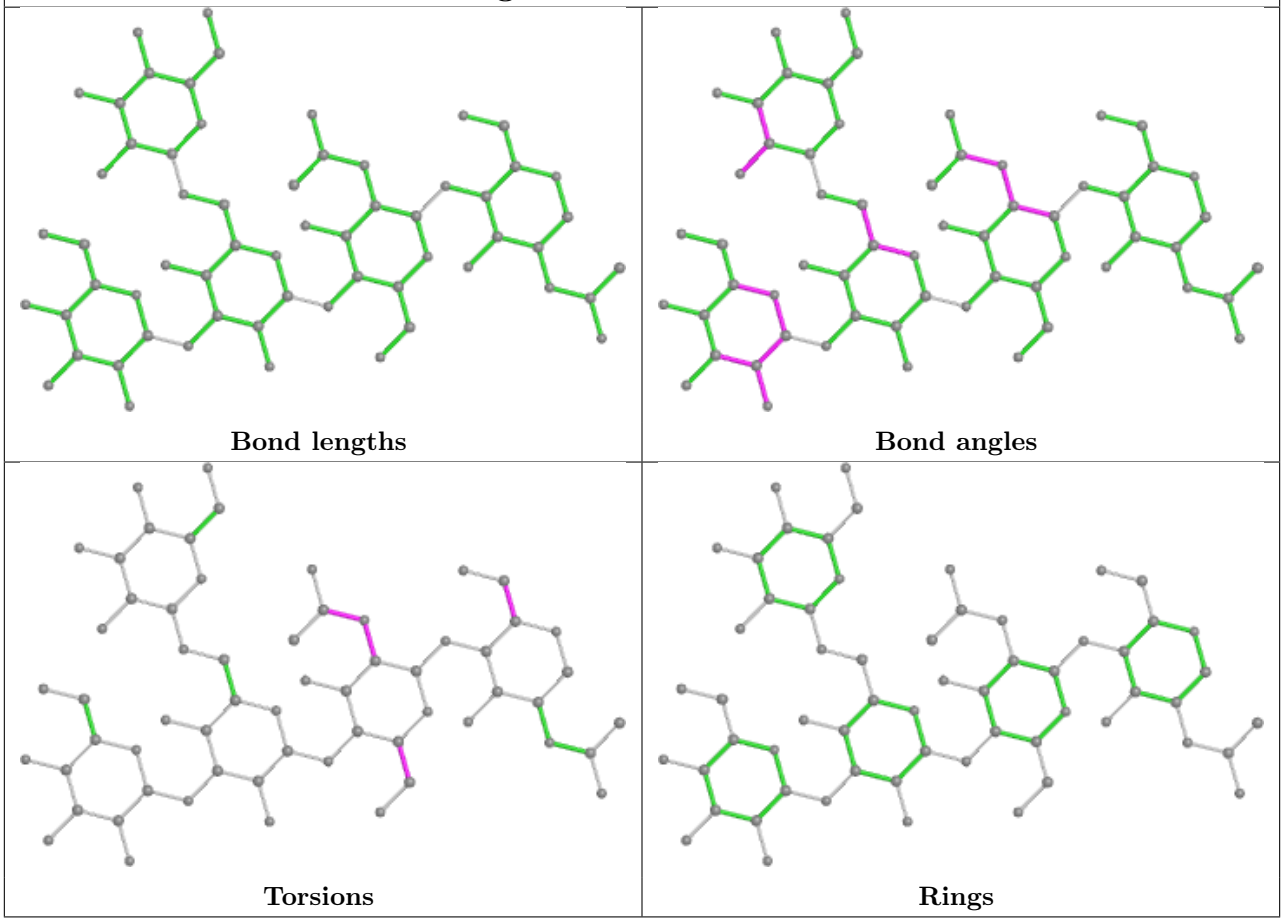
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	m	9	MAN	C1-C2-C3-C4-C5-O5
11	Y	9	MAN	C1-C2-C3-C4-C5-O5
11	0	9	MAN	C1-C2-C3-C4-C5-O5

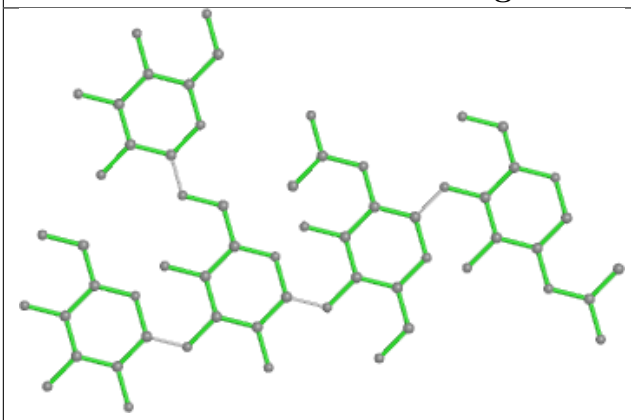
No monomer is involved in short contacts.

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

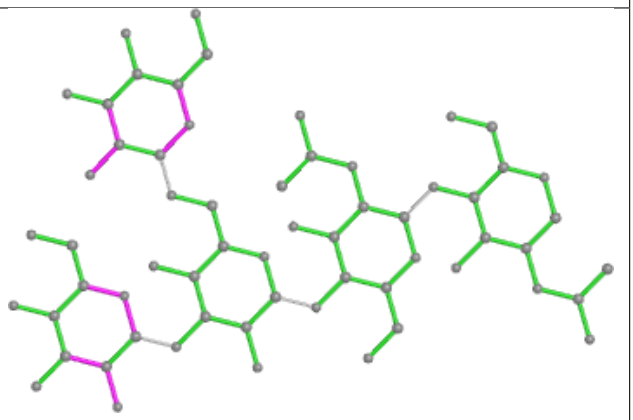
Oligosaccharide Chain P



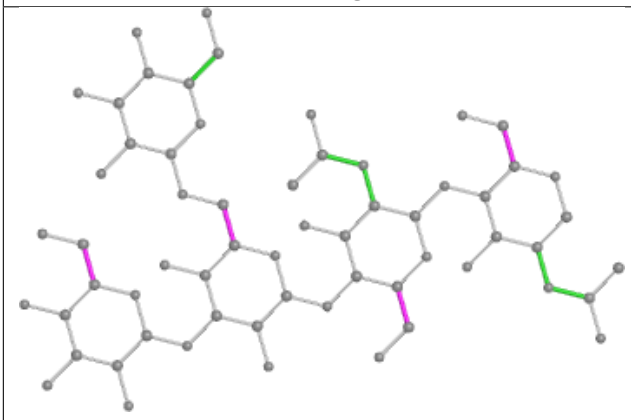
Oligosaccharide Chain R



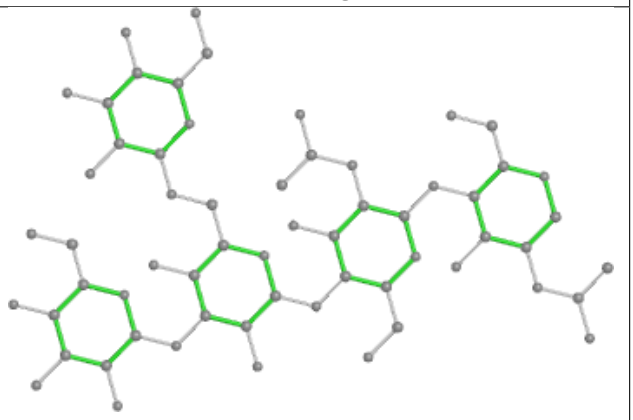
Bond lengths



Bond angles

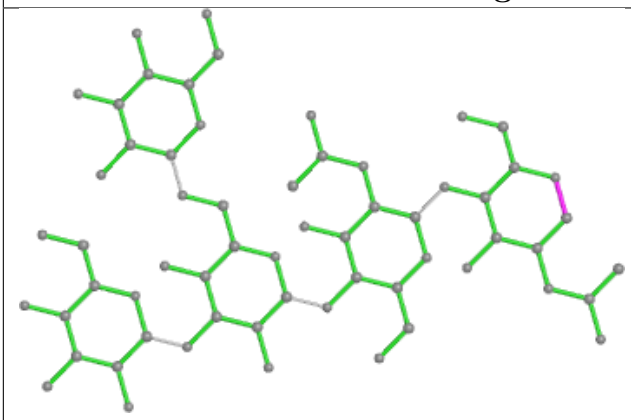


Torsions

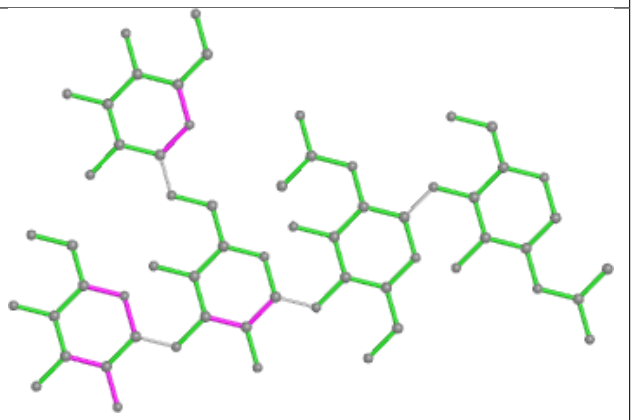


Rings

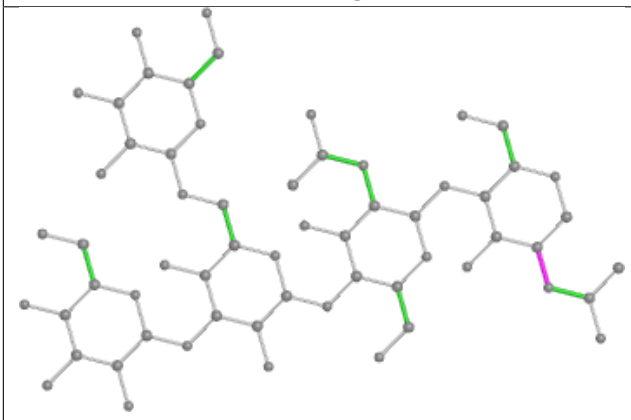
Oligosaccharide Chain V



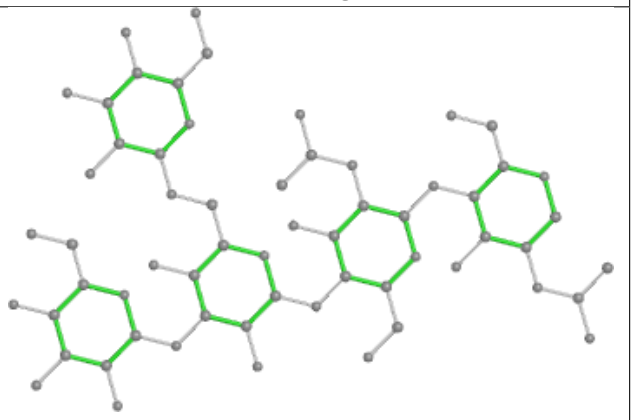
Bond lengths



Bond angles

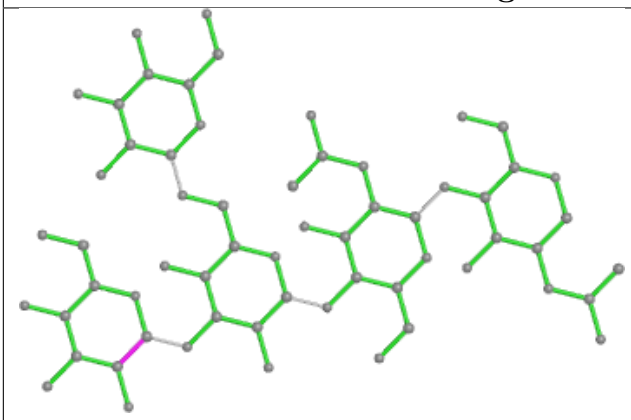


Torsions

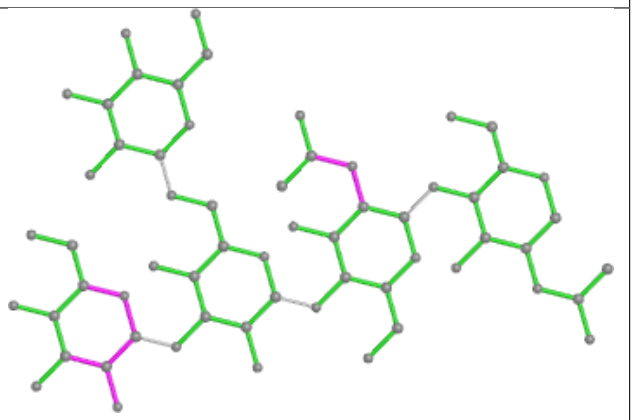


Rings

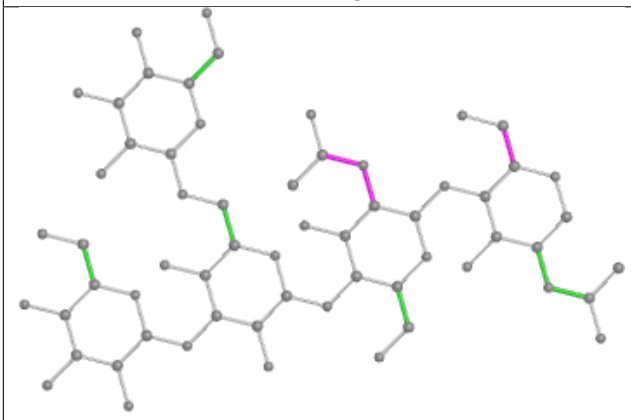
Oligosaccharide Chain d



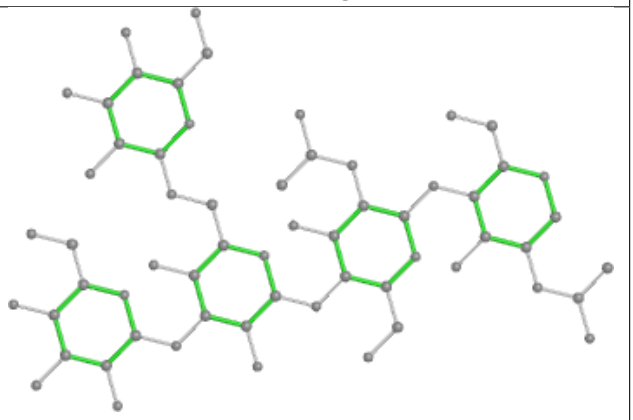
Bond lengths



Bond angles

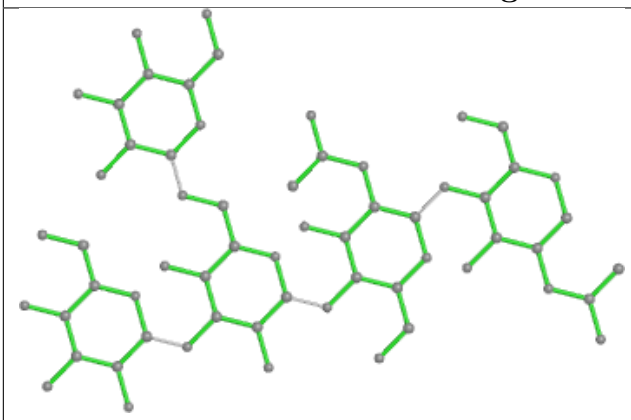


Torsions

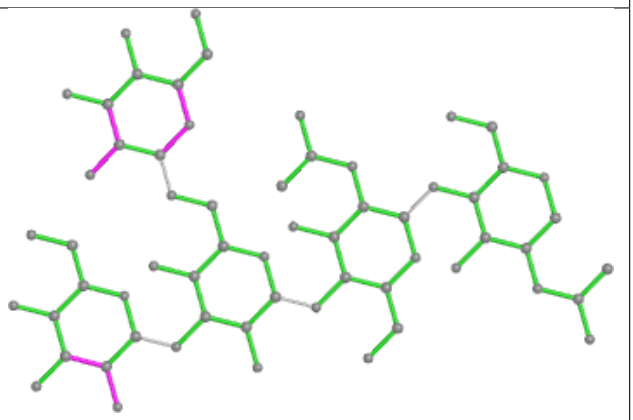


Rings

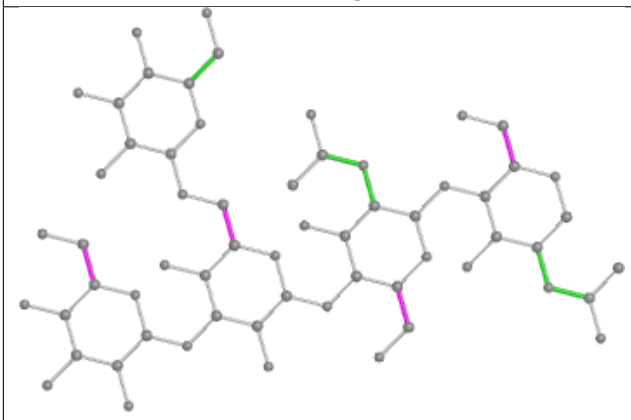
Oligosaccharide Chain f



Bond lengths



Bond angles



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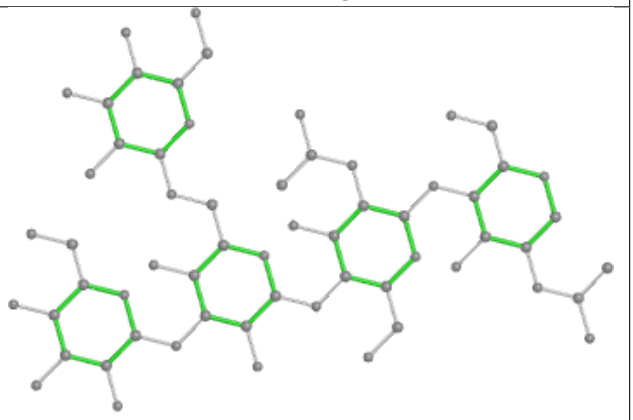
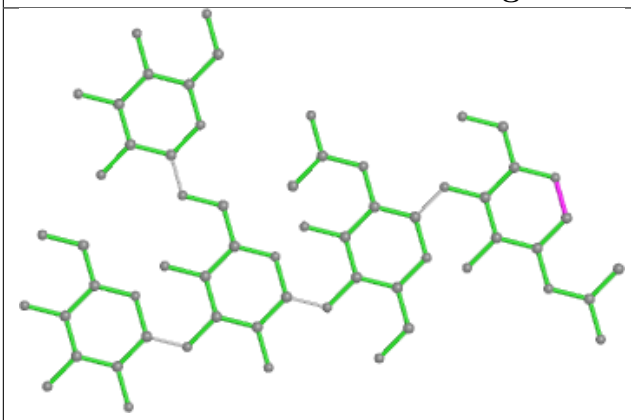


Rings

Oligosaccharide Chain j



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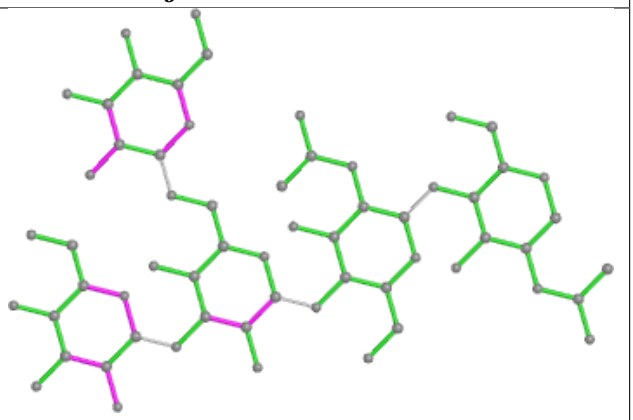

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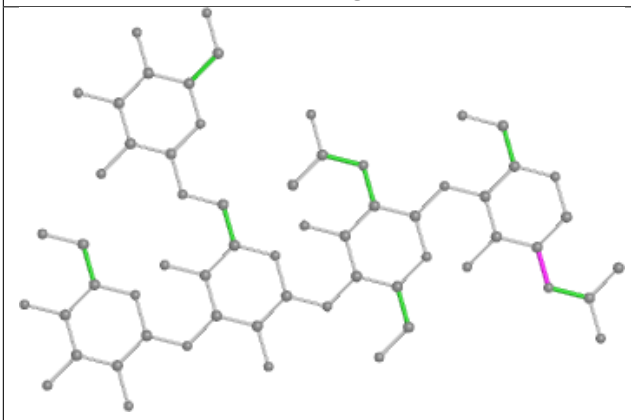

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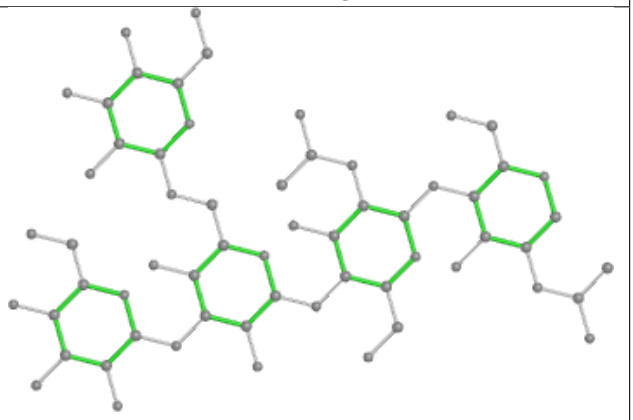
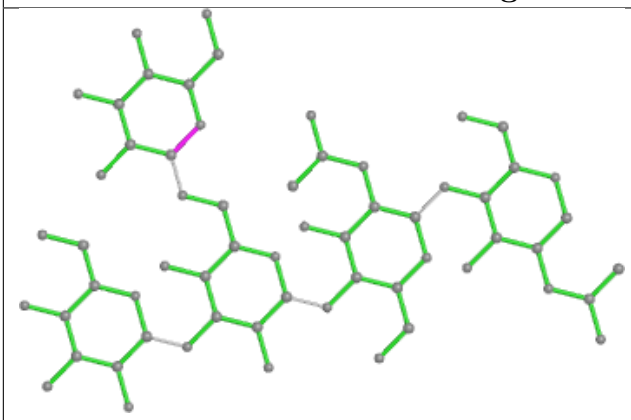


Rings

Oligosaccharide Chain r



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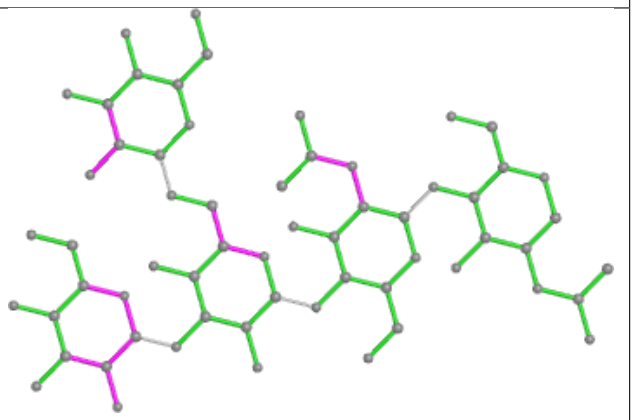

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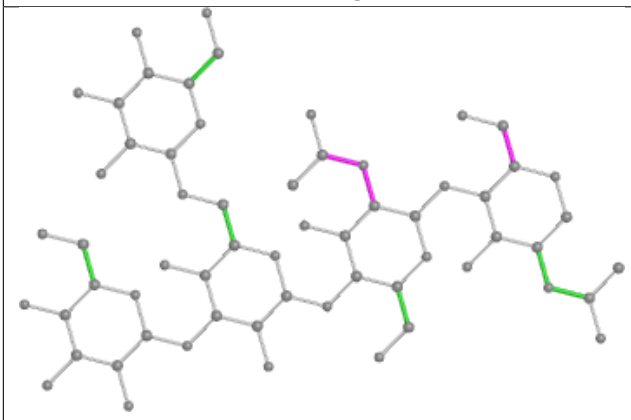
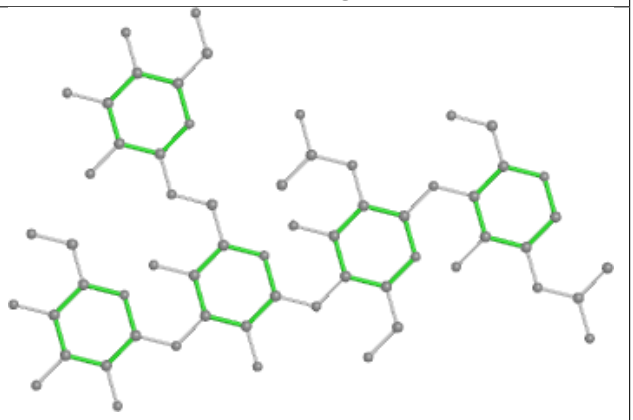
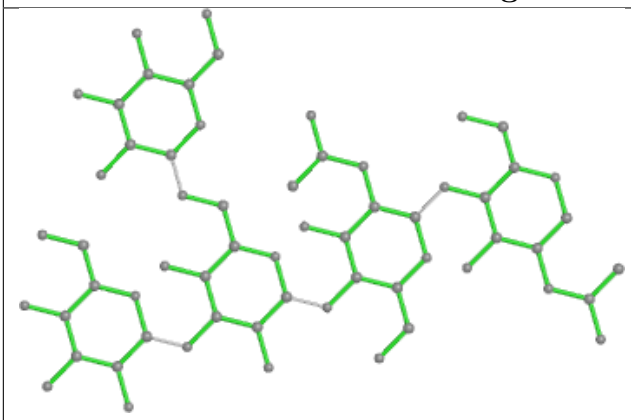


Torsions



Rings

Oligosaccharide Chain t



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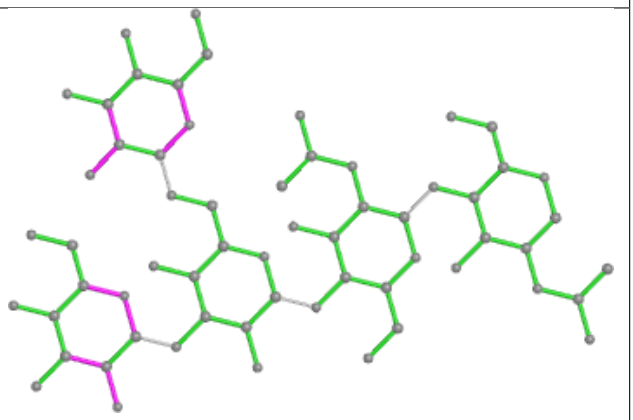
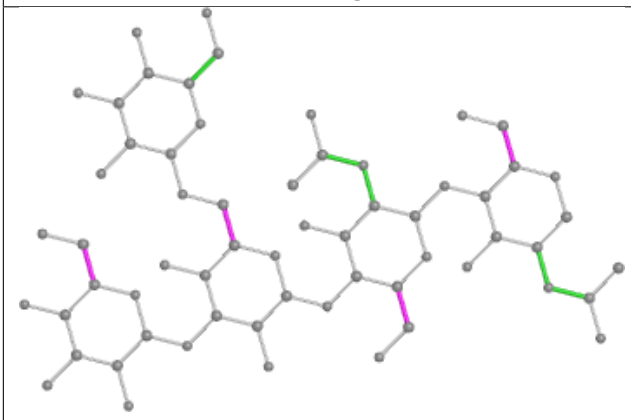


Bond angles



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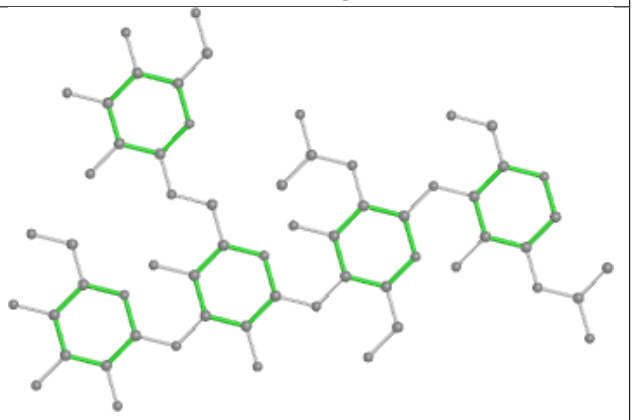
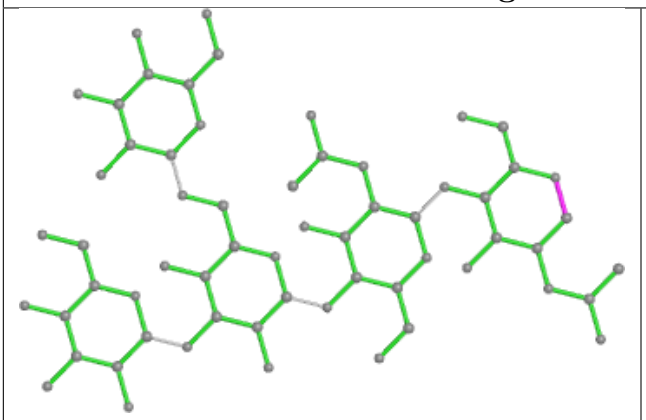


Rings

Oligosaccharide Chain x



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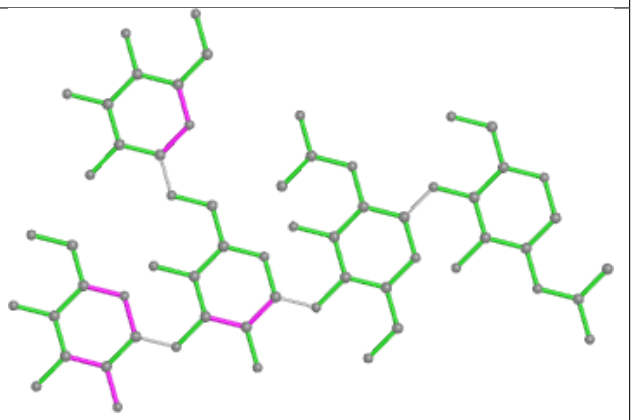
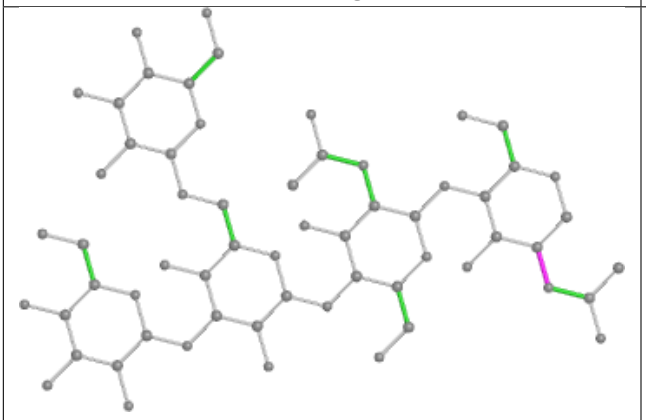


Bond angles



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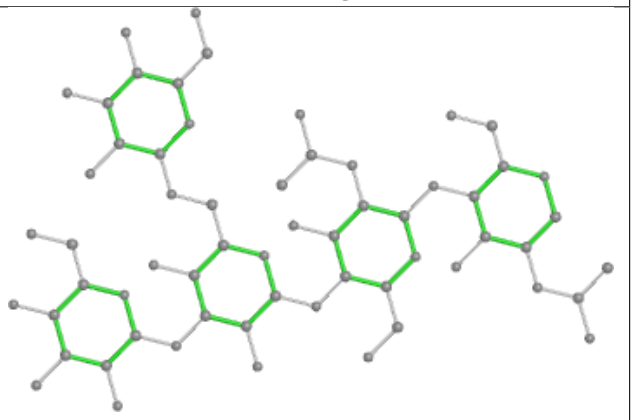
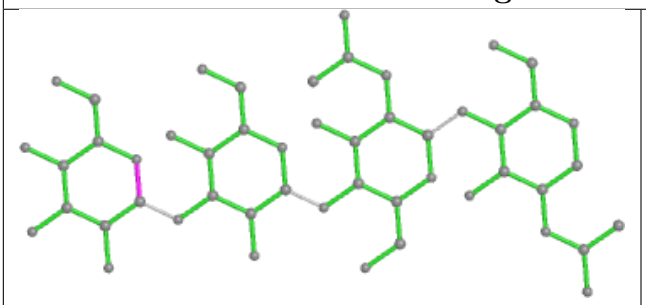


Rings

Oligosaccharide Chain Q



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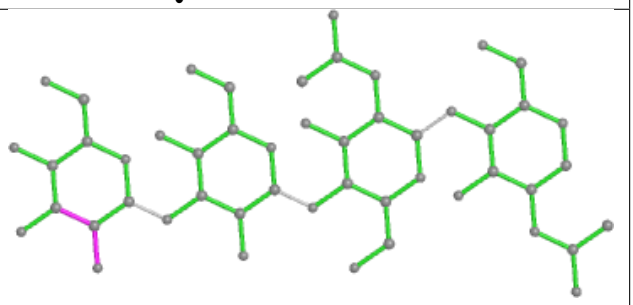

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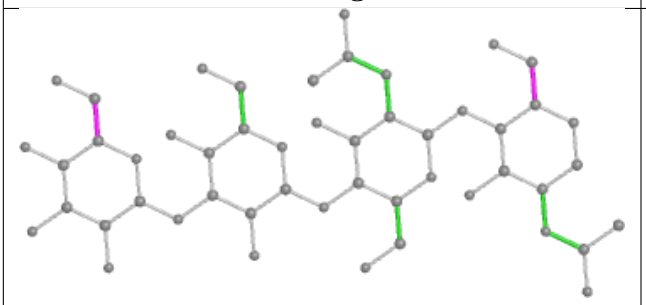

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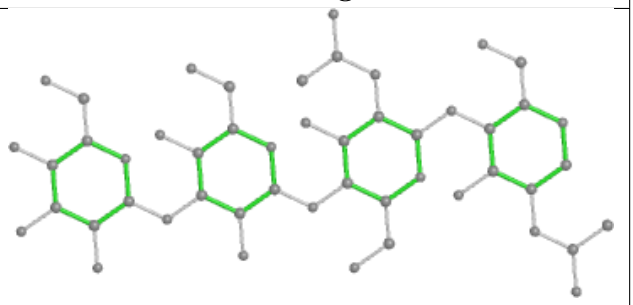
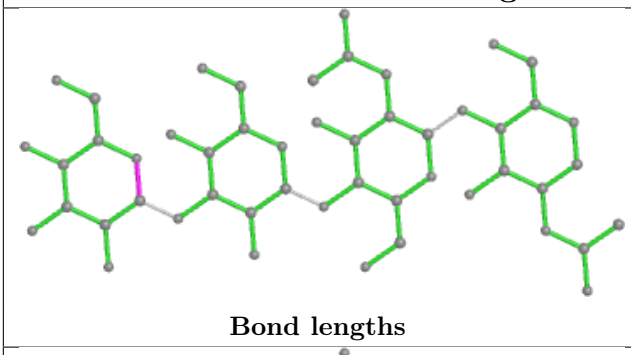


Rings

Oligosaccharide Chain e



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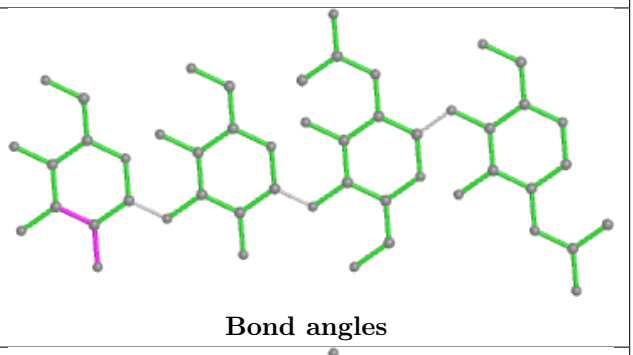
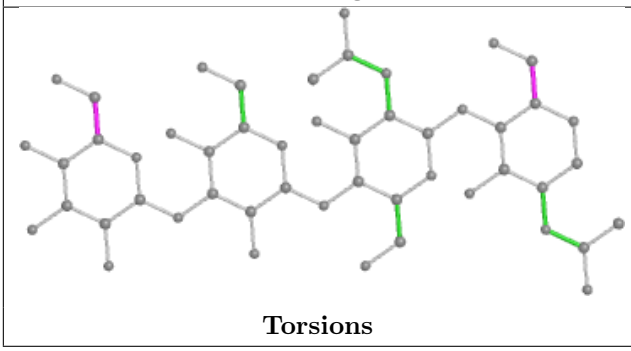


Bond angles



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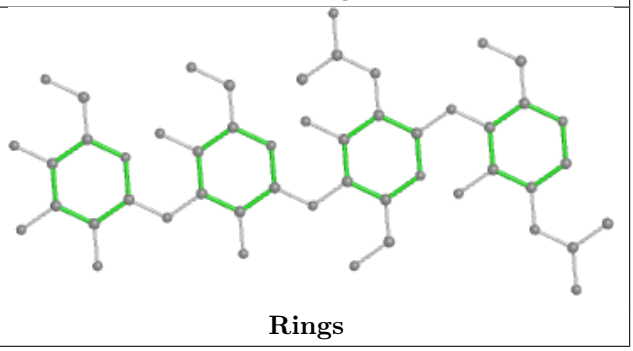
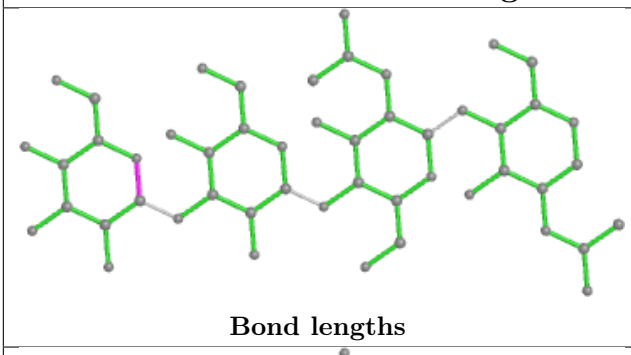


Rings

Oligosaccharide Chain s



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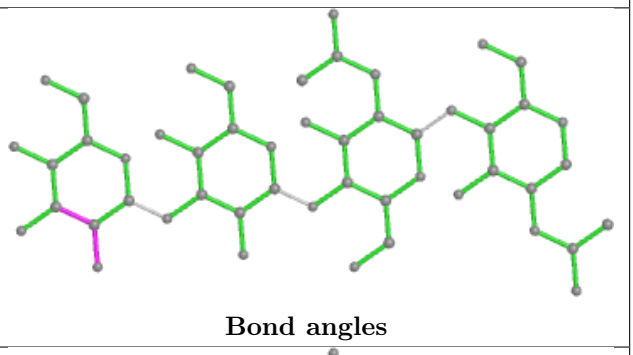
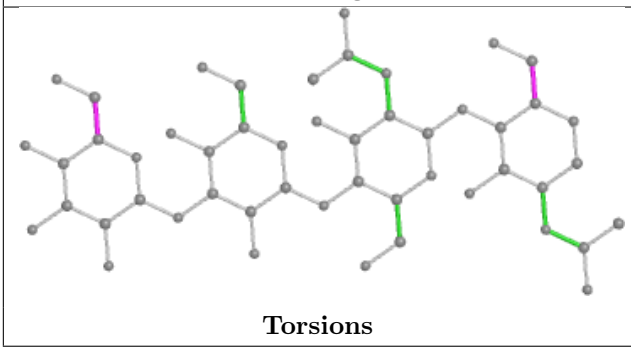


Bond angles



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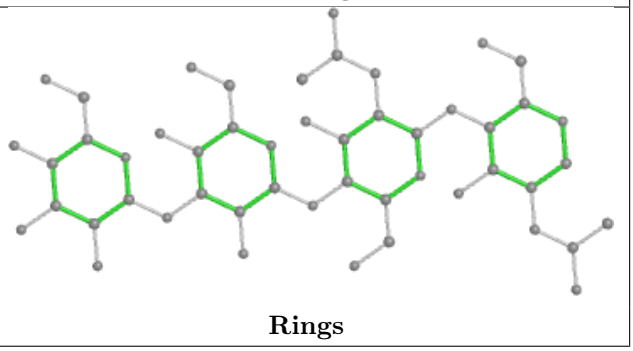
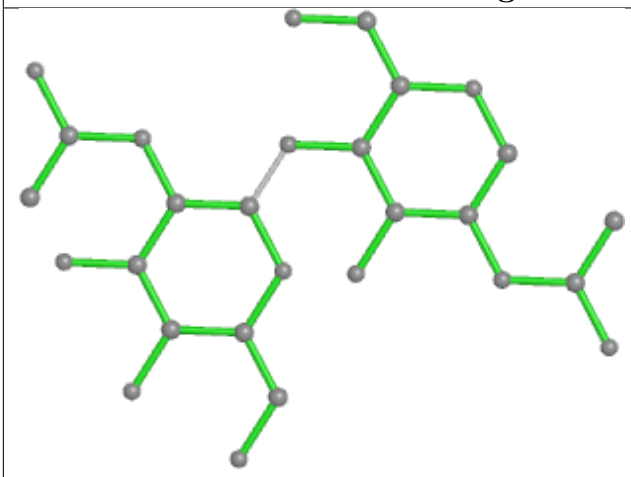


Rings

Oligosaccharide Chain S



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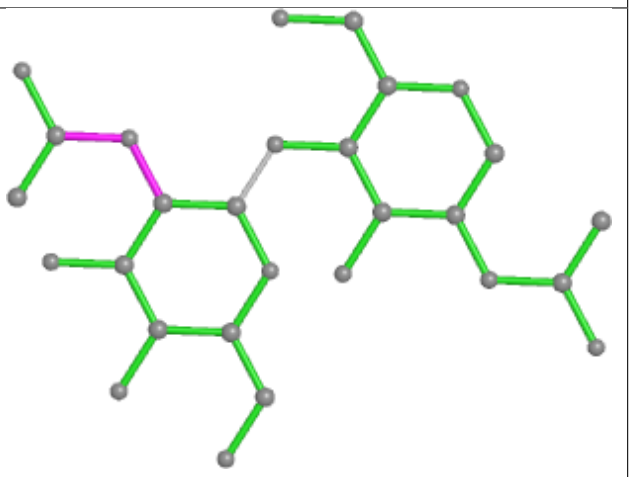
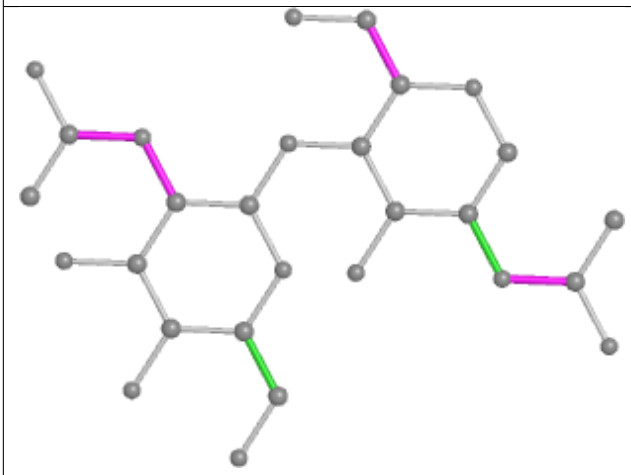


Bond angles



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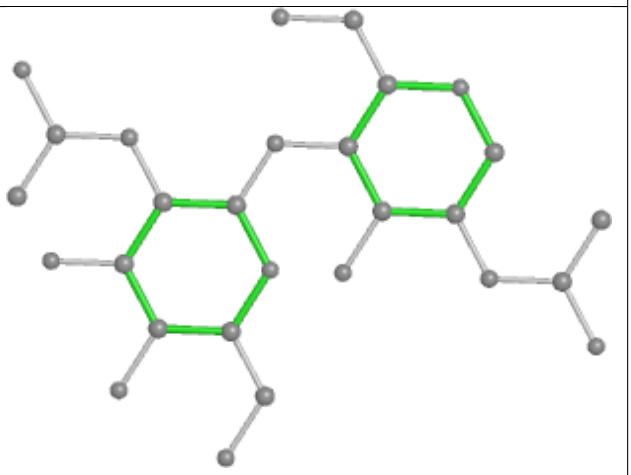
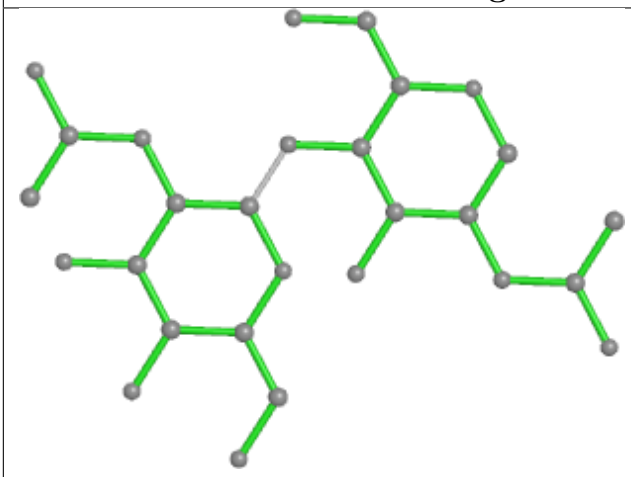


Rings

Oligosaccharide Chain W



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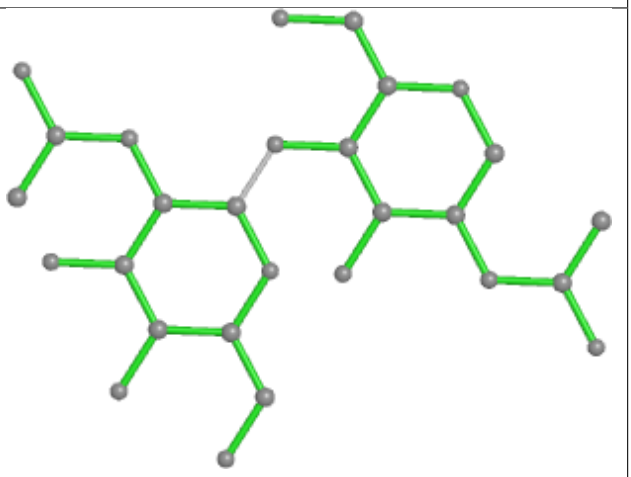
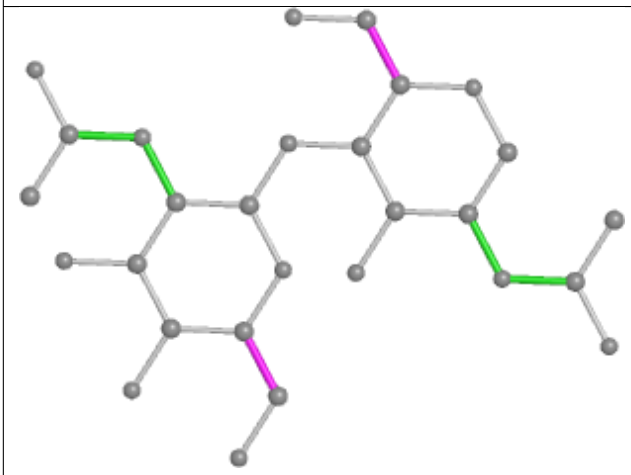


Bond angles



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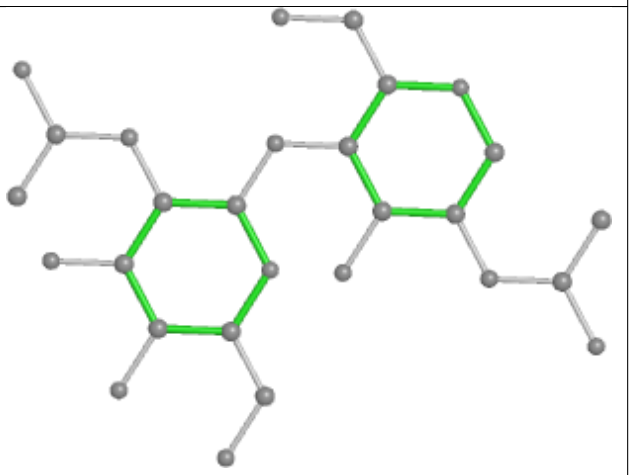
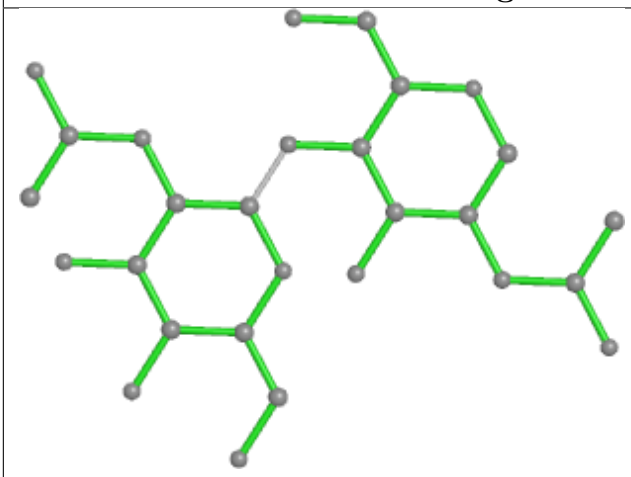


Rings

Oligosaccharide Chain Z



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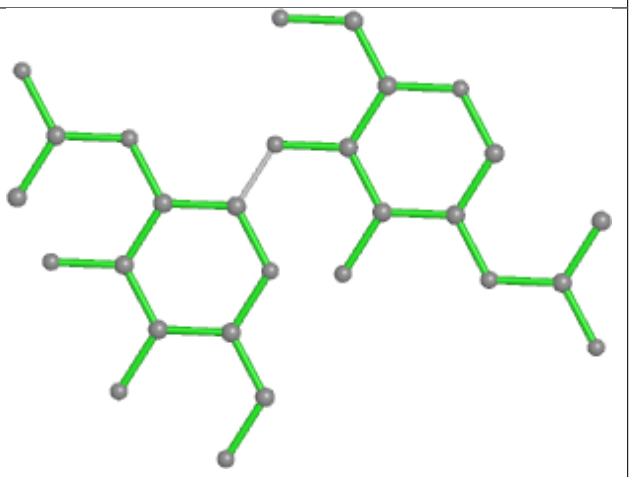
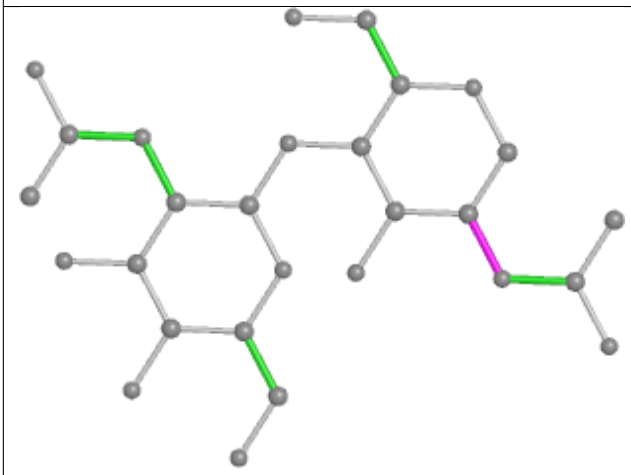


Bond angles



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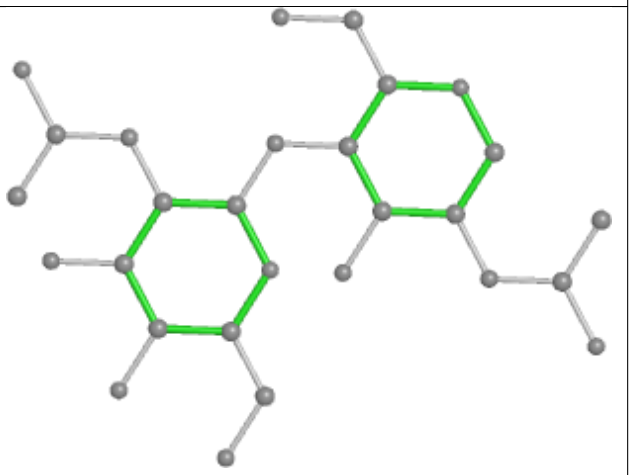
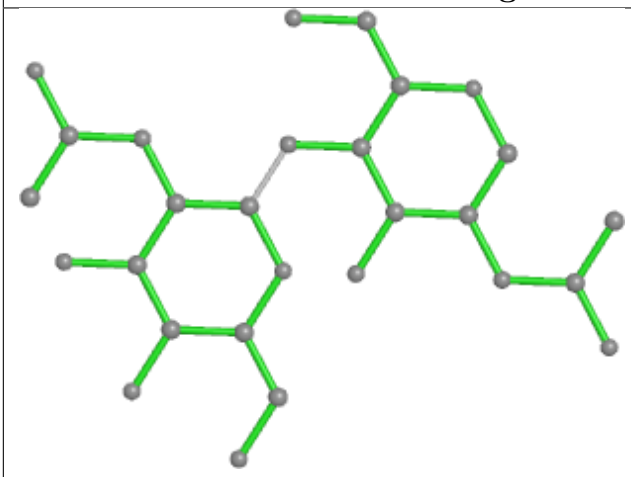


Rings

Oligosaccharide Chain a



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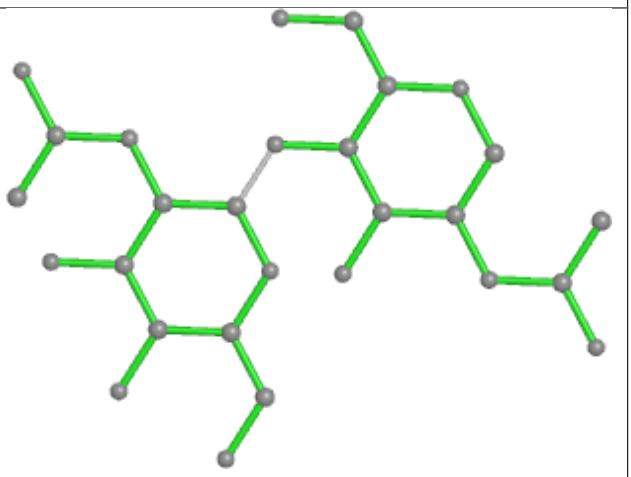

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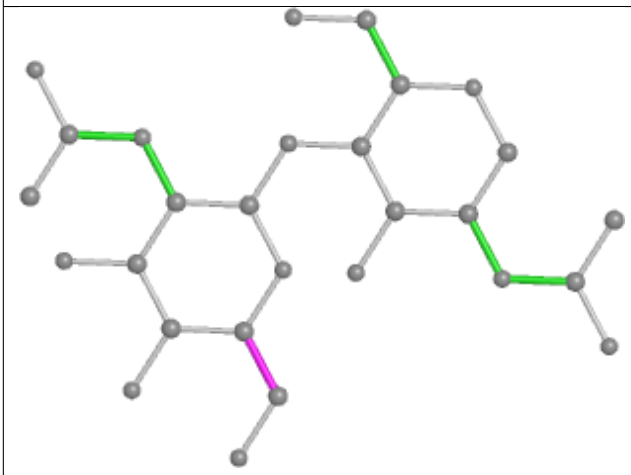

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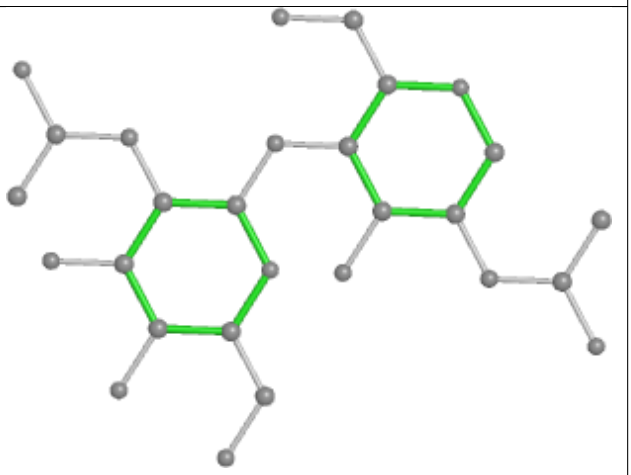
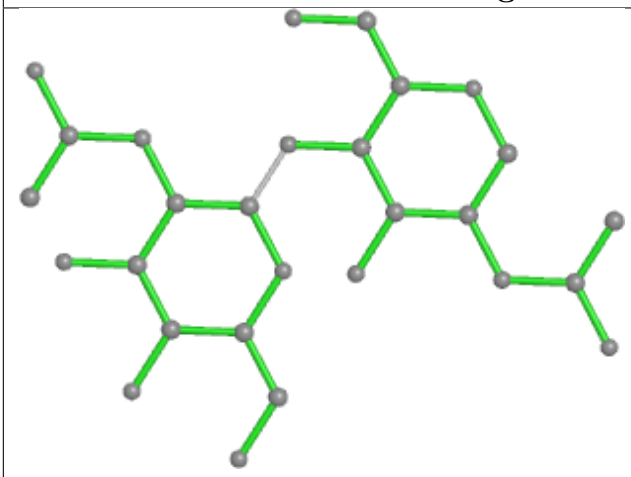
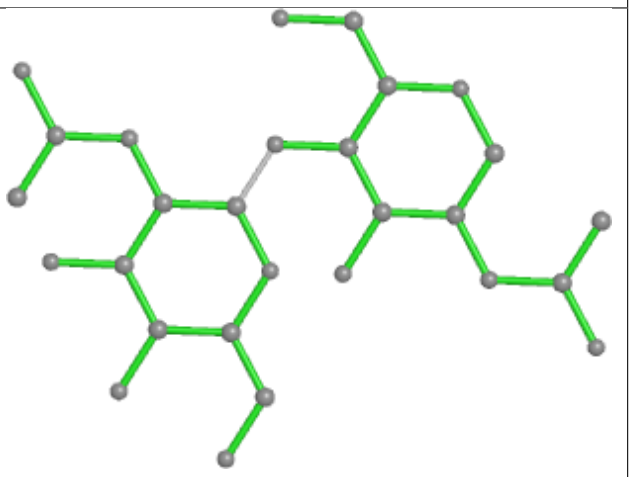


Rings

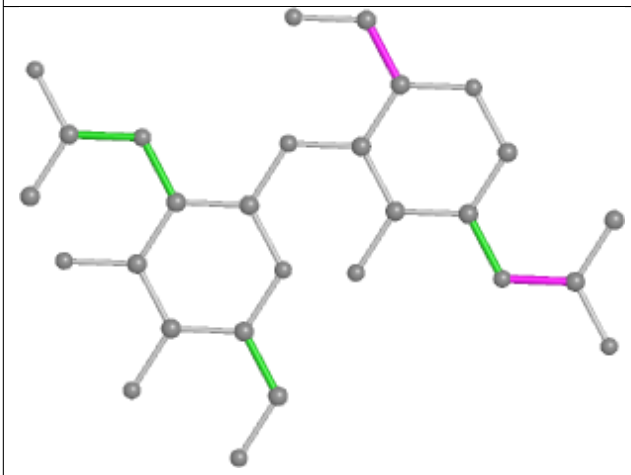
Oligosaccharide Chain b



Bond lengths



Bond angles



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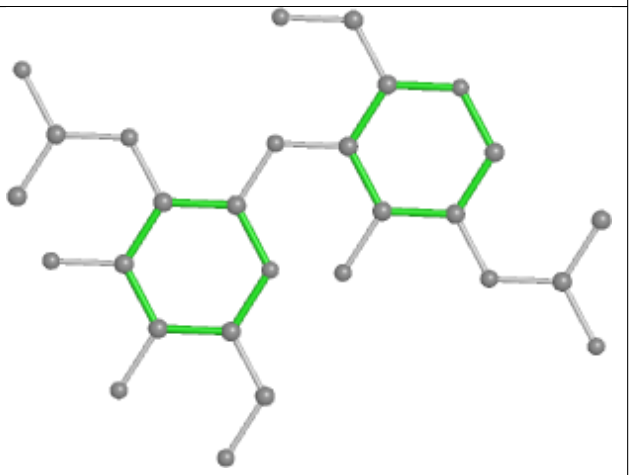
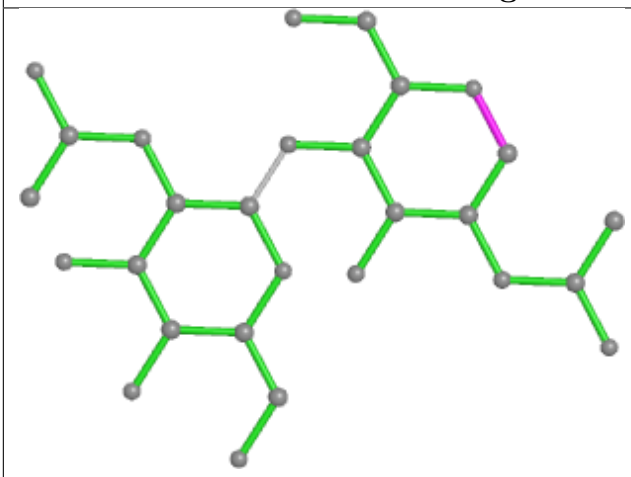
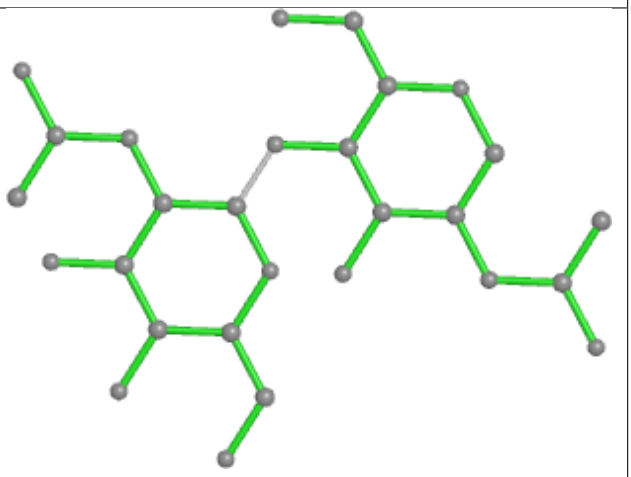


Rings

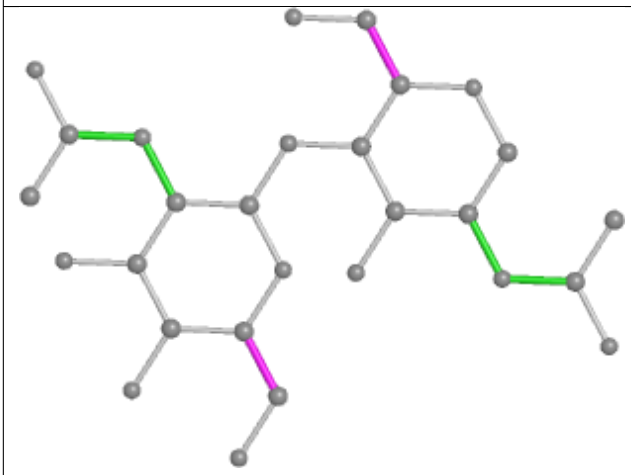
Oligosaccharide Chain c



Bond lengths



Bond angles



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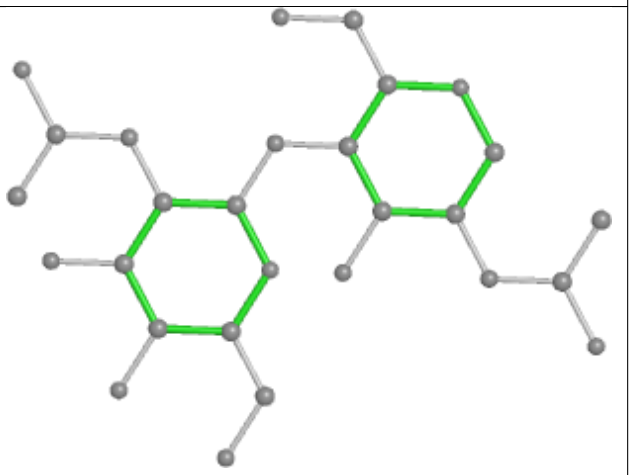
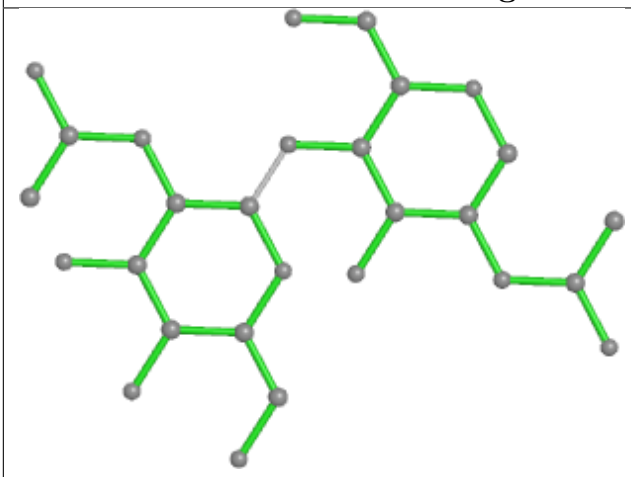


Rings

Oligosaccharide Chain g



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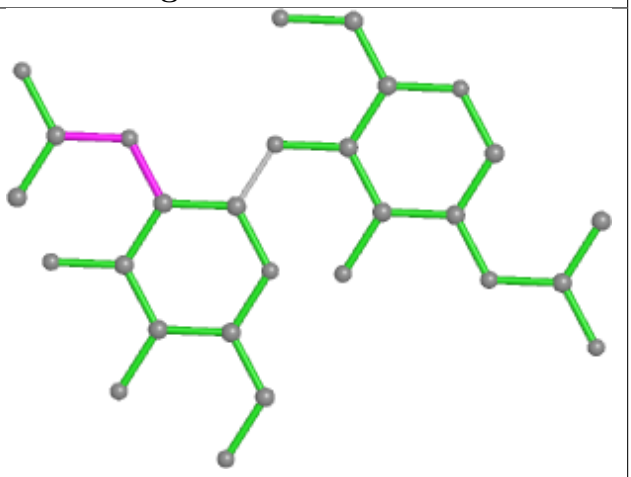
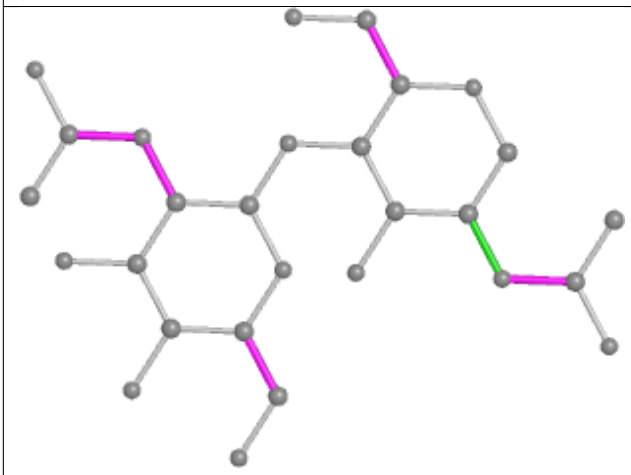
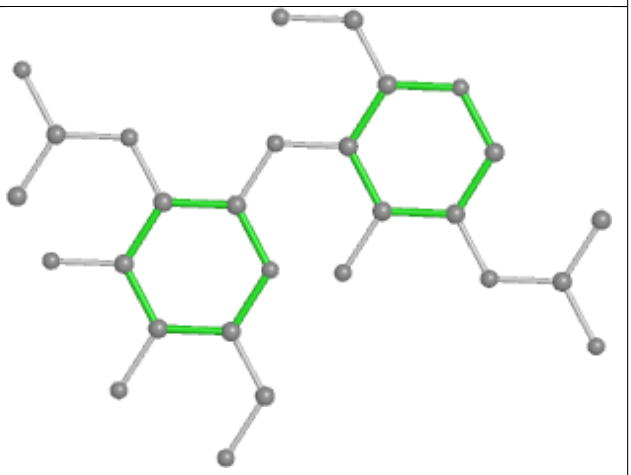


Bond angles

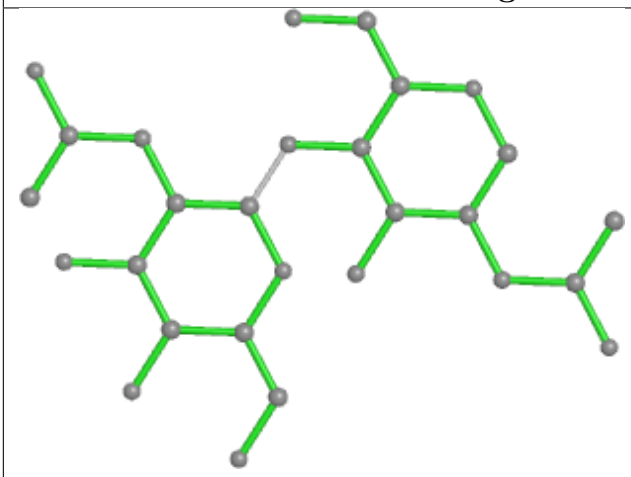


Torsions

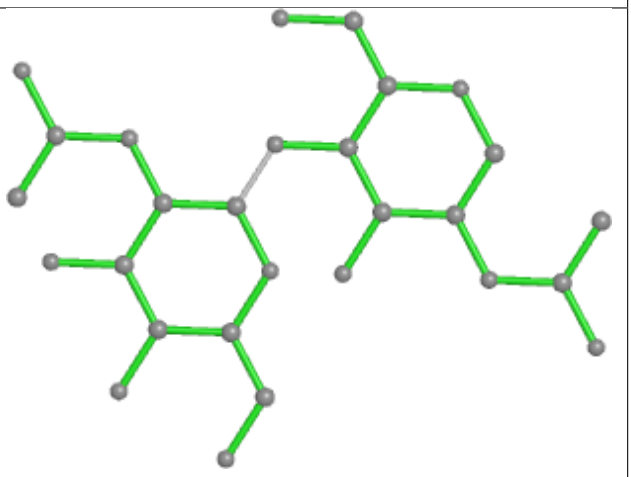


Rings

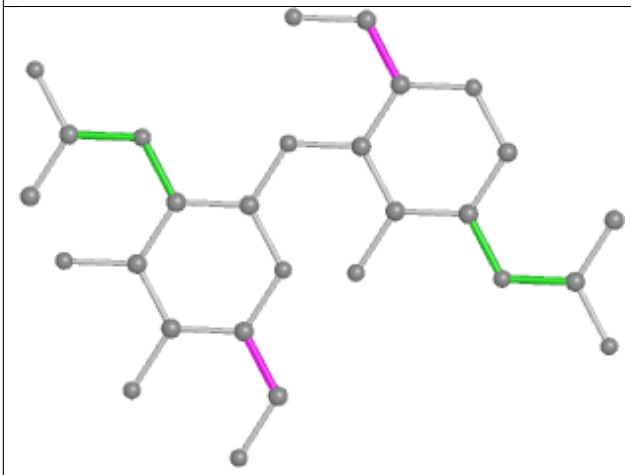
Oligosaccharide Chain k



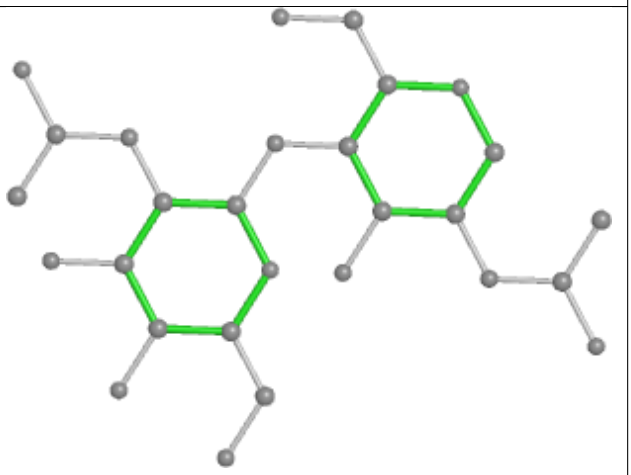
Bond lengths



Bond angles

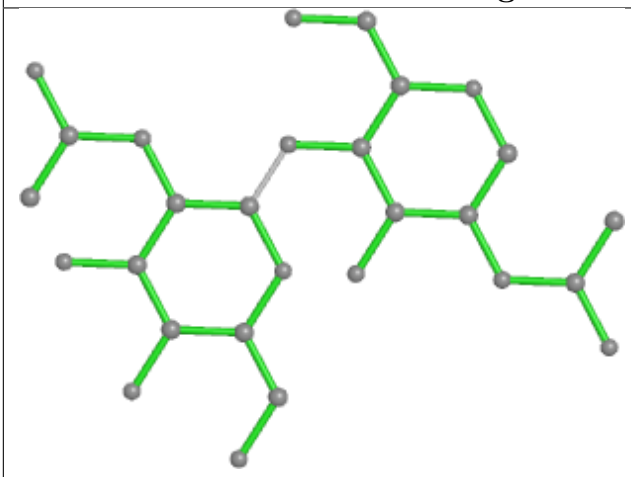


Torsions



Rings

Oligosaccharide Chain n



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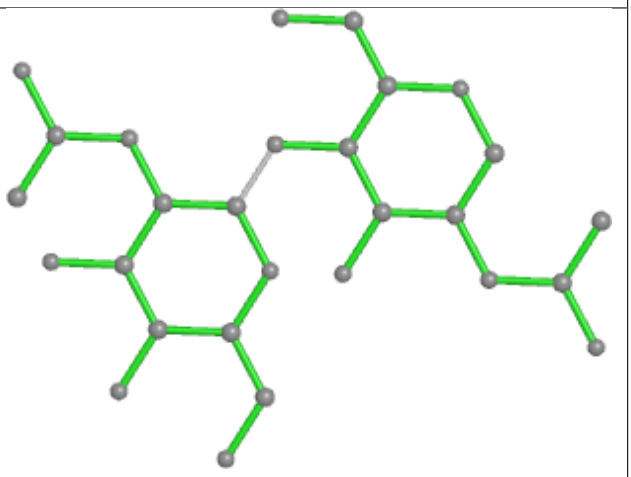
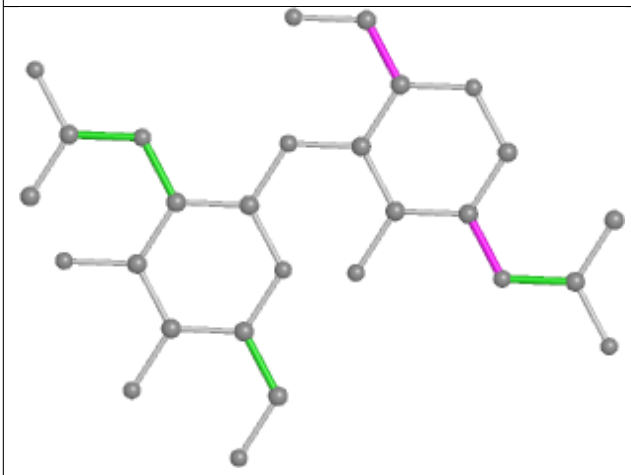


Bond angles



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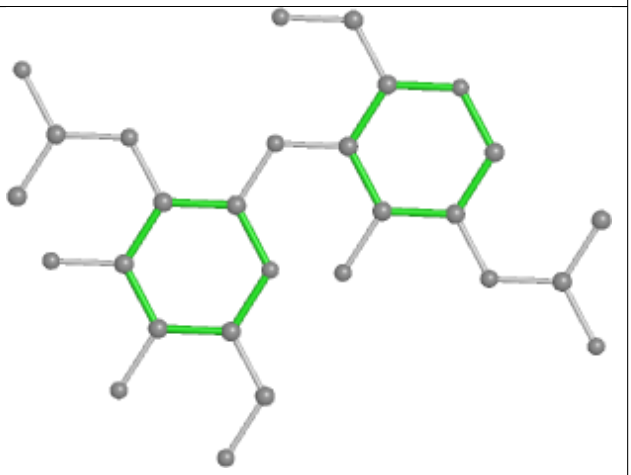
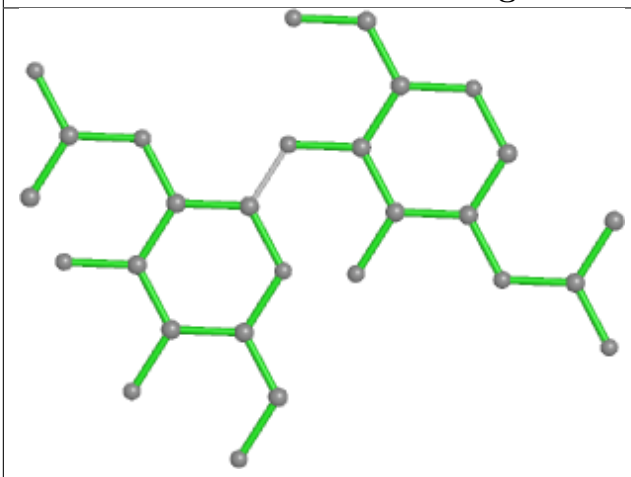


Rings

Oligosaccharide Chain o



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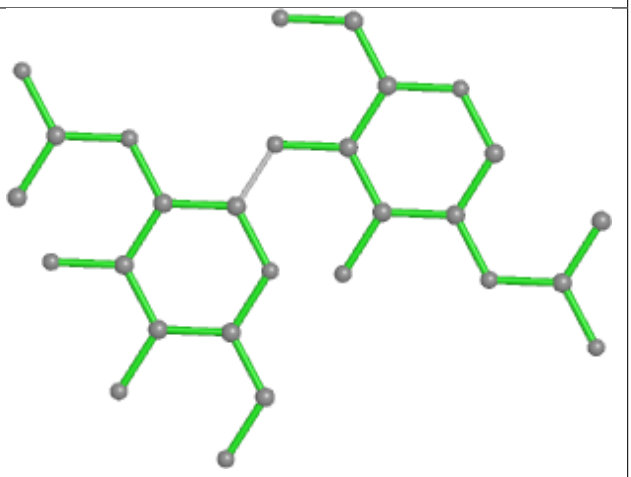
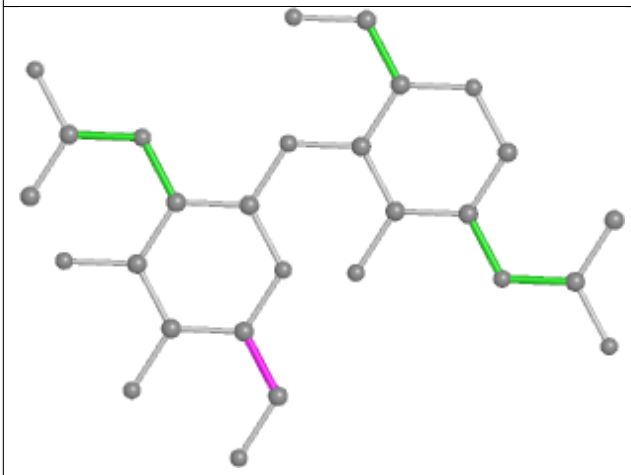


Bond angles



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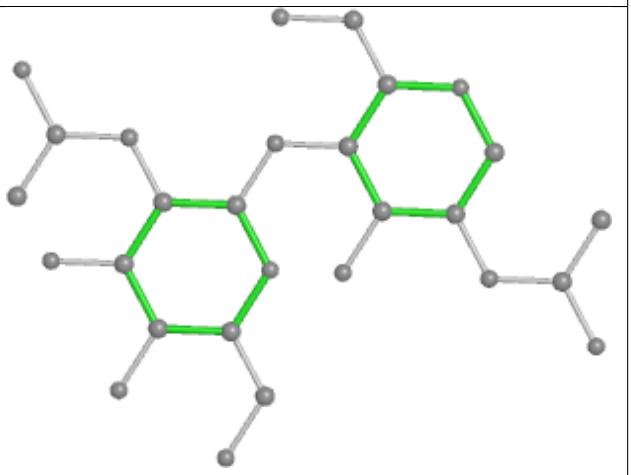
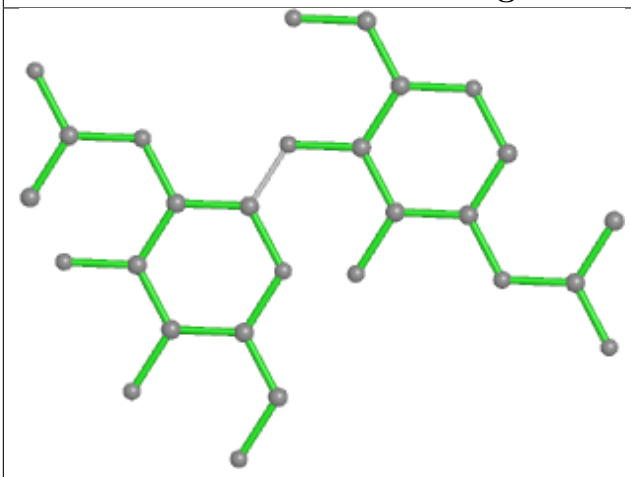


Rings

Oligosaccharide Chain p



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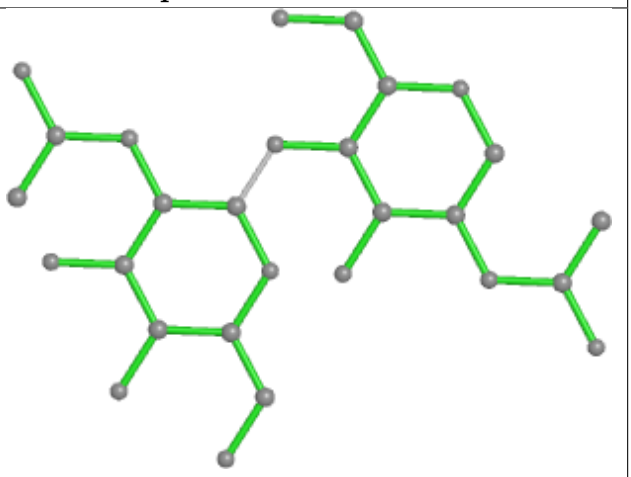
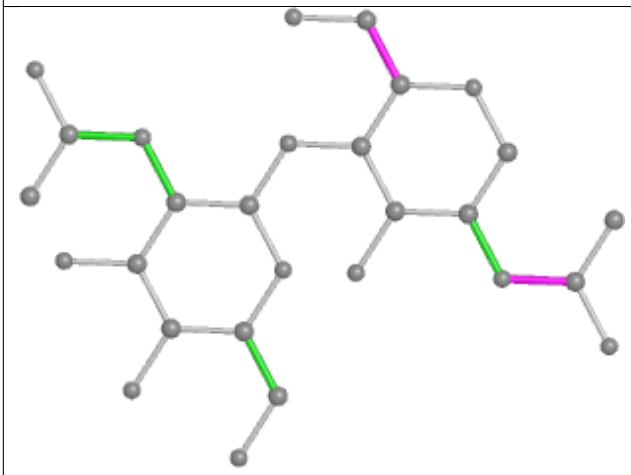


Bond angles



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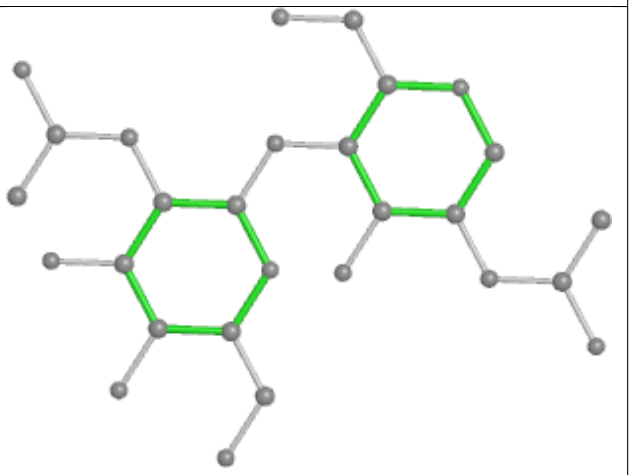
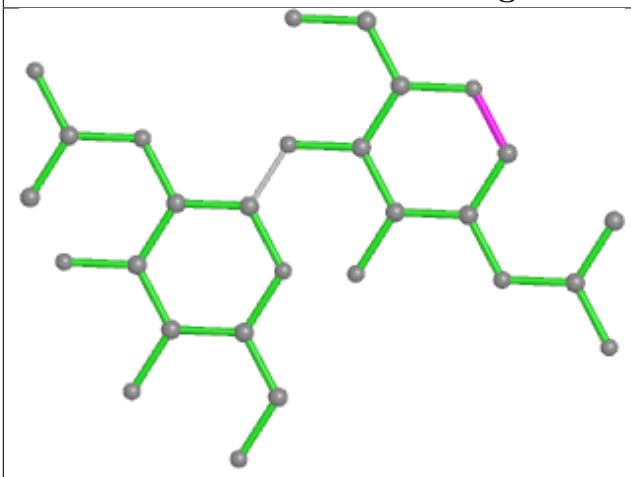


Rings

Oligosaccharide Chain q



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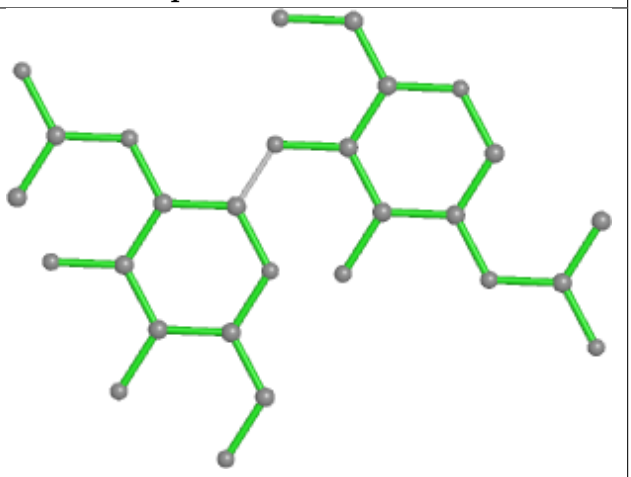
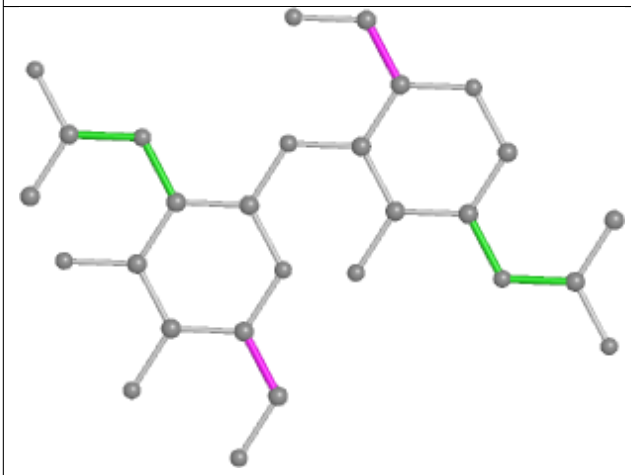


Bond angles



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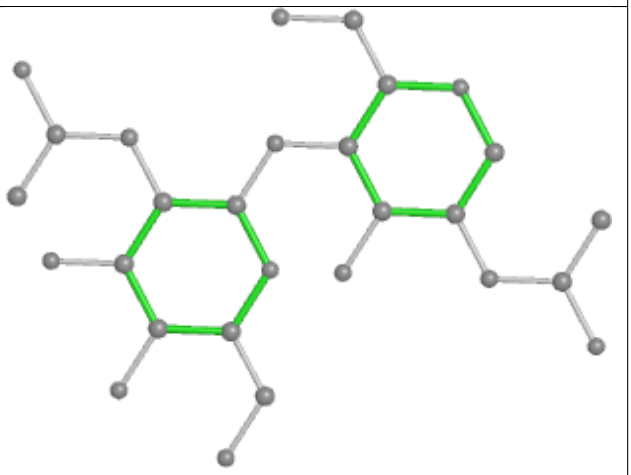
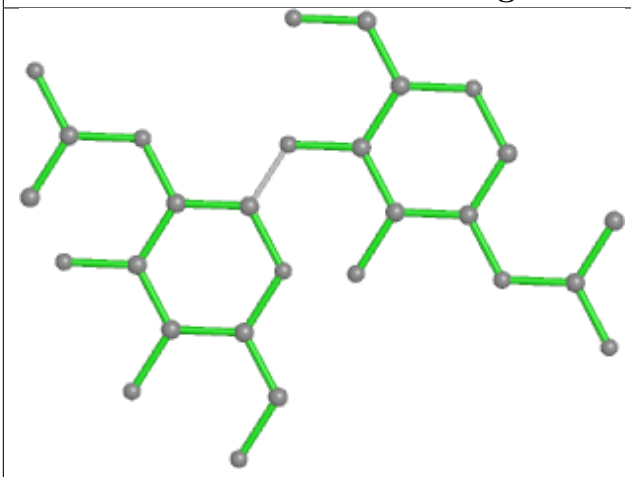


Rings

Oligosaccharide Chain u



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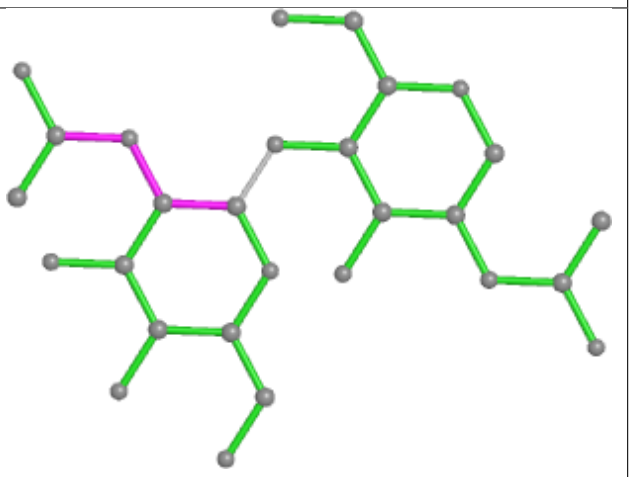
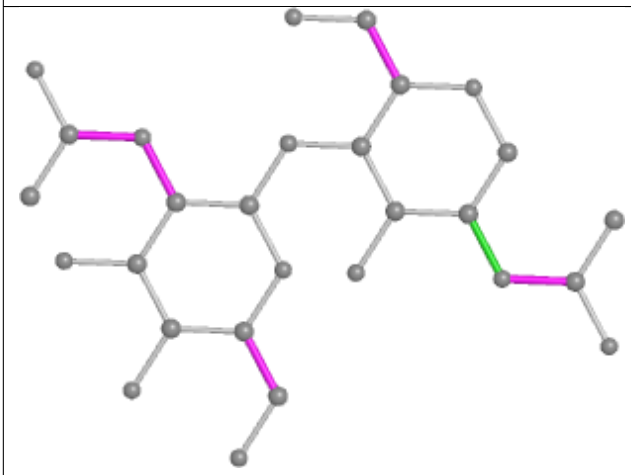


Bond angles



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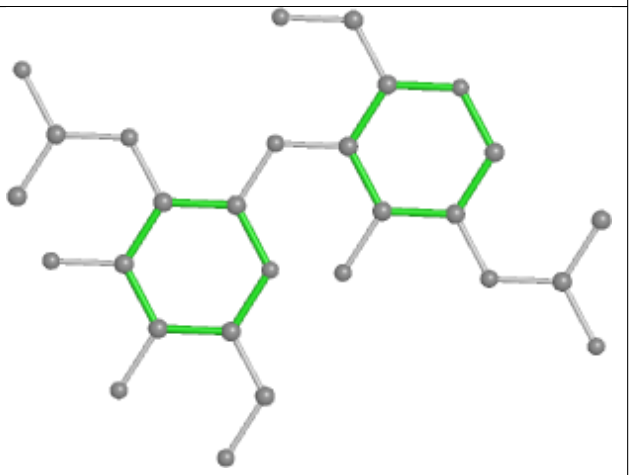
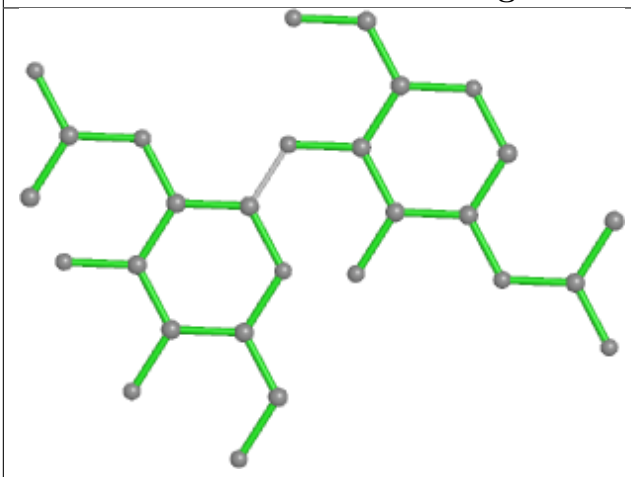


Rings

Oligosaccharide Chain y



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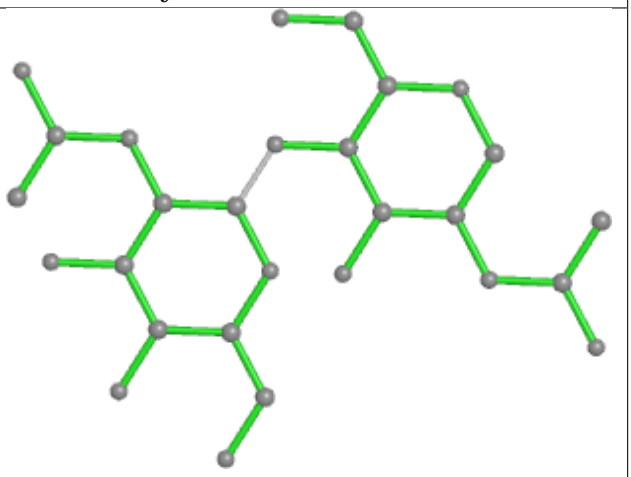
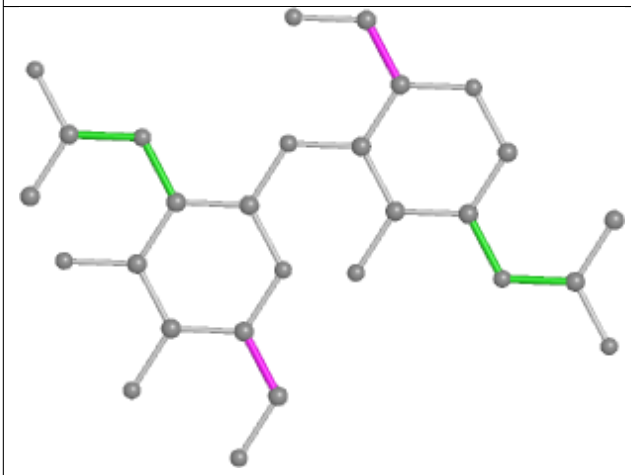


Bond angles



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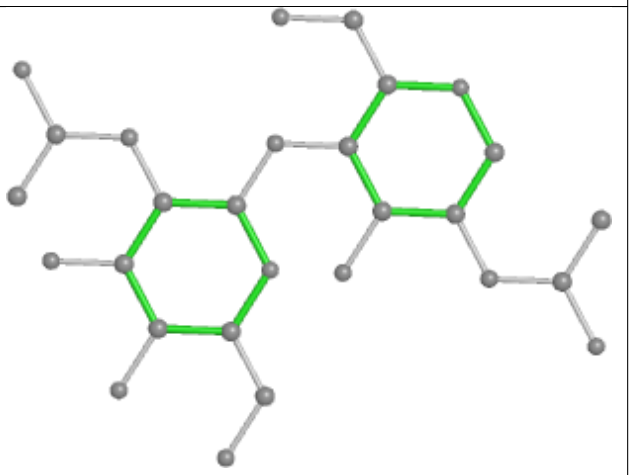
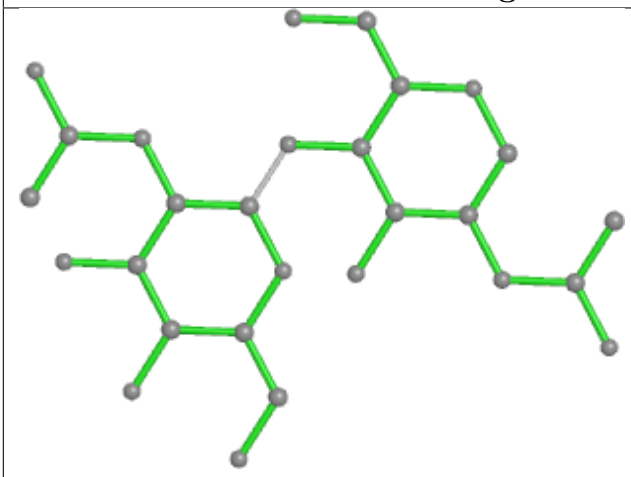


Rings

Oligosaccharide Chain 1



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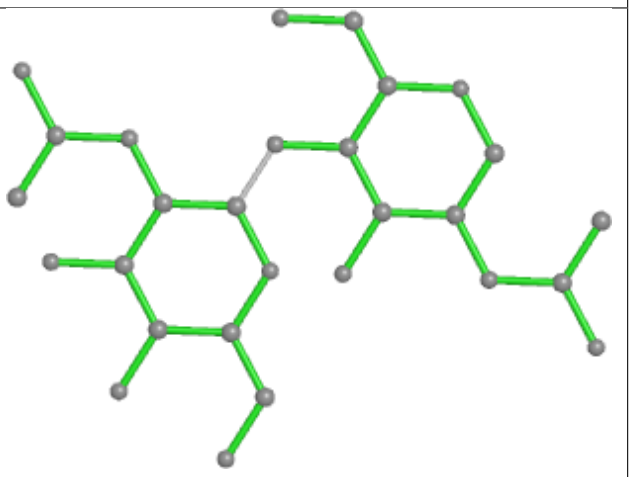
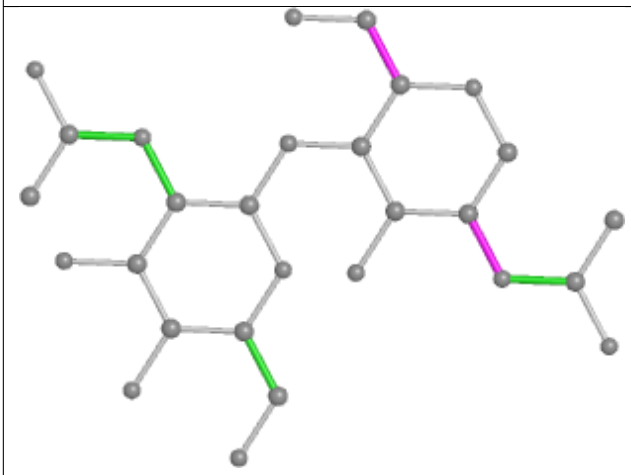


Bond angles



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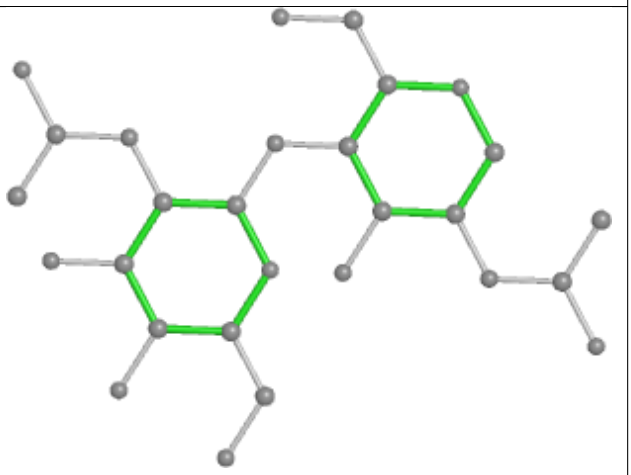
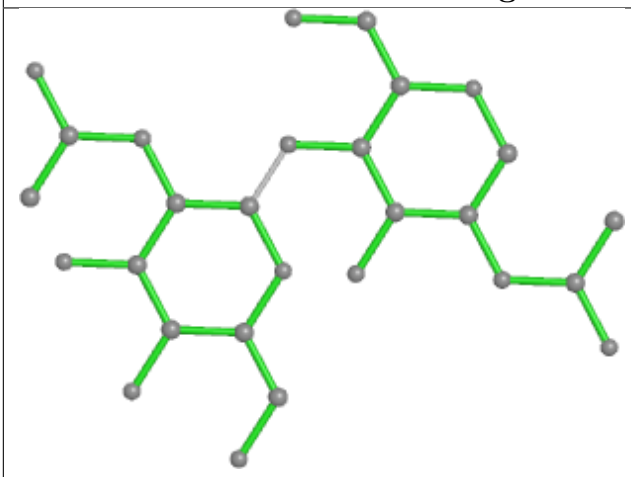


Rings

Oligosaccharide Chain 2



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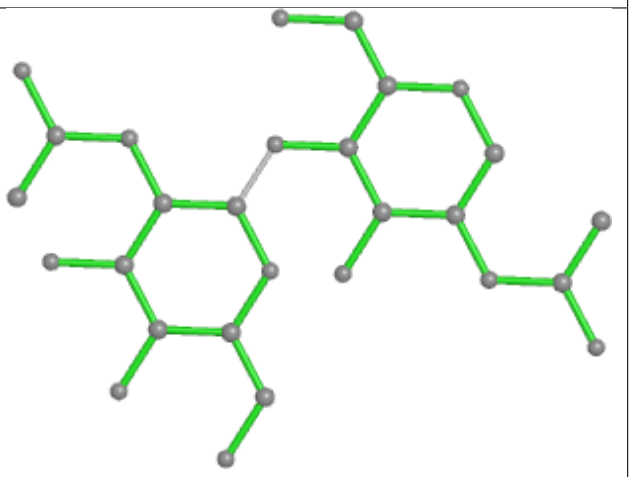
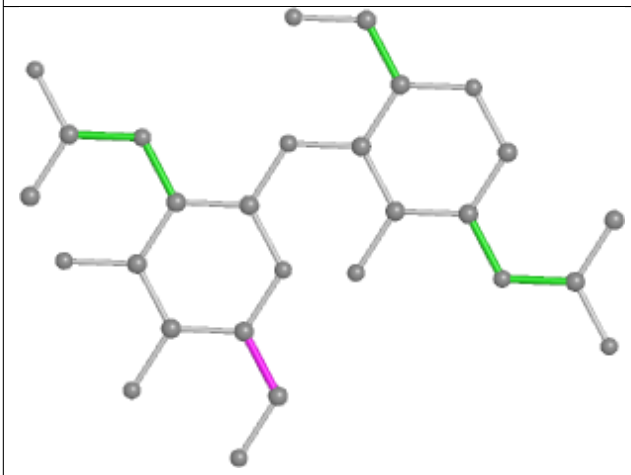


Bond angles



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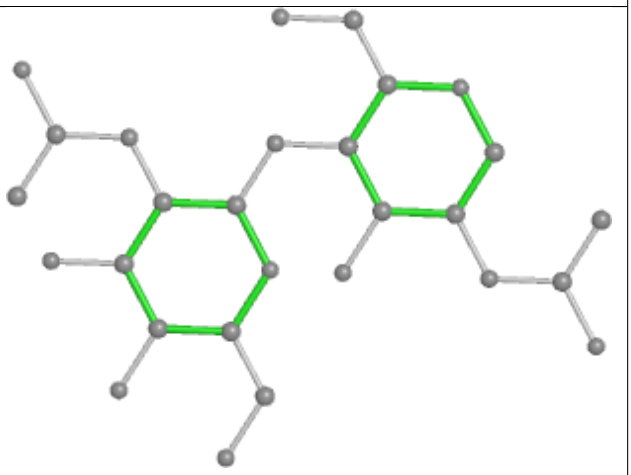
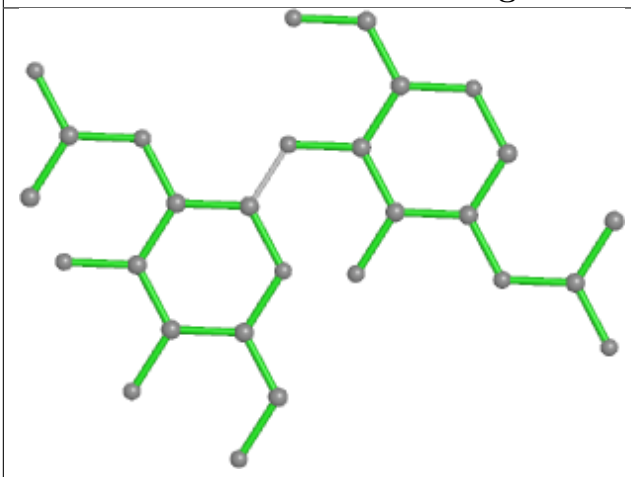


Rings

Oligosaccharide Chain 3



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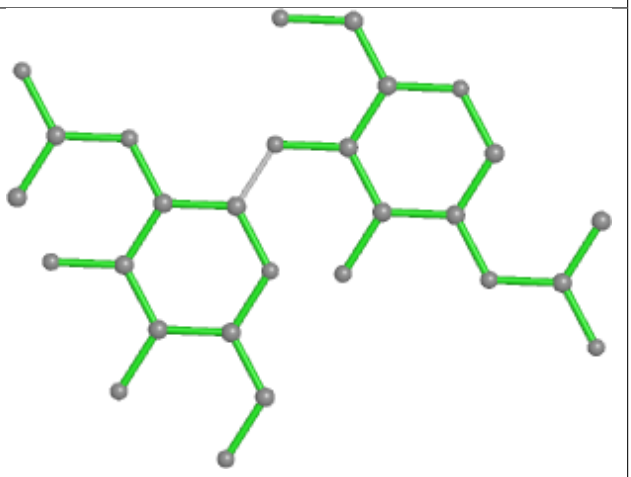
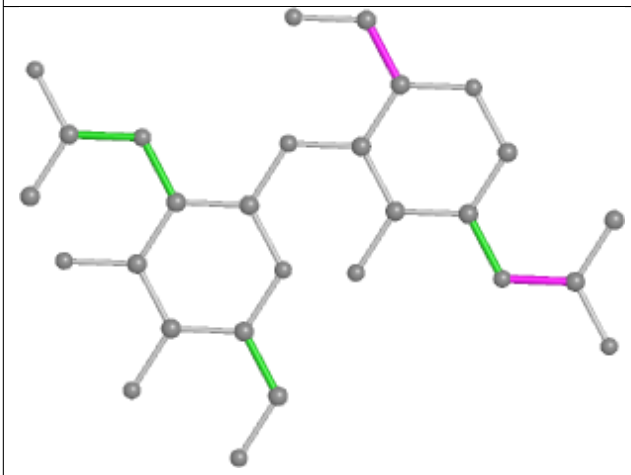


Bond angles



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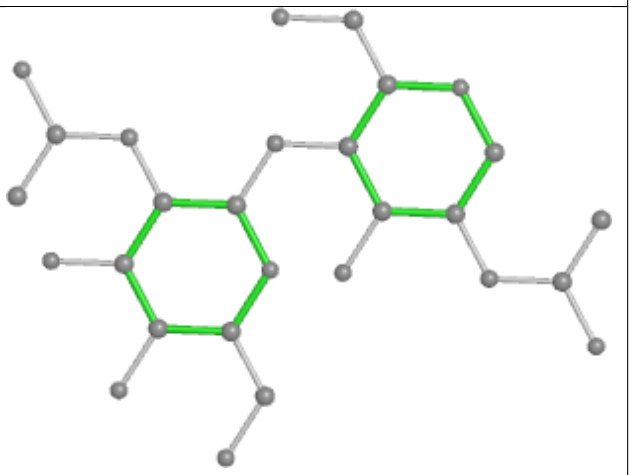
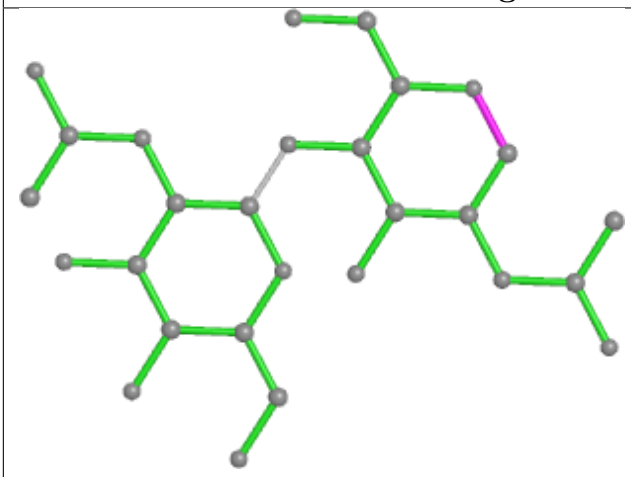


Rings

Oligosaccharide Chain 4



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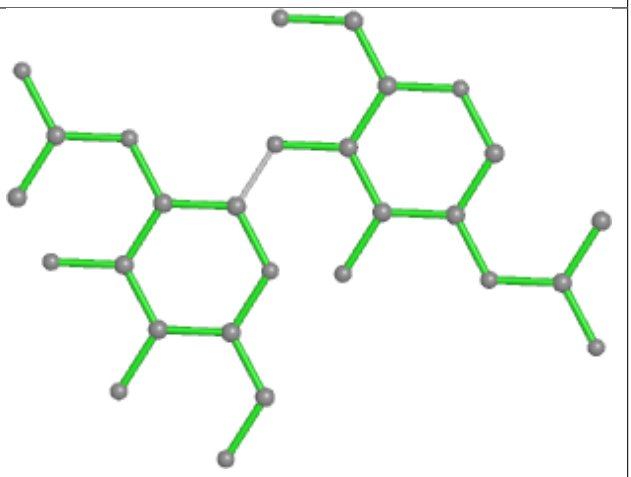
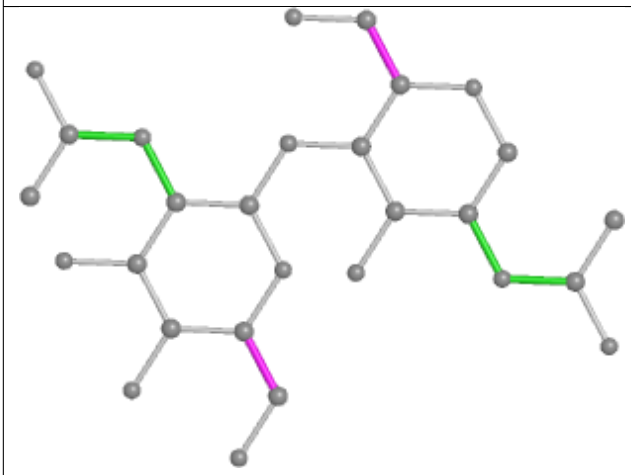


Bond angles



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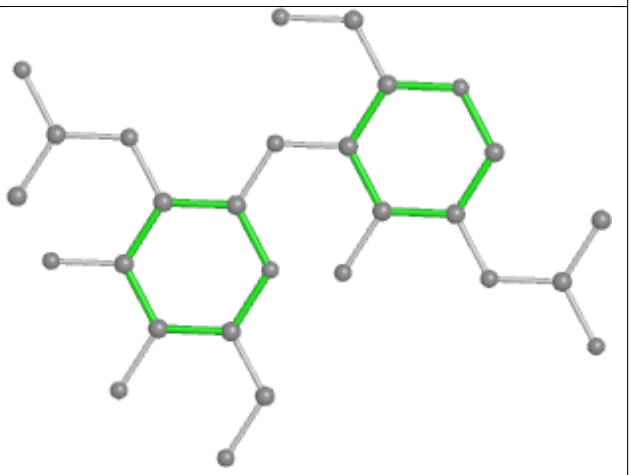
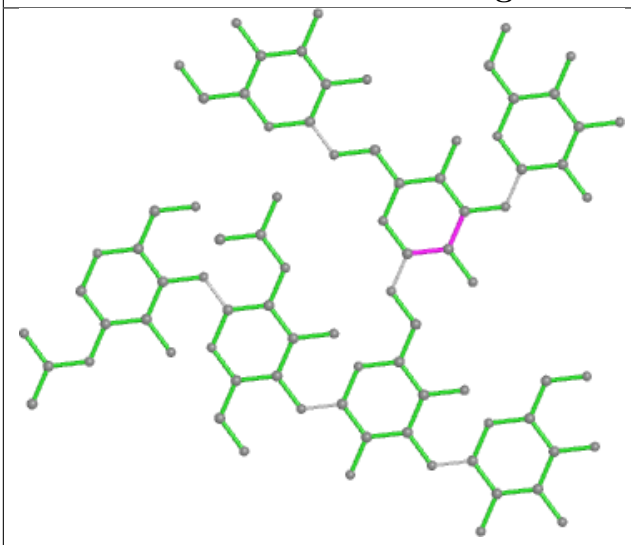
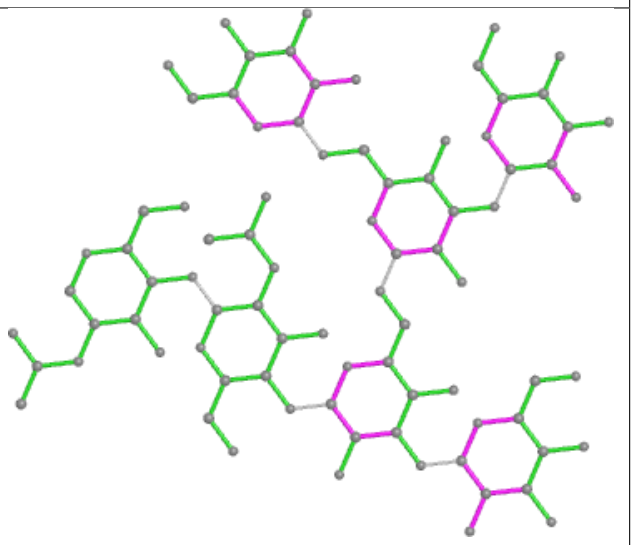


Rings

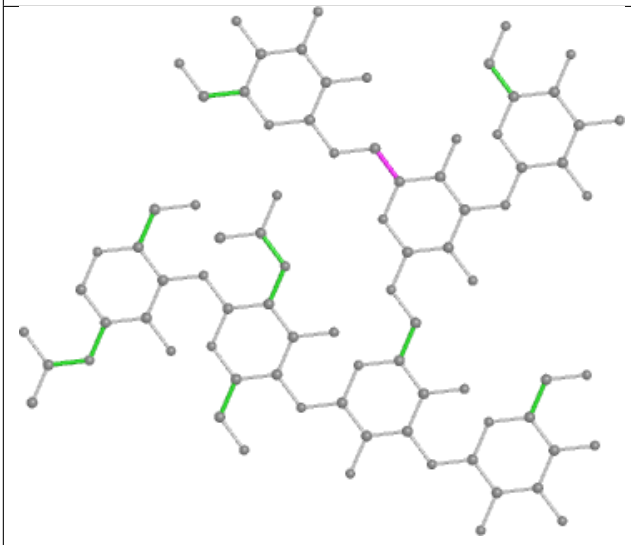
Oligosaccharide Chain T



Bond lengths



Bond angles



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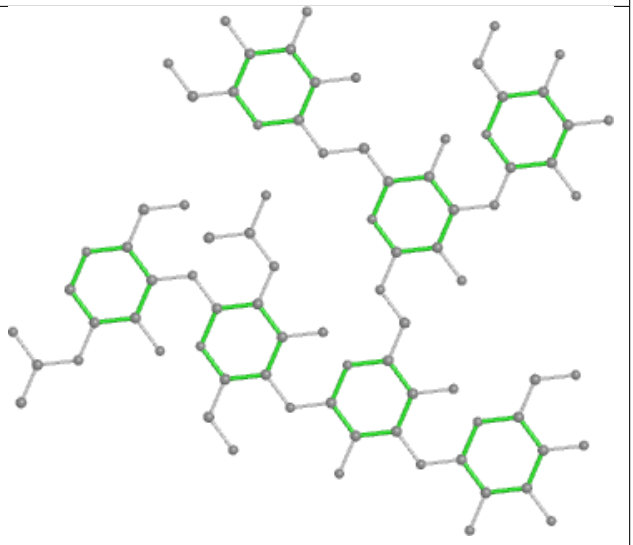
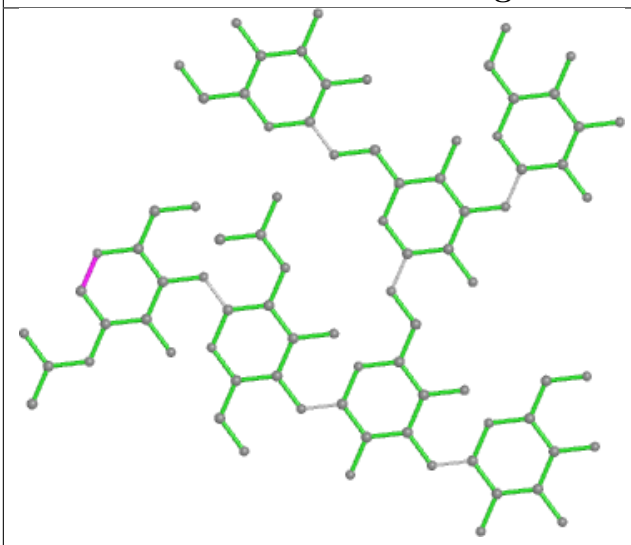
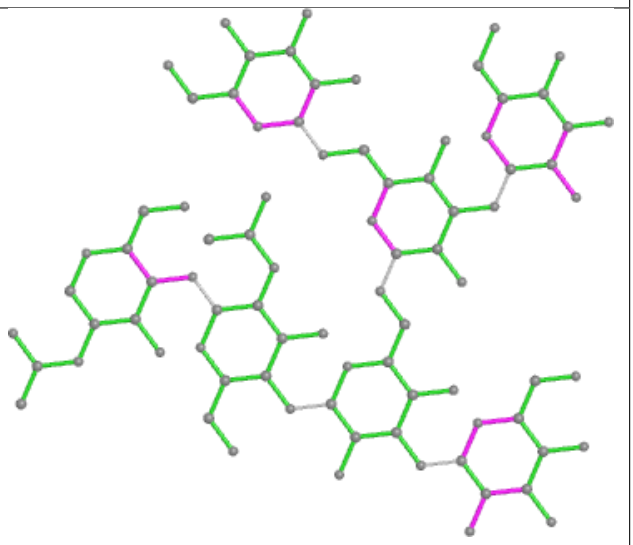


Rings

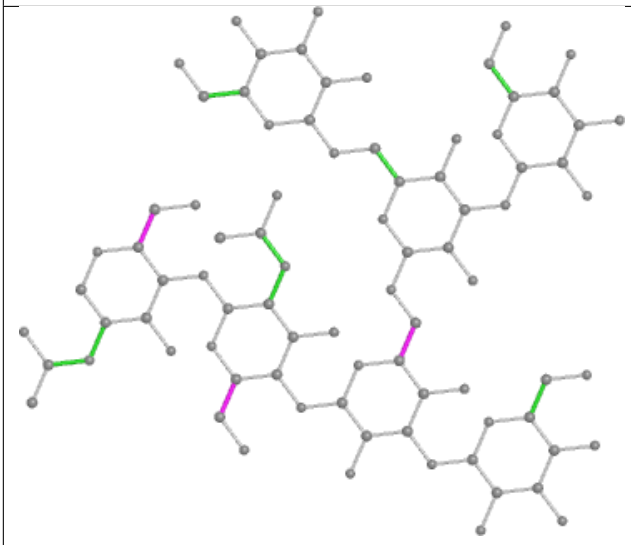
Oligosaccharide Chain X



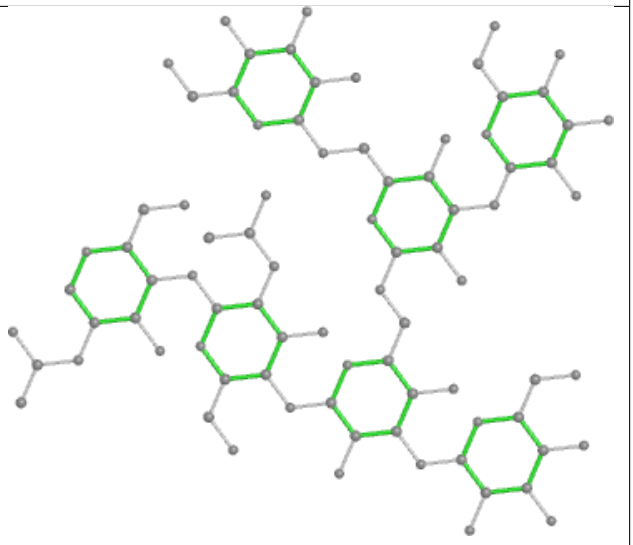
Bond lengths



Bond angles

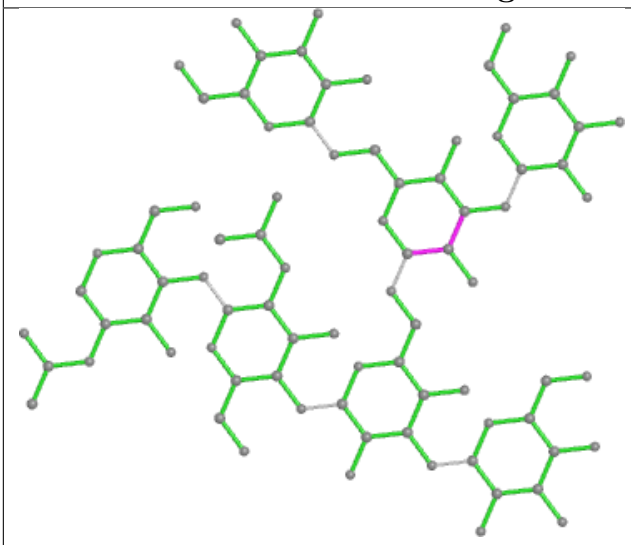


Torsions

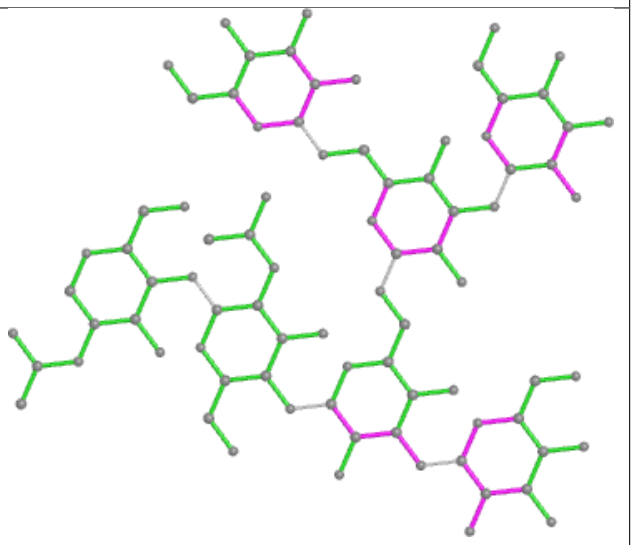


Rings

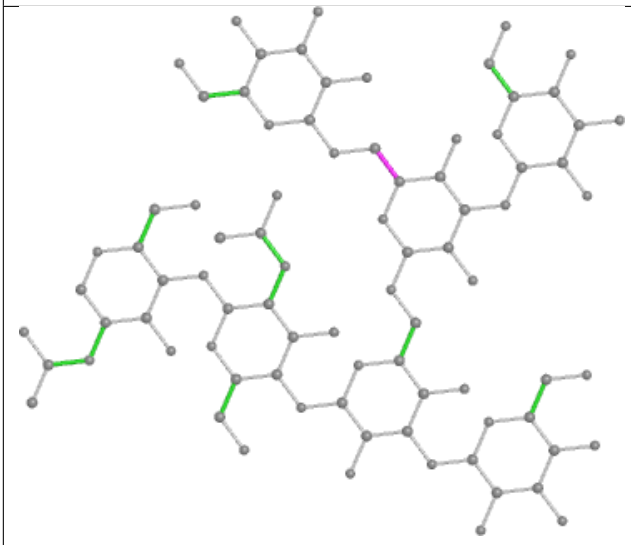
Oligosaccharide Chain h



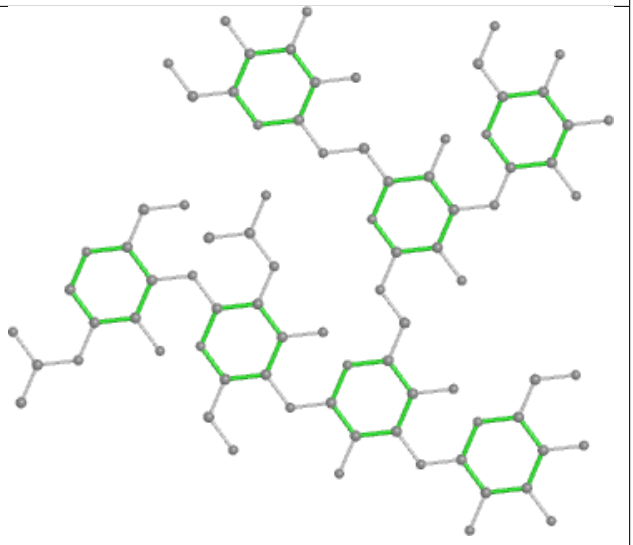
Bond lengths



Bond angles

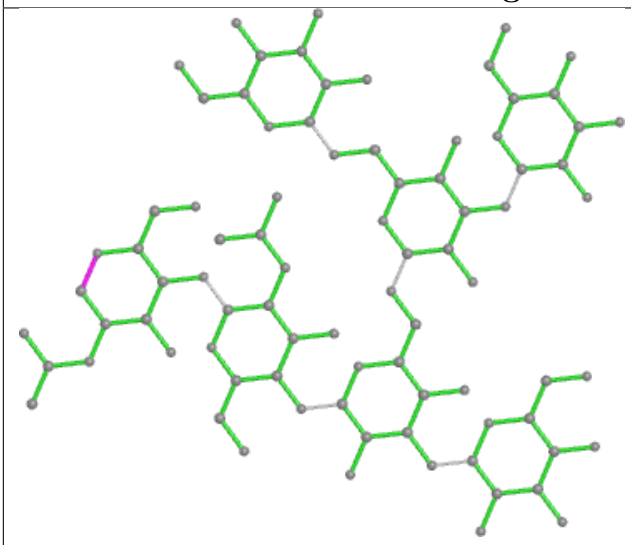


Torsions

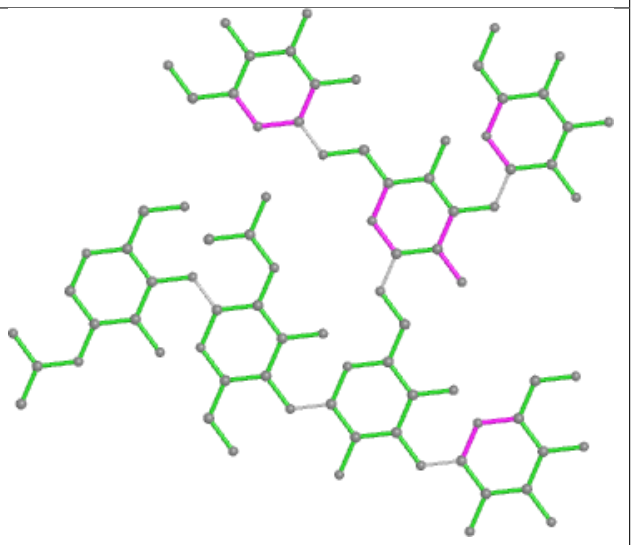


Rings

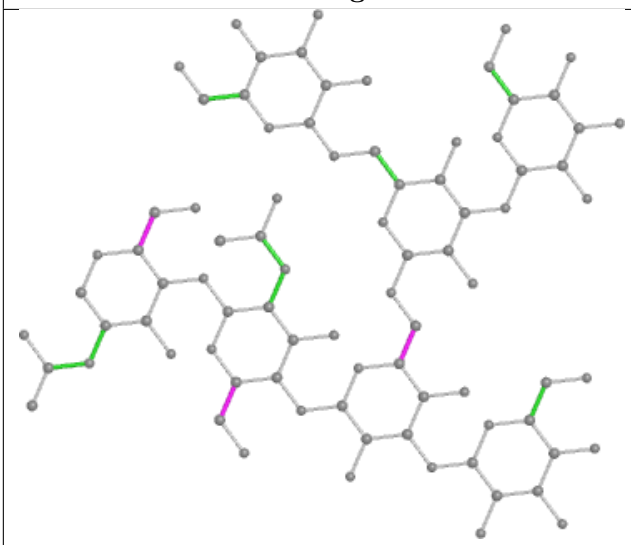
Oligosaccharide Chain l



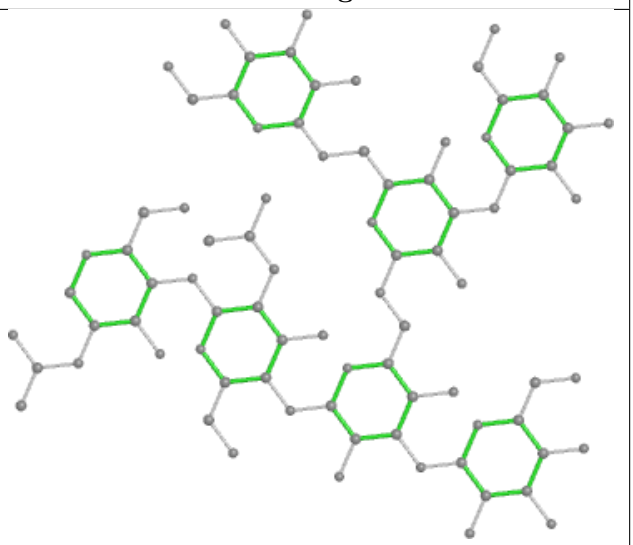
Bond lengths



Bond angles

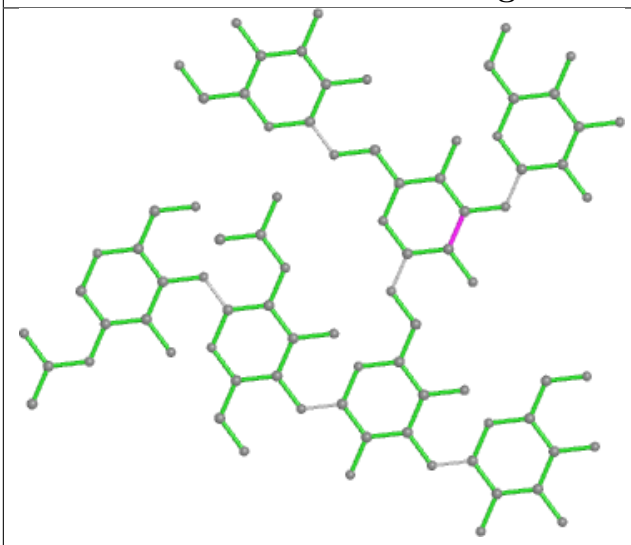


Torsions

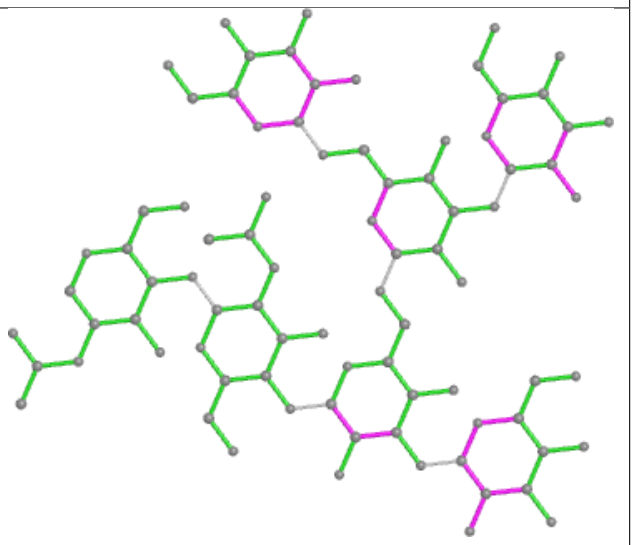


Rings

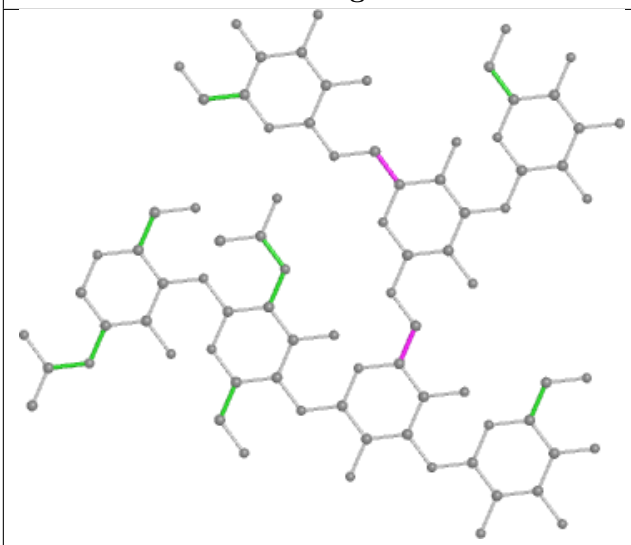
Oligosaccharide Chain v



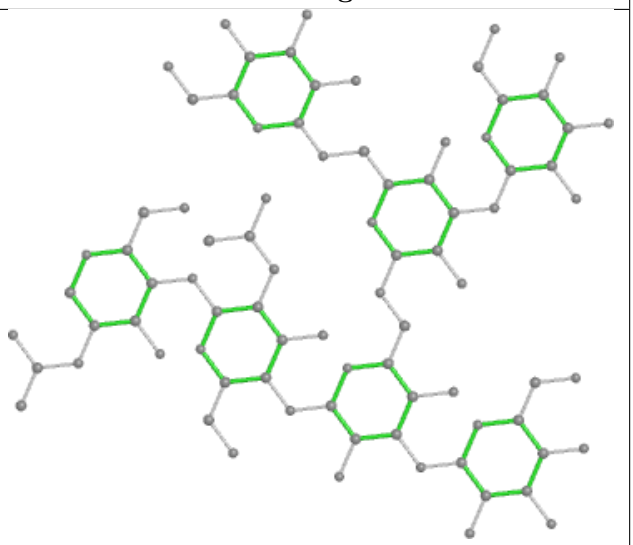
Bond lengths



Bond angles

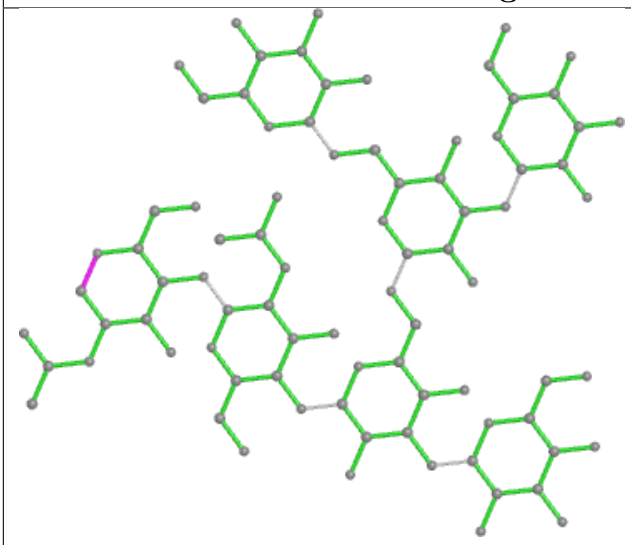


Torsions

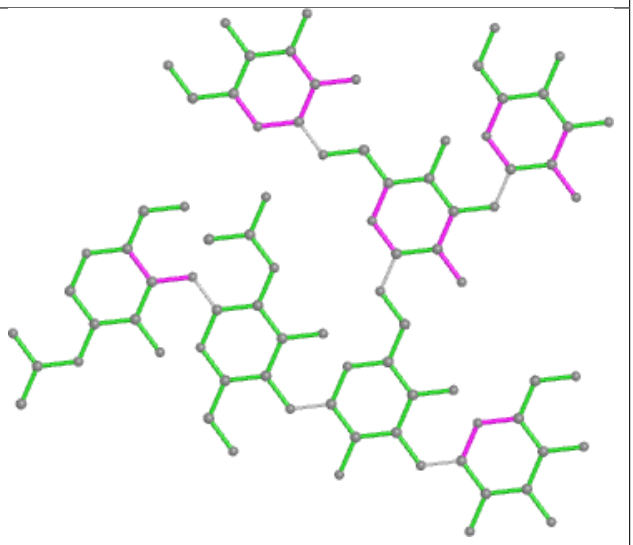


Rings

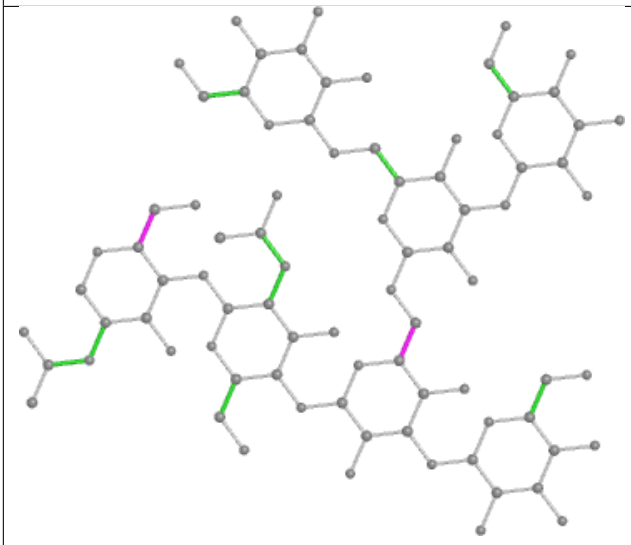
Oligosaccharide Chain z



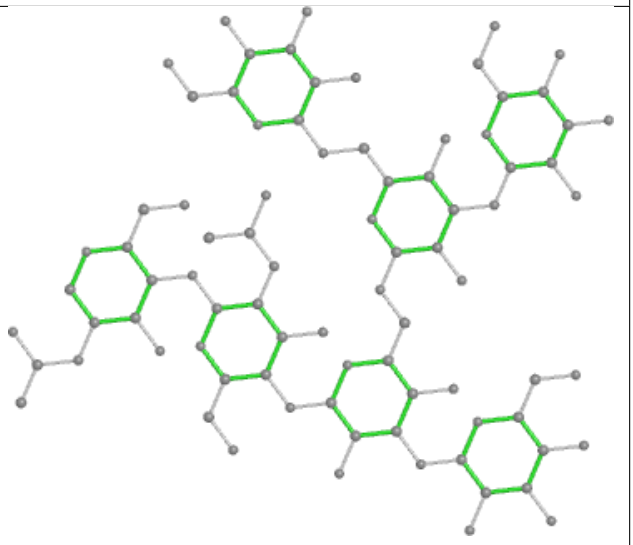
Bond lengths



Bond angles

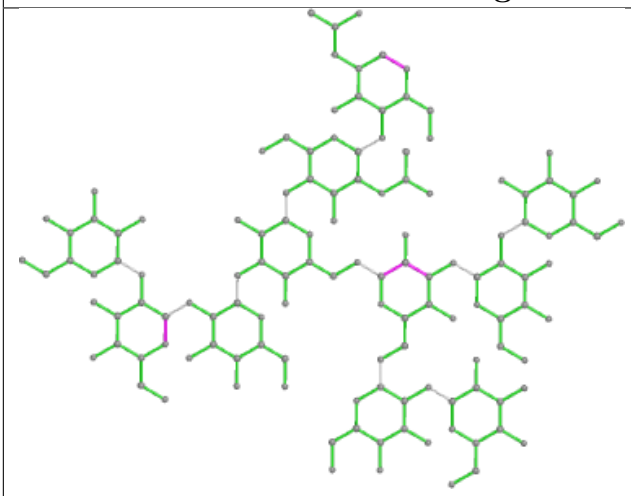


Torsions

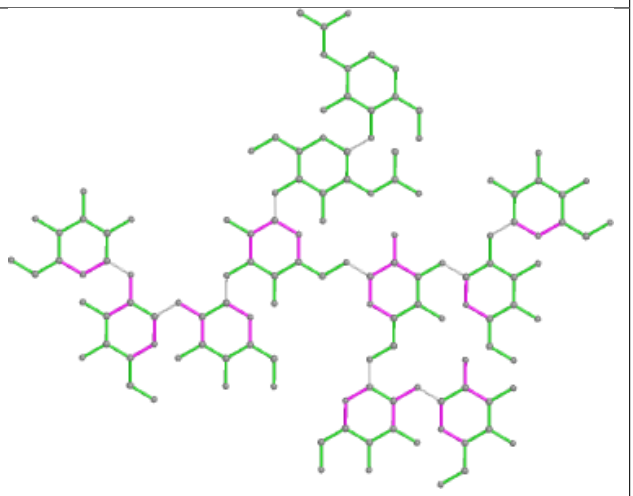


Rings

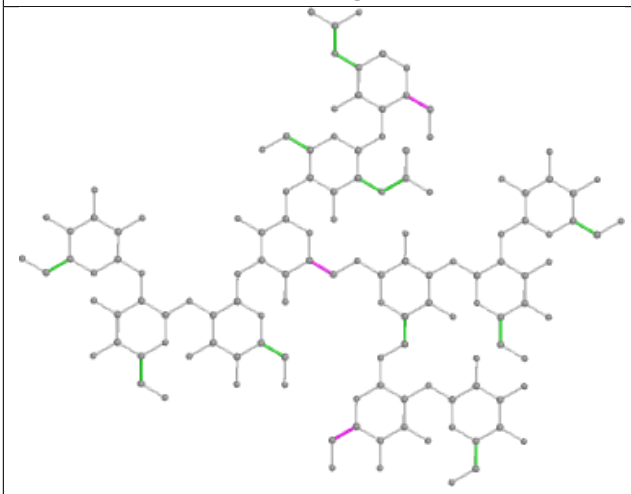
Oligosaccharide Chain U



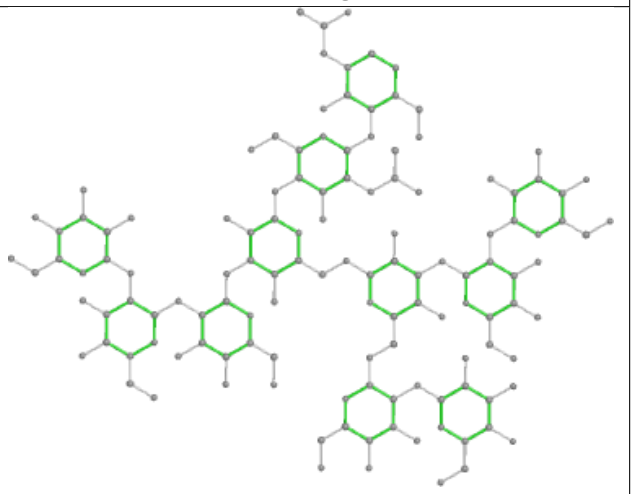
Bond lengths



Bond angles

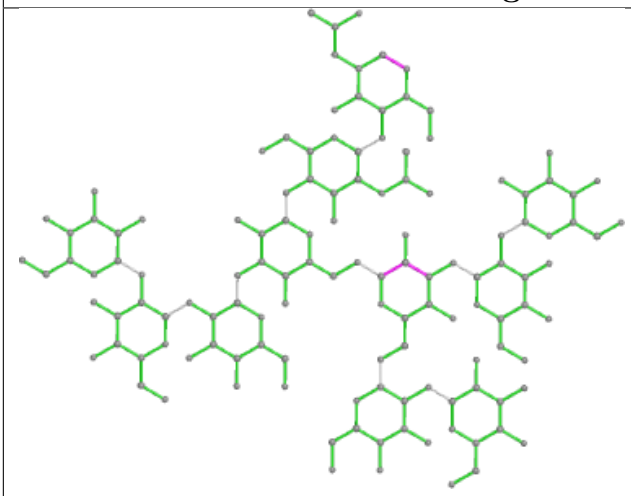


Torsions

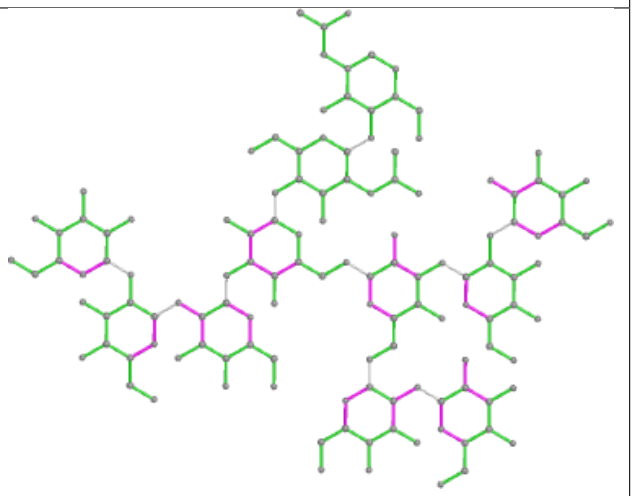


Rings

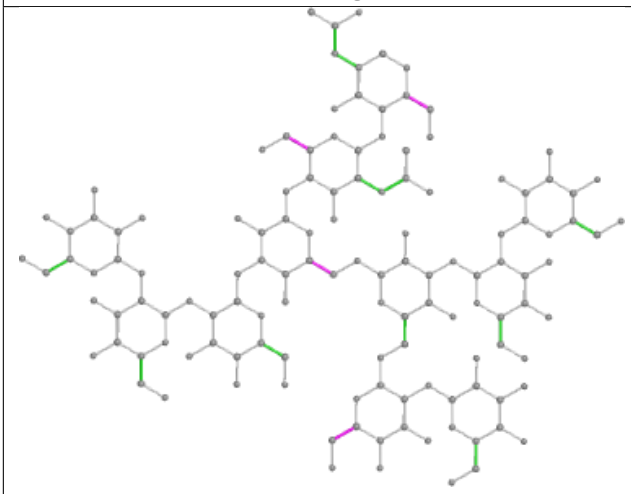
Oligosaccharide Chain i



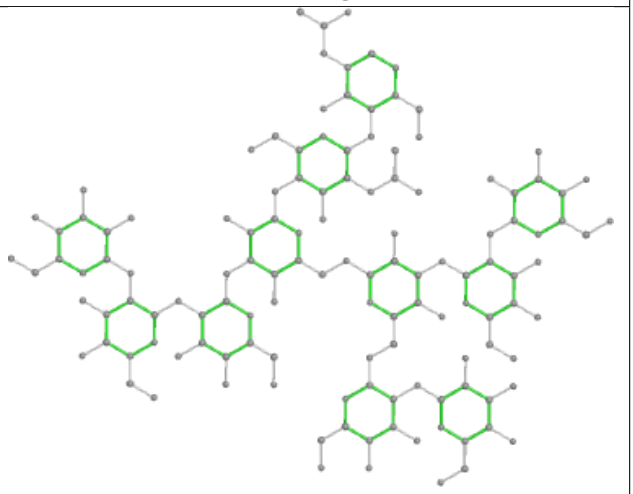
Bond lengths



Bond angles

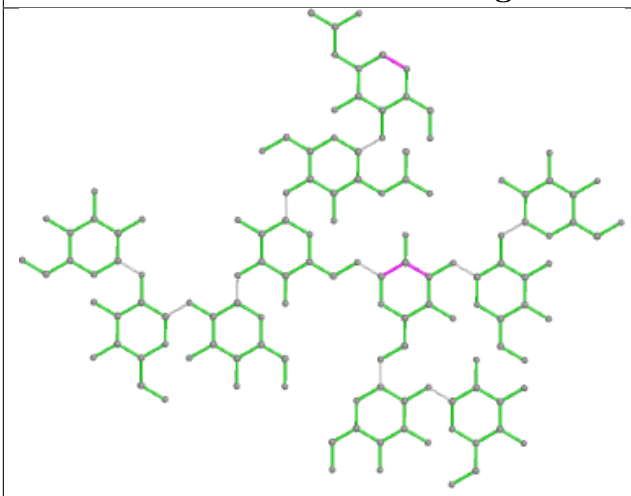


Torsions

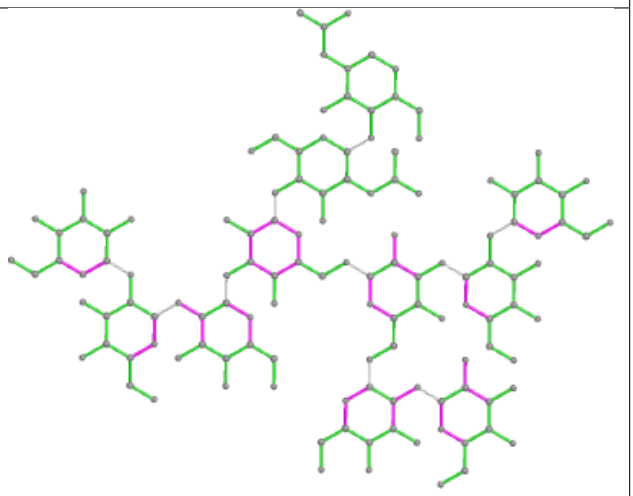


Rings

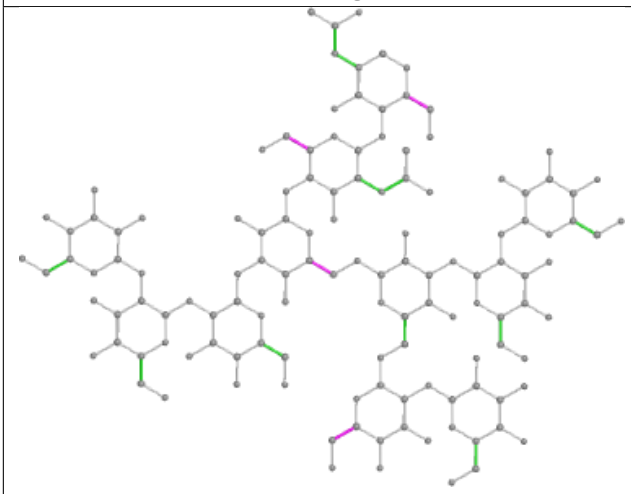
Oligosaccharide Chain w



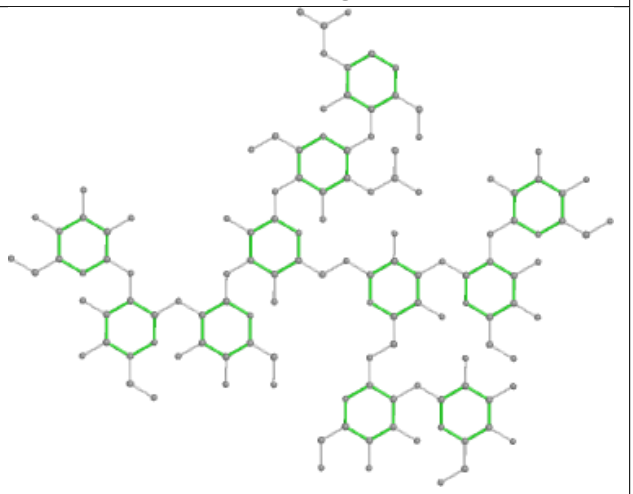
Bond lengths



Bond angles

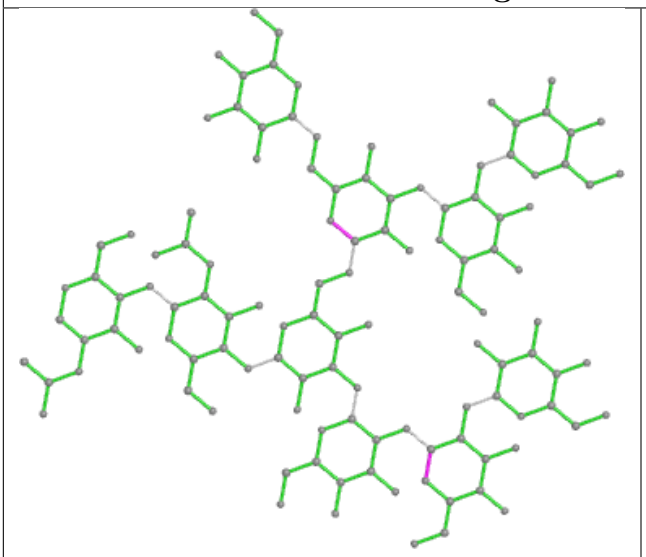


Torsions

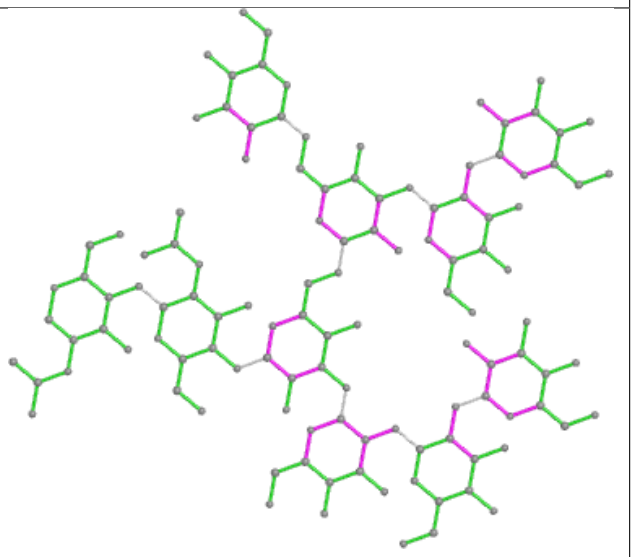


Rings

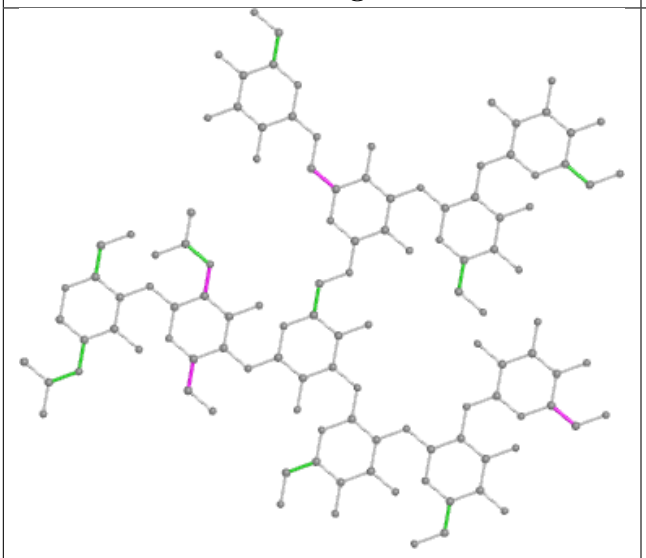
Oligosaccharide Chain Y



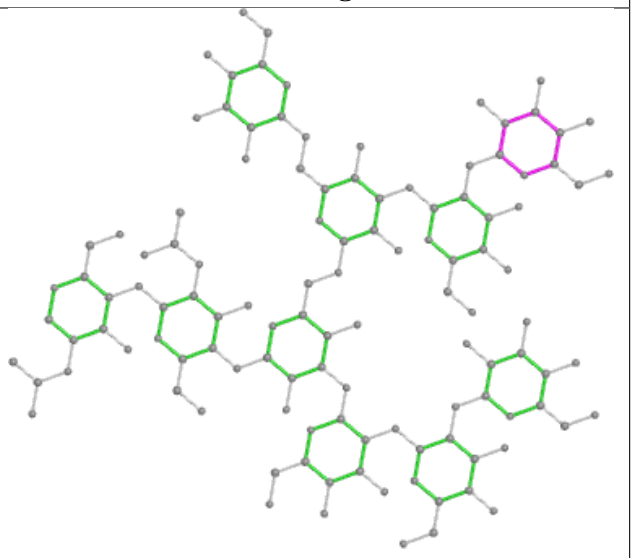
Bond lengths



Bond angles

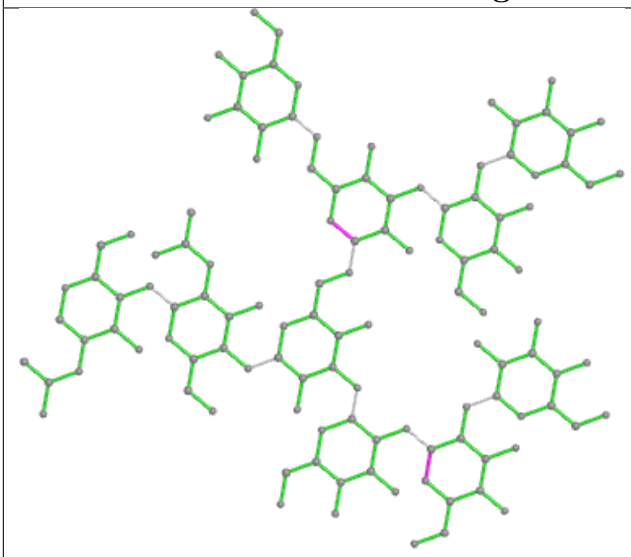


Torsions

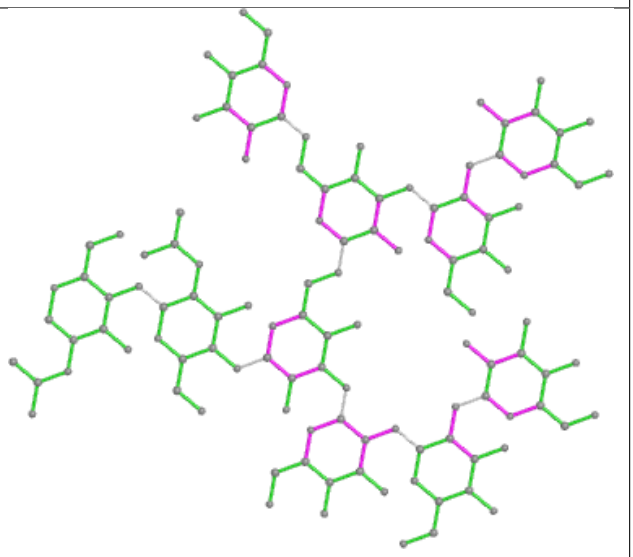


Rings

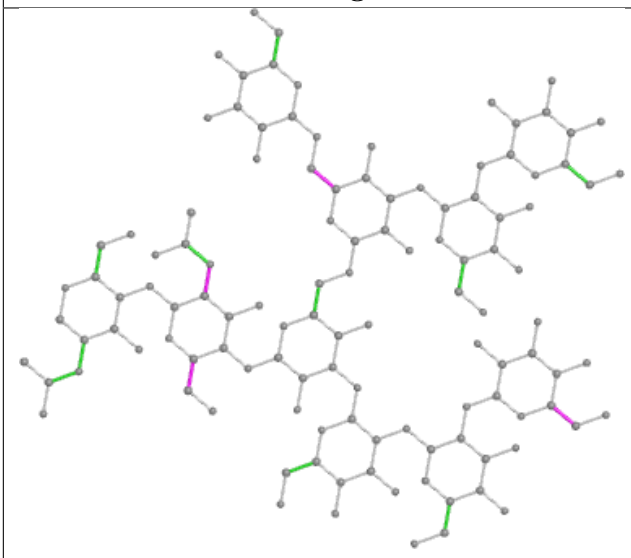
Oligosaccharide Chain m



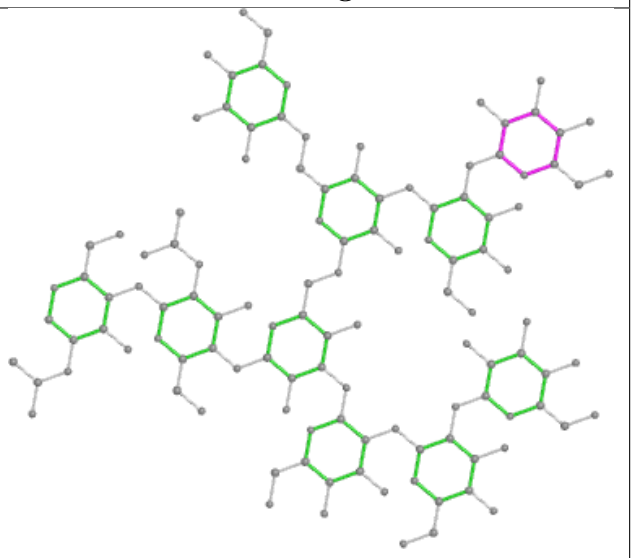
Bond lengths



Bond angles

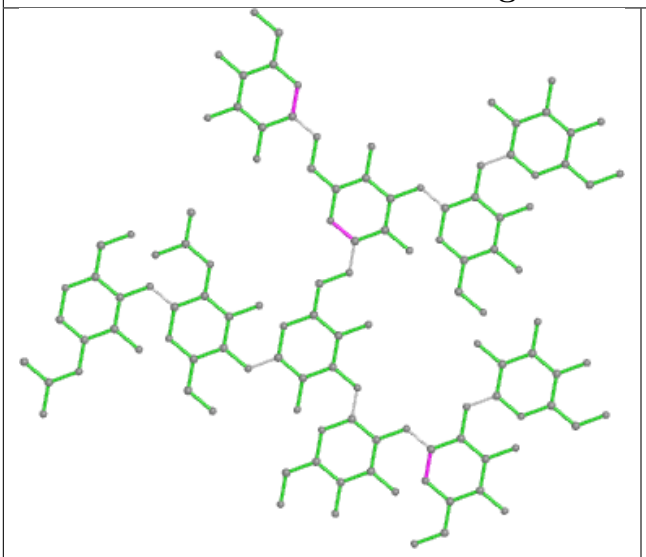


Torsions

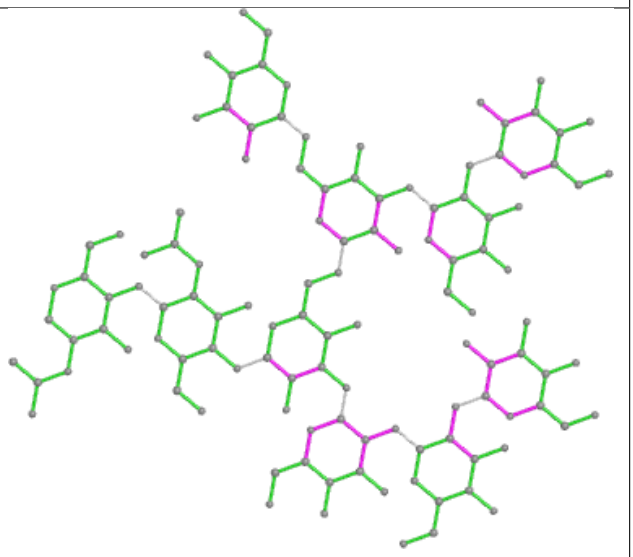


Rings

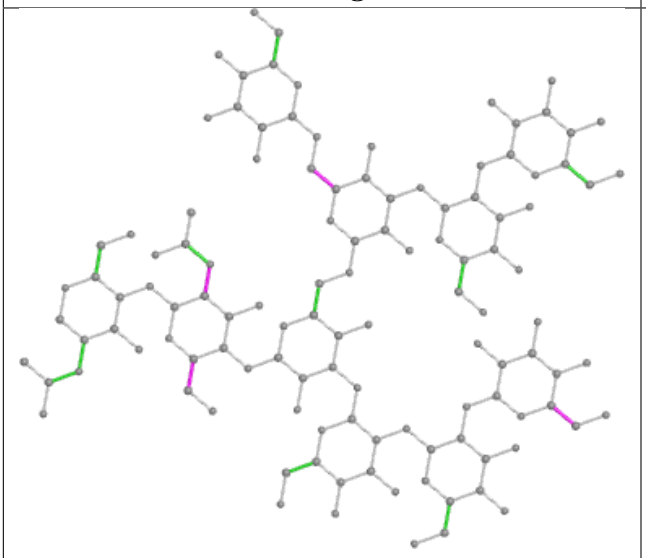
Oligosaccharide Chain 0



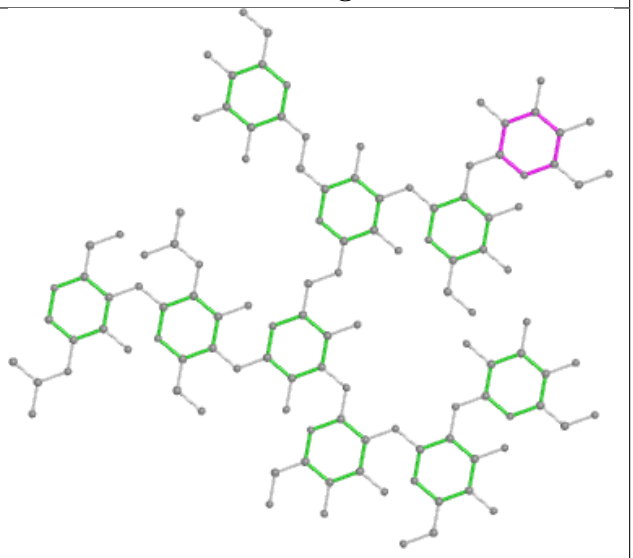
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 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	$\#\|Z\|>2$
12	NAG	C	702	2	14,14,15	0.20	0	17,19,21	0.42	0
12	NAG	B	702	2	14,14,15	0.19	0	17,19,21	0.44	0
12	NAG	A	641	1	14,14,15	0.21	0	17,19,21	0.36	0
12	NAG	A	606	1	14,14,15	0.23	0	17,19,21	0.42	0
12	NAG	J	641	1	14,14,15	0.23	0	17,19,21	0.39	0
12	NAG	K	701	2	14,14,15	0.25	0	17,19,21	0.48	0
12	NAG	G	661	1	14,14,15	0.22	0	17,19,21	0.41	0
12	NAG	G	662	1	14,14,15	0.35	0	17,19,21	0.48	0
12	NAG	C	701	2	14,14,15	0.21	0	17,19,21	0.46	0
12	NAG	A	661	1	14,14,15	0.22	0	17,19,21	0.41	0
12	NAG	J	606	1	14,14,15	0.22	0	17,19,21	0.42	0
12	NAG	B	701	2	14,14,15	0.18	0	17,19,21	0.51	0
12	NAG	A	662	1	14,14,15	0.32	0	17,19,21	0.45	0
12	NAG	K	702	2	14,14,15	0.20	0	17,19,21	0.42	0
12	NAG	J	662	1	14,14,15	0.28	0	17,19,21	0.44	0
12	NAG	G	641	1	14,14,15	0.26	0	17,19,21	0.39	0
12	NAG	G	606	1	14,14,15	0.23	0	17,19,21	0.43	0
12	NAG	J	661	1	14,14,15	0.23	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	C	702	2	-	2/6/23/26	0/1/1/1
12	NAG	B	702	2	-	2/6/23/26	0/1/1/1
12	NAG	A	641	1	-	2/6/23/26	0/1/1/1
12	NAG	A	606	1	-	1/6/23/26	0/1/1/1
12	NAG	J	641	1	-	2/6/23/26	0/1/1/1
12	NAG	K	701	2	-	1/6/23/26	0/1/1/1
12	NAG	G	661	1	-	1/6/23/26	0/1/1/1
12	NAG	G	662	1	-	0/6/23/26	0/1/1/1
12	NAG	C	701	2	-	1/6/23/26	0/1/1/1
12	NAG	A	661	1	-	0/6/23/26	0/1/1/1
12	NAG	J	606	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	2	-	1/6/23/26	0/1/1/1
12	NAG	A	662	1	-	0/6/23/26	0/1/1/1
12	NAG	K	702	2	-	2/6/23/26	0/1/1/1
12	NAG	J	662	1	-	0/6/23/26	0/1/1/1
12	NAG	G	641	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	G	606	1	-	1/6/23/26	0/1/1/1
12	NAG	J	661	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	641	NAG	O5-C5-C6-O6
12	G	641	NAG	O5-C5-C6-O6
12	J	641	NAG	O5-C5-C6-O6
12	G	641	NAG	C4-C5-C6-O6
12	J	641	NAG	C4-C5-C6-O6
12	A	641	NAG	C4-C5-C6-O6
12	K	702	NAG	O5-C5-C6-O6
12	C	702	NAG	O5-C5-C6-O6
12	B	702	NAG	O5-C5-C6-O6
12	K	702	NAG	C4-C5-C6-O6
12	J	606	NAG	O5-C5-C6-O6
12	A	606	NAG	O5-C5-C6-O6
12	G	606	NAG	O5-C5-C6-O6
12	C	702	NAG	C4-C5-C6-O6
12	B	702	NAG	C4-C5-C6-O6
12	B	701	NAG	C4-C5-C6-O6
12	G	661	NAG	O5-C5-C6-O6
12	K	701	NAG	C4-C5-C6-O6
12	C	701	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

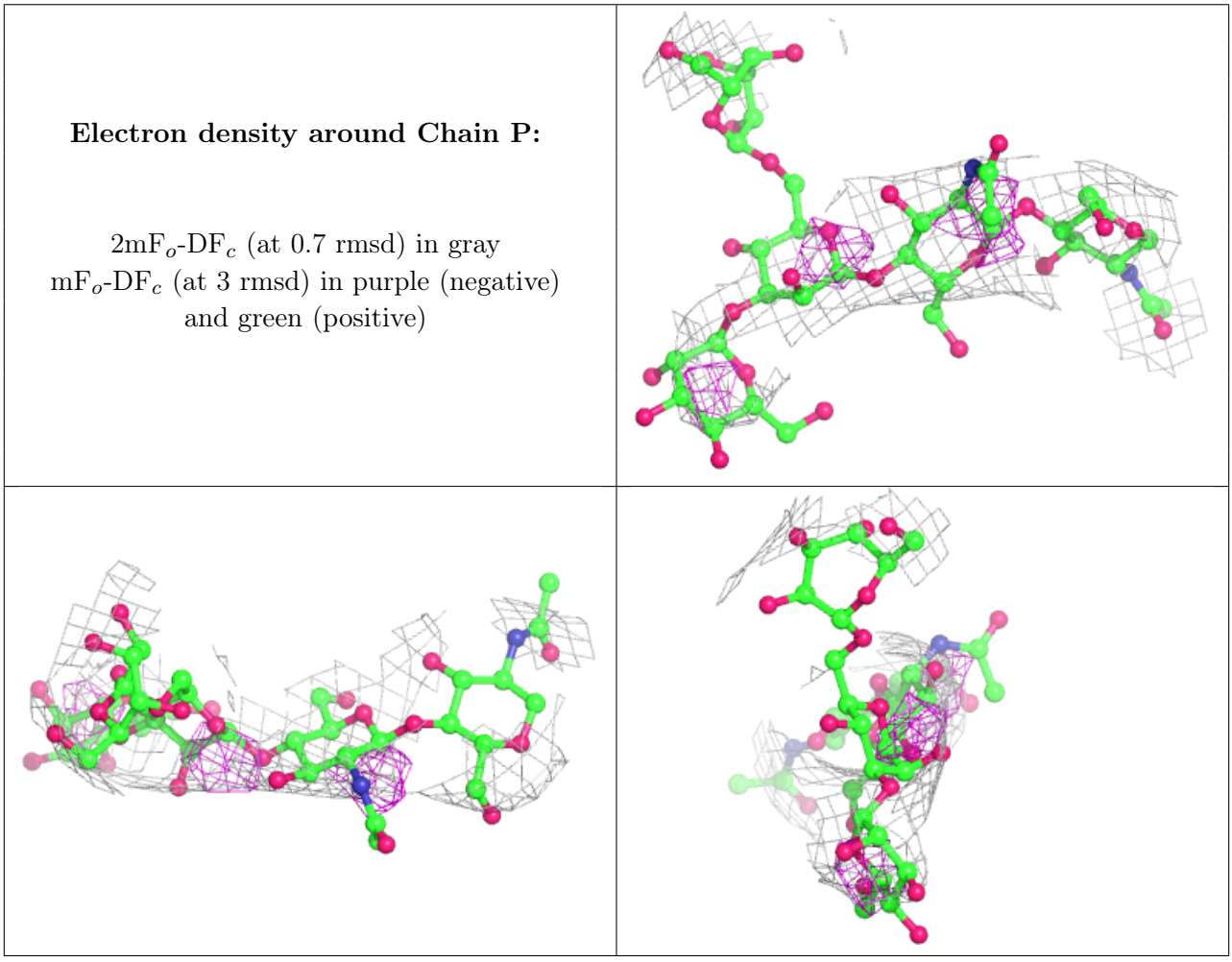
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

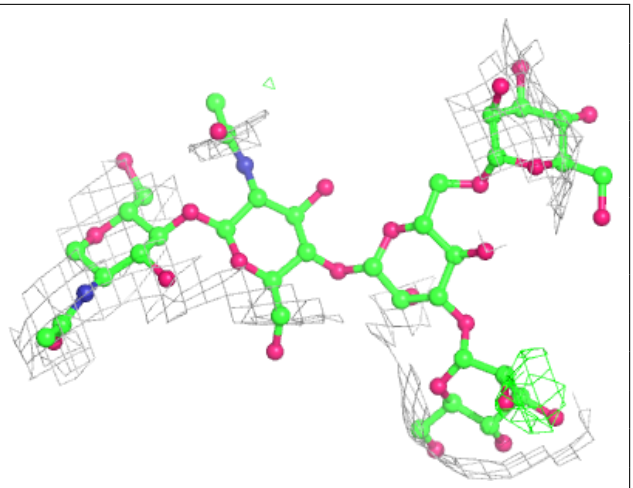
Unable to reproduce the depositors R factor - this section is therefore empty.

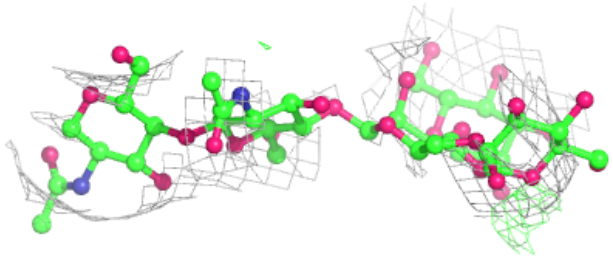
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

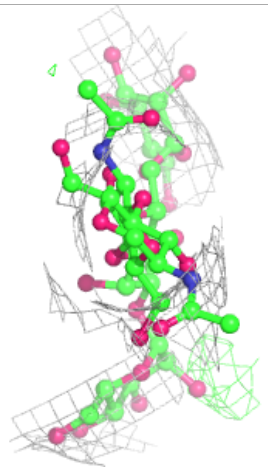


Electron density around Chain R:

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

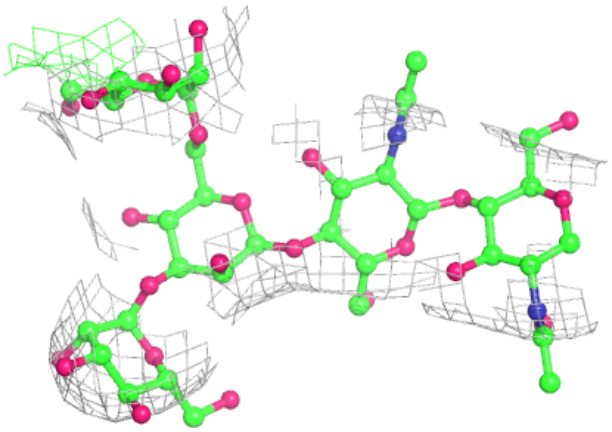


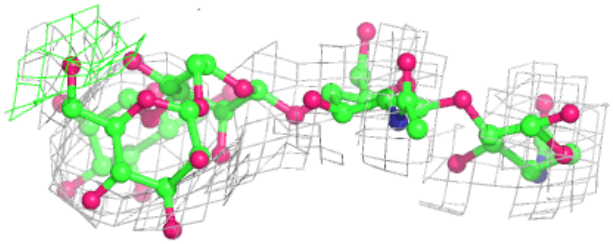


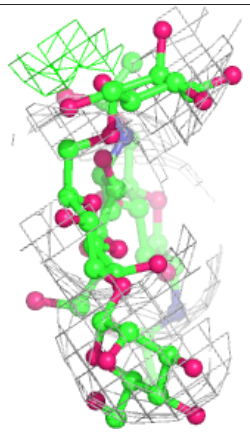


Electron density around Chain V:

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

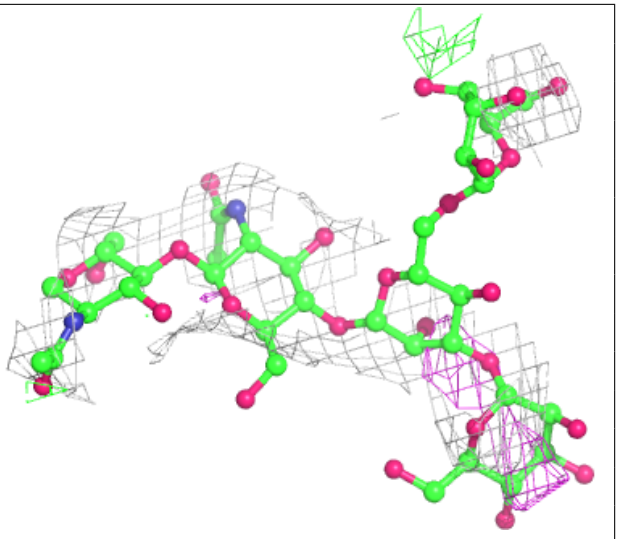


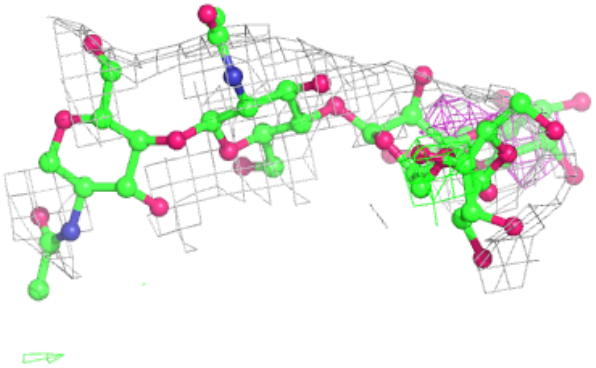


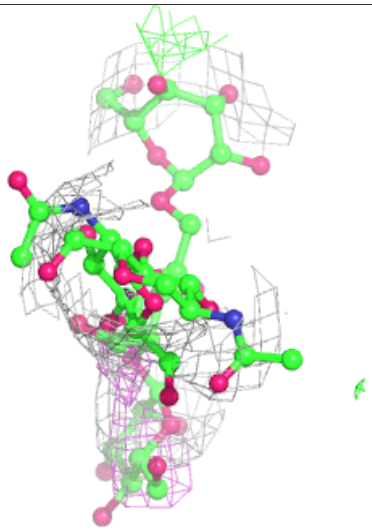


Electron density around Chain d:

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

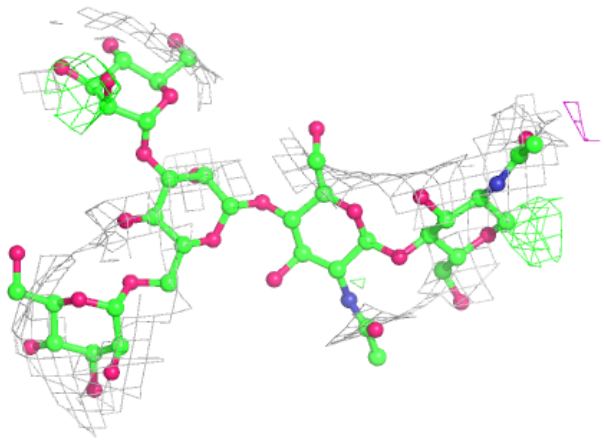


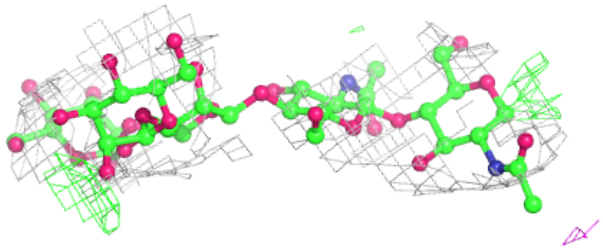


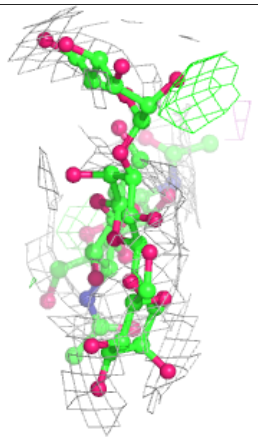


Electron density around Chain f:

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

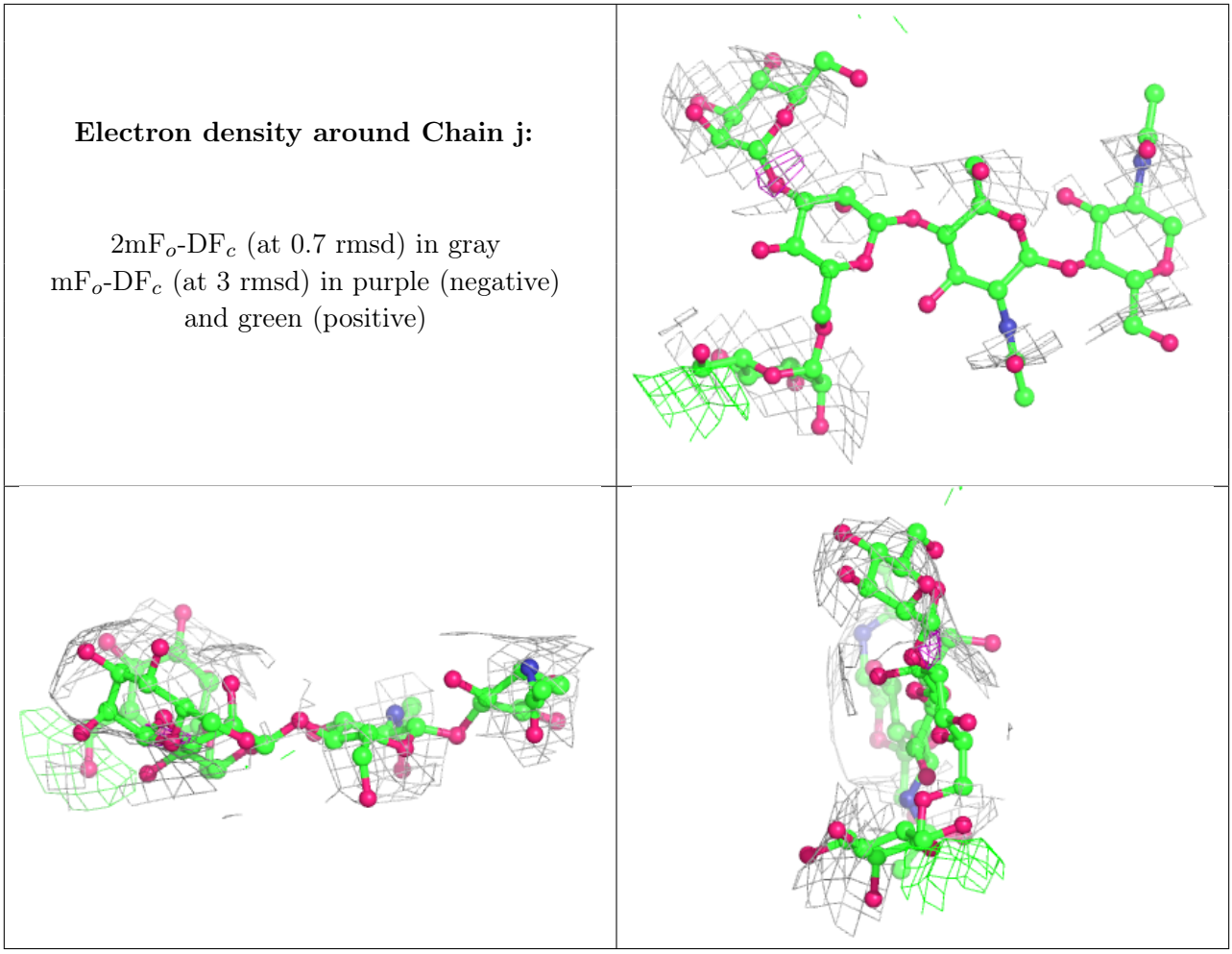






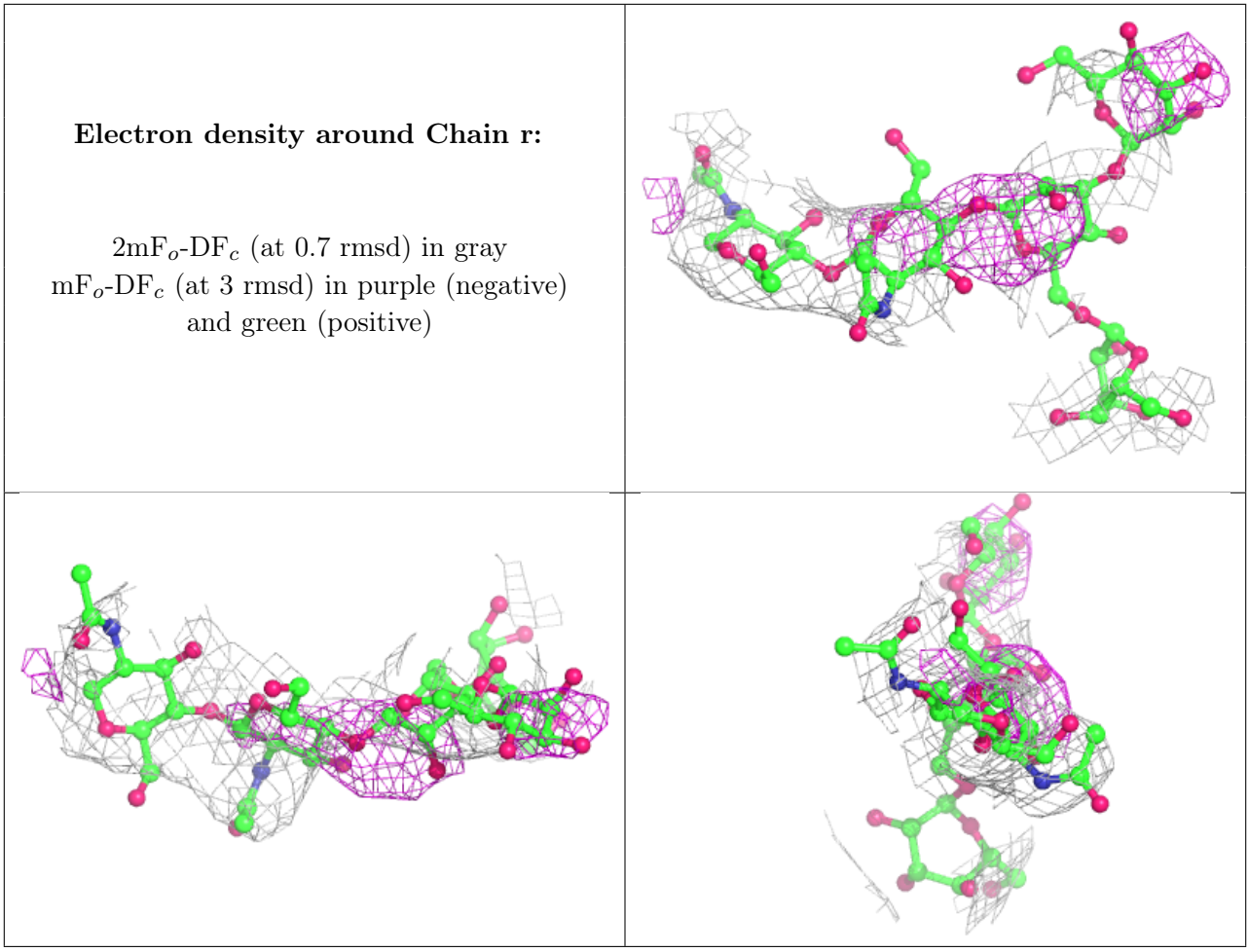
Electron density around Chain j:

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



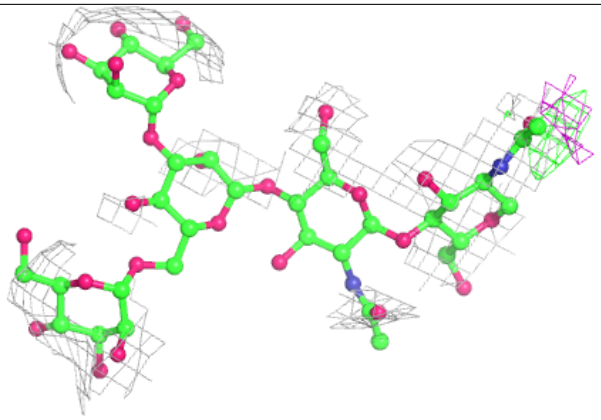
Electron density around Chain r:

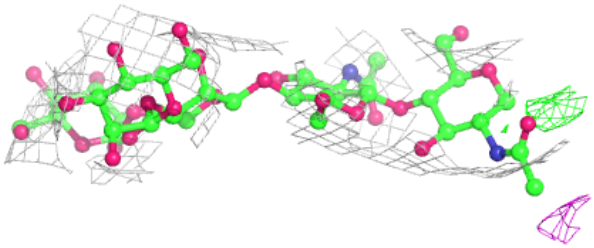
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

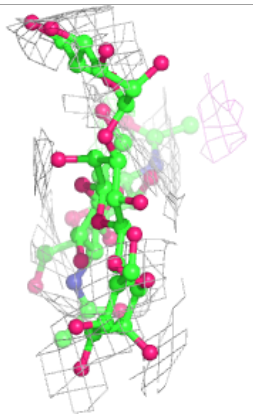


Electron density around Chain t:

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

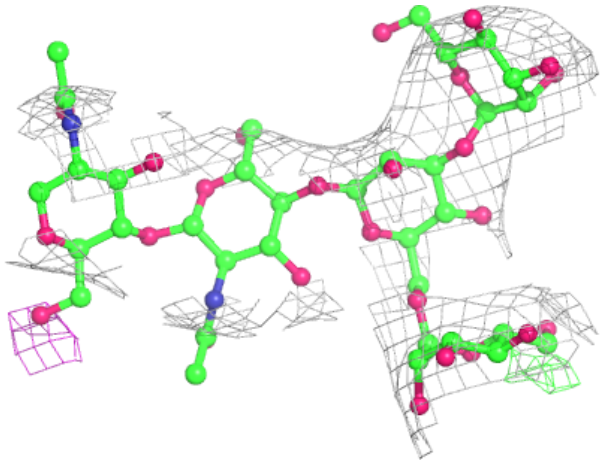


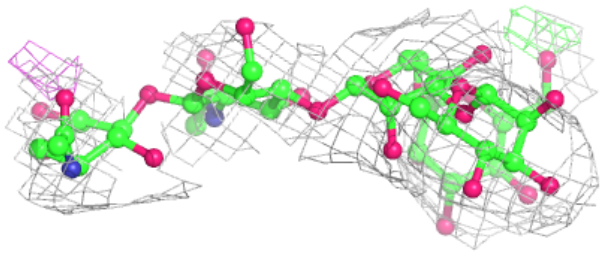


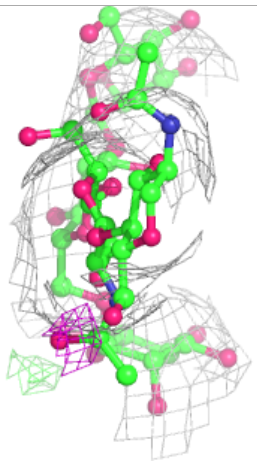


Electron density around Chain x:

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

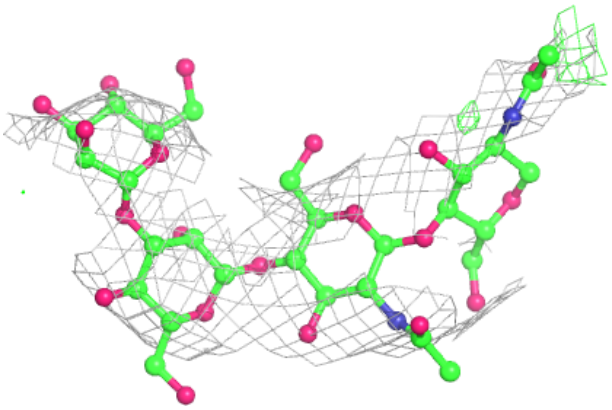


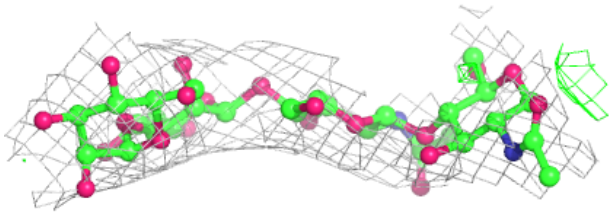


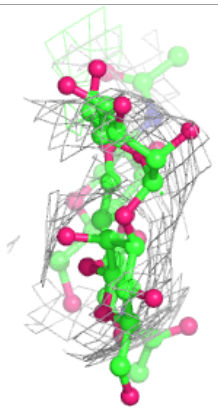


Electron density around Chain Q:

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

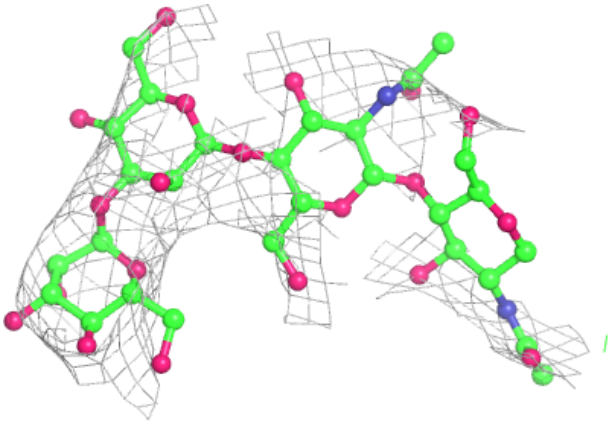


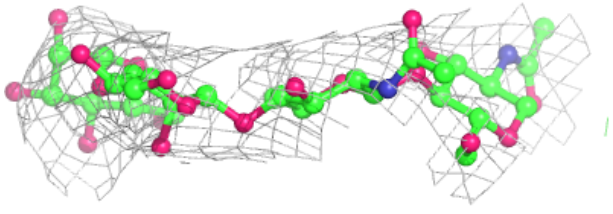


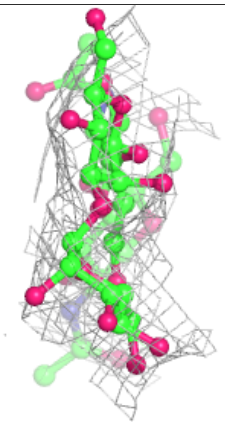


Electron density around Chain e:

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

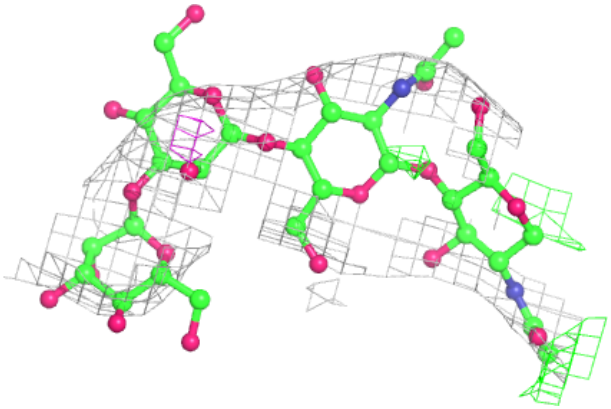


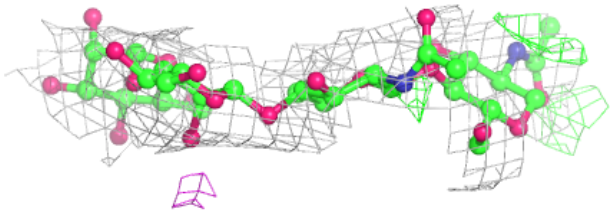


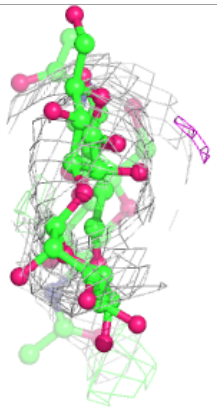


Electron density around Chain s:

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

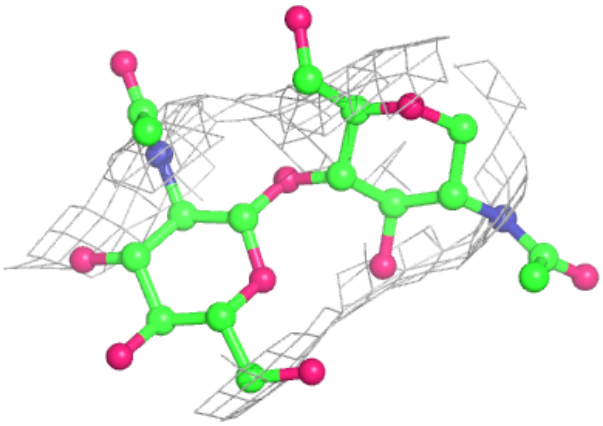


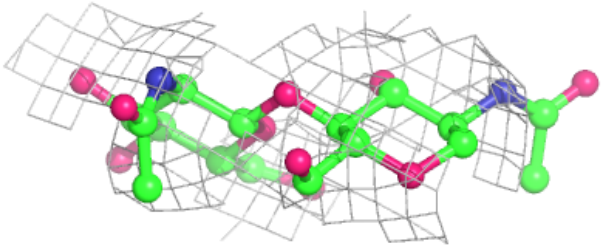


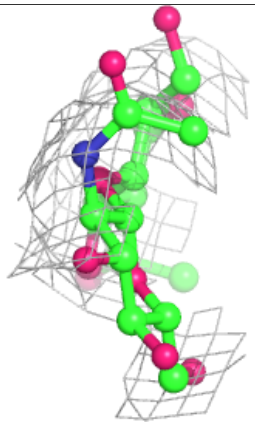


Electron density around Chain S:

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

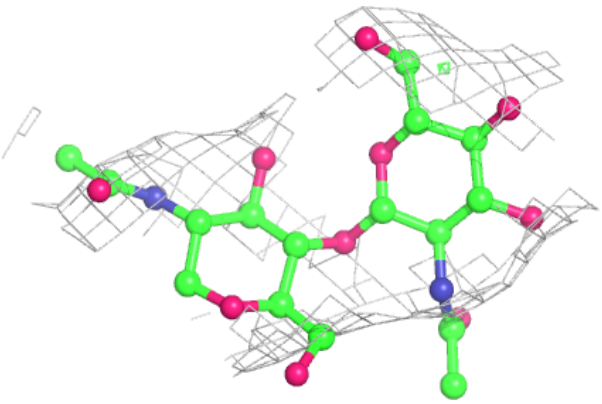


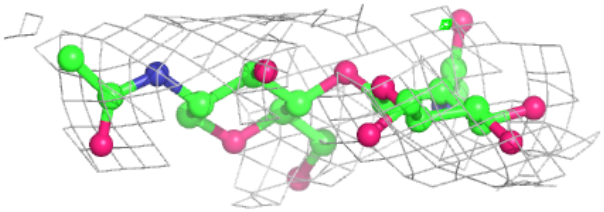


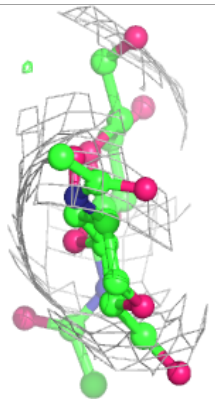


Electron density around Chain W:

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

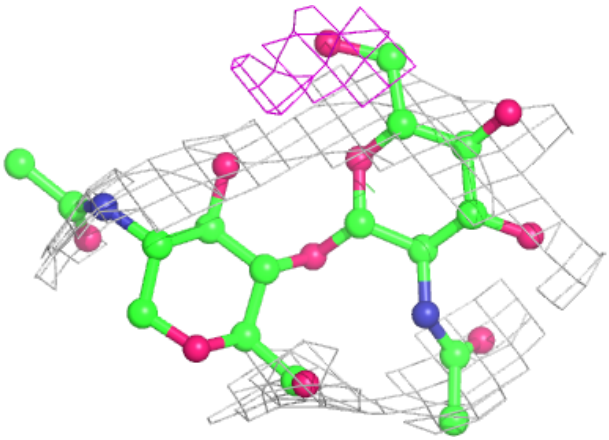


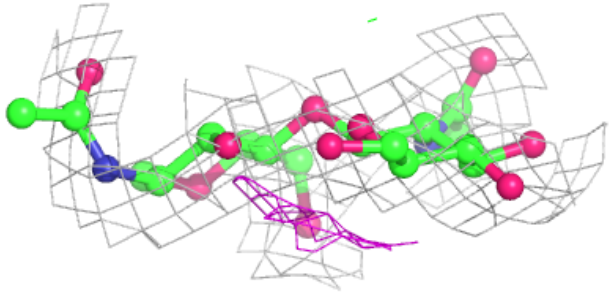


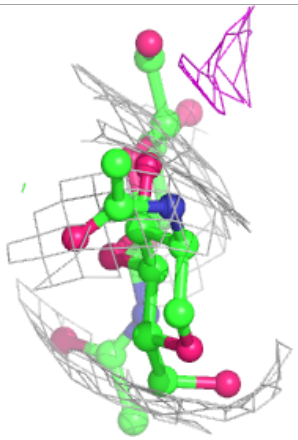


Electron density around Chain Z:

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

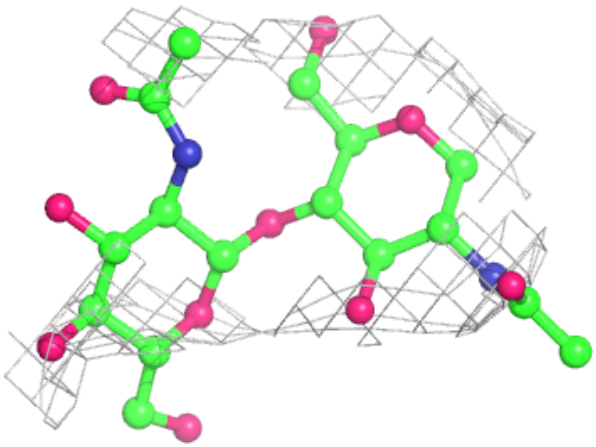


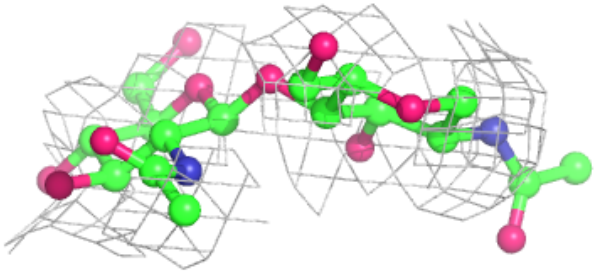


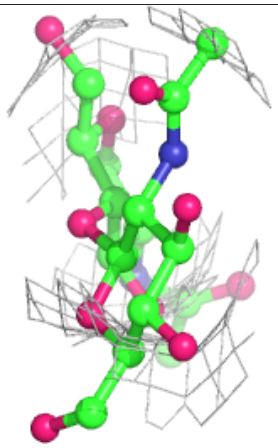


Electron density around Chain a:

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

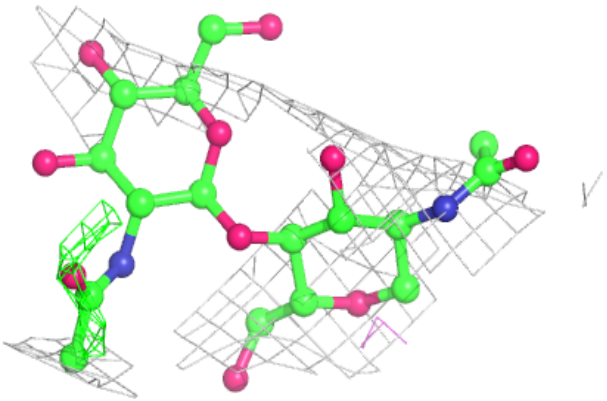


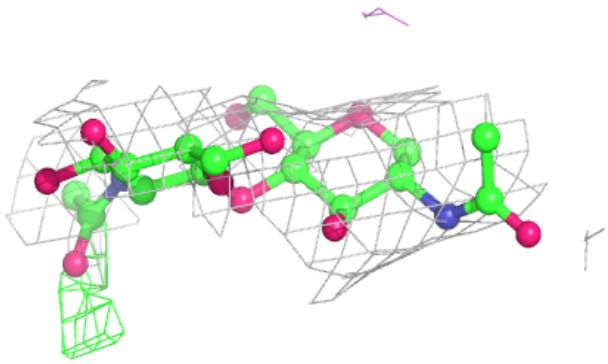


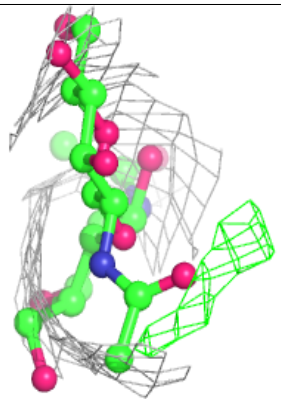


Electron density around Chain b:

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

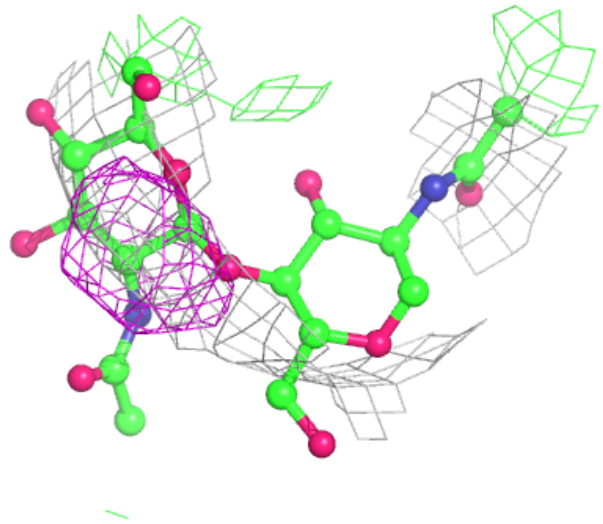


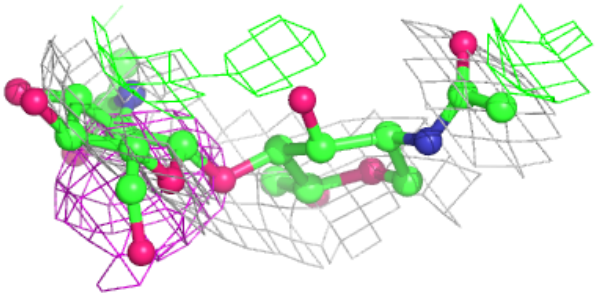




Electron density around Chain c:

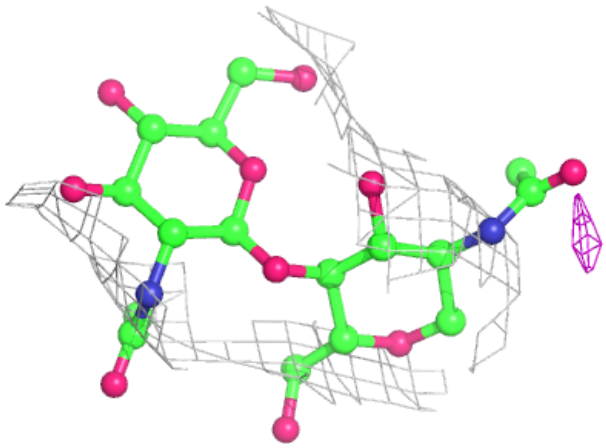
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

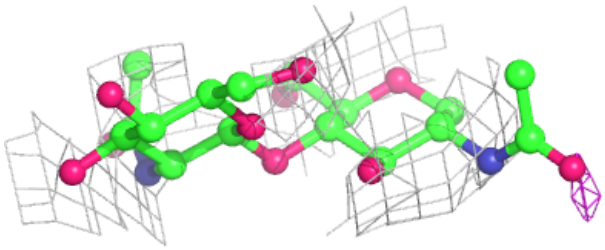


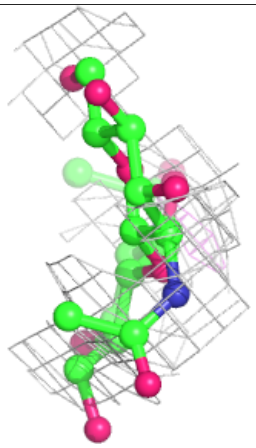


Electron density around Chain g:

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

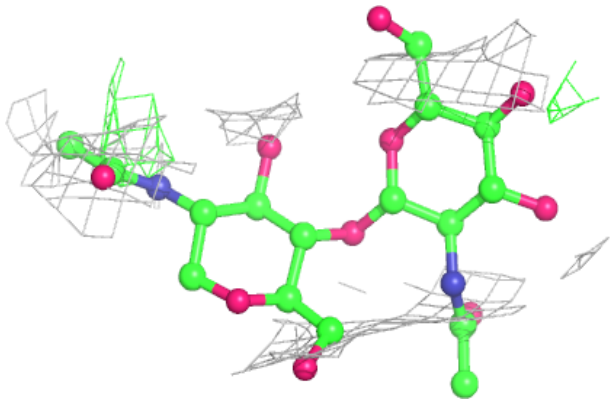


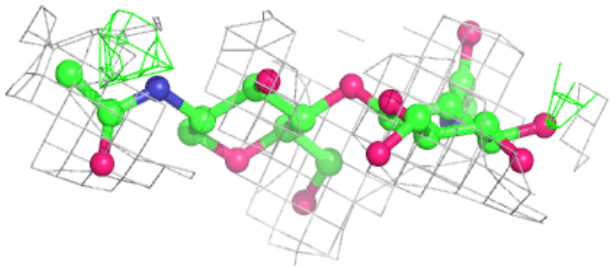


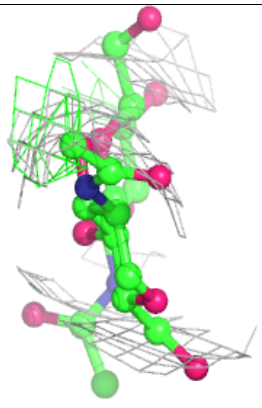


Electron density around Chain k:

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

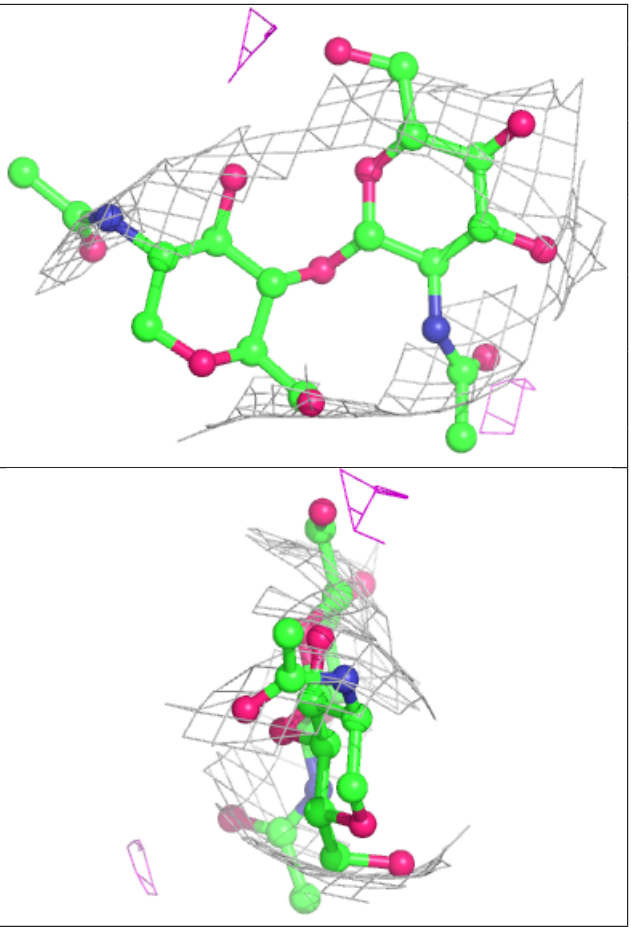


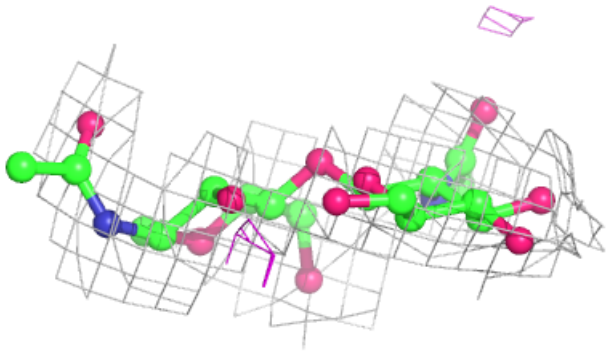




Electron density around Chain n:

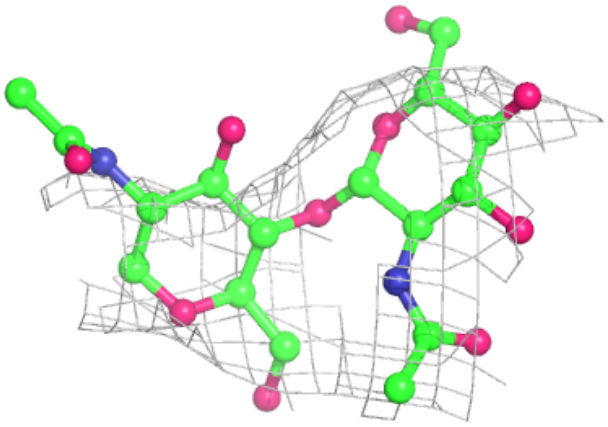
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

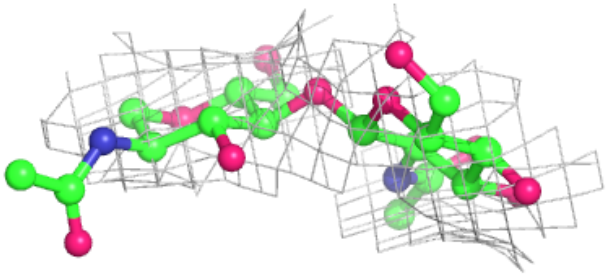


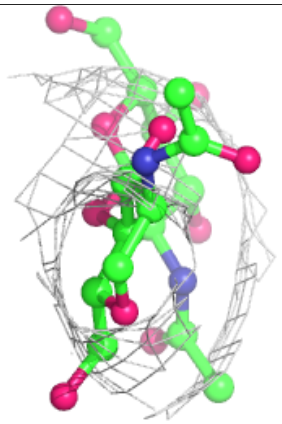


Electron density around Chain o:

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

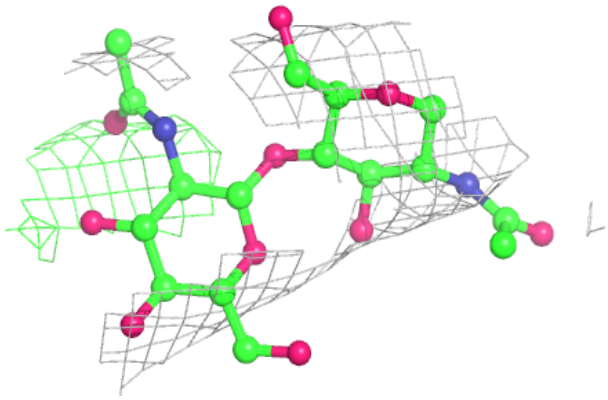


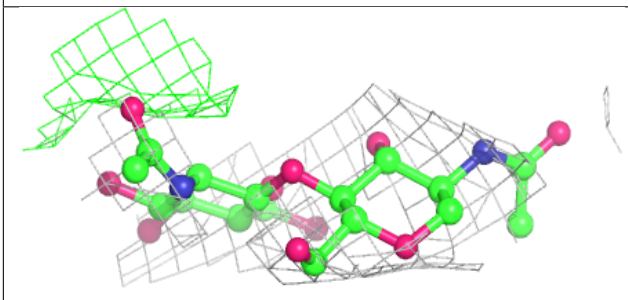


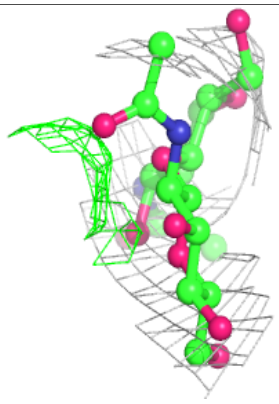


Electron density around Chain p:

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

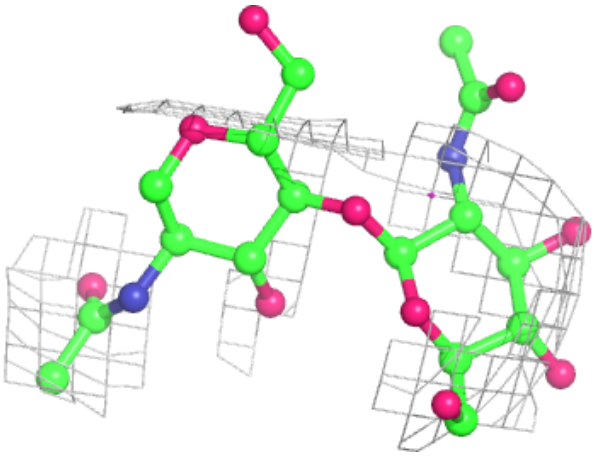


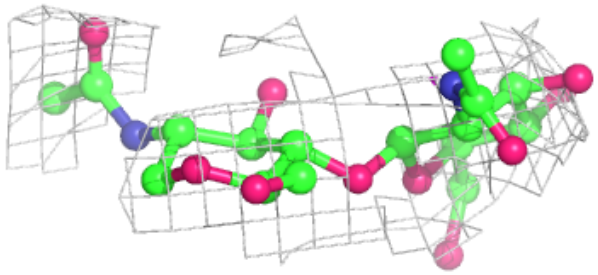


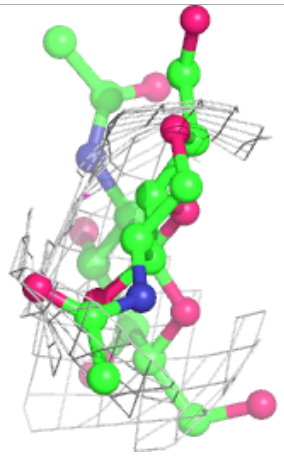


Electron density around Chain q:

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

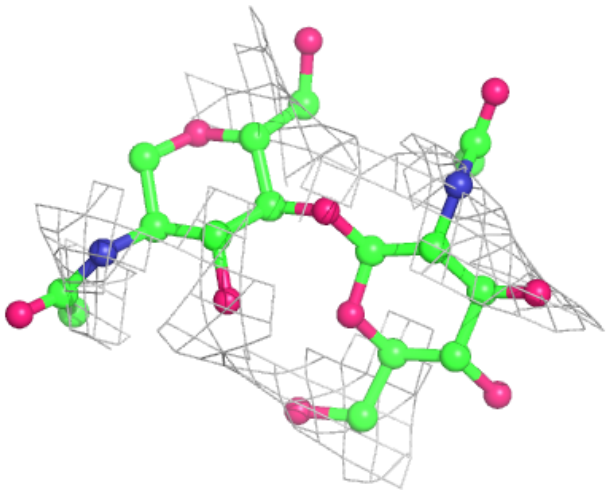


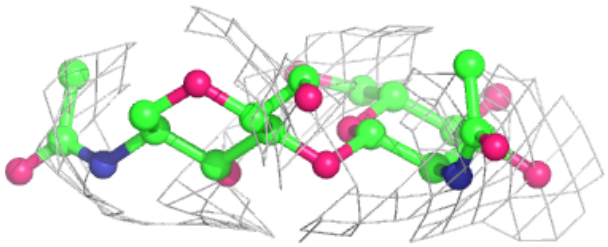


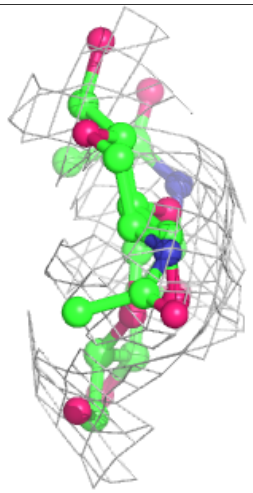


Electron density around Chain u:

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

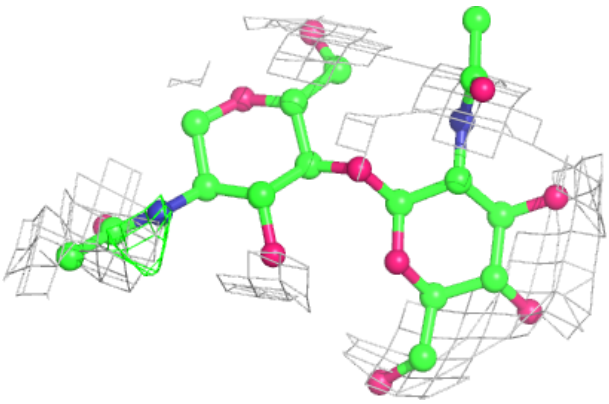


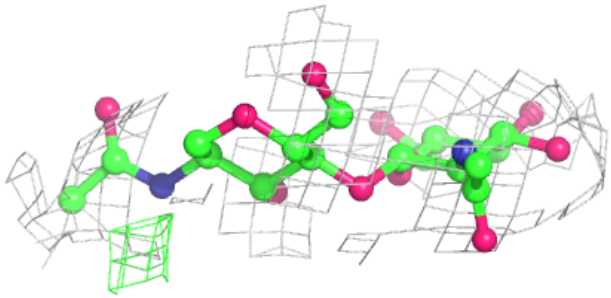


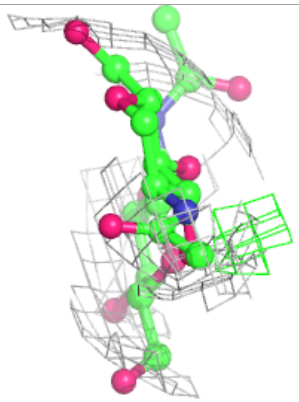


Electron density around Chain y:

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

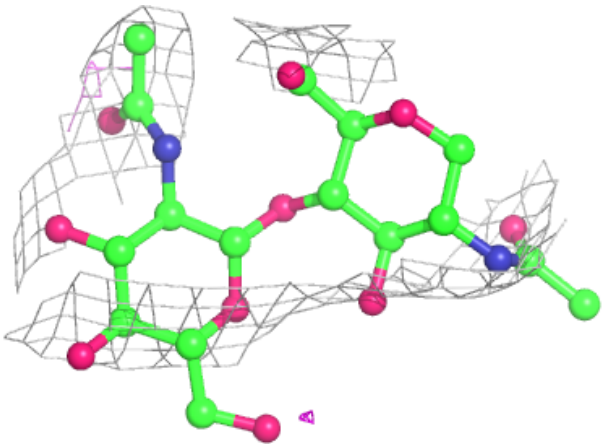


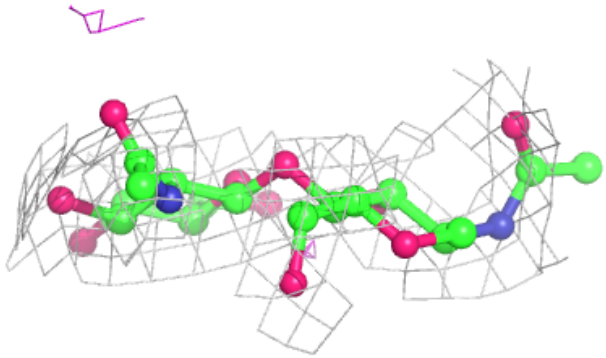


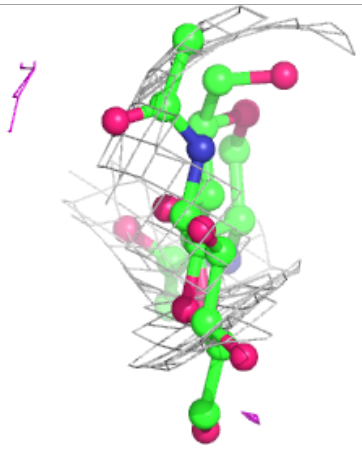


Electron density around Chain 1:

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

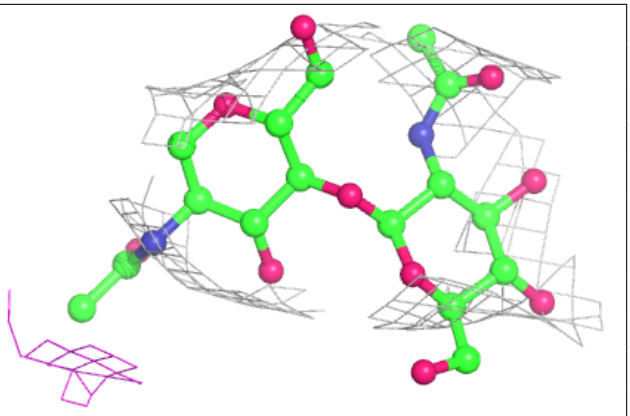


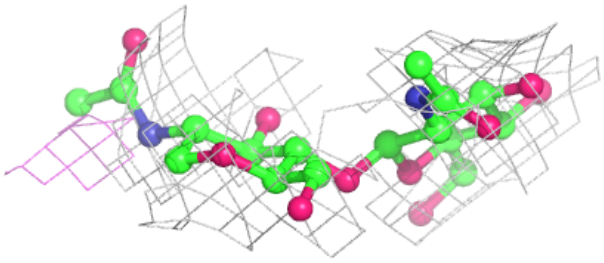


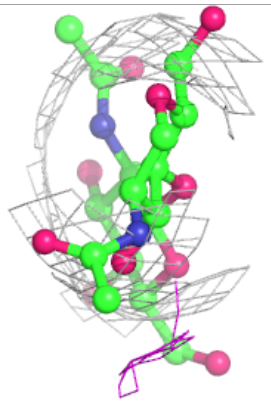


Electron density around Chain 2:

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

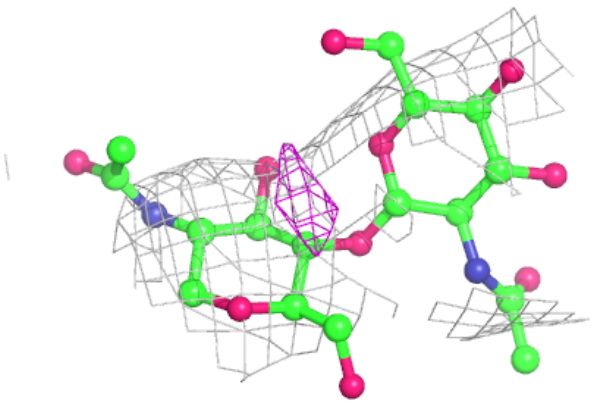


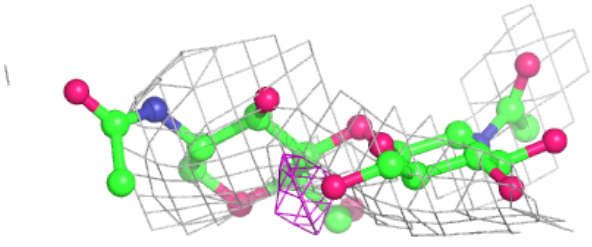


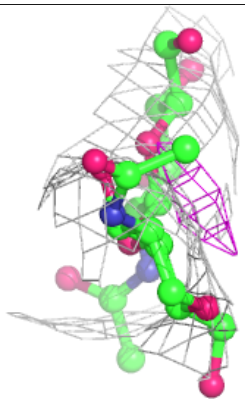


Electron density around Chain 3:

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

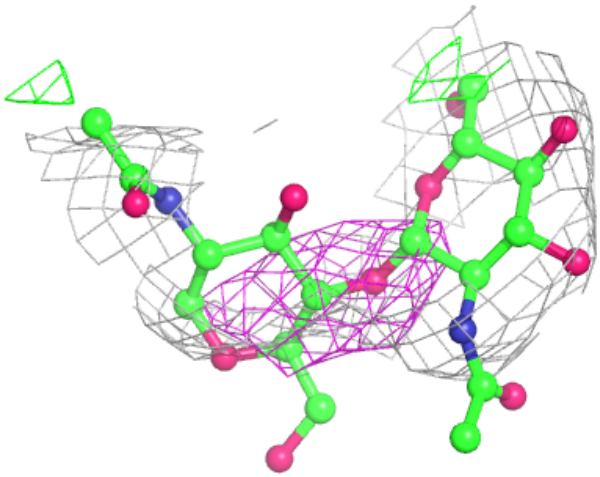


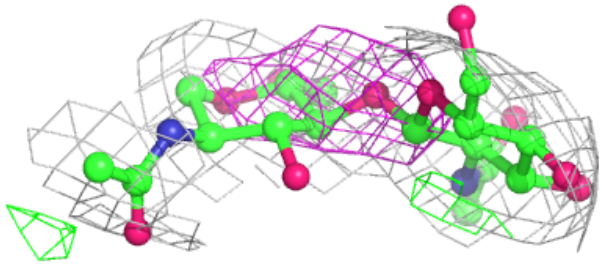


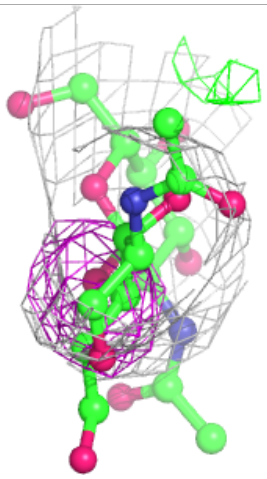


Electron density around Chain 4:

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

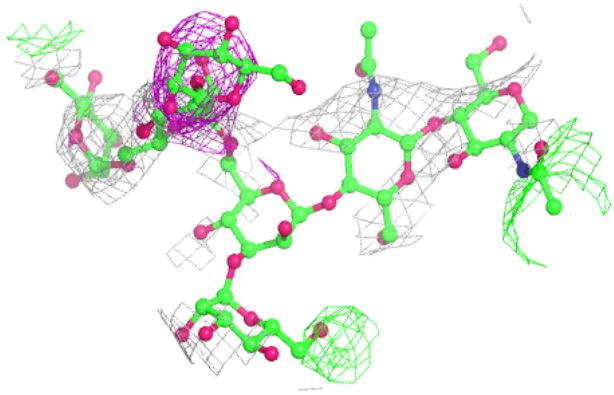


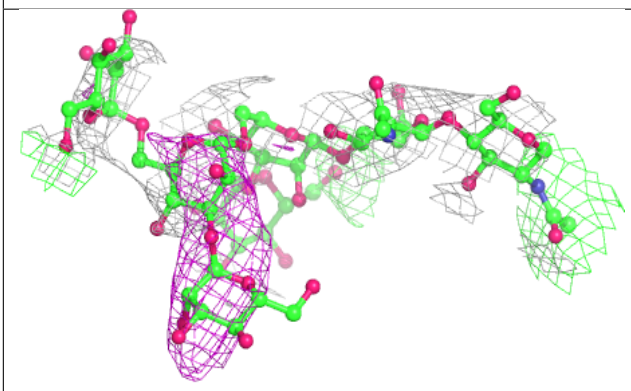


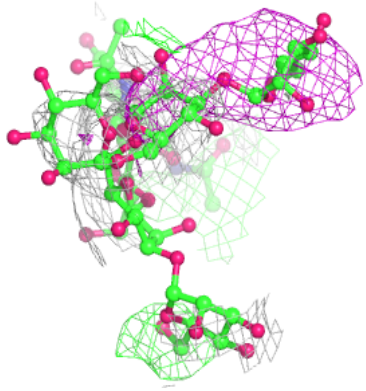


Electron density around Chain T:

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

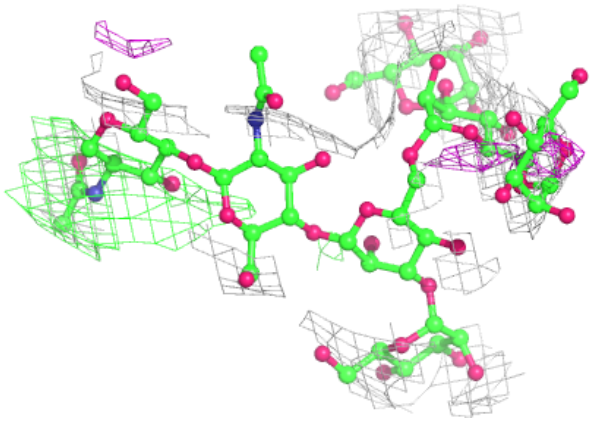


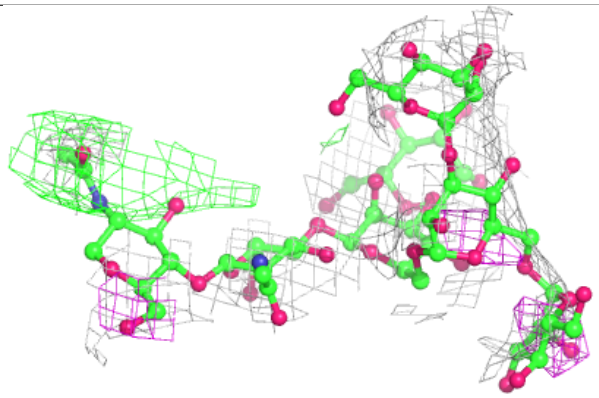


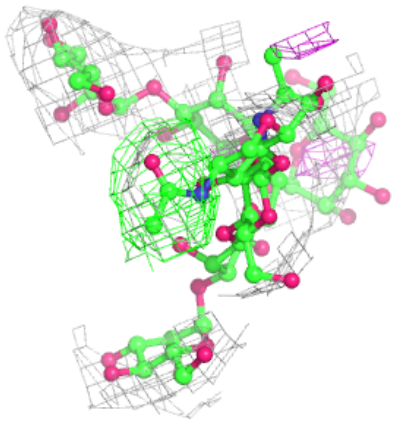


Electron density around Chain X:

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

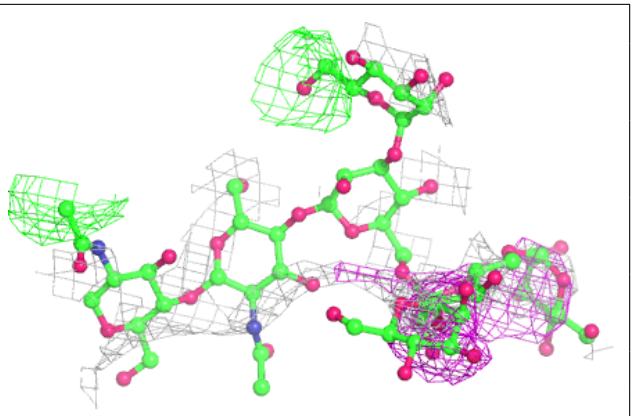


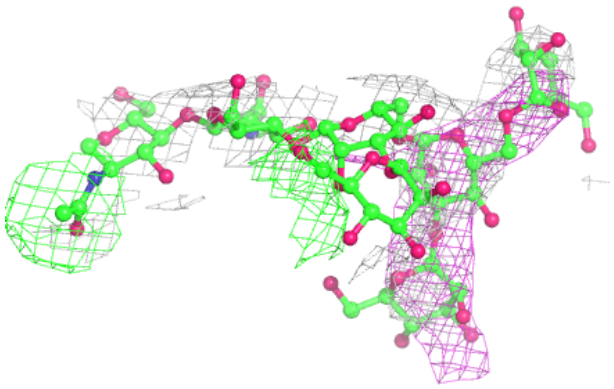


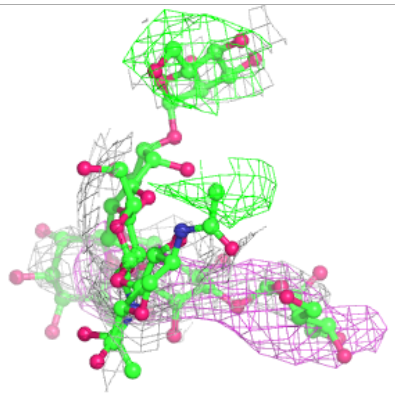


Electron density around Chain h:

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

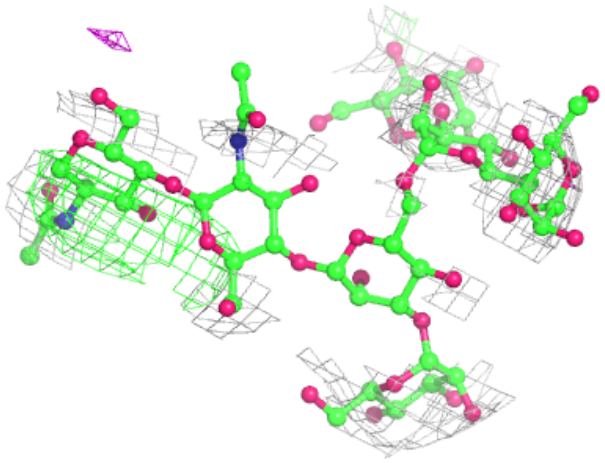


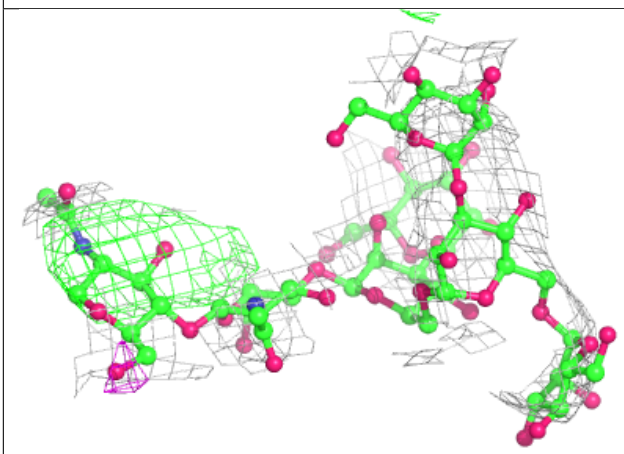


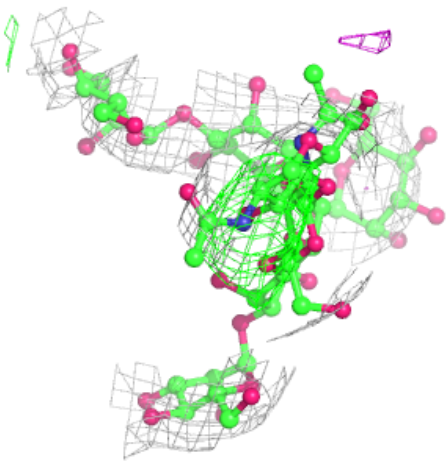


Electron density around Chain l:

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

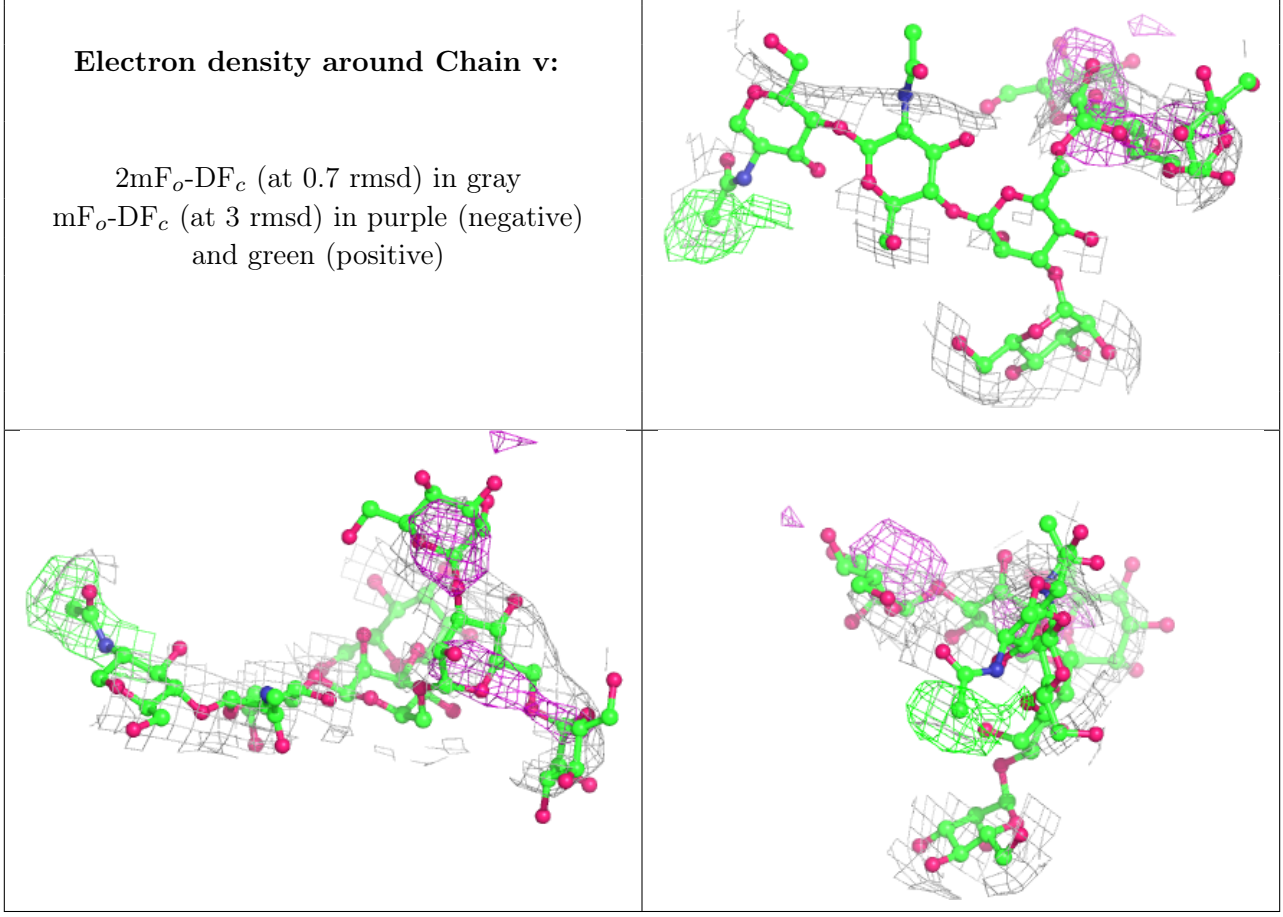






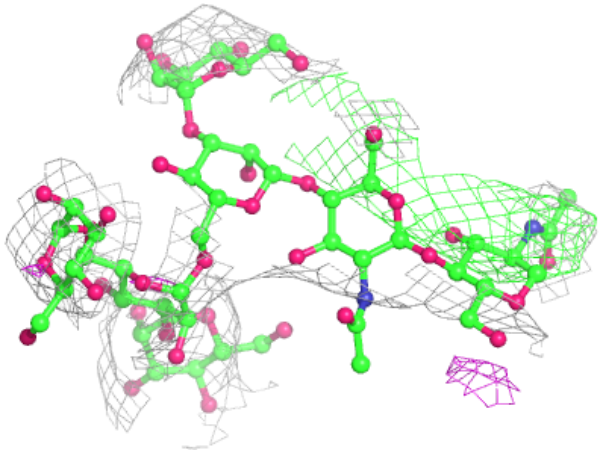
Electron density around Chain v:

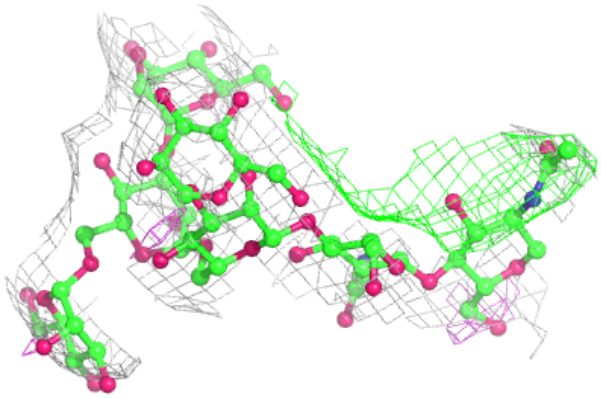
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

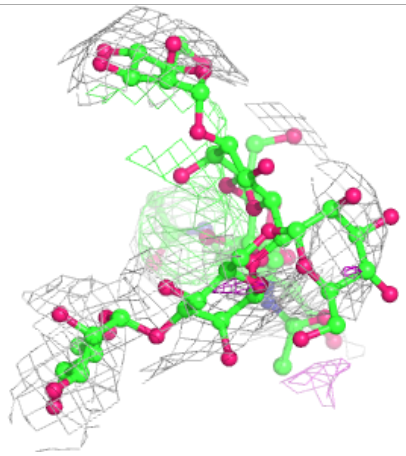


Electron density around Chain z:

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

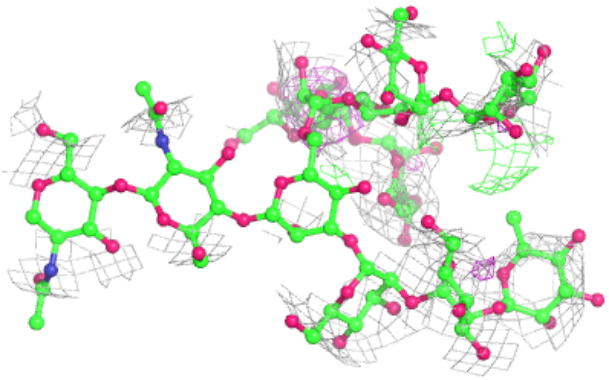


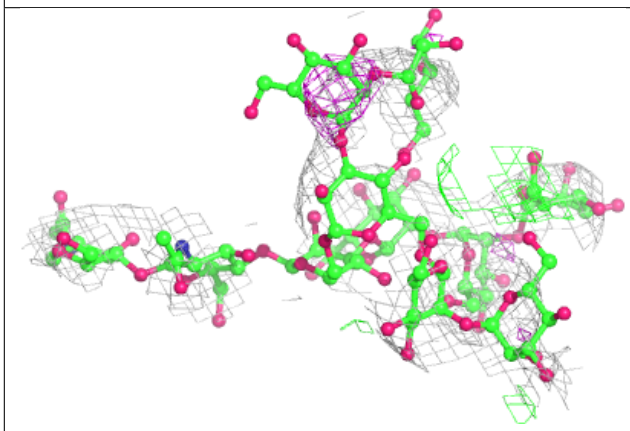


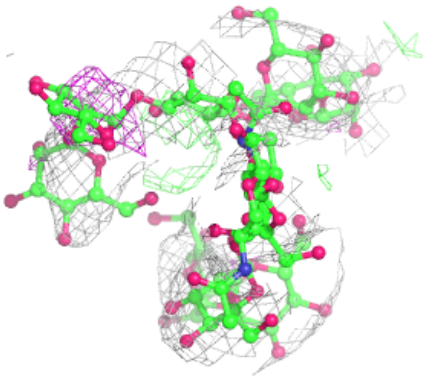


Electron density around Chain U:

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

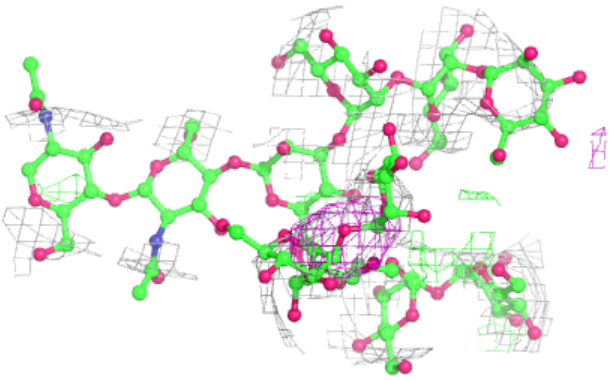


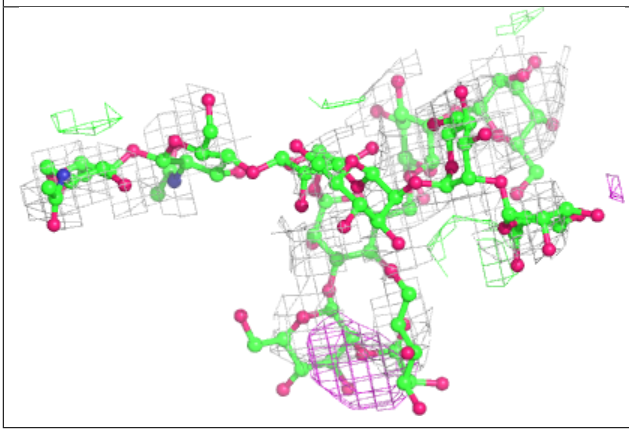


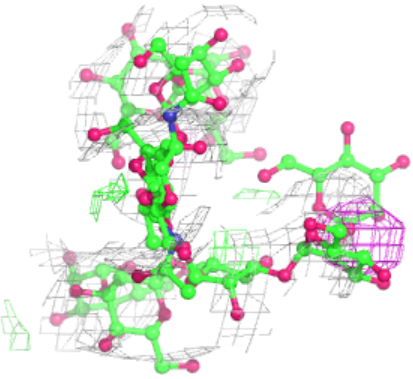


Electron density around Chain i:

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

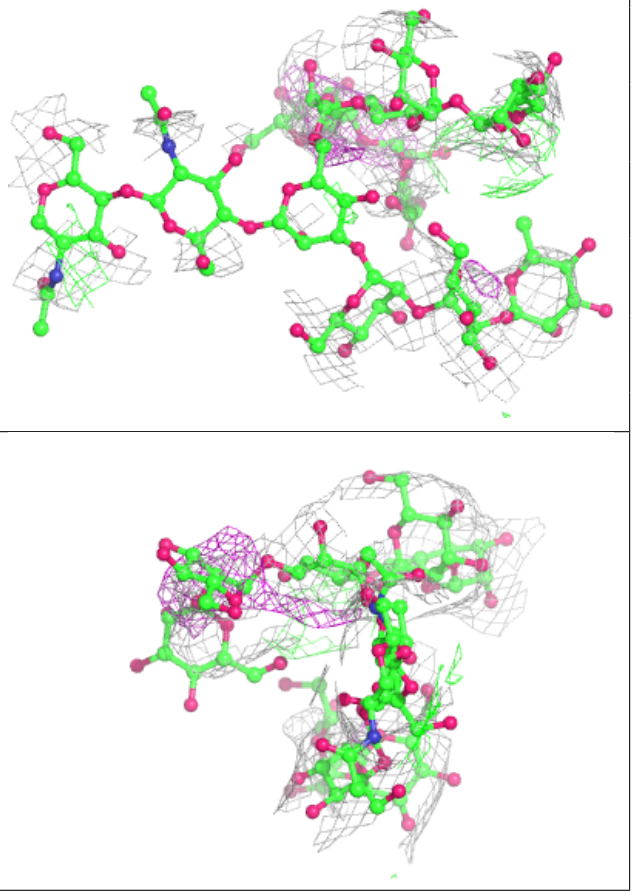






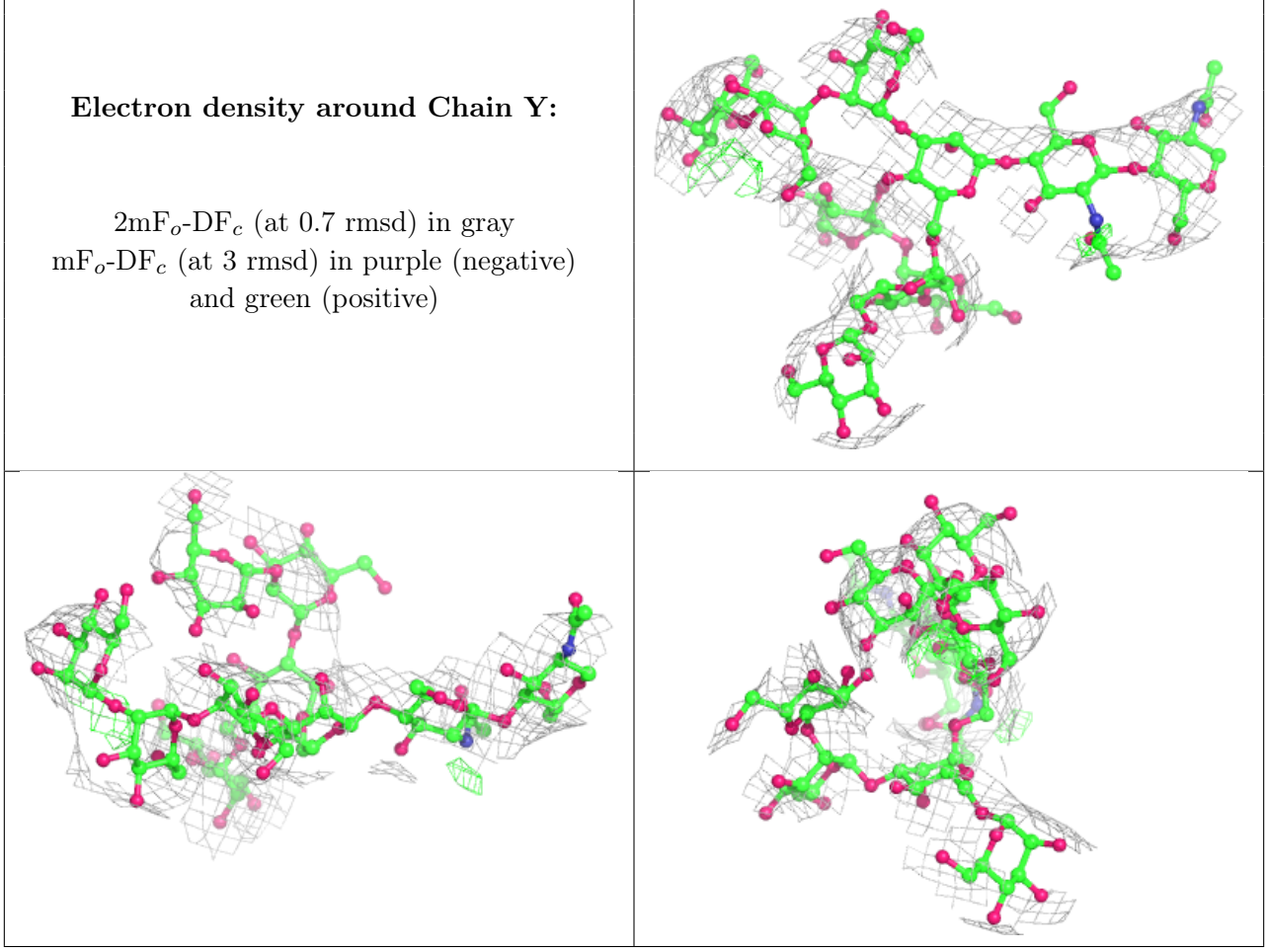
Electron density around Chain w:

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



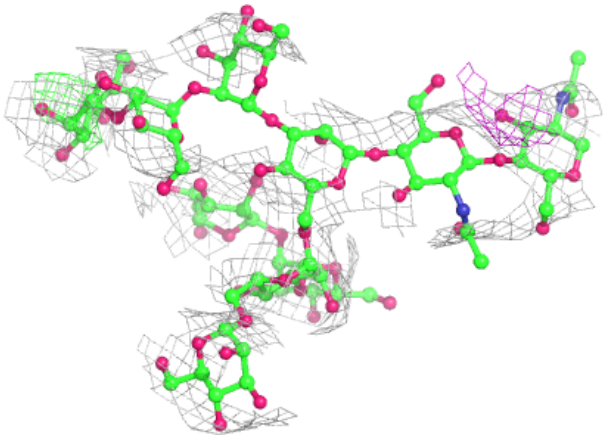
Electron density around Chain Y:

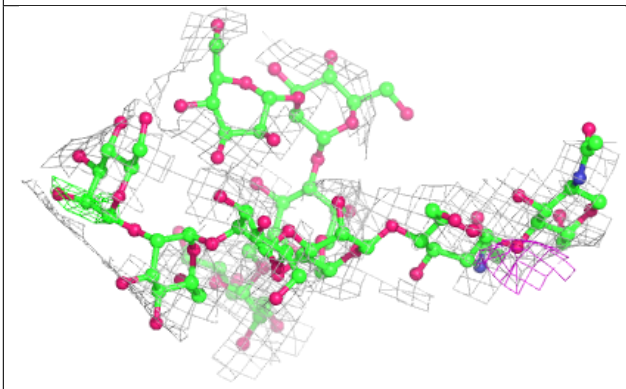
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

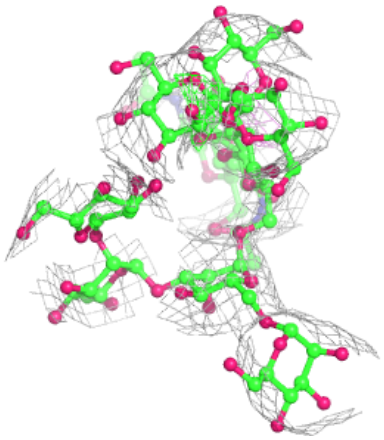


Electron density around Chain m:

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

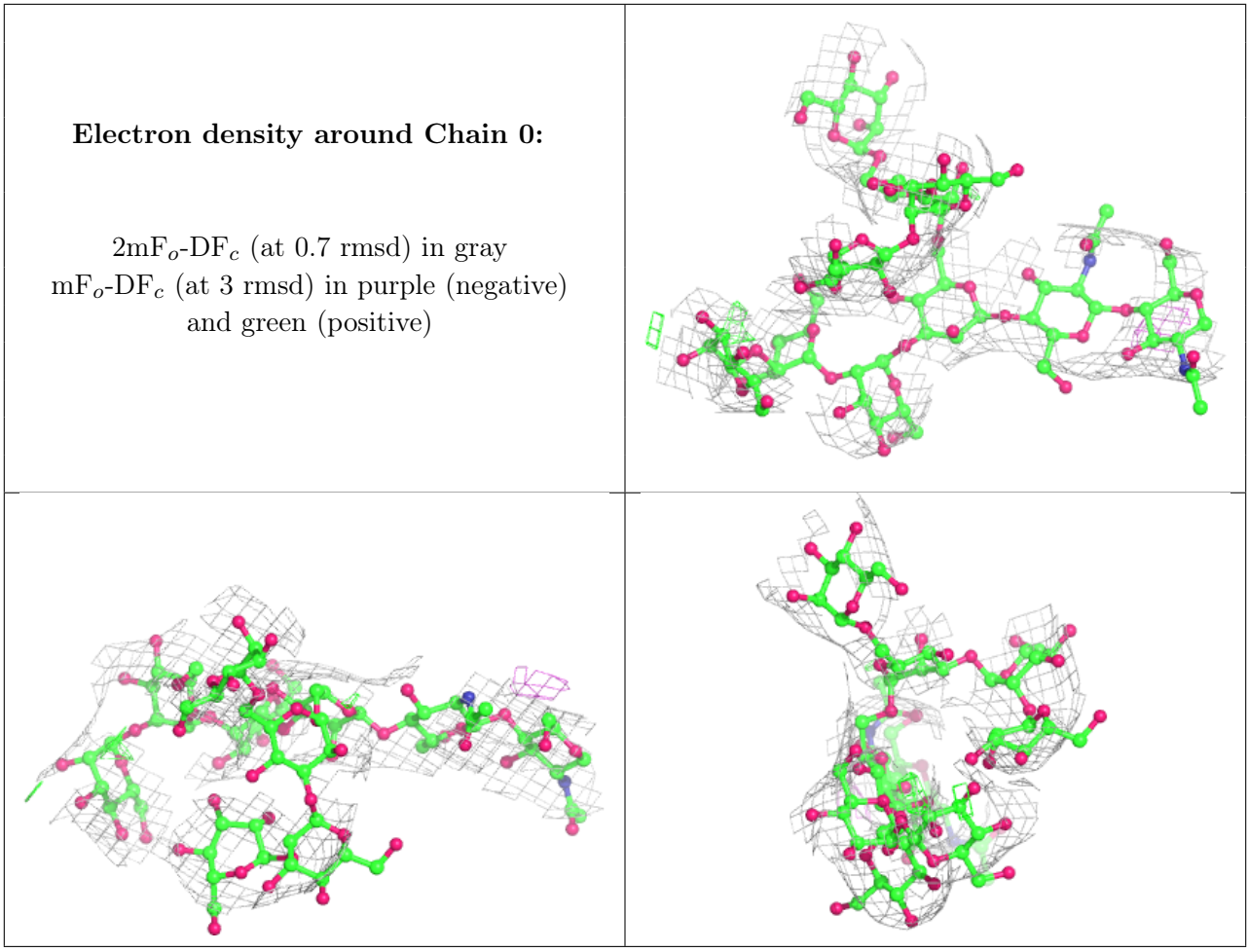






Electron density around Chain 0:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.