wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2022 – 11:58 PM EDT

PDB ID	:	3WHE
Title	:	A new conserved neutralizing epitope at the globular head of hemagglutinin in H3N2 influenza viruses
Authors	:	Fujii, Y.; Sumida, T.; Shirouzu, M.; Yokoyama, S.
Deposited on	:	2013-08-25
Resolution	:	4.00 Å(reported)

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

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

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

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

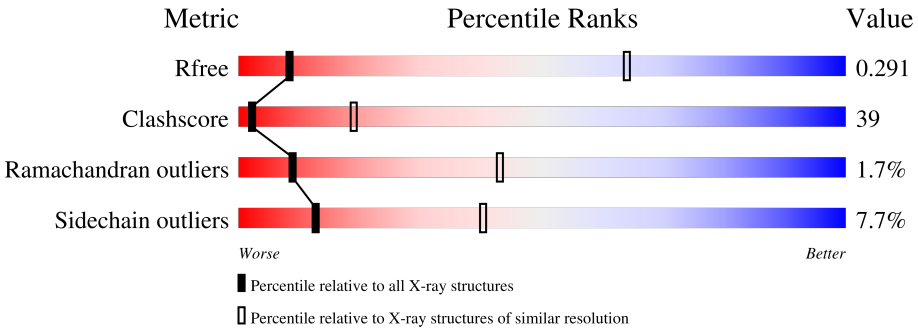
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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	493	49% 46% .
1	B	493	47% 49% .
1	C	493	47% 49% .
1	D	493	48% 48% .
1	E	493	46% 49% .
1	F	493	46% 49% 5%
1	G	493	48% 47% .

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Mol	Chain	Length	Quality of chain
1	H	493	47% 49% •
1	I	493	46% 49% •
1	J	493	47% 49% •
1	K	493	46% 50% •
1	L	493	47% 48% •
2	1	226	32% 57% 11%
2	3	226	32% 57% 11%
2	5	226	32% 57% 11%
2	7	226	32% 56% 12%
2	9	226	33% 56% 11%
2	M	226	29% 60% 11%
2	O	226	32% 57% 12%
2	Q	226	31% 58% 11%
2	S	226	31% 58% 12%
2	U	226	31% 57% 12%
2	W	226	32% 56% 12%
2	Y	226	31% 58% 11%
3	0	220	39% 52% 5% •
3	2	220	41% 50% 5% •
3	4	220	40% 52% 5% •
3	6	220	40% 52% 5% •
3	8	220	43% 49% 5% •
3	N	220	36% 55% 5% •
3	P	220	41% 51% • •
3	R	220	42% 50% 5% •

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Mol	Chain	Length	Quality of chain
3	T	220	40% 51% 5%
3	V	220	40% 51% 5%
3	X	220	39% 53% 5%
3	Z	220	40% 51% 5%
4	BA	7	43% 43% 14%
4	EA	7	29% 43% 29%
4	HA	7	29% 57% 14%
4	a	7	29% 71%
4	d	7	29% 71%
4	g	7	29% 71%
4	j	7	29% 71%
4	m	7	29% 71%
4	p	7	43% 57%
4	s	7	43% 57%
4	v	7	43% 57%
4	y	7	43% 57%
5	CA	6	67% 33%
5	FA	6	67% 33%
5	IA	6	67% 33%
5	b	6	100%
5	e	6	100%
5	h	6	100%
5	k	6	100%
5	n	6	100%
5	q	6	100%

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Mol	Chain	Length	Quality of chain
5	t	6	100%
5	w	6	17% 83%
5	z	6	100%
6	AA	3	100%
6	DA	3	100%
6	GA	3	67% 33%
6	JA	3	100%
6	c	3	33% 67%
6	f	3	33% 67%
6	i	3	33% 67%
6	l	3	33% 67%
6	o	3	67% 33%
6	r	3	67% 33%
6	u	3	100%
6	x	3	33% 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	EA	2	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 88152 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	B	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	C	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	D	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	E	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	F	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	G	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	H	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	I	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	J	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	K	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	L	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	O	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	S	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	U	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	W	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	Y	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	1	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	3	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	5	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	7	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	9	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

- Molecule 3 is a protein called immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	P	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	R	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	T	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	V	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	X	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	Z	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	2	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	4	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

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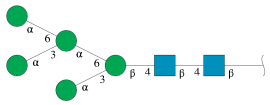
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	6	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	8	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	0	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

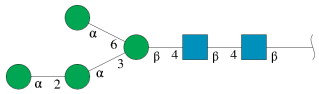
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	d	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	g	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	j	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	m	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	p	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	s	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	v	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	y	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	BA	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	EA	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	HA	7	Total	C	N	O	0	0	0
			83	46	2	35			

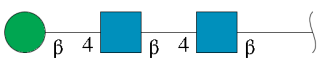
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(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
5	b	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	e	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	h	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	k	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	n	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	q	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	t	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	w	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	z	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	CA	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	FA	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	IA	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	c	3	Total	C	N	O	0	0	0
			39	22	2	15			

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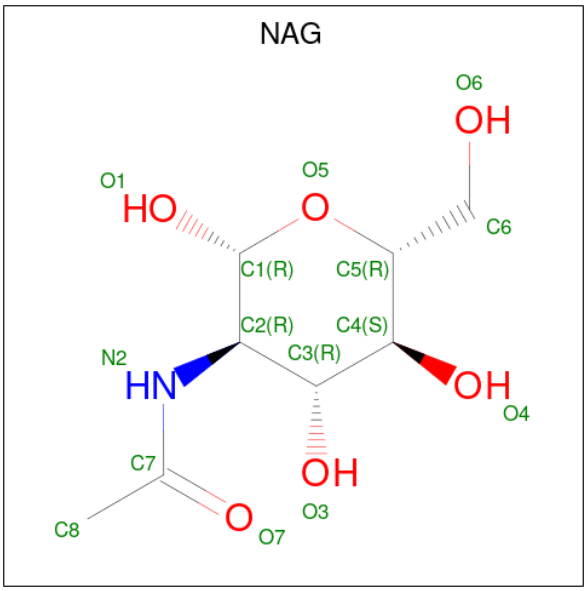
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	f	3	Total C N O 39 22 2 15	0	0	0
6	i	3	Total C N O 39 22 2 15	0	0	0
6	l	3	Total C N O 39 22 2 15	0	0	0
6	o	3	Total C N O 39 22 2 15	0	0	0
6	r	3	Total C N O 39 22 2 15	0	0	0
6	u	3	Total C N O 39 22 2 15	0	0	0
6	x	3	Total C N O 39 22 2 15	0	0	0
6	AA	3	Total C N O 39 22 2 15	0	0	0
6	DA	3	Total C N O 39 22 2 15	0	0	0
6	GA	3	Total C N O 39 22 2 15	0	0	0
6	JA	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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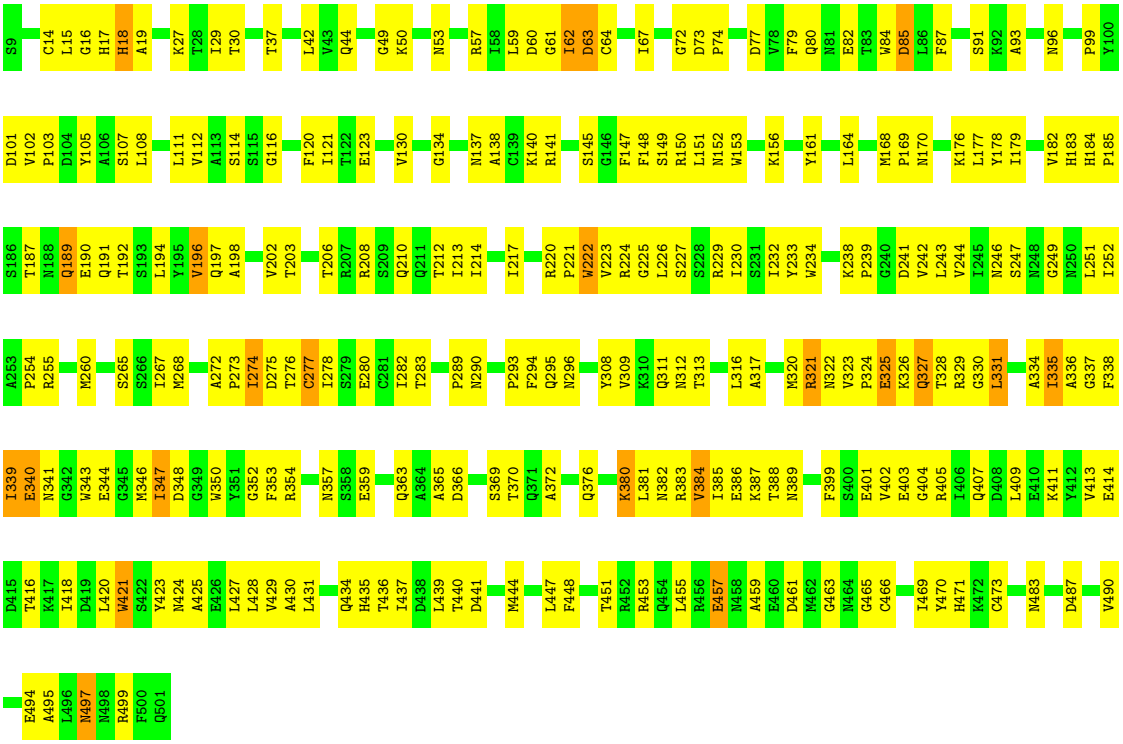
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

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: Hemagglutinin

Chain A:

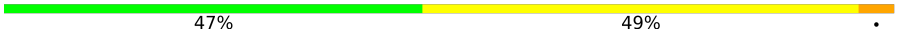


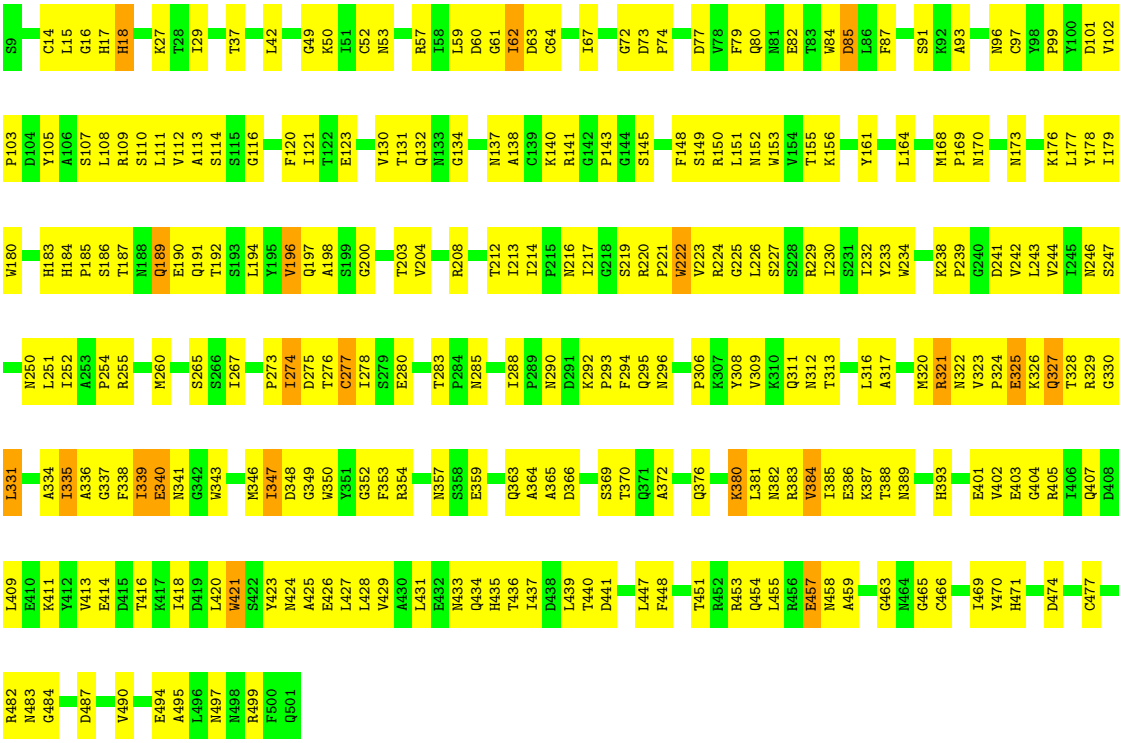
- Molecule 1: Hemagglutinin

Chain B:

• Molecule 1: Hemagglutinin

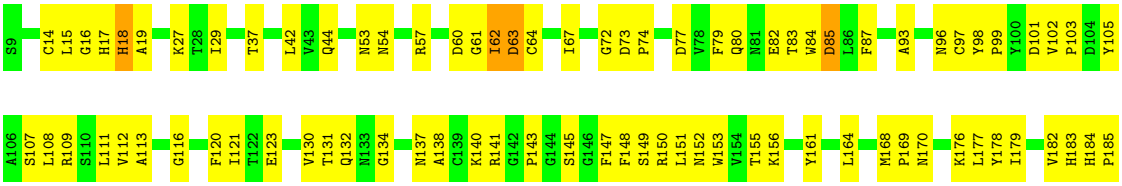
Chain C:

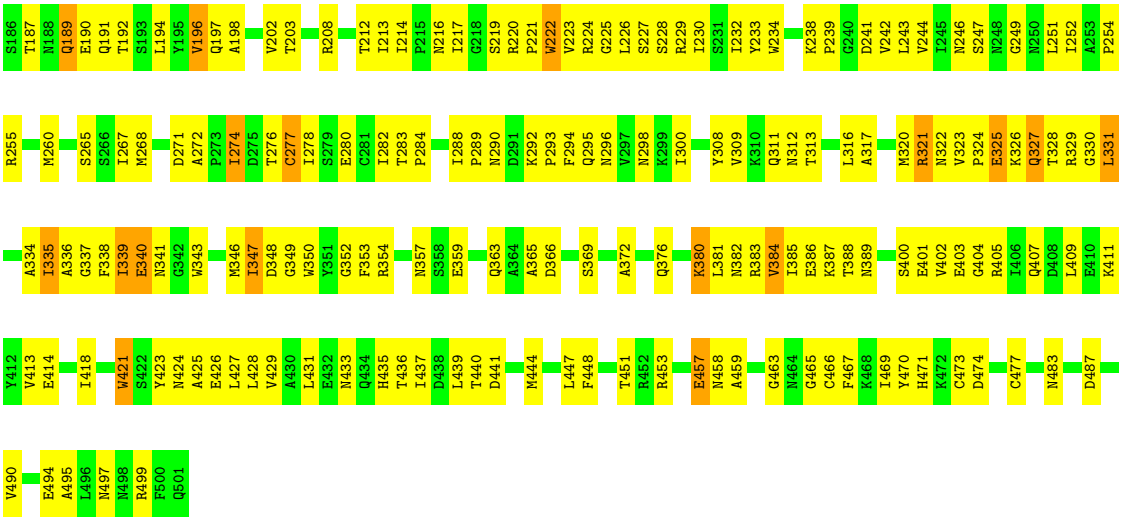




• Molecule 1: Hemagglutinin

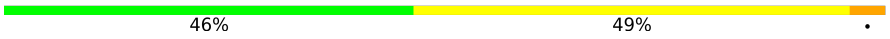
Chain D:

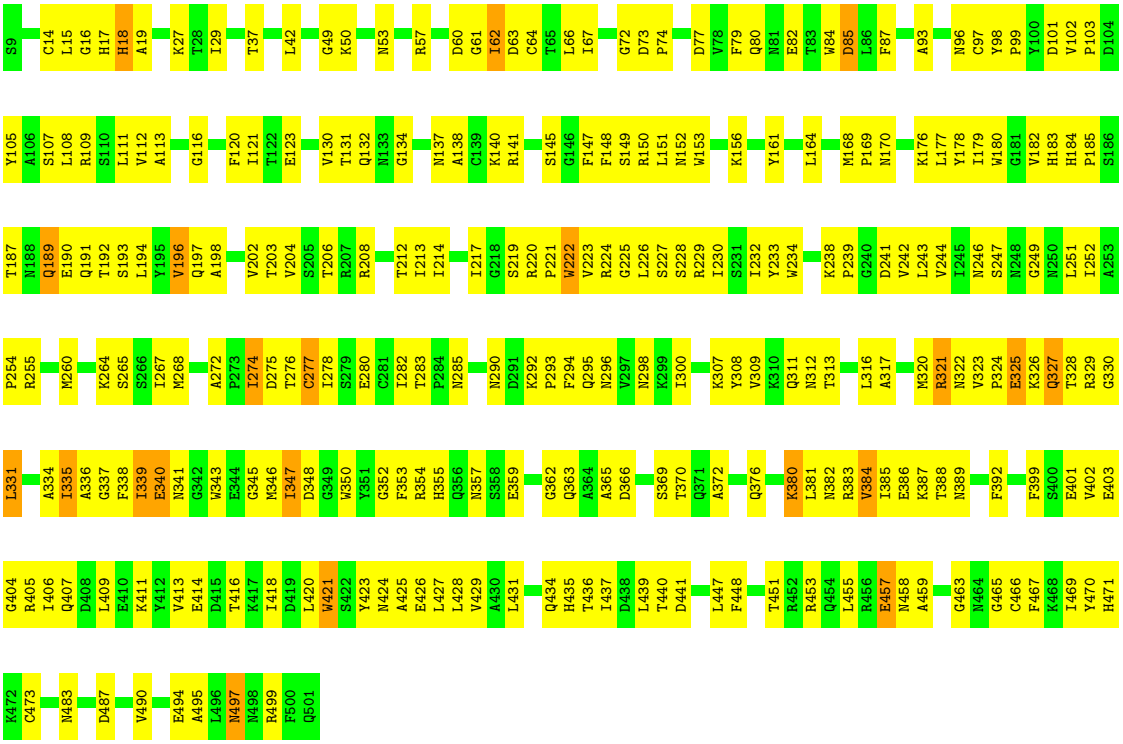




• Molecule 1: Hemagglutinin

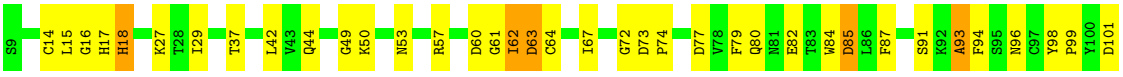
Chain E:

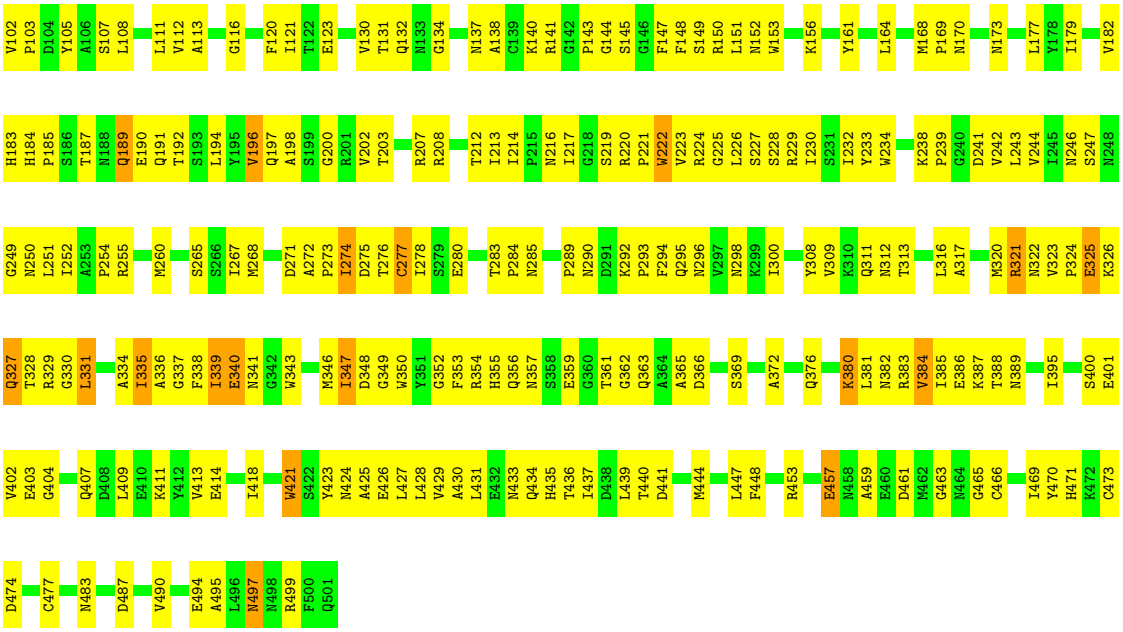




• Molecule 1: Hemagglutinin

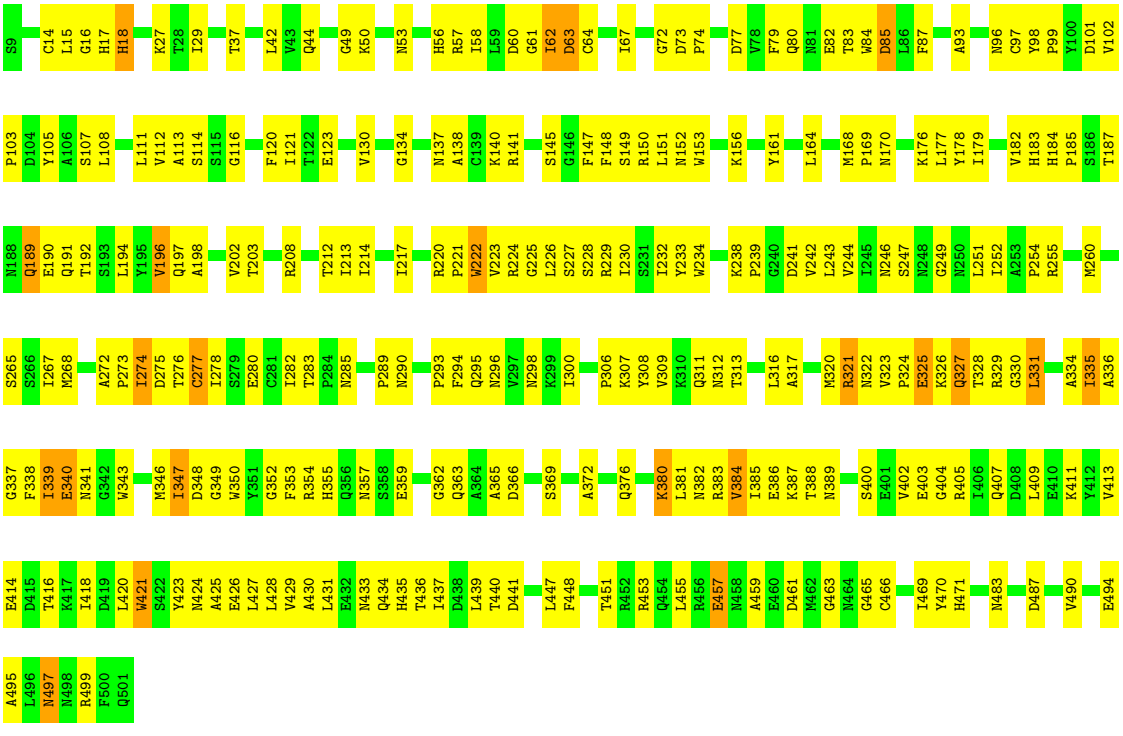
Chain F:





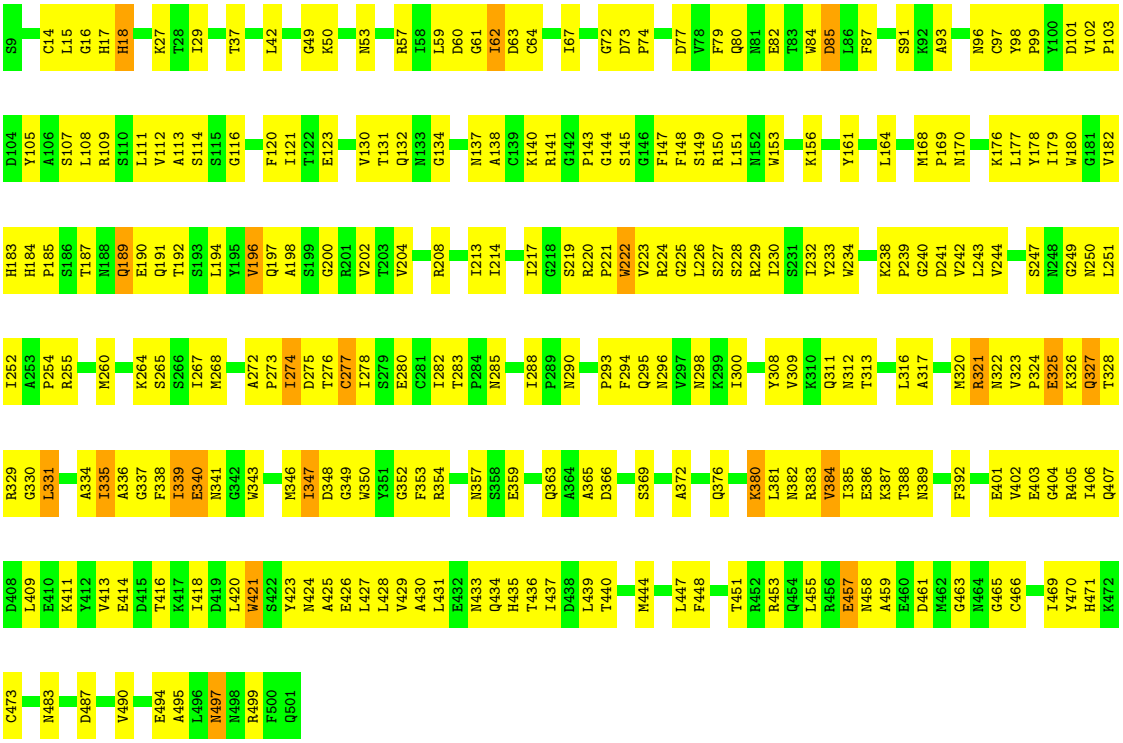
• Molecule 1: Hemagglutinin

Chain G:



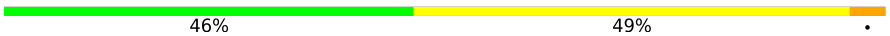
• Molecule 1: Hemagglutinin

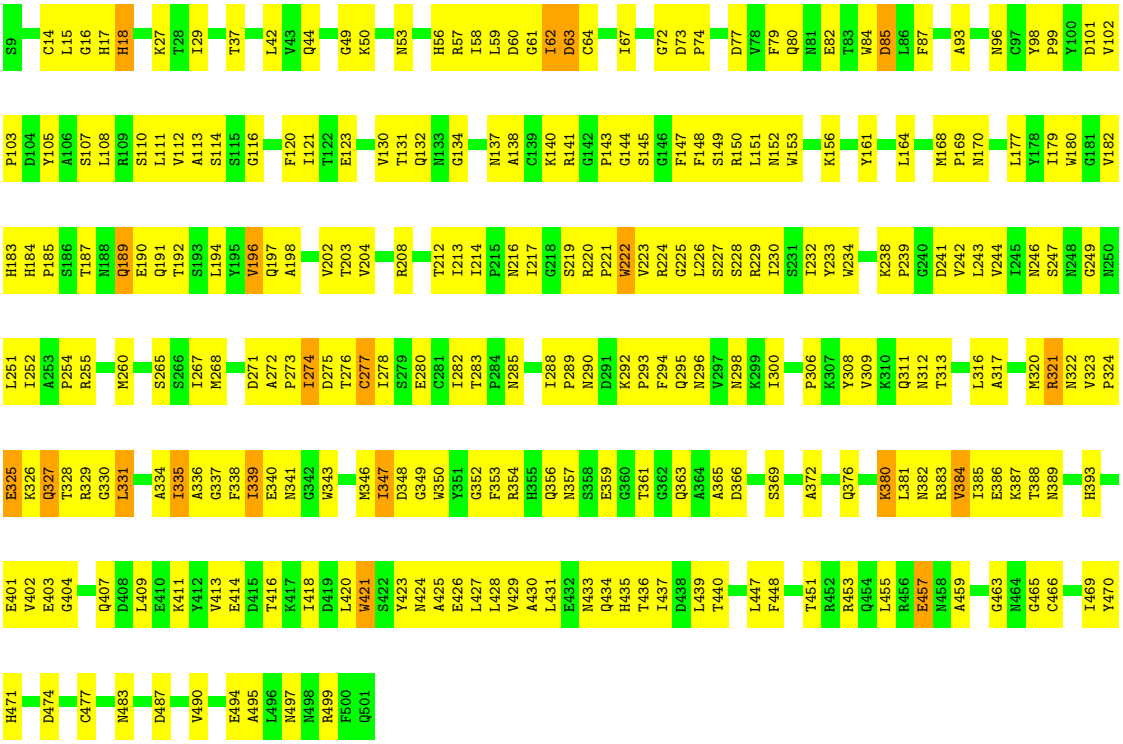
Chain H:



• Molecule 1: Hemagglutinin

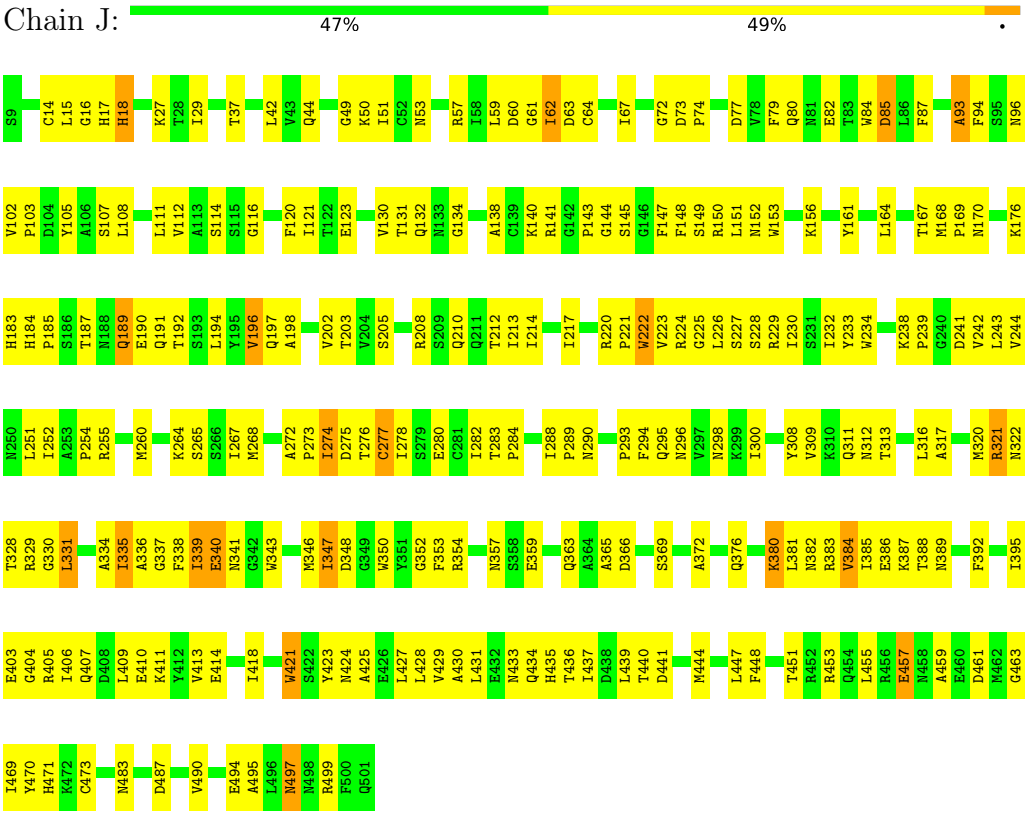
Chain I:





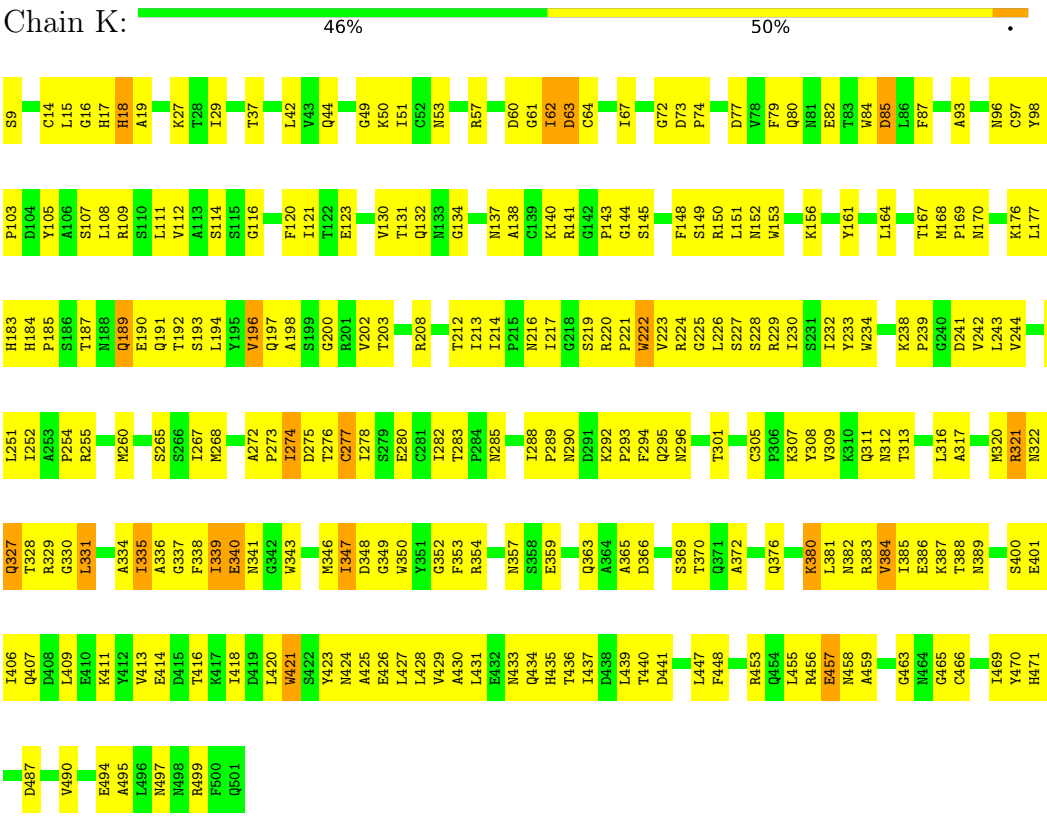
• Molecule 1: Hemagglutinin

Chain J:



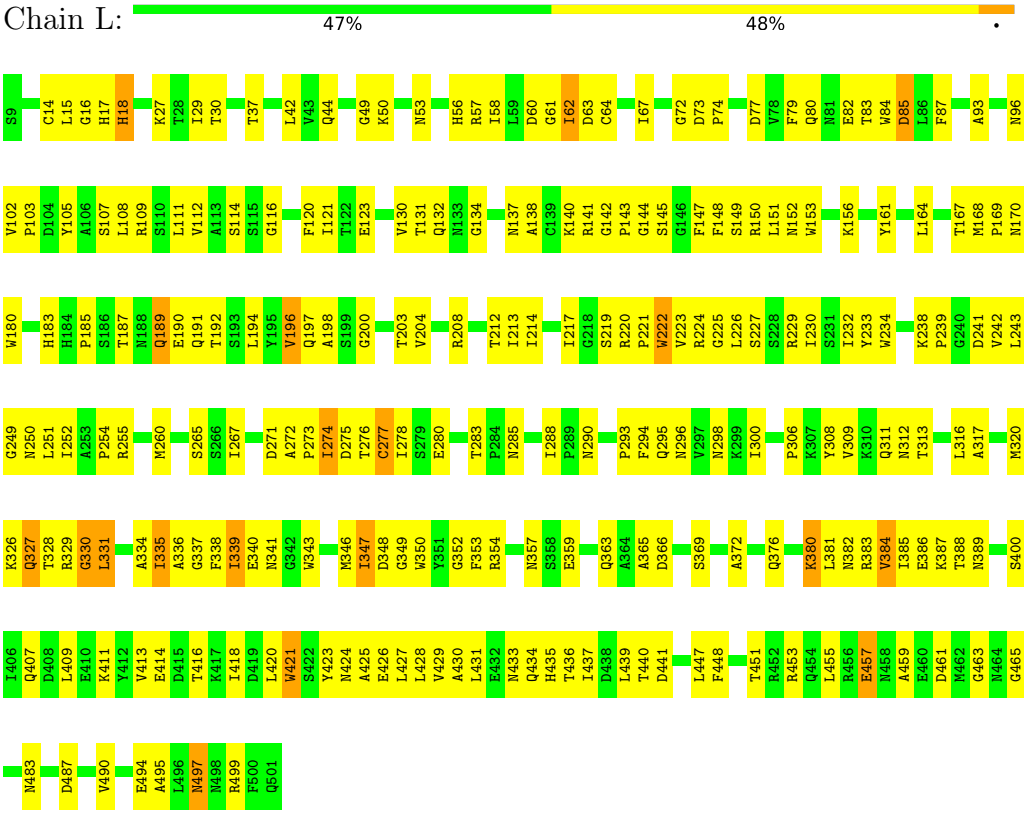
• Molecule 1: Hemagglutinin

Chain K:



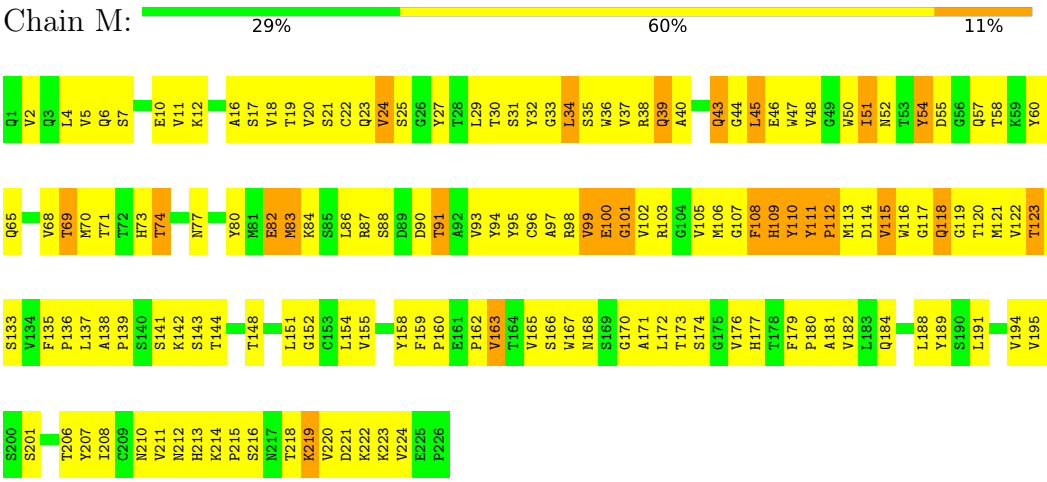
• Molecule 1: Hemagglutinin

Chain L:



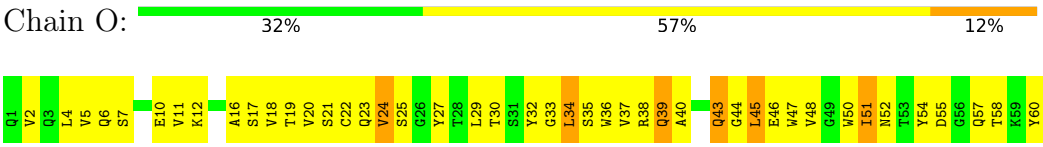
• Molecule 2: immunoglobulin heavy chain

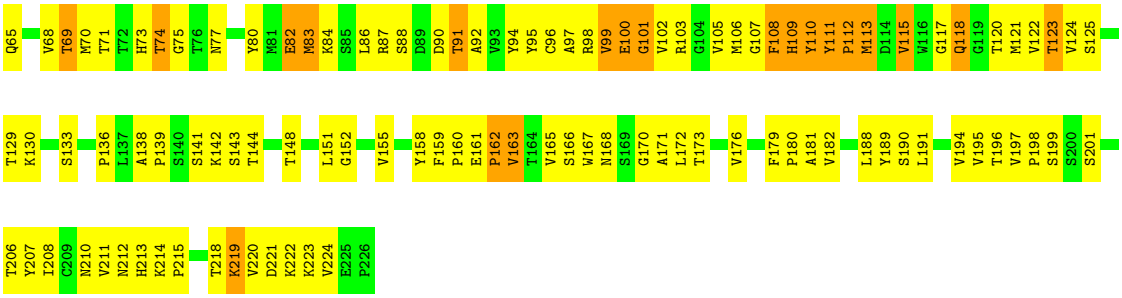
Chain M:



• Molecule 2: immunoglobulin heavy chain

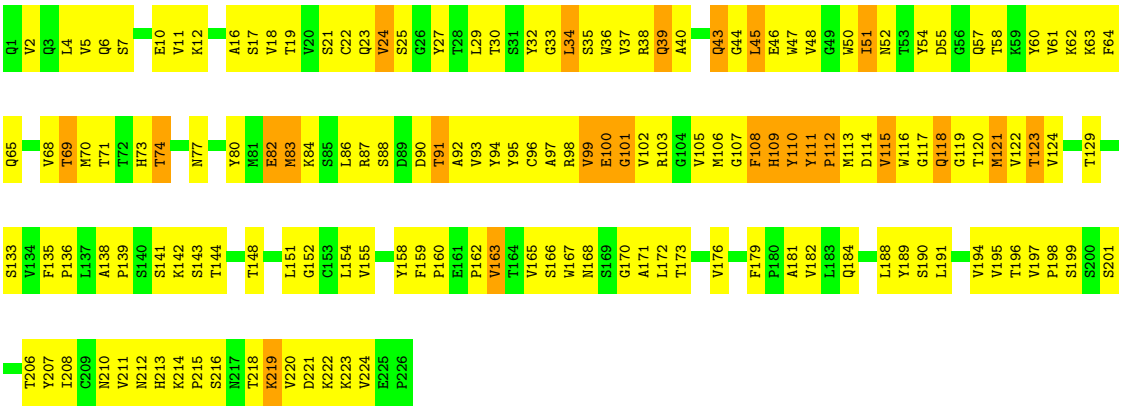
Chain O:





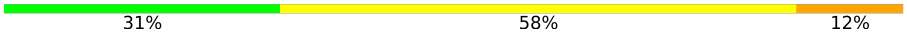
• Molecule 2: immunoglobulin heavy chain

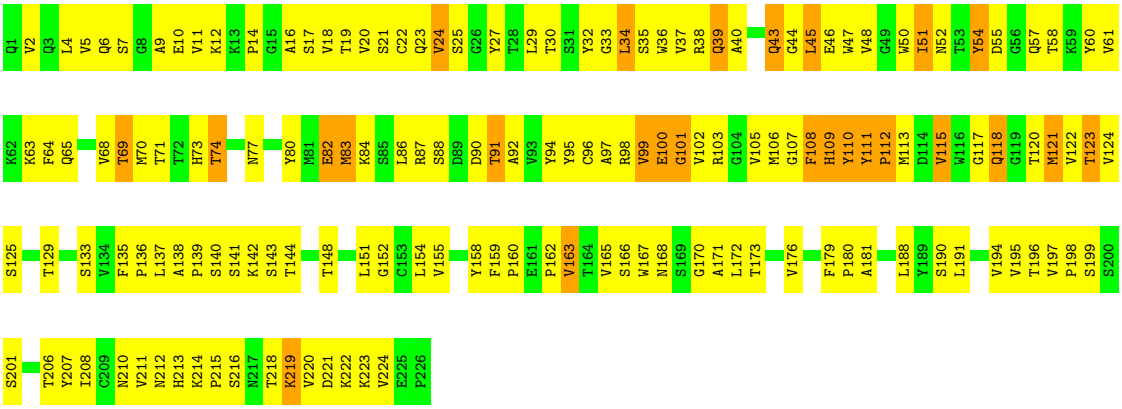
Chain Q:



• Molecule 2: immunoglobulin heavy chain

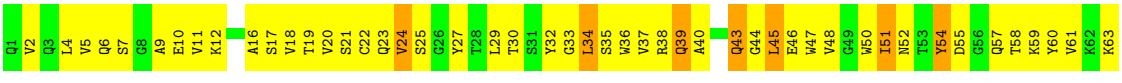
Chain S:

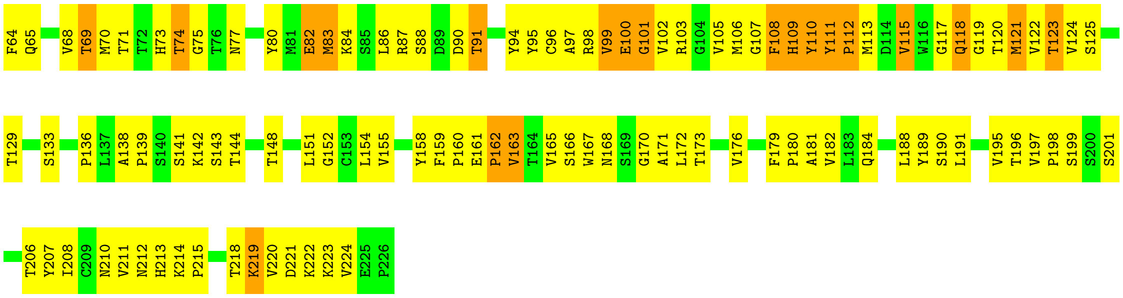




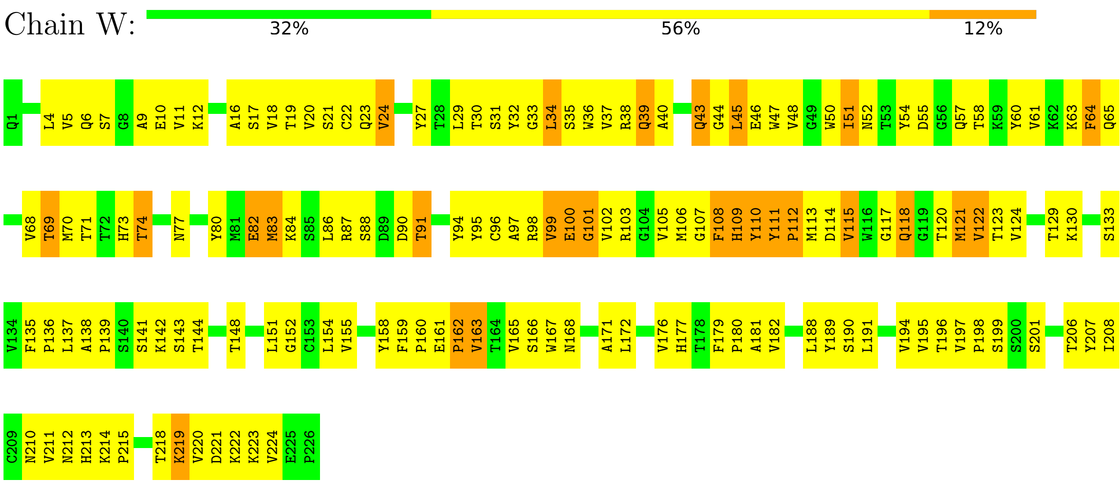
• Molecule 2: immunoglobulin heavy chain

Chain U:

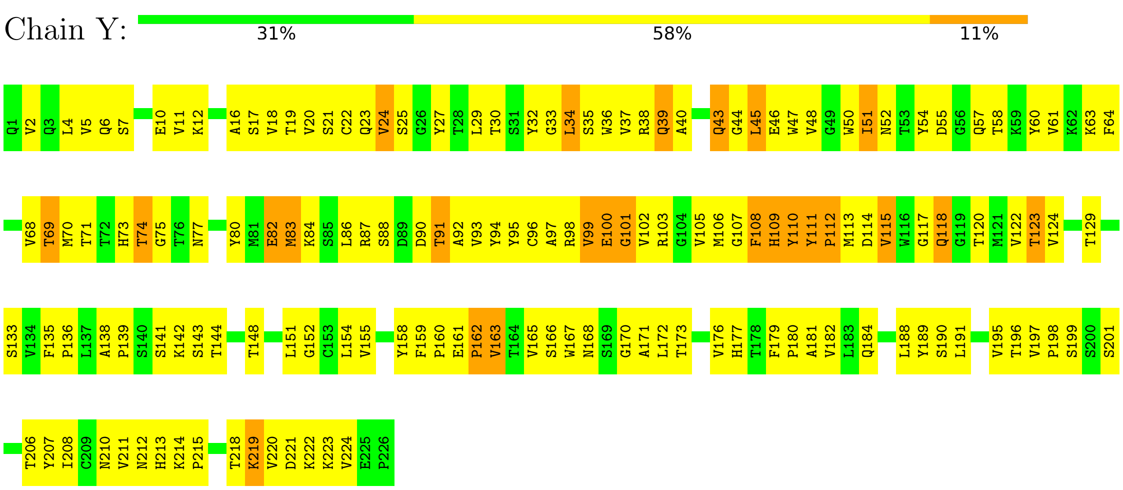




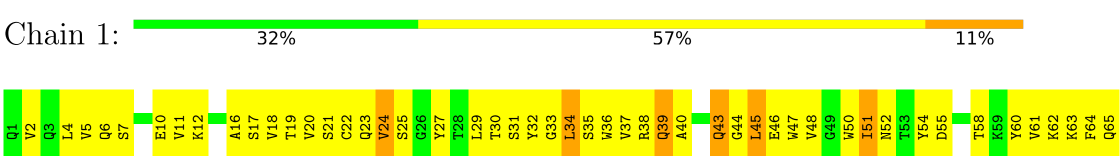
- Molecule 2: immunoglobulin heavy chain

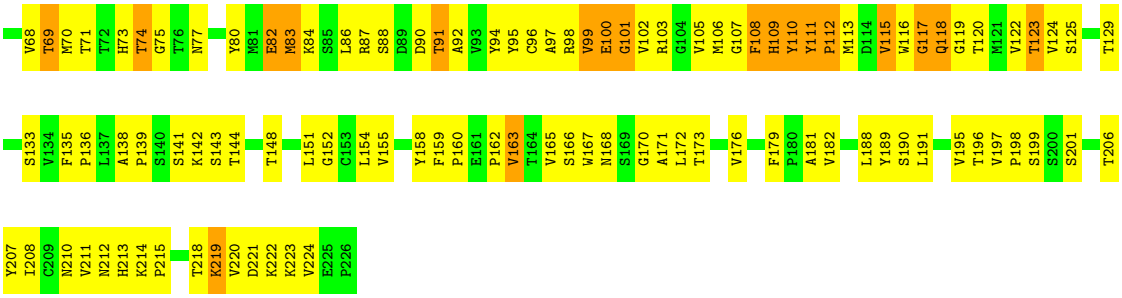


- Molecule 2: immunoglobulin heavy chain



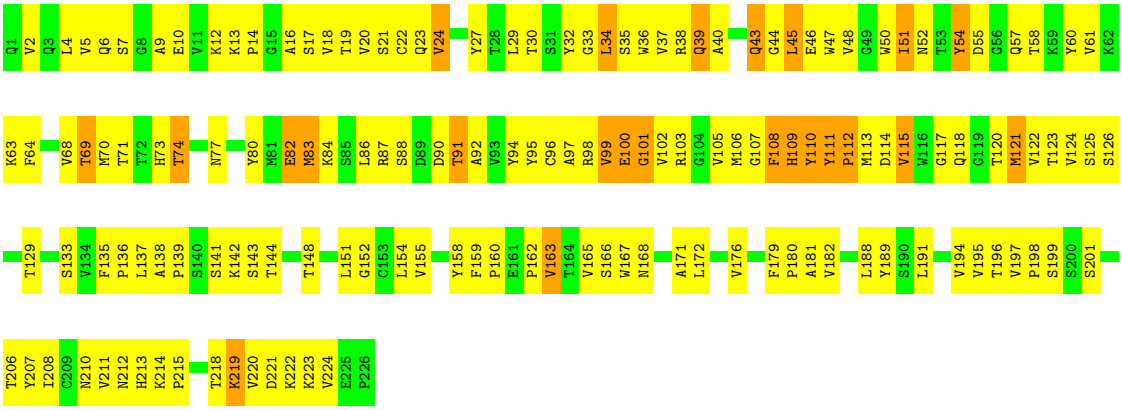
- Molecule 2: immunoglobulin heavy chain





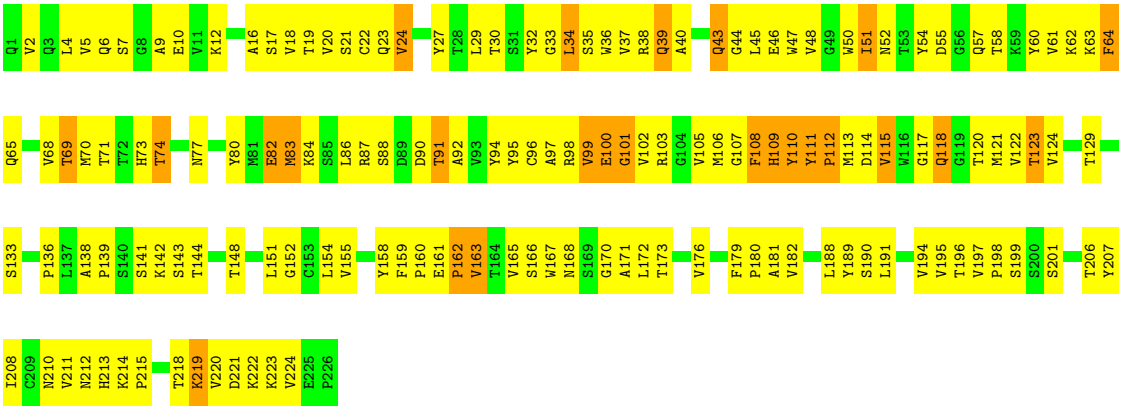
• Molecule 2: immunoglobulin heavy chain

Chain 3:



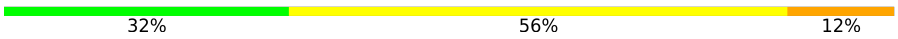
• Molecule 2: immunoglobulin heavy chain

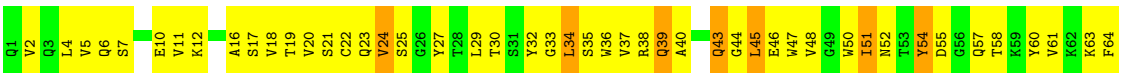
Chain 5:

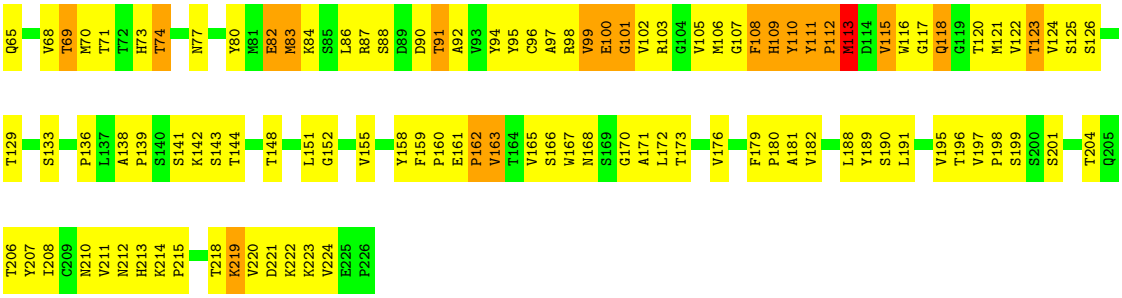


• Molecule 2: immunoglobulin heavy chain

Chain 7:

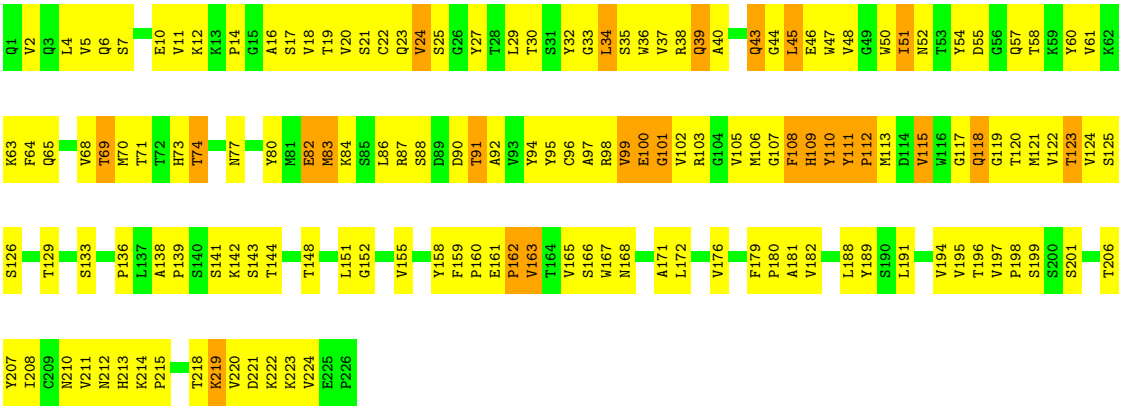






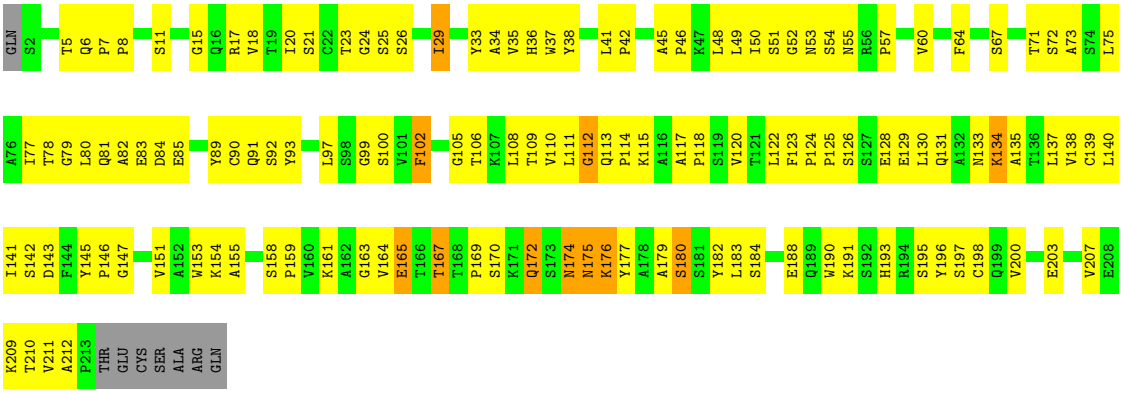
• Molecule 2: immunoglobulin heavy chain

Chain 9:



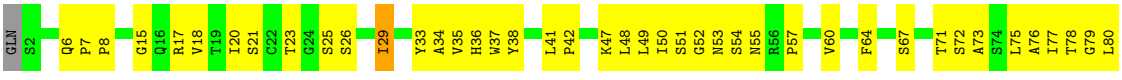
• Molecule 3: immunoglobulin light chain

Chain N:



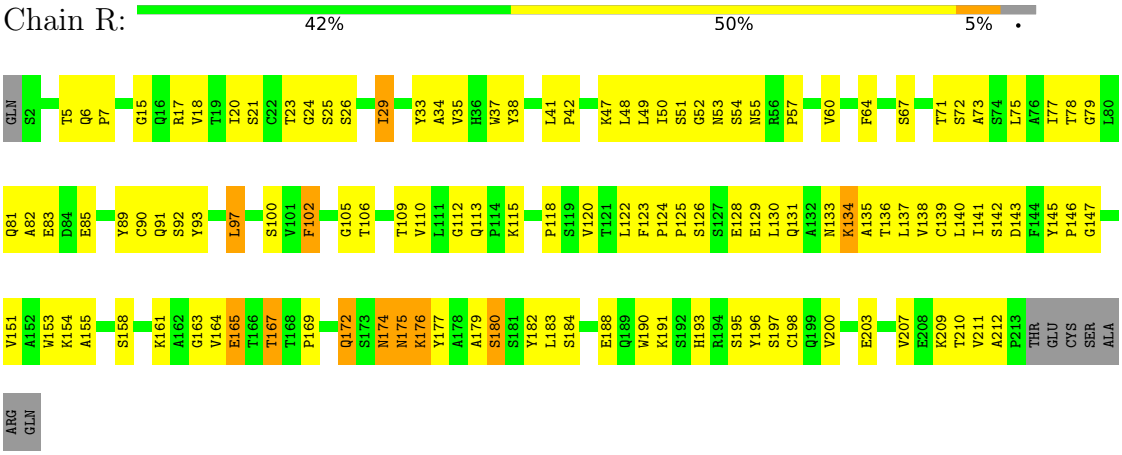
• Molecule 3: immunoglobulin light chain

Chain P:



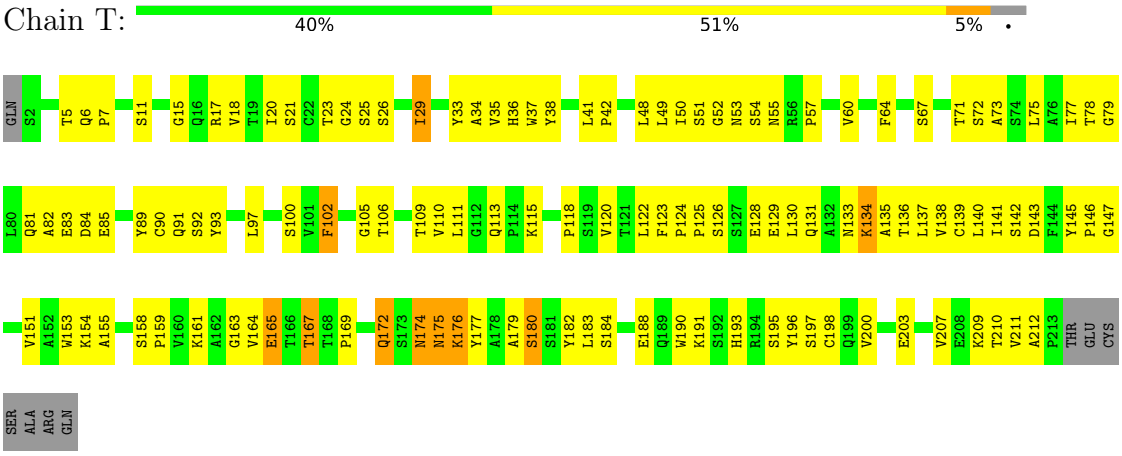
• Molecule 3: immunoglobulin light chain

Chain R:



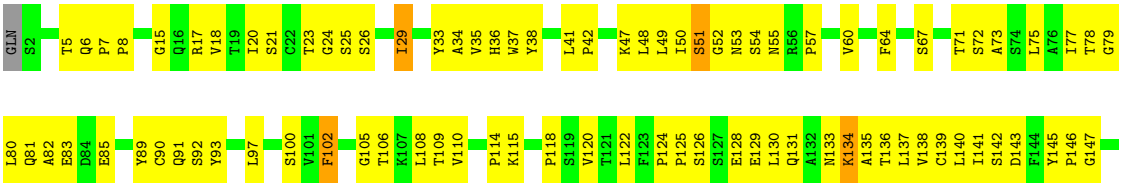
• Molecule 3: immunoglobulin light chain

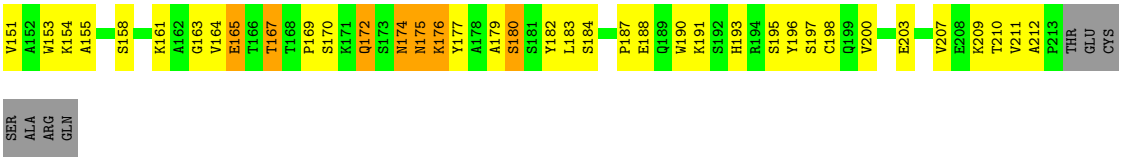
Chain T:



• Molecule 3: immunoglobulin light chain

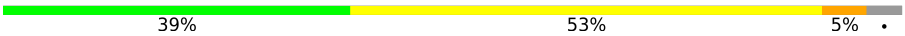
Chain V:

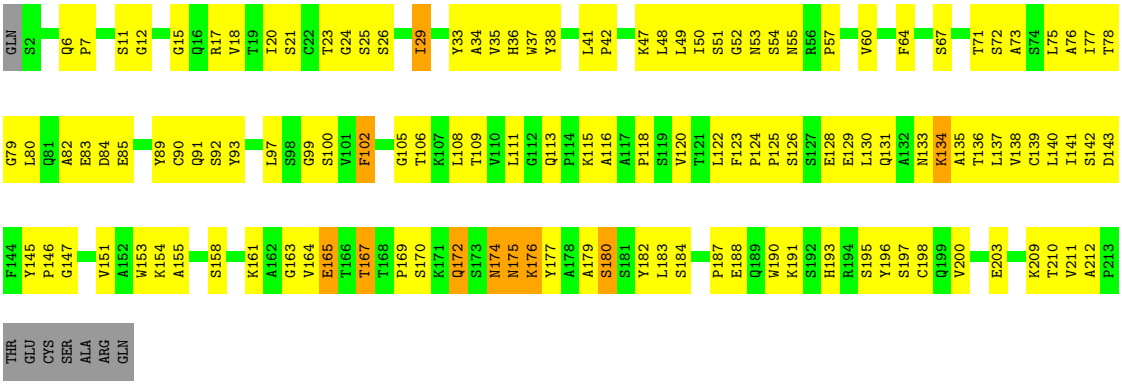




• Molecule 3: immunoglobulin light chain

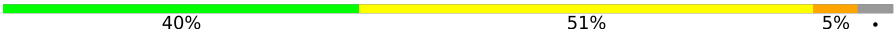
Chain X:

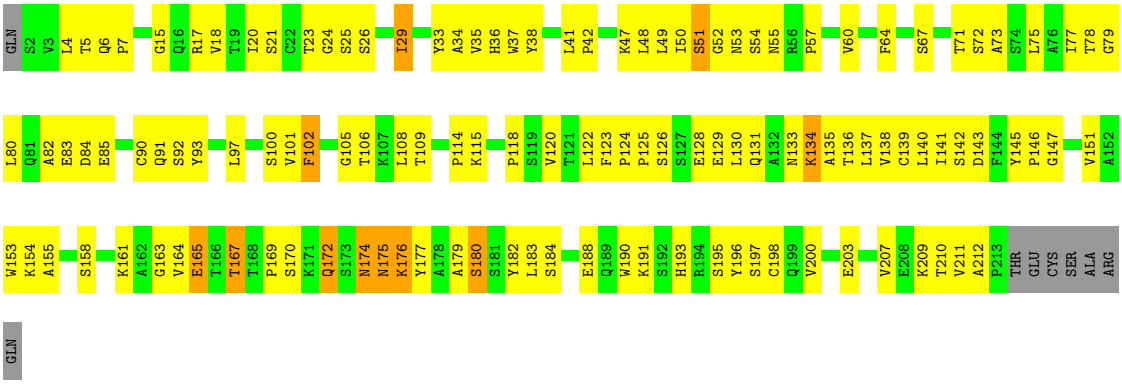




• Molecule 3: immunoglobulin light chain

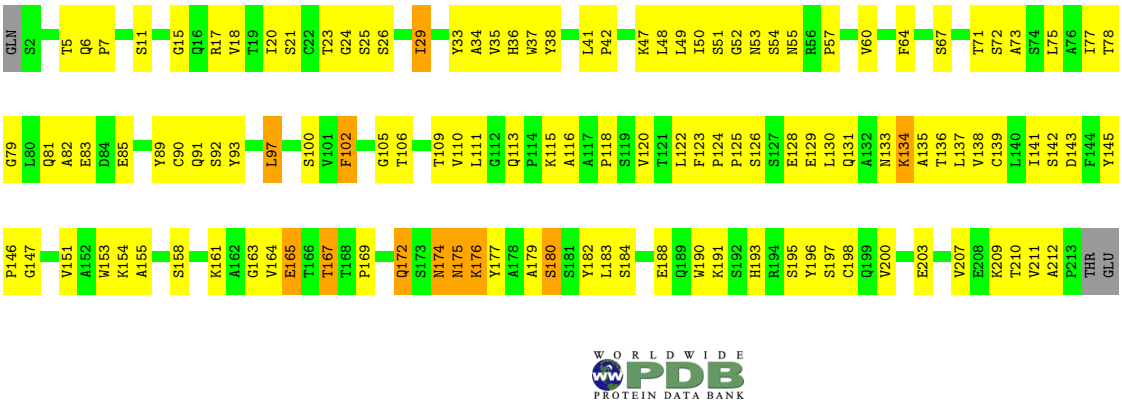
Chain Z:





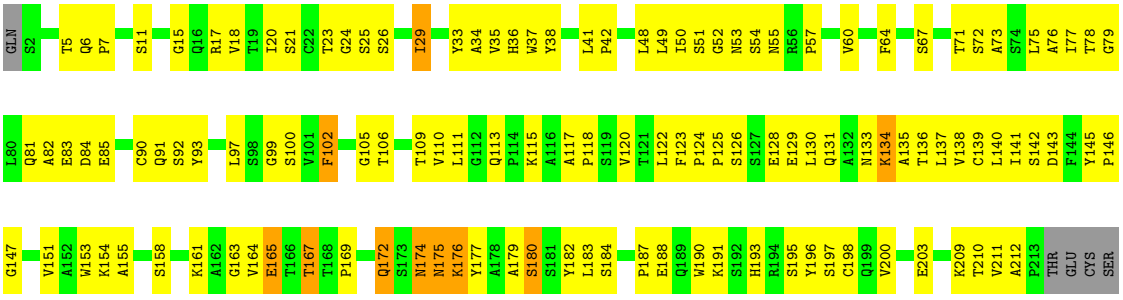
• Molecule 3: immunoglobulin light chain

Chain 2:



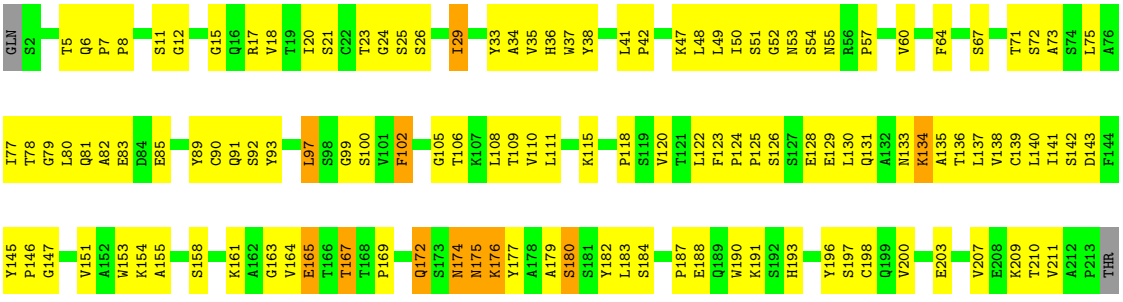
• Molecule 3: immunoglobulin light chain

Chain 4:



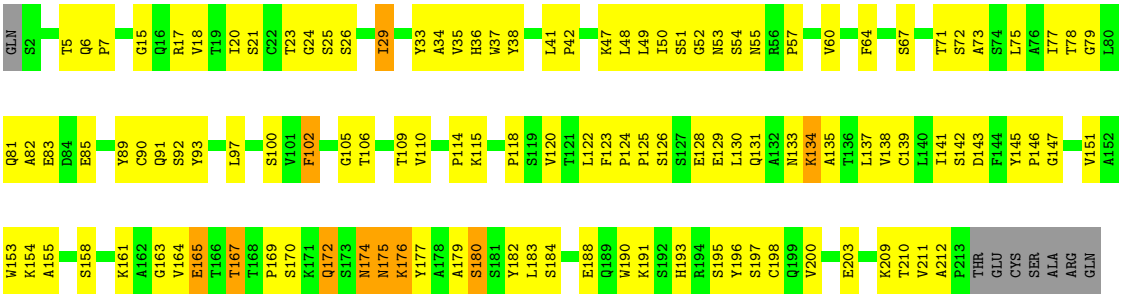
• Molecule 3: immunoglobulin light chain

Chain 6:



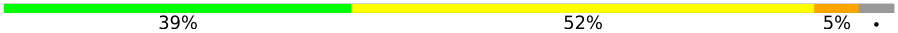
• Molecule 3: immunoglobulin light chain

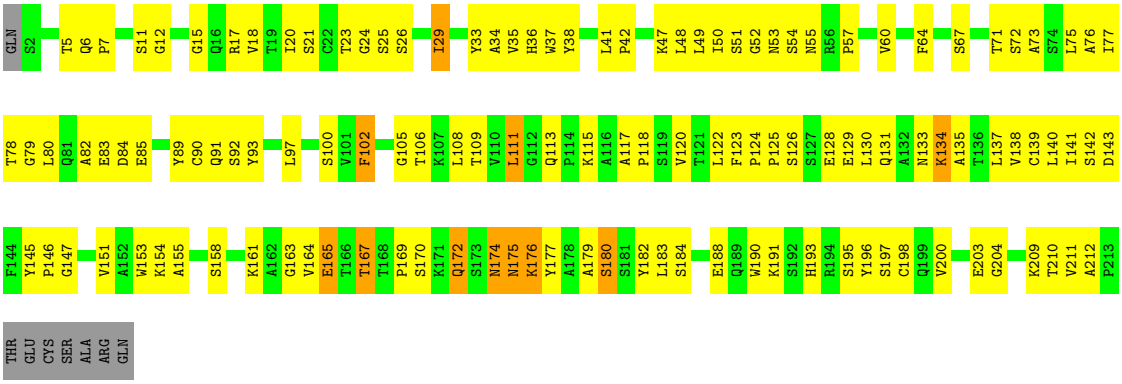
Chain 8:



• Molecule 3: immunoglobulin light chain

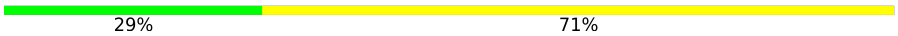
Chain 0:





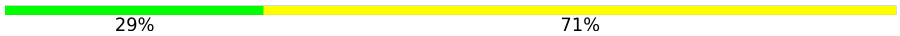
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



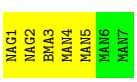
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



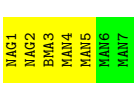
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



• Molecule 4: 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 j:



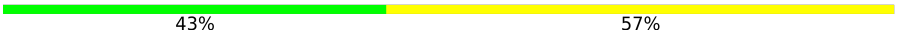
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-

D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 4: 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 p:

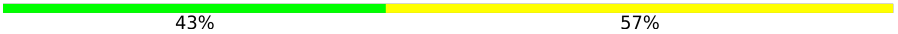


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

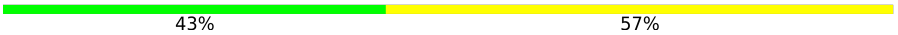
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



• Molecule 4: 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 y:

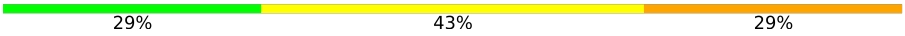


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:

• Molecule 4: 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 EA:

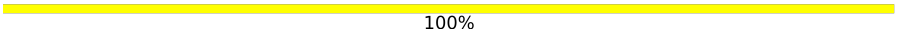


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:

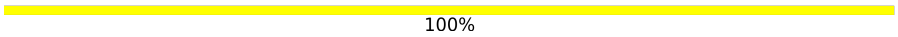
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



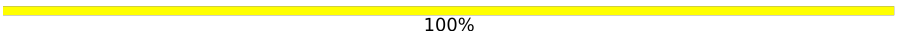
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



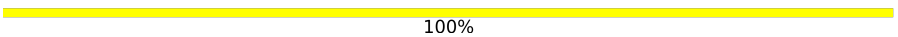
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



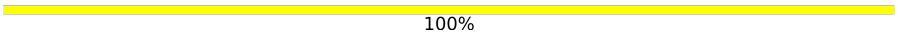
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



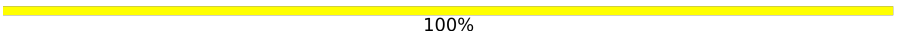
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



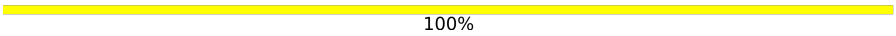
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



• Molecule 5: alpha-D-mannopyranose-(1-2)-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:

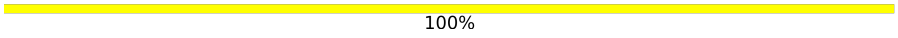


• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

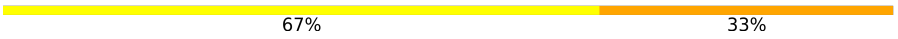
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



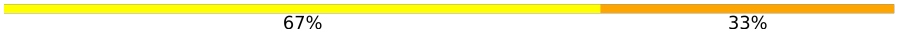
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:



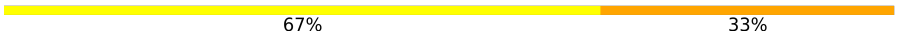
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:



• Molecule 5: alpha-D-mannopyranose-(1-2)-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 IA:

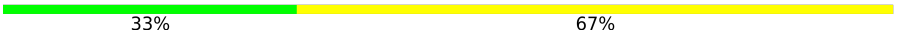


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

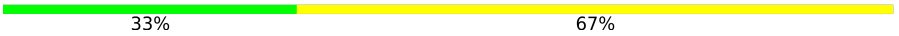
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



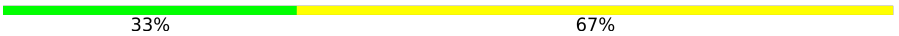
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



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

Chain l:



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

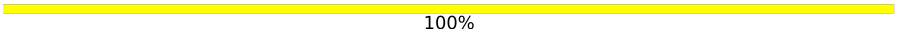
Chain o:

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

Chain r:

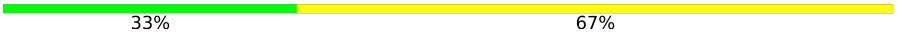
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



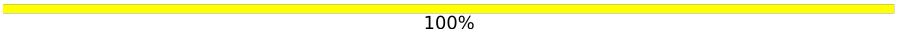
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



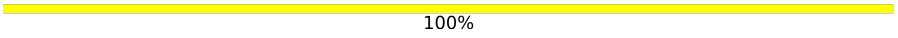
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



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

Chain DA:

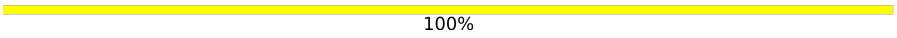


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:

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

Chain JA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	391.04Å 241.17Å 223.21Å 90.00° 123.62° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 29.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-4.00) 98.2 (29.98-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 3.98Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.235 , 0.308 0.284 , 0.291	Depositor DCC
R_{free} test set	7106 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	180.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 149.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.063 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	88152	wwPDB-VP
Average B, all atoms (Å^2)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/3959	0.50	0/5369
1	B	0.25	0/3959	0.50	0/5369
1	C	0.25	0/3959	0.50	0/5369
1	D	0.25	0/3959	0.50	0/5369
1	E	0.25	0/3959	0.50	0/5369
1	F	0.25	0/3959	0.49	0/5369
1	G	0.25	0/3959	0.50	0/5369
1	H	0.25	0/3959	0.50	0/5369
1	I	0.25	0/3959	0.50	0/5369
1	J	0.25	0/3959	0.50	0/5369
1	K	0.25	0/3959	0.50	0/5369
1	L	0.25	0/3959	0.50	0/5369
2	1	0.25	0/1739	0.52	0/2371
2	3	0.26	0/1739	0.52	0/2371
2	5	0.25	0/1739	0.52	0/2371
2	7	0.25	0/1739	0.52	0/2371
2	9	0.26	0/1739	0.52	0/2371
2	M	0.25	0/1739	0.52	0/2371
2	O	0.25	0/1739	0.52	0/2371
2	Q	0.25	0/1739	0.53	0/2371
2	S	0.25	0/1739	0.52	0/2371
2	U	0.25	0/1739	0.52	0/2371
2	W	0.26	0/1739	0.52	0/2371
2	Y	0.25	0/1739	0.52	0/2371
3	0	0.26	0/1586	0.53	0/2166
3	2	0.26	0/1586	0.53	0/2166
3	4	0.26	0/1586	0.53	0/2166
3	6	0.26	0/1586	0.53	0/2166
3	8	0.26	0/1586	0.53	0/2166
3	N	0.26	0/1586	0.55	1/2166 (0.0%)
3	P	0.26	0/1586	0.53	0/2166
3	R	0.26	0/1586	0.55	1/2166 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	T	0.26	0/1586	0.53	0/2166
3	V	0.28	0/1586	0.55	0/2166
3	X	0.26	0/1586	0.53	0/2166
3	Z	0.26	0/1586	0.53	0/2166
All	All	0.25	0/87408	0.51	2/118872 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	112	GLY	N-CA-C	-5.23	100.03	113.10
3	N	112	GLY	N-CA-C	-5.11	100.33	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3743	258	0
1	B	3878	0	3743	272	0
1	C	3878	0	3743	276	0
1	D	3878	0	3743	276	0
1	E	3878	0	3743	272	0
1	F	3878	0	3743	278	0
1	G	3878	0	3743	248	0
1	H	3878	0	3743	257	0
1	I	3878	0	3743	255	0
1	J	3878	0	3743	263	0
1	K	3878	0	3743	262	0
1	L	3878	0	3743	268	0
2	1	1697	0	1668	191	0
2	3	1697	0	1668	191	2
2	5	1697	0	1668	193	0
2	7	1697	0	1668	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	1697	0	1668	192	0
2	M	1697	0	1668	214	0
2	O	1697	0	1668	193	0
2	Q	1697	0	1668	191	0
2	S	1697	0	1668	197	0
2	U	1697	0	1668	209	0
2	W	1697	0	1668	210	0
2	Y	1697	0	1668	188	0
3	0	1549	0	1503	133	0
3	2	1549	0	1503	133	0
3	4	1549	0	1503	136	0
3	6	1549	0	1503	137	0
3	8	1549	0	1503	127	0
3	N	1549	0	1503	154	0
3	P	1549	0	1503	132	0
3	R	1549	0	1503	137	0
3	T	1549	0	1503	135	0
3	V	1549	0	1503	144	0
3	X	1549	0	1503	143	0
3	Z	1549	0	1503	133	0
4	BA	83	0	70	4	0
4	EA	83	0	70	7	0
4	HA	83	0	70	5	0
4	a	83	0	70	0	0
4	d	83	0	70	0	0
4	g	83	0	70	0	0
4	j	83	0	70	0	0
4	m	83	0	70	0	0
4	p	83	0	70	0	0
4	s	83	0	70	0	0
4	v	83	0	70	0	0
4	y	83	0	70	0	0
5	CA	72	0	61	3	0
5	FA	72	0	61	3	0
5	IA	72	0	61	4	0
5	b	72	0	61	0	0
5	e	72	0	61	0	0
5	h	72	0	61	0	0
5	k	72	0	61	0	0
5	n	72	0	61	0	0
5	q	72	0	61	0	0
5	t	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	w	72	0	61	0	0
5	z	72	0	61	0	0
6	AA	39	0	34	1	0
6	DA	39	0	34	1	0
6	GA	39	0	34	1	0
6	JA	39	0	34	1	0
6	c	39	0	34	0	0
6	f	39	0	34	0	0
6	i	39	0	34	0	0
6	l	39	0	34	0	0
6	o	39	0	34	0	0
6	r	39	0	34	0	0
6	u	39	0	34	0	0
6	x	39	0	34	0	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
7	E	28	0	26	0	0
7	F	28	0	26	0	0
7	G	28	0	26	0	0
7	H	28	0	26	0	0
7	I	28	0	26	0	0
7	J	28	0	26	0	0
7	K	28	0	26	0	0
7	L	28	0	26	0	0
All	All	88152	0	85260	6696	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 6696 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:136:PRO:O	3:6:126:SER:HB3	1.52	1.09
3:2:143:ASP:HA	3:2:176:LYS:HG3	1.35	1.08
3:T:143:ASP:HA	3:T:176:LYS:HG3	1.35	1.08
3:0:143:ASP:HA	3:0:176:LYS:HG3	1.34	1.08
1:G:331:LEU:HD22	1:G:331:LEU:H	1.19	1.08

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:171:ALA:CB	2:3:171:ALA:CB[2_556]	1.73	0.47
2:3:206:THR:OG1	2:3:206:THR:OG1[2_556]	1.74	0.46

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	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	13	49
1	B	491/493 (100%)	425 (87%)	60 (12%)	6 (1%)	13	49
1	C	491/493 (100%)	427 (87%)	57 (12%)	7 (1%)	11	46
1	D	491/493 (100%)	429 (87%)	55 (11%)	7 (1%)	11	46
1	E	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	11	46
1	F	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	11	46
1	G	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	13	49
1	H	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	11	46
1	I	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	13	49
1	J	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	11	46
1	K	491/493 (100%)	424 (86%)	60 (12%)	7 (1%)	11	46
1	L	491/493 (100%)	429 (87%)	56 (11%)	6 (1%)	13	49
2	1	224/226 (99%)	200 (89%)	18 (8%)	6 (3%)	5	34
2	3	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	6	37
2	5	224/226 (99%)	202 (90%)	17 (8%)	5 (2%)	6	37
2	7	224/226 (99%)	198 (88%)	20 (9%)	6 (3%)	5	34
2	9	224/226 (99%)	201 (90%)	18 (8%)	5 (2%)	6	37
2	M	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	6	37
2	O	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	6	37
2	S	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	6	37
2	U	224/226 (99%)	199 (89%)	20 (9%)	5 (2%)	6	37
2	W	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	6	37
2	Y	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	6	37
3	0	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	6	36
3	2	210/220 (96%)	191 (91%)	16 (8%)	3 (1%)	11	46
3	4	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	8	40
3	6	210/220 (96%)	192 (91%)	15 (7%)	3 (1%)	11	46
3	8	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	8	40
3	N	210/220 (96%)	189 (90%)	16 (8%)	5 (2%)	6	36
3	P	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	8	40
3	R	210/220 (96%)	190 (90%)	17 (8%)	3 (1%)	11	46
3	T	210/220 (96%)	192 (91%)	14 (7%)	4 (2%)	8	40
3	V	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	8	40
3	X	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	8	40
3	Z	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	6	36
All	All	11100/11268 (98%)	9822 (88%)	1089 (10%)	189 (2%)	9	43

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	330	GLY
2	5	115	VAL
3	N	175	ASN
3	P	175	ASN
3	R	175	ASN

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	430/430 (100%)	406 (94%)	24 (6%)	21	49
1	B	430/430 (100%)	406 (94%)	24 (6%)	21	49
1	C	430/430 (100%)	407 (95%)	23 (5%)	22	51
1	D	430/430 (100%)	405 (94%)	25 (6%)	20	48
1	E	430/430 (100%)	407 (95%)	23 (5%)	22	51
1	F	430/430 (100%)	405 (94%)	25 (6%)	20	48
1	G	430/430 (100%)	405 (94%)	25 (6%)	20	48
1	H	430/430 (100%)	407 (95%)	23 (5%)	22	51
1	I	430/430 (100%)	406 (94%)	24 (6%)	21	49
1	J	430/430 (100%)	406 (94%)	24 (6%)	21	49
1	K	430/430 (100%)	405 (94%)	25 (6%)	20	48
1	L	430/430 (100%)	406 (94%)	24 (6%)	21	49
2	1	191/191 (100%)	166 (87%)	25 (13%)	4	21
2	3	191/191 (100%)	166 (87%)	25 (13%)	4	21
2	5	191/191 (100%)	168 (88%)	23 (12%)	5	23
2	7	191/191 (100%)	163 (85%)	28 (15%)	3	18
2	9	191/191 (100%)	165 (86%)	26 (14%)	3	21
2	M	191/191 (100%)	167 (87%)	24 (13%)	4	22
2	O	191/191 (100%)	164 (86%)	27 (14%)	3	19
2	Q	191/191 (100%)	166 (87%)	25 (13%)	4	21
2	S	191/191 (100%)	166 (87%)	25 (13%)	4	21
2	U	191/191 (100%)	165 (86%)	26 (14%)	3	21
2	W	191/191 (100%)	166 (87%)	25 (13%)	4	21
2	Y	191/191 (100%)	167 (87%)	24 (13%)	4	22
3	0	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	2	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	4	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	6	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	8	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	N	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	P	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	R	174/181 (96%)	162 (93%)	12 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	V	174/181 (96%)	161 (92%)	13 (8%)	13	41
3	X	174/181 (96%)	162 (93%)	12 (7%)	15	43
3	Z	174/181 (96%)	161 (92%)	13 (8%)	13	41
All	All	9540/9624 (99%)	8802 (92%)	738 (8%)	13	40

5 of 738 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	163	VAL
2	9	64	PHE
2	1	82	GLU
2	Y	143	SER
2	5	54	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 369 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	322	ASN
2	7	210	ASN
2	M	1	GLN
2	U	210	ASN
3	P	81	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

192 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	$\#\|Z\| > 2$
6	NAG	AA	1	1,6	14,14,15	0.89	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	AA	2	6	14,14,15	0.76	0	17,19,21	0.67	0
6	BMA	AA	3	6	11,11,12	0.76	0	15,15,17	0.30	0
4	NAG	BA	1	1,4	14,14,15	0.63	0	17,19,21	0.69	1 (5%)
4	NAG	BA	2	4	14,14,15	0.50	0	17,19,21	0.71	0
4	BMA	BA	3	4	11,11,12	0.84	0	15,15,17	0.56	0
4	MAN	BA	4	4	11,11,12	1.04	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	BA	5	4	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
4	MAN	BA	6	4	11,11,12	0.60	0	15,15,17	0.69	0
4	MAN	BA	7	4	11,11,12	0.72	0	15,15,17	0.62	0
5	NAG	CA	1	1,5	14,14,15	0.89	0	17,19,21	1.09	1 (5%)
5	NAG	CA	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.26	2 (11%)
5	BMA	CA	3	5	11,11,12	0.81	0	15,15,17	0.78	1 (6%)
5	MAN	CA	4	5	11,11,12	0.84	0	15,15,17	1.28	1 (6%)
5	MAN	CA	5	5	11,11,12	0.67	0	15,15,17	0.81	1 (6%)
5	MAN	CA	6	5	11,11,12	0.77	0	15,15,17	0.79	1 (6%)
6	NAG	DA	1	1,6	14,14,15	0.86	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	DA	2	6	14,14,15	0.74	0	17,19,21	0.71	0
6	BMA	DA	3	6	11,11,12	0.79	0	15,15,17	0.32	0
4	NAG	EA	1	1,4	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
4	NAG	EA	2	4	14,14,15	0.59	0	17,19,21	0.71	1 (5%)
4	BMA	EA	3	4	11,11,12	0.92	1 (9%)	15,15,17	0.52	0
4	MAN	EA	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.26	1 (6%)
4	MAN	EA	5	4	11,11,12	0.69	0	15,15,17	0.89	1 (6%)
4	MAN	EA	6	4	11,11,12	0.64	0	15,15,17	0.71	0
4	MAN	EA	7	4	11,11,12	0.65	0	15,15,17	0.65	0
5	NAG	FA	1	1,5	14,14,15	0.90	0	17,19,21	1.06	1 (5%)
5	NAG	FA	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.19	2 (11%)
5	BMA	FA	3	5	11,11,12	0.90	1 (9%)	15,15,17	0.77	1 (6%)
5	MAN	FA	4	5	11,11,12	0.86	0	15,15,17	1.27	1 (6%)
5	MAN	FA	5	5	11,11,12	0.68	0	15,15,17	0.80	1 (6%)
5	MAN	FA	6	5	11,11,12	0.73	0	15,15,17	0.74	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	GA	1	1,6	14,14,15	0.97	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	GA	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.67	0
6	BMA	GA	3	6	11,11,12	0.74	0	15,15,17	0.30	0
4	NAG	HA	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	0.69	1 (5%)
4	NAG	HA	2	4	14,14,15	0.56	0	17,19,21	0.71	0
4	BMA	HA	3	4	11,11,12	0.86	1 (9%)	15,15,17	0.52	0
4	MAN	HA	4	4	11,11,12	1.16	1 (9%)	15,15,17	1.32	1 (6%)
4	MAN	HA	5	4	11,11,12	0.78	0	15,15,17	0.95	1 (6%)
4	MAN	HA	6	4	11,11,12	0.68	0	15,15,17	0.67	0
4	MAN	HA	7	4	11,11,12	0.76	0	15,15,17	0.64	0
5	NAG	IA	1	1,5	14,14,15	0.88	0	17,19,21	1.05	1 (5%)
5	NAG	IA	2	5	14,14,15	0.89	1 (7%)	17,19,21	1.23	2 (11%)
5	BMA	IA	3	5	11,11,12	0.83	0	15,15,17	0.79	1 (6%)
5	MAN	IA	4	5	11,11,12	0.86	0	15,15,17	1.27	1 (6%)
5	MAN	IA	5	5	11,11,12	0.69	0	15,15,17	0.83	1 (6%)
5	MAN	IA	6	5	11,11,12	0.70	0	15,15,17	0.76	1 (6%)
6	NAG	JA	1	1,6	14,14,15	0.93	1 (7%)	17,19,21	1.16	2 (11%)
6	NAG	JA	2	6	14,14,15	0.74	0	17,19,21	0.70	0
6	BMA	JA	3	6	11,11,12	0.77	0	15,15,17	0.32	0
4	NAG	a	1	1,4	14,14,15	0.57	0	17,19,21	0.72	1 (5%)
4	NAG	a	2	4	14,14,15	0.55	0	17,19,21	0.70	1 (5%)
4	BMA	a	3	4	11,11,12	0.95	1 (9%)	15,15,17	0.51	0
4	MAN	a	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.27	1 (6%)
4	MAN	a	5	4	11,11,12	0.74	0	15,15,17	0.90	1 (6%)
4	MAN	a	6	4	11,11,12	0.64	0	15,15,17	0.68	0
4	MAN	a	7	4	11,11,12	0.77	0	15,15,17	0.64	0
5	NAG	b	1	1,5	14,14,15	0.78	0	17,19,21	1.04	1 (5%)
5	NAG	b	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
5	BMA	b	3	5	11,11,12	0.95	1 (9%)	15,15,17	0.78	1 (6%)
5	MAN	b	4	5	11,11,12	0.92	0	15,15,17	1.21	1 (6%)
5	MAN	b	5	5	11,11,12	0.67	0	15,15,17	0.85	1 (6%)
5	MAN	b	6	5	11,11,12	0.65	0	15,15,17	0.78	1 (6%)
6	NAG	c	1	1,6	14,14,15	0.79	0	17,19,21	1.21	2 (11%)
6	NAG	c	2	6	14,14,15	0.78	1 (7%)	17,19,21	0.69	0
6	BMA	c	3	6	11,11,12	0.76	0	15,15,17	0.32	0
4	NAG	d	1	1,4	14,14,15	0.62	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	d	2	4	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
4	BMA	d	3	4	11,11,12	0.94	1 (9%)	15,15,17	0.56	0
4	MAN	d	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	d	5	4	11,11,12	0.82	0	15,15,17	0.95	1 (6%)
4	MAN	d	6	4	11,11,12	0.64	0	15,15,17	0.68	0
4	MAN	d	7	4	11,11,12	0.76	0	15,15,17	0.59	0
5	NAG	e	1	1,5	14,14,15	0.90	0	17,19,21	1.06	1 (5%)
5	NAG	e	2	5	14,14,15	0.94	1 (7%)	17,19,21	1.17	2 (11%)
5	BMA	e	3	5	11,11,12	0.79	0	15,15,17	0.78	1 (6%)
5	MAN	e	4	5	11,11,12	0.92	1 (9%)	15,15,17	1.26	1 (6%)
5	MAN	e	5	5	11,11,12	0.69	0	15,15,17	0.82	1 (6%)
5	MAN	e	6	5	11,11,12	0.72	0	15,15,17	0.76	1 (6%)
6	NAG	f	1	1,6	14,14,15	0.82	0	17,19,21	1.24	2 (11%)
6	NAG	f	2	6	14,14,15	0.76	1 (7%)	17,19,21	0.70	0
6	BMA	f	3	6	11,11,12	0.76	0	15,15,17	0.29	0
4	NAG	g	1	1,4	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
4	NAG	g	2	4	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
4	BMA	g	3	4	11,11,12	0.94	1 (9%)	15,15,17	0.54	0
4	MAN	g	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.26	1 (6%)
4	MAN	g	5	4	11,11,12	0.75	0	15,15,17	0.90	1 (6%)
4	MAN	g	6	4	11,11,12	0.64	0	15,15,17	0.70	0
4	MAN	g	7	4	11,11,12	0.77	0	15,15,17	0.63	0
5	NAG	h	1	1,5	14,14,15	0.79	0	17,19,21	1.11	1 (5%)
5	NAG	h	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.29	2 (11%)
5	BMA	h	3	5	11,11,12	0.75	0	15,15,17	0.86	1 (6%)
5	MAN	h	4	5	11,11,12	0.84	0	15,15,17	1.27	1 (6%)
5	MAN	h	5	5	11,11,12	0.64	0	15,15,17	0.81	1 (6%)
5	MAN	h	6	5	11,11,12	0.70	0	15,15,17	0.81	1 (6%)
6	NAG	i	1	1,6	14,14,15	0.89	1 (7%)	17,19,21	1.17	2 (11%)
6	NAG	i	2	6	14,14,15	0.86	1 (7%)	17,19,21	0.71	0
6	BMA	i	3	6	11,11,12	0.77	0	15,15,17	0.33	0
4	NAG	j	1	1,4	14,14,15	0.62	0	17,19,21	0.66	1 (5%)
4	NAG	j	2	4	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
4	BMA	j	3	4	11,11,12	0.86	1 (9%)	15,15,17	0.50	0
4	MAN	j	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.29	1 (6%)
4	MAN	j	5	4	11,11,12	0.77	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	j	6	4	11,11,12	0.63	0	15,15,17	0.67	0
4	MAN	j	7	4	11,11,12	0.69	0	15,15,17	0.59	0
5	NAG	k	1	1,5	14,14,15	0.84	0	17,19,21	1.11	1 (5%)
5	NAG	k	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.23	2 (11%)
5	BMA	k	3	5	11,11,12	0.90	1 (9%)	15,15,17	0.80	1 (6%)
5	MAN	k	4	5	11,11,12	0.92	1 (9%)	15,15,17	1.25	1 (6%)
5	MAN	k	5	5	11,11,12	0.68	0	15,15,17	0.83	1 (6%)
5	MAN	k	6	5	11,11,12	0.73	0	15,15,17	0.77	1 (6%)
6	NAG	l	1	1,6	14,14,15	0.87	1 (7%)	17,19,21	1.16	2 (11%)
6	NAG	l	2	6	14,14,15	0.79	1 (7%)	17,19,21	0.67	0
6	BMA	l	3	6	11,11,12	0.73	0	15,15,17	0.30	0
4	NAG	m	1	1,4	14,14,15	0.51	0	17,19,21	0.68	1 (5%)
4	NAG	m	2	4	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
4	BMA	m	3	4	11,11,12	1.03	1 (9%)	15,15,17	0.54	0
4	MAN	m	4	4	11,11,12	1.13	1 (9%)	15,15,17	1.27	1 (6%)
4	MAN	m	5	4	11,11,12	0.74	0	15,15,17	0.88	2 (13%)
4	MAN	m	6	4	11,11,12	0.59	0	15,15,17	0.68	0
4	MAN	m	7	4	11,11,12	0.81	0	15,15,17	0.67	0
5	NAG	n	1	1,5	14,14,15	0.81	0	17,19,21	1.06	1 (5%)
5	NAG	n	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.25	2 (11%)
5	BMA	n	3	5	11,11,12	0.87	0	15,15,17	0.79	1 (6%)
5	MAN	n	4	5	11,11,12	0.89	0	15,15,17	1.25	1 (6%)
5	MAN	n	5	5	11,11,12	0.72	0	15,15,17	0.85	1 (6%)
5	MAN	n	6	5	11,11,12	0.66	0	15,15,17	0.78	1 (6%)
6	NAG	o	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.23	2 (11%)
6	NAG	o	2	6	14,14,15	0.72	0	17,19,21	0.71	0
6	BMA	o	3	6	11,11,12	0.73	0	15,15,17	0.32	0
4	NAG	p	1	1,4	14,14,15	0.68	0	17,19,21	0.75	0
4	NAG	p	2	4	14,14,15	0.45	0	17,19,21	0.78	1 (5%)
4	BMA	p	3	4	11,11,12	1.02	1 (9%)	15,15,17	0.55	0
4	MAN	p	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.30	1 (6%)
4	MAN	p	5	4	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
4	MAN	p	6	4	11,11,12	0.58	0	15,15,17	0.67	0
4	MAN	p	7	4	11,11,12	0.74	0	15,15,17	0.63	0
5	NAG	q	1	1,5	14,14,15	0.84	0	17,19,21	1.01	1 (5%)
5	NAG	q	2	5	14,14,15	0.92	1 (7%)	17,19,21	1.17	2 (11%)
5	BMA	q	3	5	11,11,12	0.90	1 (9%)	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	q	4	5	11,11,12	0.87	0	15,15,17	1.26	1 (6%)
5	MAN	q	5	5	11,11,12	0.69	0	15,15,17	0.85	1 (6%)
5	MAN	q	6	5	11,11,12	0.66	0	15,15,17	0.77	1 (6%)
6	NAG	r	1	1,6	14,14,15	0.81	0	17,19,21	1.23	2 (11%)
6	NAG	r	2	6	14,14,15	0.69	0	17,19,21	0.71	0
6	BMA	r	3	6	11,11,12	0.72	0	15,15,17	0.31	0
4	NAG	s	1	1,4	14,14,15	0.64	0	17,19,21	0.69	0
4	NAG	s	2	4	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
4	BMA	s	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.58	0
4	MAN	s	4	4	11,11,12	1.03	1 (9%)	15,15,17	1.25	1 (6%)
4	MAN	s	5	4	11,11,12	0.70	0	15,15,17	0.89	2 (13%)
4	MAN	s	6	4	11,11,12	0.61	0	15,15,17	0.69	0
4	MAN	s	7	4	11,11,12	0.71	0	15,15,17	0.64	0
5	NAG	t	1	1,5	14,14,15	0.92	0	17,19,21	1.05	1 (5%)
5	NAG	t	2	5	14,14,15	0.90	1 (7%)	17,19,21	1.21	2 (11%)
5	BMA	t	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.76	1 (6%)
5	MAN	t	4	5	11,11,12	0.78	0	15,15,17	1.30	1 (6%)
5	MAN	t	5	5	11,11,12	0.68	0	15,15,17	0.81	1 (6%)
5	MAN	t	6	5	11,11,12	0.71	0	15,15,17	0.76	1 (6%)
6	NAG	u	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	1.23	2 (11%)
6	NAG	u	2	6	14,14,15	0.83	1 (7%)	17,19,21	0.68	0
6	BMA	u	3	6	11,11,12	0.79	1 (9%)	15,15,17	0.36	0
4	NAG	v	1	1,4	14,14,15	0.65	0	17,19,21	0.66	1 (5%)
4	NAG	v	2	4	14,14,15	0.69	0	17,19,21	0.69	0
4	BMA	v	3	4	11,11,12	0.91	1 (9%)	15,15,17	0.46	0
4	MAN	v	4	4	11,11,12	1.11	1 (9%)	15,15,17	1.27	1 (6%)
4	MAN	v	5	4	11,11,12	0.74	0	15,15,17	0.94	1 (6%)
4	MAN	v	6	4	11,11,12	0.66	0	15,15,17	0.70	0
4	MAN	v	7	4	11,11,12	0.74	0	15,15,17	0.60	0
5	NAG	w	1	1,5	14,14,15	0.89	0	17,19,21	1.05	1 (5%)
5	NAG	w	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.21	2 (11%)
5	BMA	w	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.79	1 (6%)
5	MAN	w	4	5	11,11,12	0.90	0	15,15,17	1.26	1 (6%)
5	MAN	w	5	5	11,11,12	0.69	0	15,15,17	0.81	0
5	MAN	w	6	5	11,11,12	0.64	0	15,15,17	0.76	1 (6%)
6	NAG	x	1	1,6	14,14,15	1.05	1 (7%)	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	x	2	6	14,14,15	0.76	1 (7%)	17,19,21	0.64	0
6	BMA	x	3	6	11,11,12	0.75	0	15,15,17	0.33	0
4	NAG	y	1	1,4	14,14,15	0.61	0	17,19,21	0.70	0
4	NAG	y	2	4	14,14,15	0.44	0	17,19,21	0.74	0
4	BMA	y	3	4	11,11,12	1.11	1 (9%)	15,15,17	0.55	0
4	MAN	y	4	4	11,11,12	1.12	1 (9%)	15,15,17	1.31	1 (6%)
4	MAN	y	5	4	11,11,12	0.74	0	15,15,17	0.95	2 (13%)
4	MAN	y	6	4	11,11,12	0.66	0	15,15,17	0.69	0
4	MAN	y	7	4	11,11,12	0.85	1 (9%)	15,15,17	0.67	0
5	NAG	z	1	1,5	14,14,15	0.89	0	17,19,21	1.07	1 (5%)
5	NAG	z	2	5	14,14,15	0.92	1 (7%)	17,19,21	1.19	2 (11%)
5	BMA	z	3	5	11,11,12	0.76	0	15,15,17	0.80	1 (6%)
5	MAN	z	4	5	11,11,12	0.84	0	15,15,17	1.28	1 (6%)
5	MAN	z	5	5	11,11,12	0.69	0	15,15,17	0.80	1 (6%)
5	MAN	z	6	5	11,11,12	0.71	0	15,15,17	0.79	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
6	NAG	AA	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	AA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	AA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	BA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	5/6/23/26	0/1/1/1
4	BMA	BA	3	4	-	1/2/19/22	0/1/1/1
4	MAN	BA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	BA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	BA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	BA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	CA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	CA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	CA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	CA	6	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	DA	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	EA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	EA	2	4	-	5/6/23/26	0/1/1/1
4	BMA	EA	3	4	-	1/2/19/22	0/1/1/1
4	MAN	EA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	EA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	EA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	EA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	FA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	FA	6	5	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	HA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	HA	2	4	-	5/6/23/26	0/1/1/1
4	BMA	HA	3	4	-	2/2/19/22	0/1/1/1
4	MAN	HA	4	4	-	2/2/19/22	0/1/1/1
4	MAN	HA	5	4	-	1/2/19/22	0/1/1/1
4	MAN	HA	6	4	-	0/2/19/22	0/1/1/1
4	MAN	HA	7	4	-	0/2/19/22	0/1/1/1
5	NAG	IA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	IA	2	5	-	4/6/23/26	0/1/1/1
5	BMA	IA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	4	5	-	0/2/19/22	0/1/1/1
5	MAN	IA	5	5	-	2/2/19/22	0/1/1/1
5	MAN	IA	6	5	-	0/2/19/22	0/1/1/1
6	NAG	JA	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	JA	3	6	-	1/2/19/22	0/1/1/1
4	NAG	a	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	a	2	4	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	a	3	4	-	1/2/19/22	0/1/1/1
4	MAN	a	4	4	-	2/2/19/22	0/1/1/1
4	MAN	a	5	4	-	1/2/19/22	0/1/1/1
4	MAN	a	6	4	-	0/2/19/22	0/1/1/1
4	MAN	a	7	4	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	b	2	5	-	4/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	0/2/19/22	0/1/1/1
5	MAN	b	5	5	-	2/2/19/22	0/1/1/1
5	MAN	b	6	5	-	0/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	1/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	d	2	4	-	5/6/23/26	0/1/1/1
4	BMA	d	3	4	-	2/2/19/22	0/1/1/1
4	MAN	d	4	4	-	2/2/19/22	0/1/1/1
4	MAN	d	5	4	-	2/2/19/22	0/1/1/1
4	MAN	d	6	4	-	0/2/19/22	0/1/1/1
4	MAN	d	7	4	-	0/2/19/22	0/1/1/1
5	NAG	e	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	e	2	5	-	4/6/23/26	0/1/1/1
5	BMA	e	3	5	-	0/2/19/22	0/1/1/1
5	MAN	e	4	5	-	0/2/19/22	0/1/1/1
5	MAN	e	5	5	-	2/2/19/22	0/1/1/1
5	MAN	e	6	5	-	0/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	f	2	6	-	4/6/23/26	0/1/1/1
6	BMA	f	3	6	-	1/2/19/22	0/1/1/1
4	NAG	g	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	5/6/23/26	0/1/1/1
4	BMA	g	3	4	-	2/2/19/22	0/1/1/1
4	MAN	g	4	4	-	2/2/19/22	0/1/1/1
4	MAN	g	5	4	-	1/2/19/22	0/1/1/1
4	MAN	g	6	4	-	0/2/19/22	0/1/1/1
4	MAN	g	7	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	h	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	h	2	5	-	4/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	MAN	h	4	5	-	0/2/19/22	0/1/1/1
5	MAN	h	5	5	-	2/2/19/22	0/1/1/1
5	MAN	h	6	5	-	0/2/19/22	0/1/1/1
6	NAG	i	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	i	2	6	-	4/6/23/26	0/1/1/1
6	BMA	i	3	6	-	1/2/19/22	0/1/1/1
4	NAG	j	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	j	2	4	-	5/6/23/26	0/1/1/1
4	BMA	j	3	4	-	1/2/19/22	0/1/1/1
4	MAN	j	4	4	-	2/2/19/22	0/1/1/1
4	MAN	j	5	4	-	1/2/19/22	0/1/1/1
4	MAN	j	6	4	-	0/2/19/22	0/1/1/1
4	MAN	j	7	4	-	0/2/19/22	0/1/1/1
5	NAG	k	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	k	2	5	-	4/6/23/26	0/1/1/1
5	BMA	k	3	5	-	0/2/19/22	0/1/1/1
5	MAN	k	4	5	-	0/2/19/22	0/1/1/1
5	MAN	k	5	5	-	2/2/19/22	0/1/1/1
5	MAN	k	6	5	-	0/2/19/22	0/1/1/1
6	NAG	l	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	l	2	6	-	4/6/23/26	0/1/1/1
6	BMA	l	3	6	-	1/2/19/22	0/1/1/1
4	NAG	m	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	m	2	4	-	5/6/23/26	0/1/1/1
4	BMA	m	3	4	-	2/2/19/22	0/1/1/1
4	MAN	m	4	4	-	2/2/19/22	0/1/1/1
4	MAN	m	5	4	-	1/2/19/22	0/1/1/1
4	MAN	m	6	4	-	0/2/19/22	0/1/1/1
4	MAN	m	7	4	-	0/2/19/22	0/1/1/1
5	NAG	n	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	n	2	5	-	4/6/23/26	0/1/1/1
5	BMA	n	3	5	-	0/2/19/22	0/1/1/1
5	MAN	n	4	5	-	0/2/19/22	0/1/1/1
5	MAN	n	5	5	-	2/2/19/22	0/1/1/1
5	MAN	n	6	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	o	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	o	2	6	-	4/6/23/26	0/1/1/1
6	BMA	o	3	6	-	1/2/19/22	0/1/1/1
4	NAG	p	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	5/6/23/26	0/1/1/1
4	BMA	p	3	4	-	2/2/19/22	0/1/1/1
4	MAN	p	4	4	-	2/2/19/22	0/1/1/1
4	MAN	p	5	4	-	1/2/19/22	0/1/1/1
4	MAN	p	6	4	-	0/2/19/22	0/1/1/1
4	MAN	p	7	4	-	0/2/19/22	0/1/1/1
5	NAG	q	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	q	2	5	-	4/6/23/26	0/1/1/1
5	BMA	q	3	5	-	0/2/19/22	0/1/1/1
5	MAN	q	4	5	-	0/2/19/22	0/1/1/1
5	MAN	q	5	5	-	2/2/19/22	0/1/1/1
5	MAN	q	6	5	-	0/2/19/22	0/1/1/1
6	NAG	r	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	r	2	6	-	4/6/23/26	0/1/1/1
6	BMA	r	3	6	-	1/2/19/22	0/1/1/1
4	NAG	s	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	s	2	4	-	5/6/23/26	0/1/1/1
4	BMA	s	3	4	-	1/2/19/22	0/1/1/1
4	MAN	s	4	4	-	2/2/19/22	0/1/1/1
4	MAN	s	5	4	-	1/2/19/22	0/1/1/1
4	MAN	s	6	4	-	0/2/19/22	0/1/1/1
4	MAN	s	7	4	-	0/2/19/22	0/1/1/1
5	NAG	t	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	t	2	5	-	4/6/23/26	0/1/1/1
5	BMA	t	3	5	-	0/2/19/22	0/1/1/1
5	MAN	t	4	5	-	0/2/19/22	0/1/1/1
5	MAN	t	5	5	-	2/2/19/22	0/1/1/1
5	MAN	t	6	5	-	0/2/19/22	0/1/1/1
6	NAG	u	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	u	2	6	-	4/6/23/26	0/1/1/1
6	BMA	u	3	6	-	1/2/19/22	0/1/1/1
4	NAG	v	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	v	2	4	-	5/6/23/26	0/1/1/1

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

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	y	3	BMA	C4-C3	3.05	1.60	1.52
6	x	1	NAG	C4-C3	2.97	1.59	1.52
4	m	3	BMA	C4-C3	2.74	1.59	1.52
4	p	3	BMA	C4-C3	2.70	1.59	1.52
4	HA	4	MAN	C4-C3	2.60	1.58	1.52

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	4	MAN	C1-C2-C3	4.15	114.77	109.67
4	BA	4	MAN	C1-C2-C3	4.12	114.73	109.67
4	s	4	MAN	C1-C2-C3	4.11	114.71	109.67
5	t	4	MAN	C1-C2-C3	4.10	114.70	109.67
4	g	4	MAN	C1-C2-C3	4.09	114.70	109.67

There are no chirality outliers.

5 of 385 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2

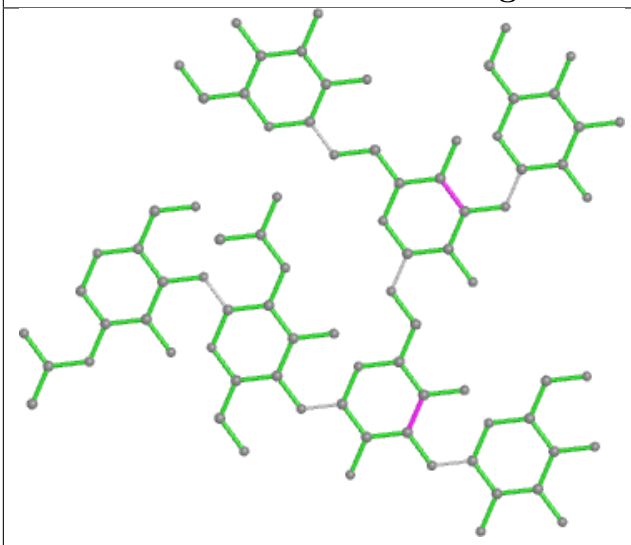
There are no ring outliers.

20 monomers are involved in 30 short contacts:

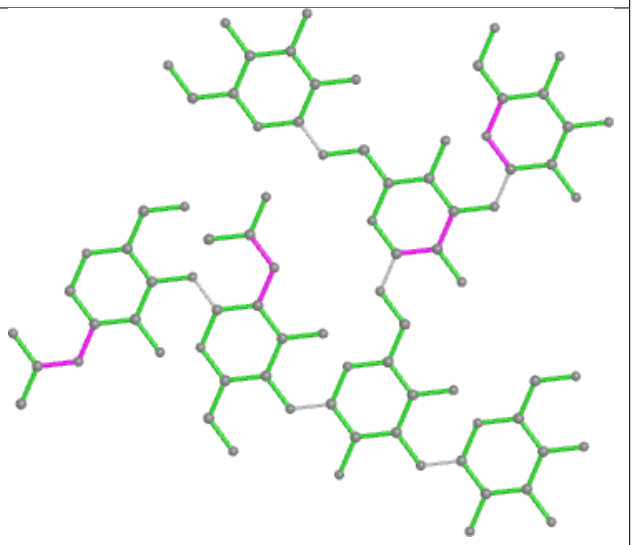
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BA	1	NAG	1	0
5	IA	2	NAG	3	0
4	HA	2	NAG	5	0
6	GA	3	BMA	1	0
6	AA	2	NAG	1	0
4	EA	1	NAG	1	0
5	IA	1	NAG	3	0
5	CA	1	NAG	3	0
6	DA	3	BMA	1	0
4	EA	2	NAG	7	0
6	DA	2	NAG	1	0
6	JA	3	BMA	1	0
4	BA	2	NAG	4	0
4	HA	1	NAG	1	0
5	FA	2	NAG	2	0
6	JA	2	NAG	1	0
6	AA	3	BMA	1	0
5	CA	2	NAG	2	0
5	FA	1	NAG	3	0
6	GA	2	NAG	1	0

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

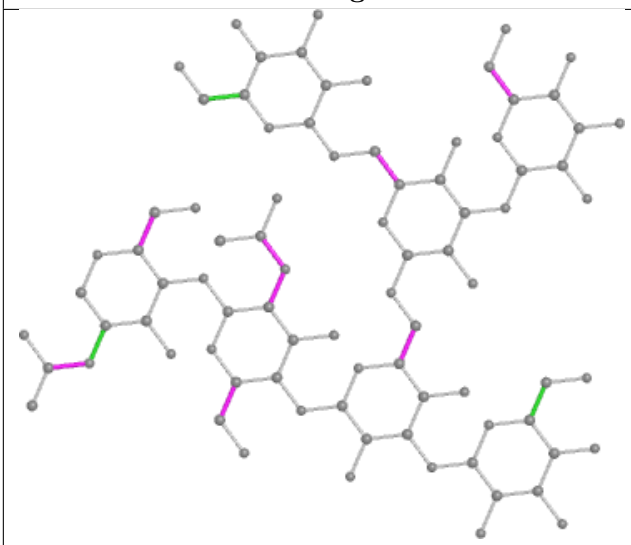
Oligosaccharide Chain a



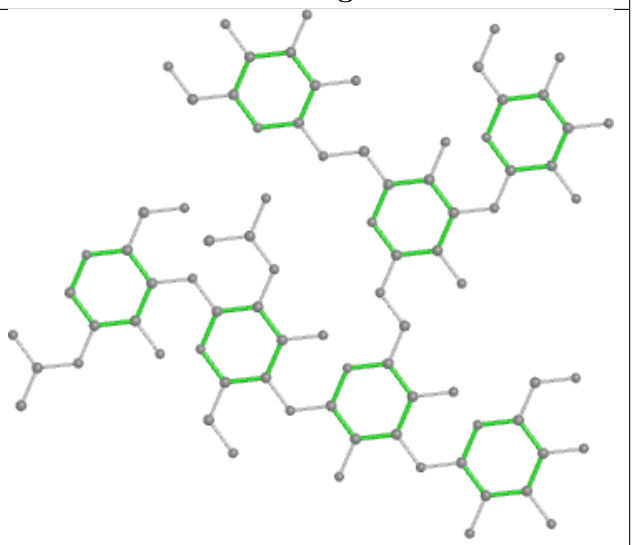
Bond lengths



Bond angles

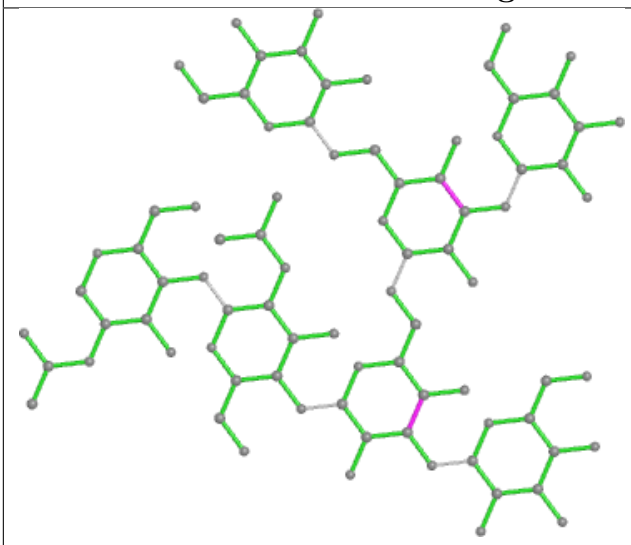


Torsions



Rings

Oligosaccharide Chain d



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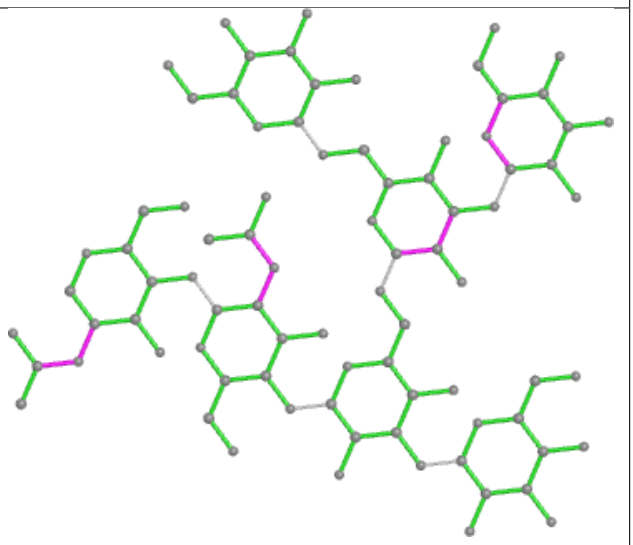
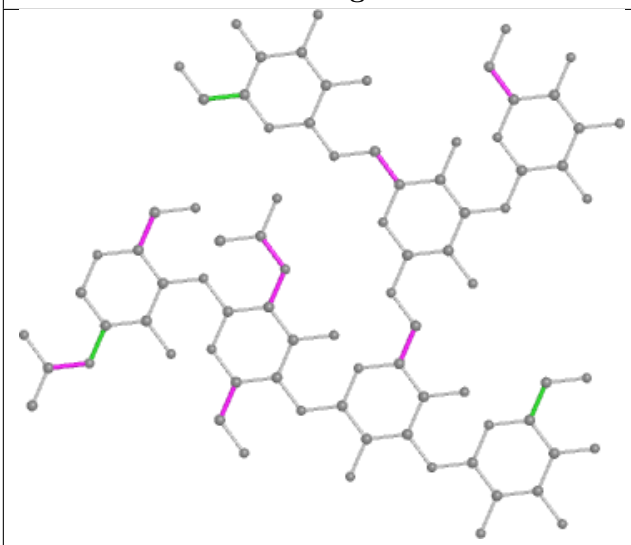


Bond angles



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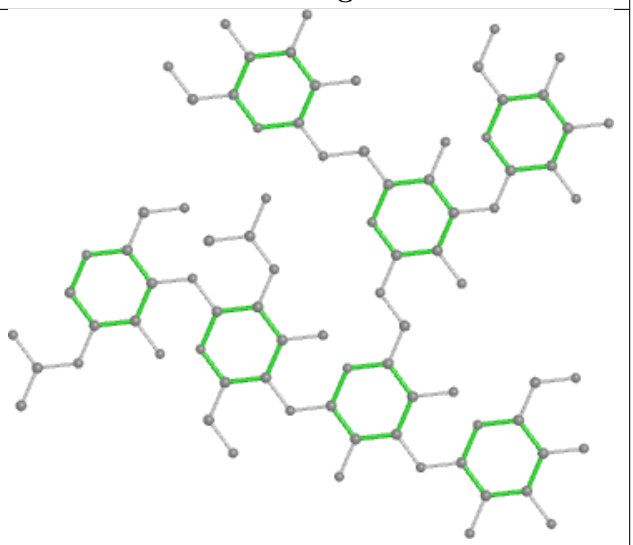
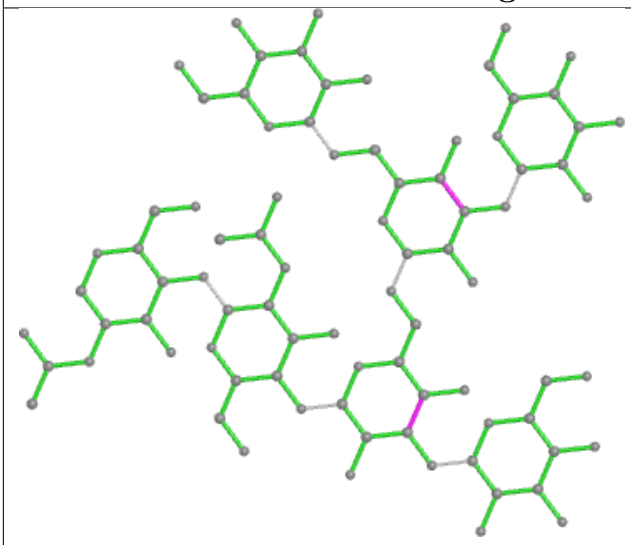
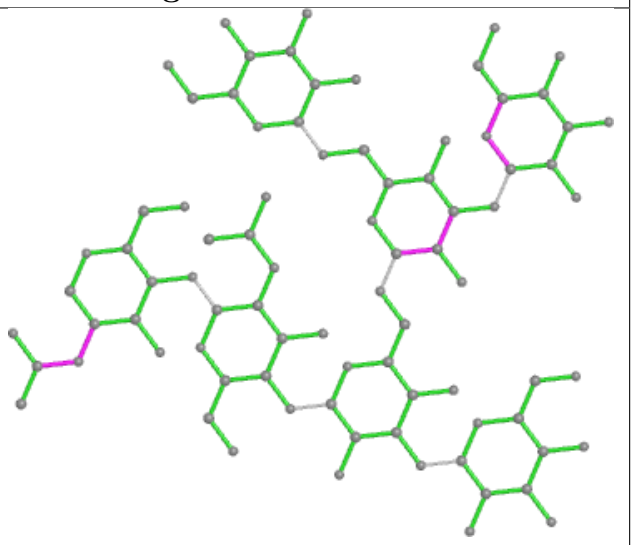


Rings

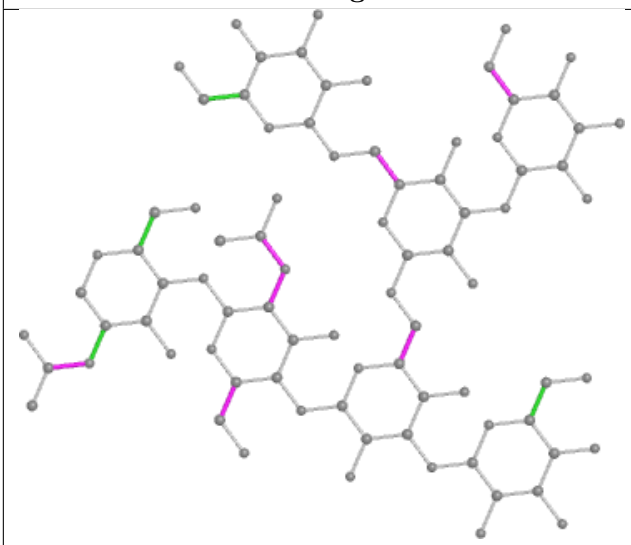
Oligosaccharide Chain g



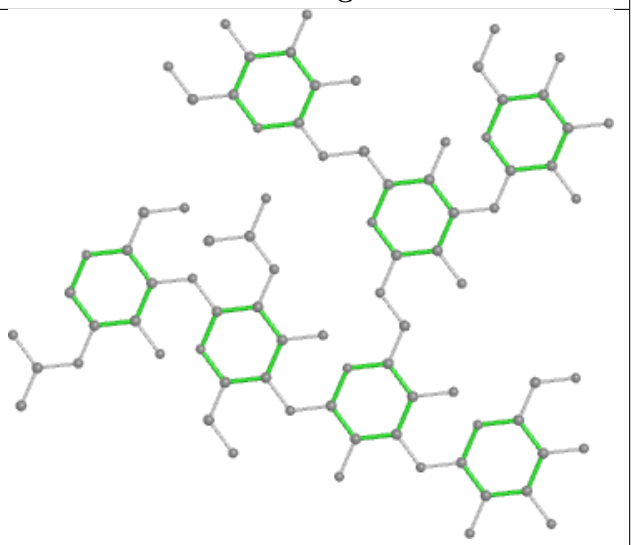
Bond lengths



Bond angles

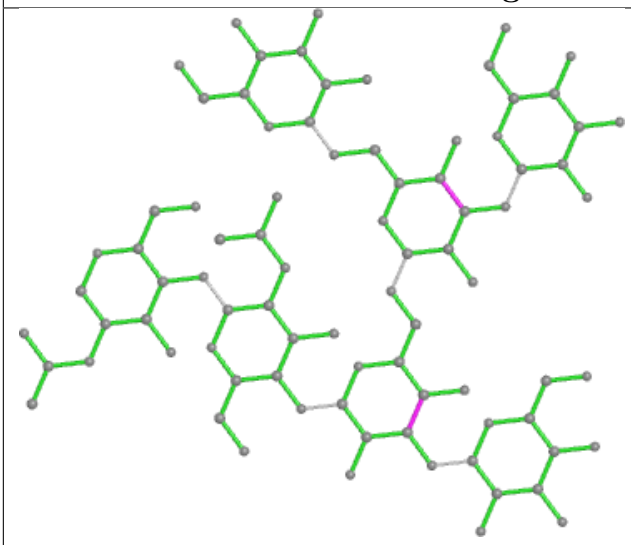


Torsions

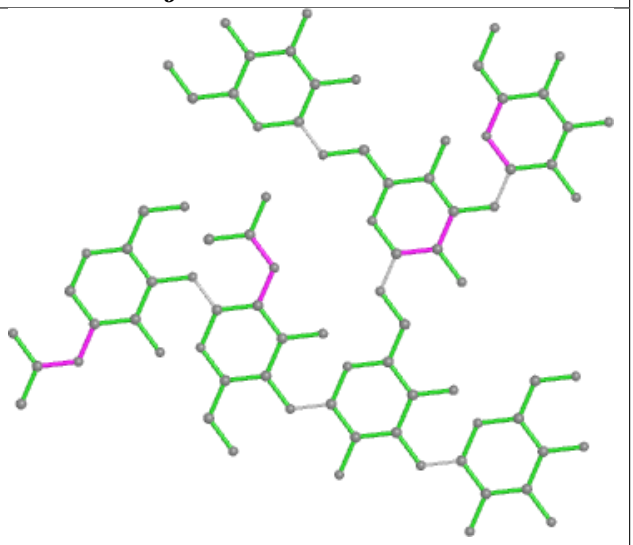


Rings

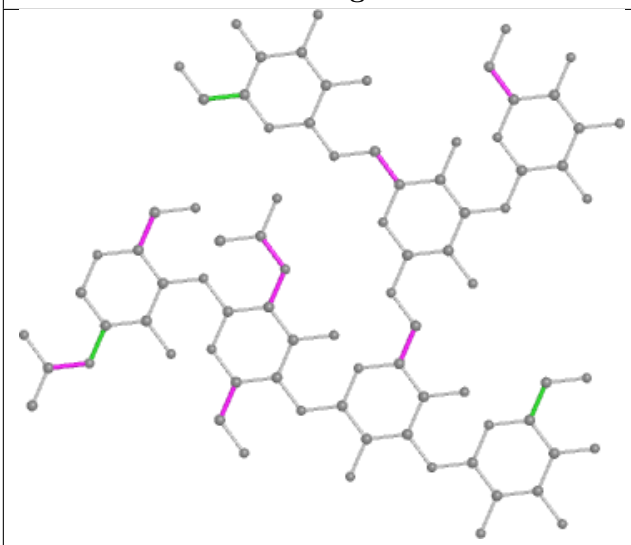
Oligosaccharide Chain j



Bond lengths



Bond angles



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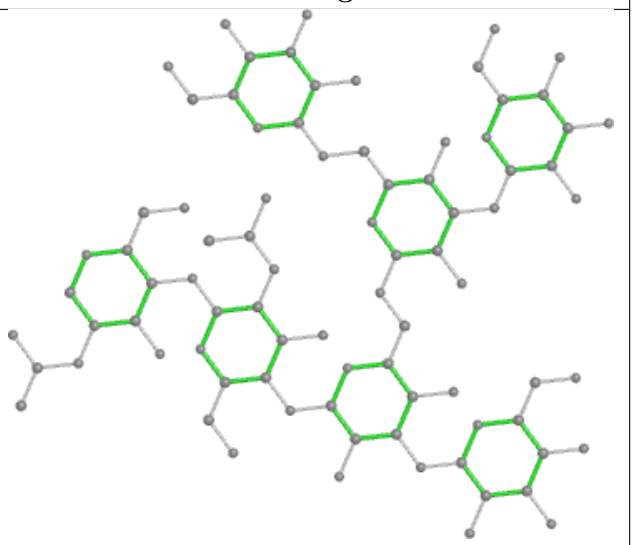
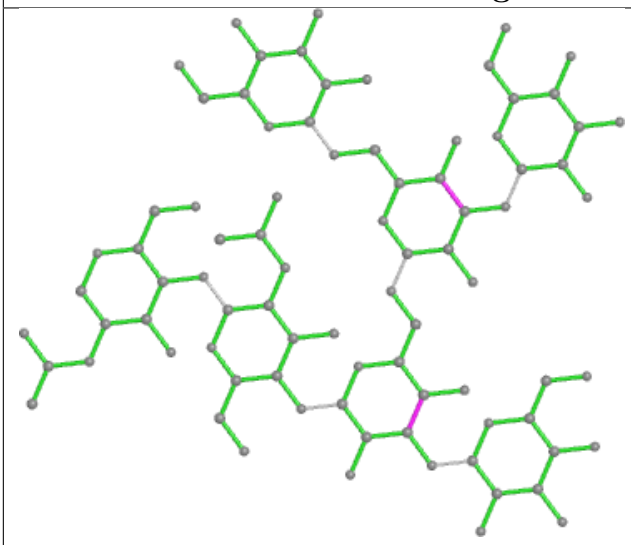


Rings

Oligosaccharide Chain m



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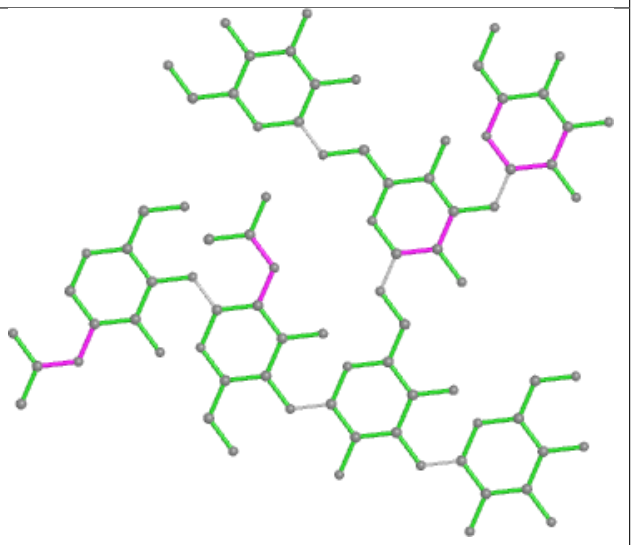

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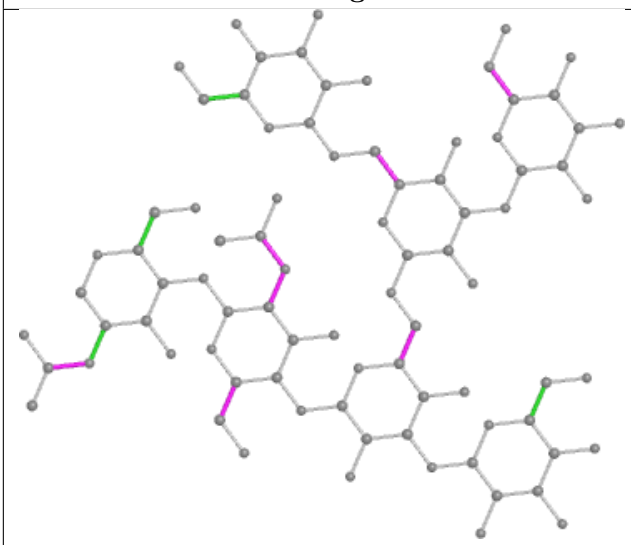

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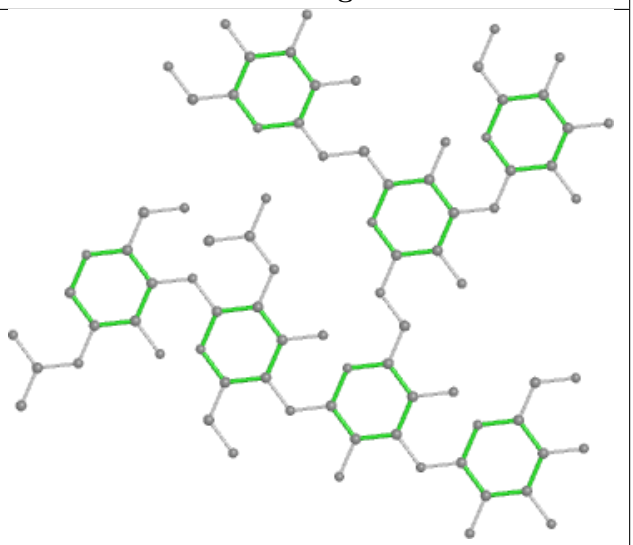
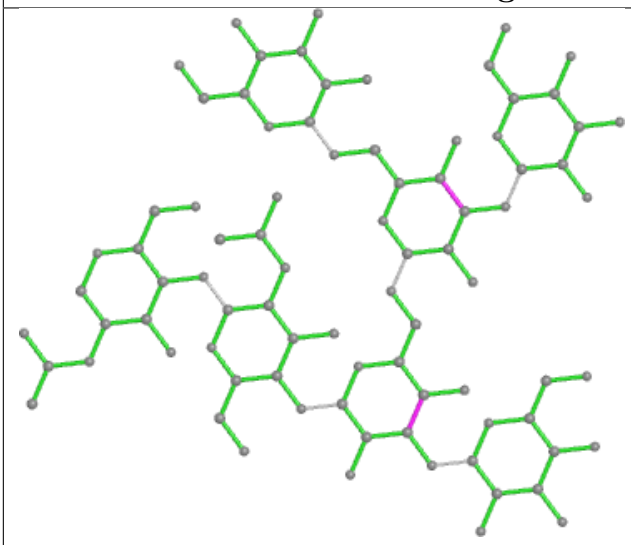


Rings

Oligosaccharide Chain p



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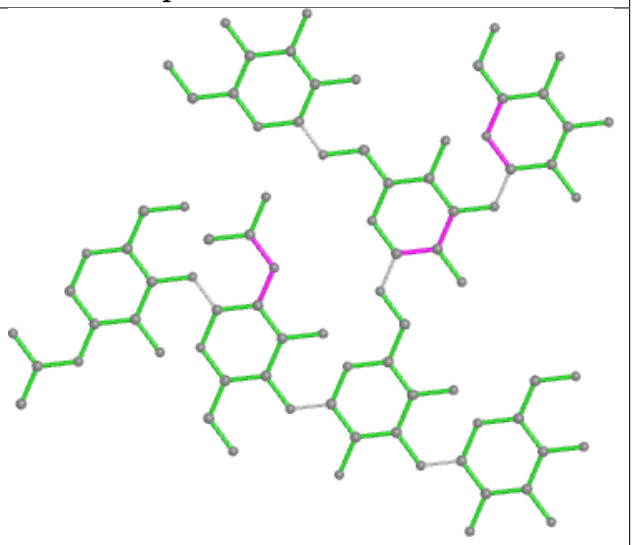

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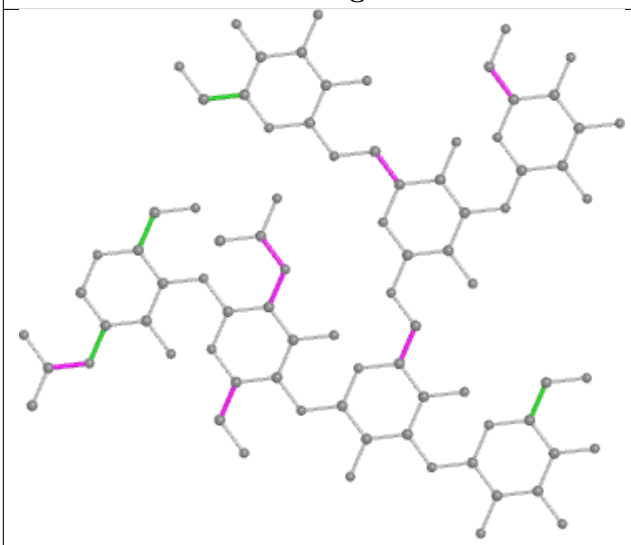

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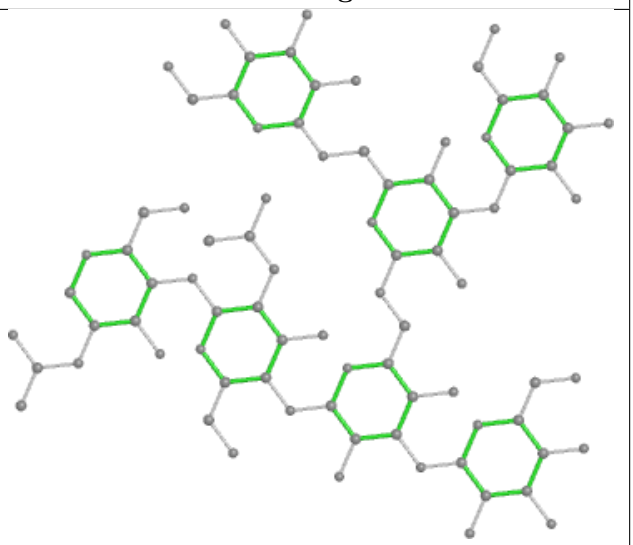
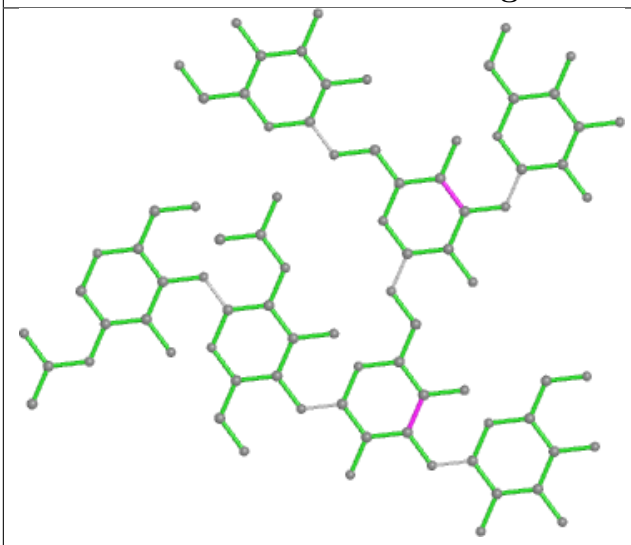
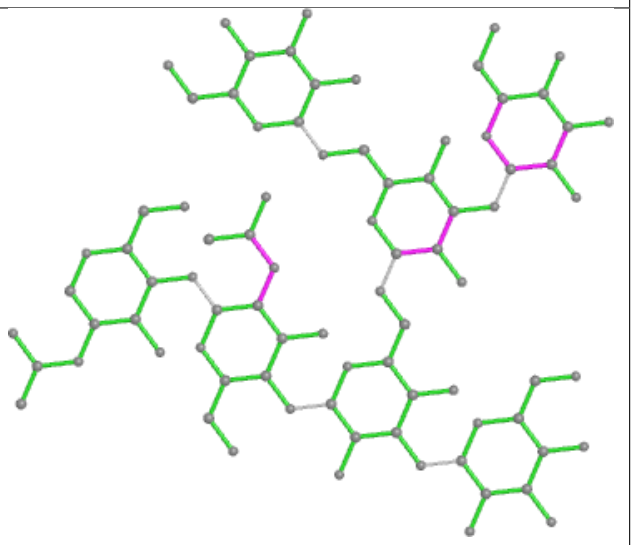


Rings

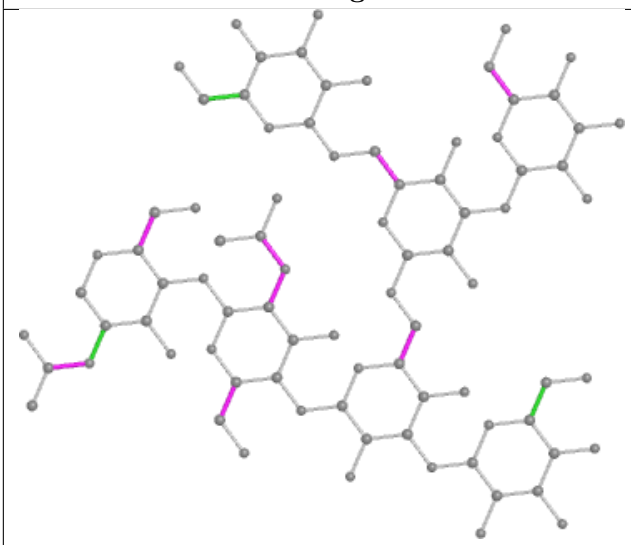
Oligosaccharide Chain s



Bond lengths



Bond angles



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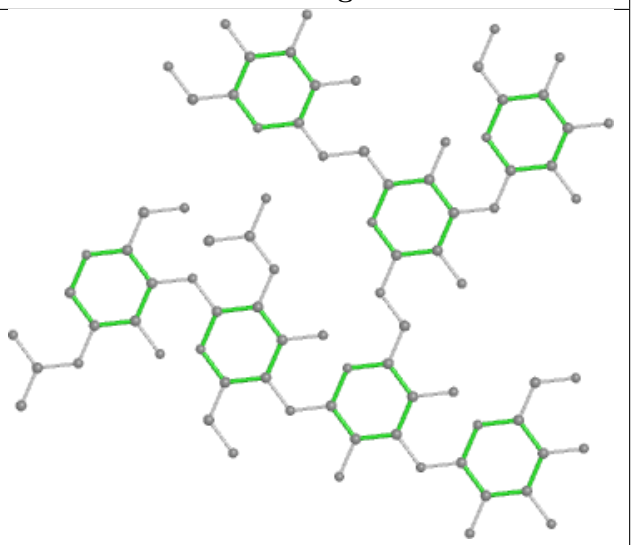
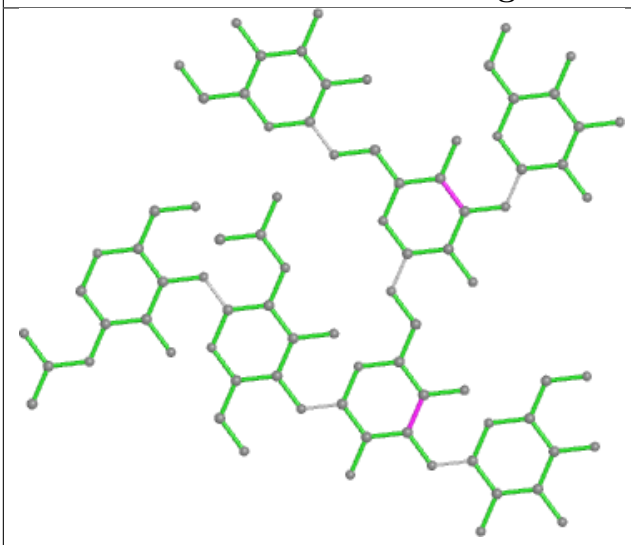


Rings

Oligosaccharide Chain v



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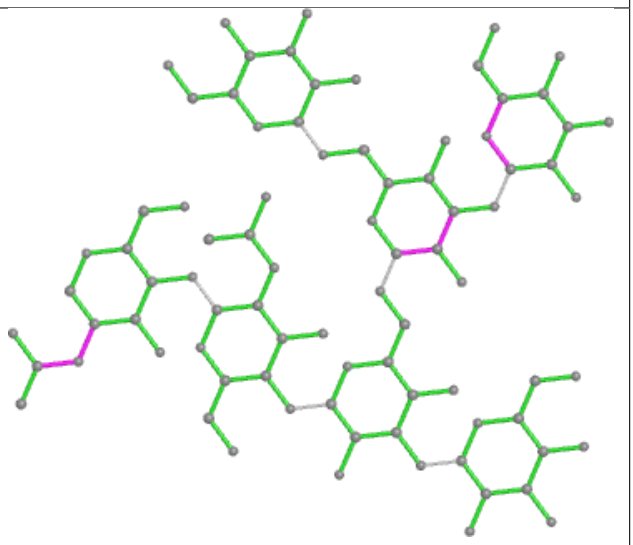
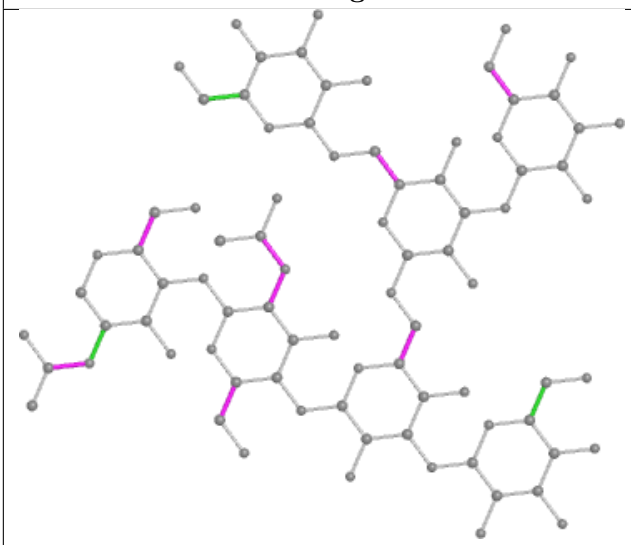


Bond angles



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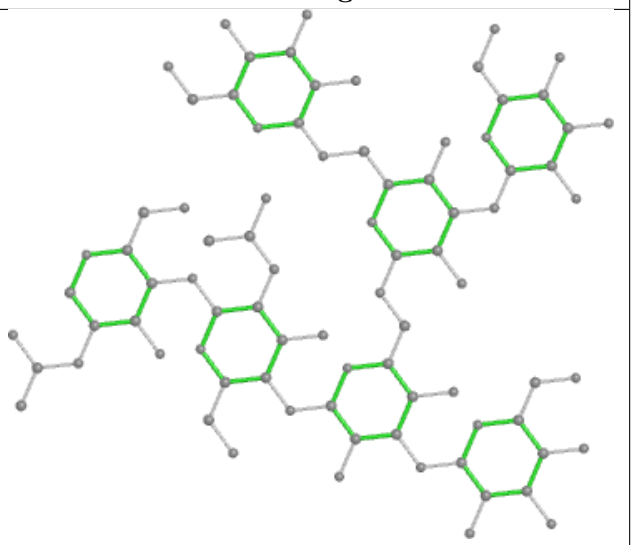
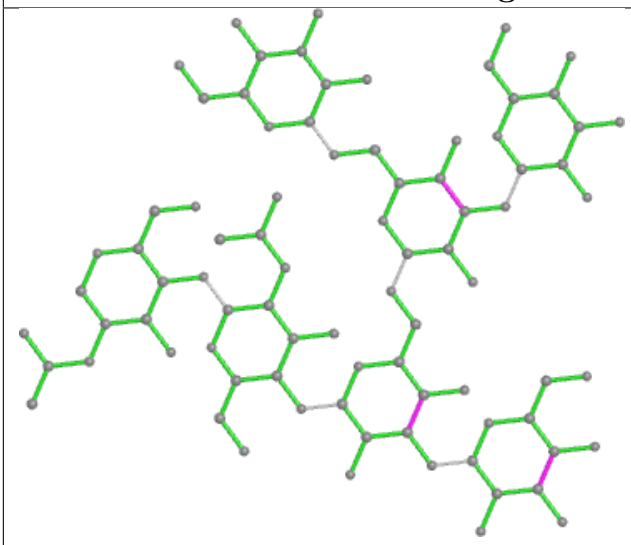


Rings

Oligosaccharide Chain y



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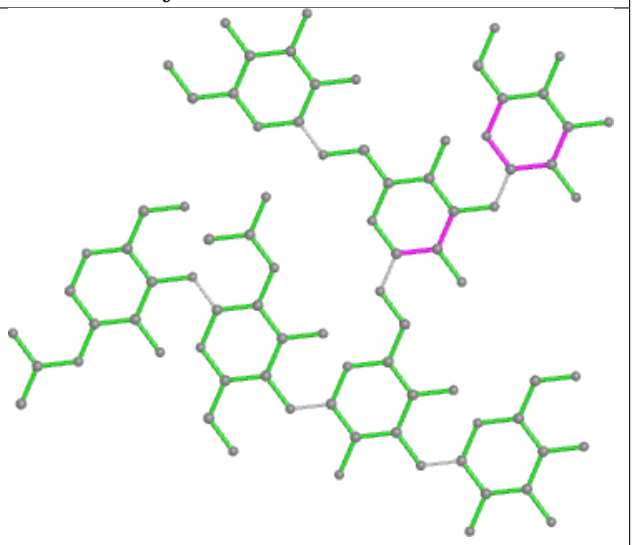

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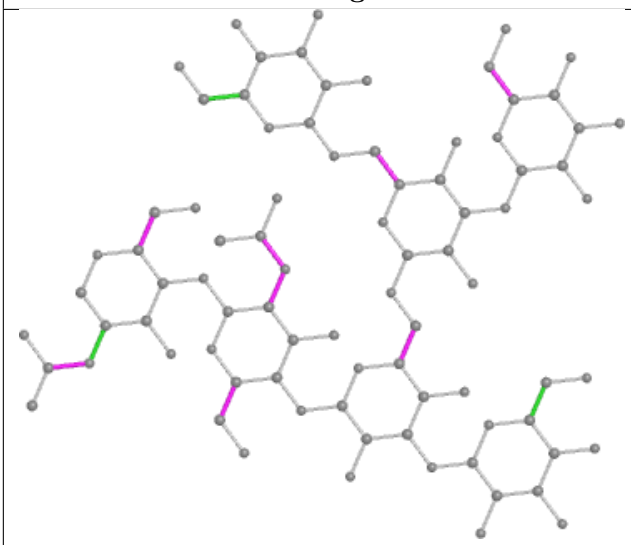
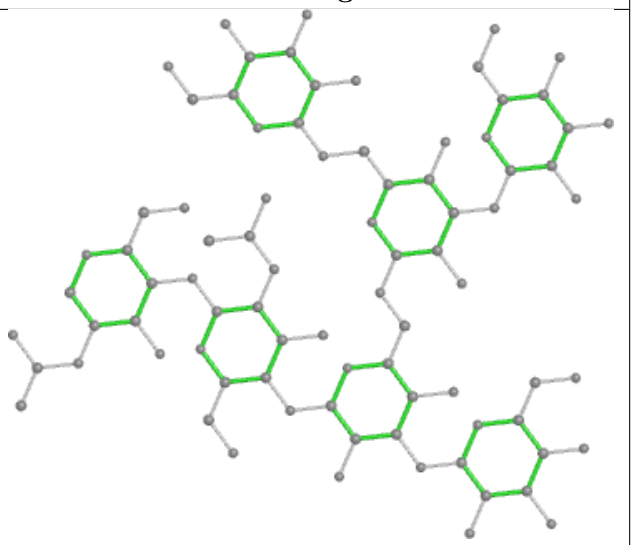
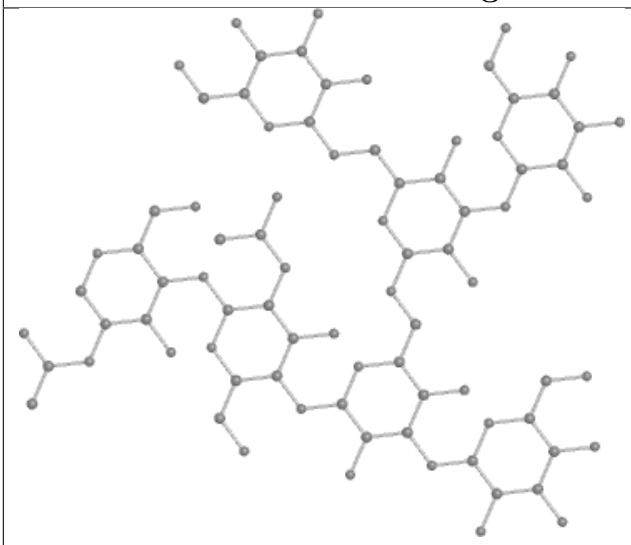


Torsions

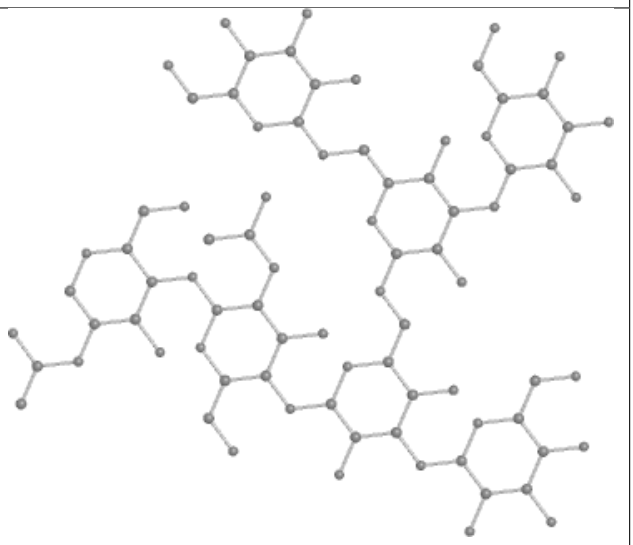


Rings

Oligosaccharide Chain BA



Bond lengths



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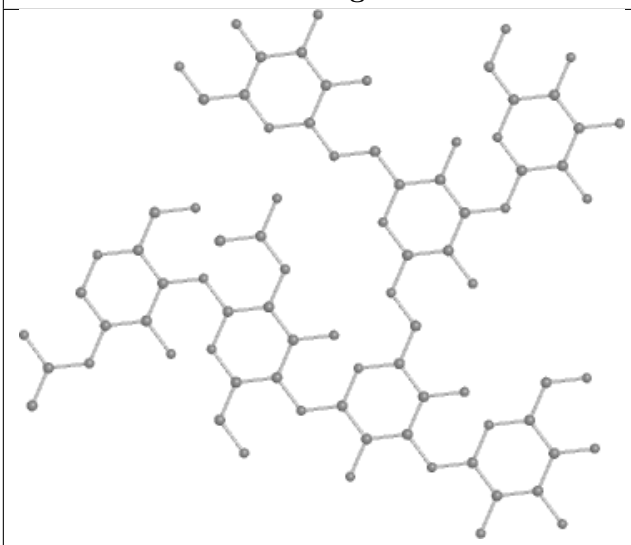
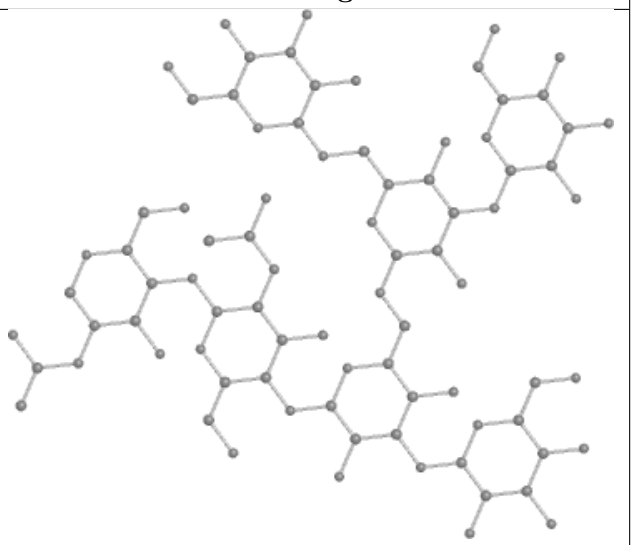
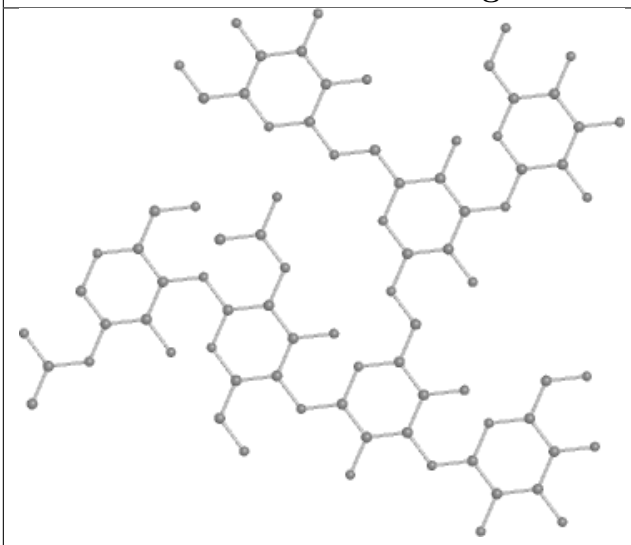


Torsions

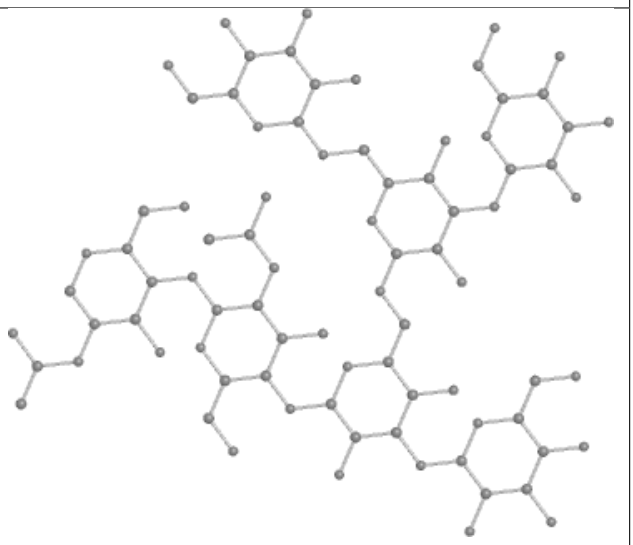


Rings

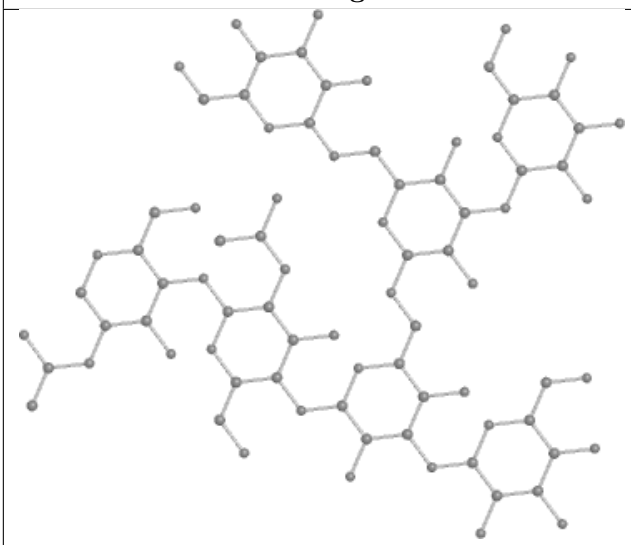
Oligosaccharide Chain EA



Bond lengths



Bond angles



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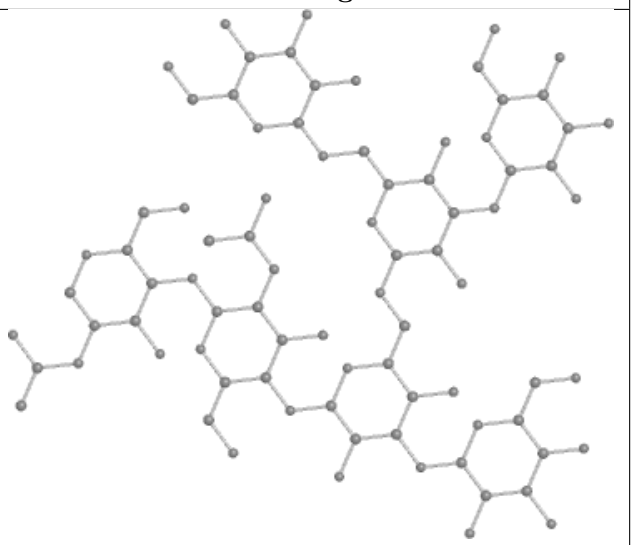
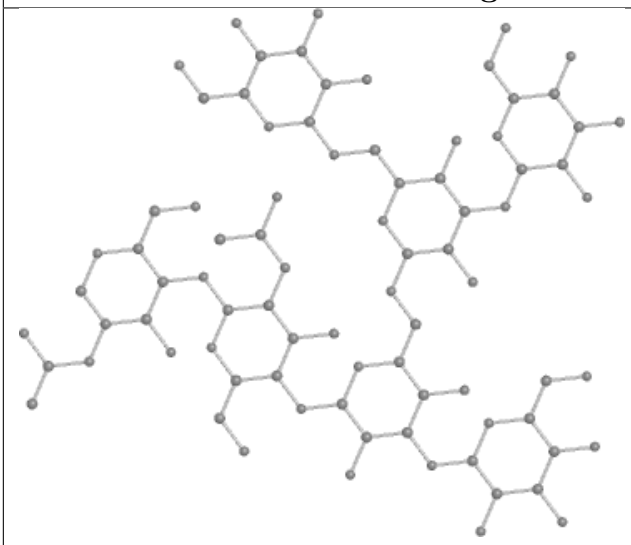
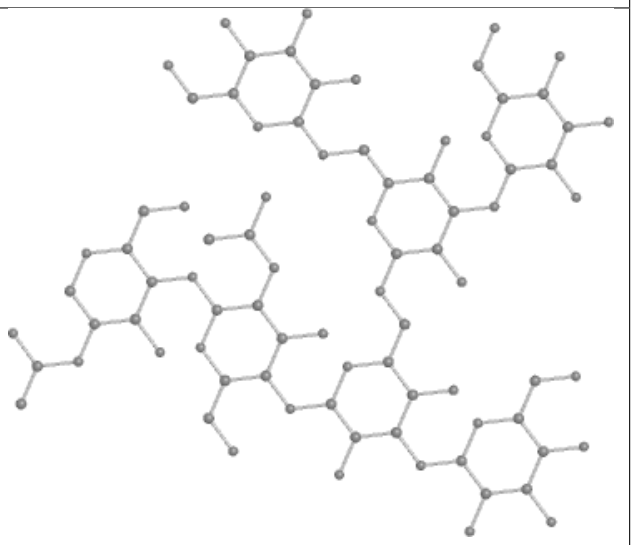


Rings

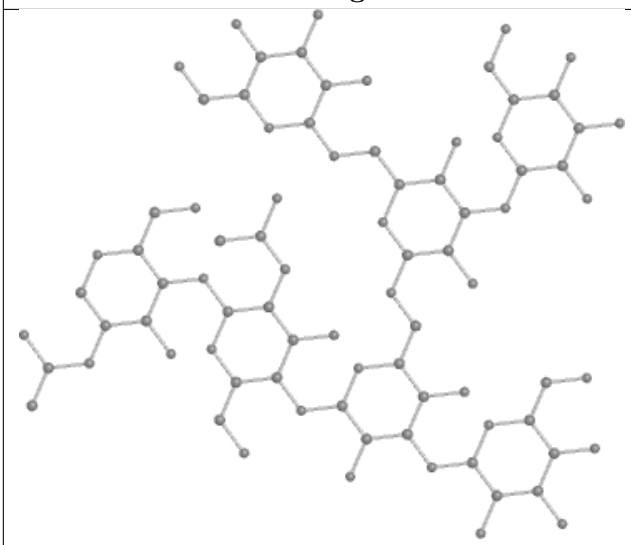
Oligosaccharide Chain HA



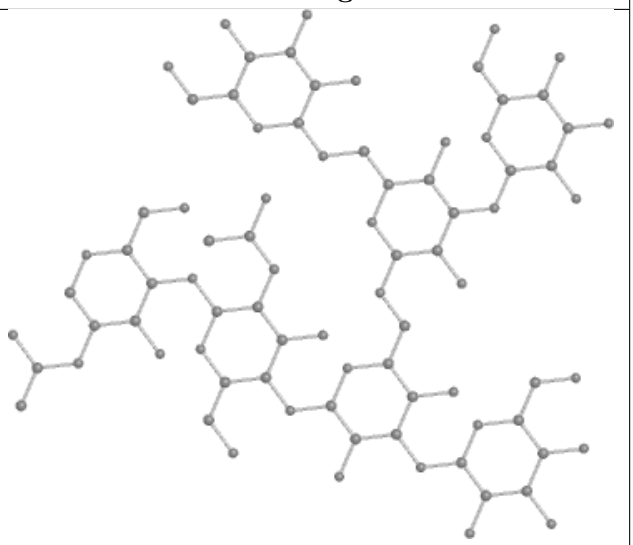
Bond lengths



Bond angles

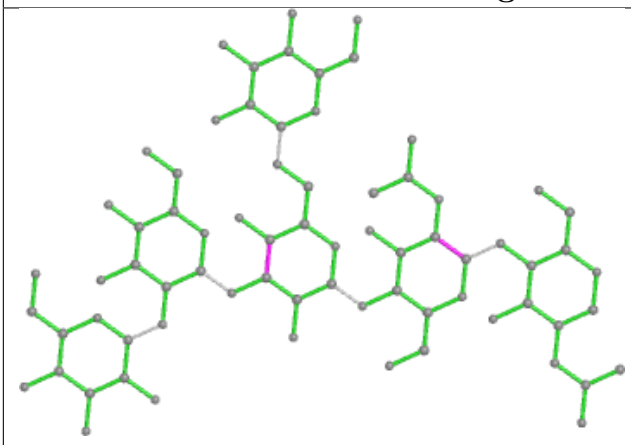


Torsions



Rings

Oligosaccharide Chain b



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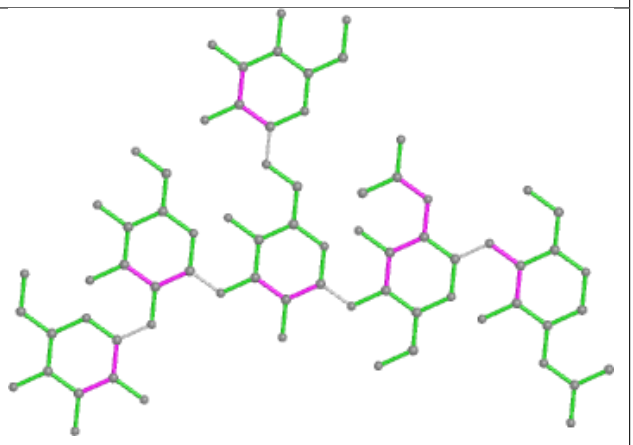

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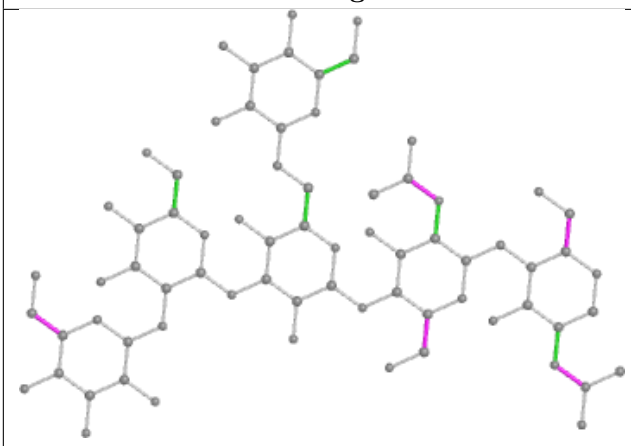

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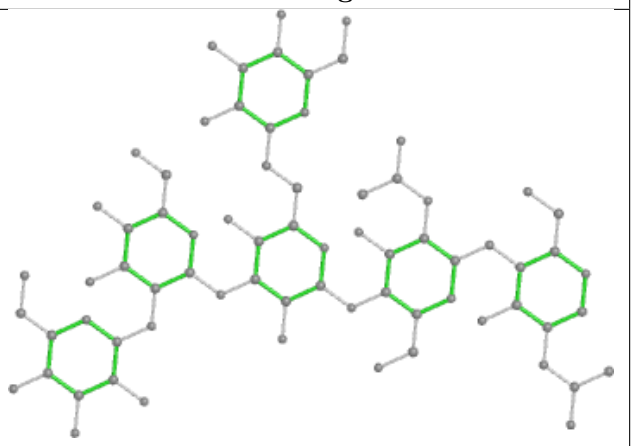
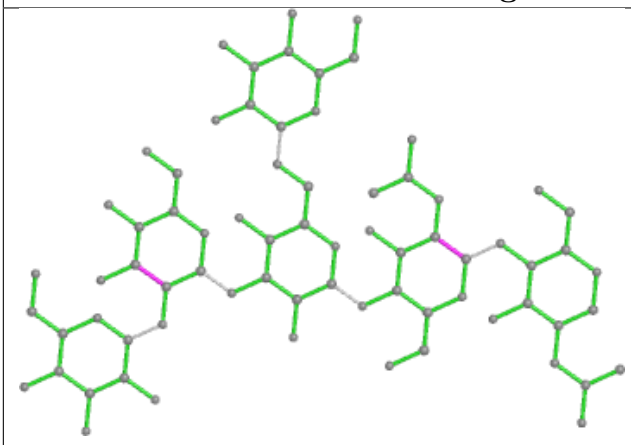


Rings

Oligosaccharide Chain e



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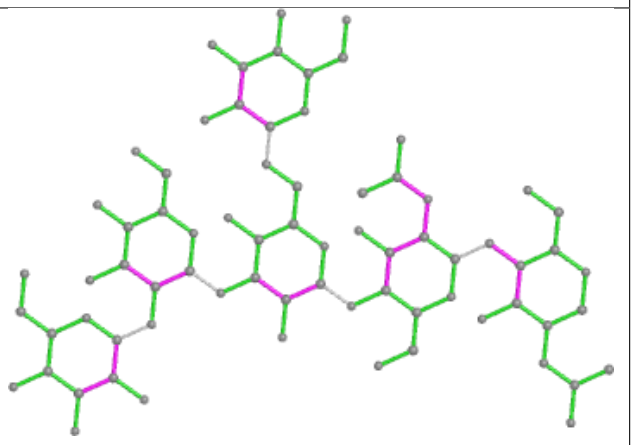
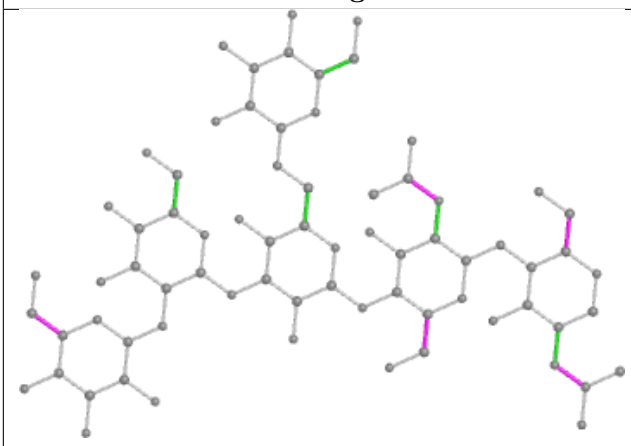


Bond angles



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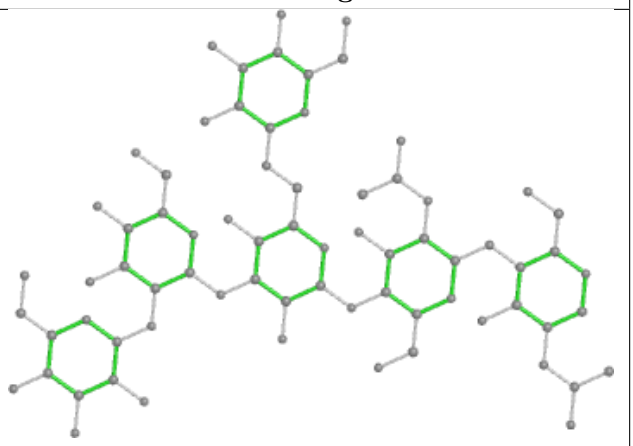
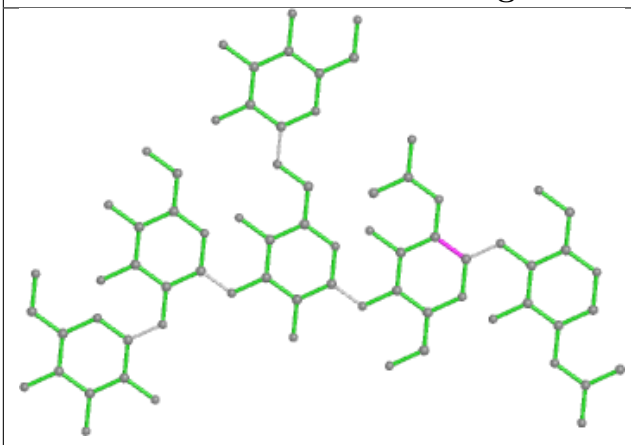


Rings

Oligosaccharide Chain h



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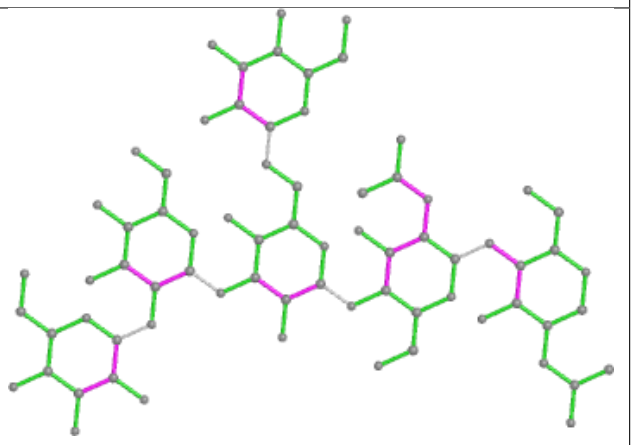

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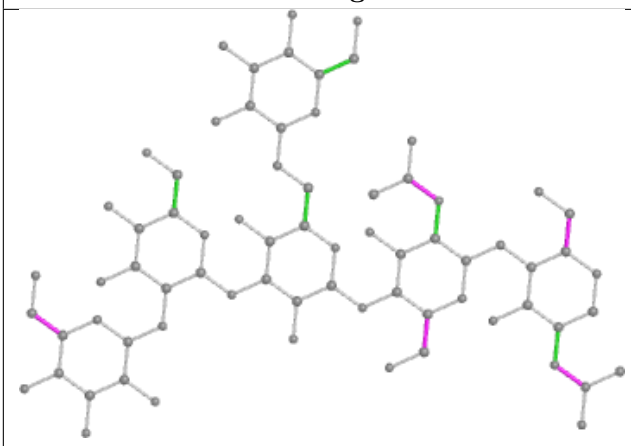

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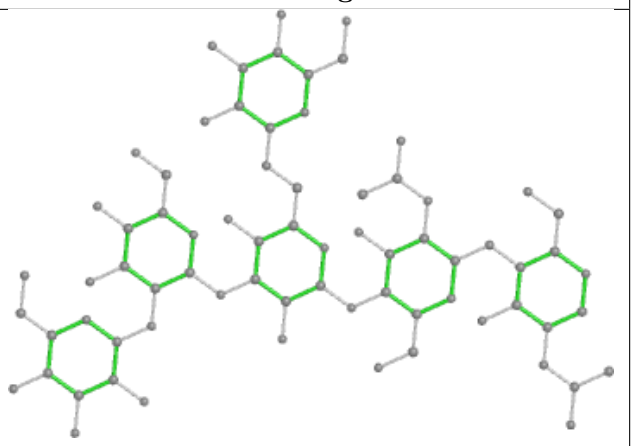
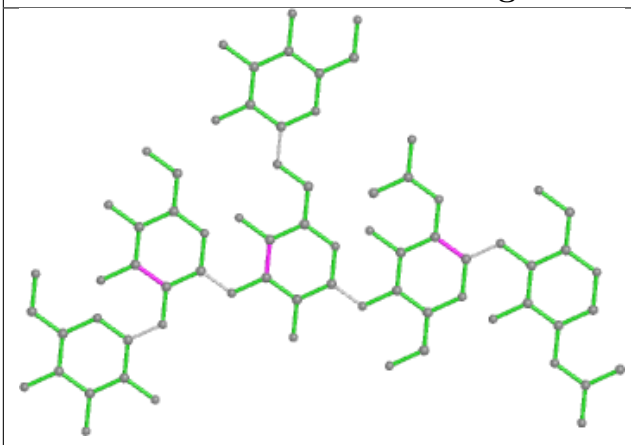


Rings

Oligosaccharide Chain k



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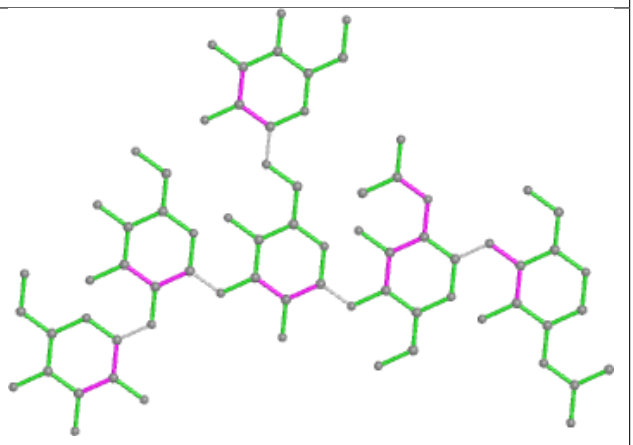
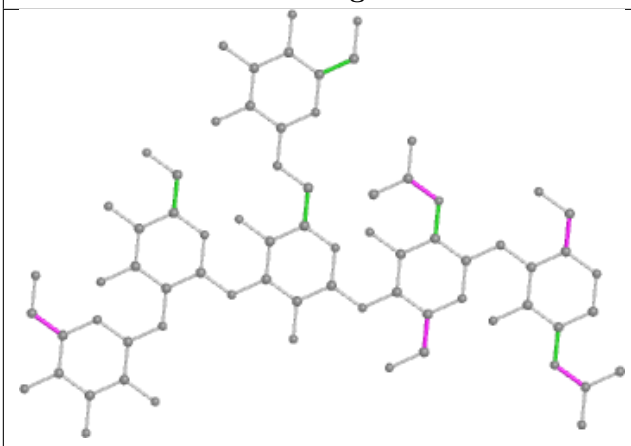


Bond angles



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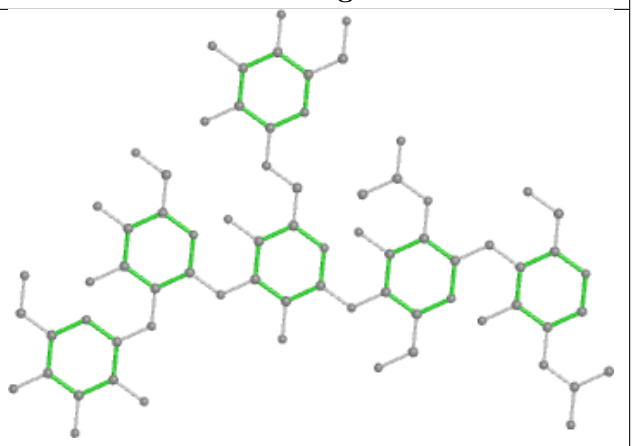
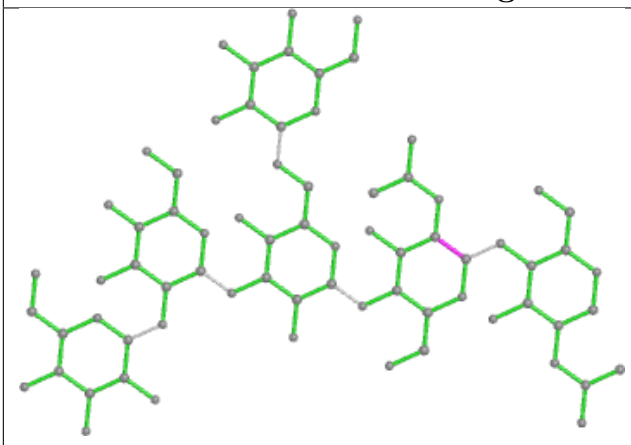


Rings

Oligosaccharide Chain n



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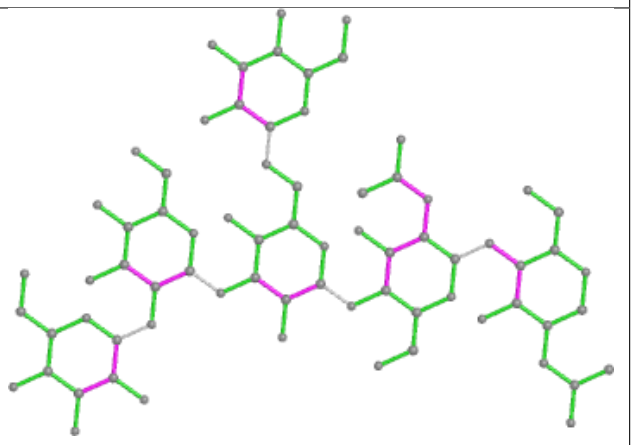

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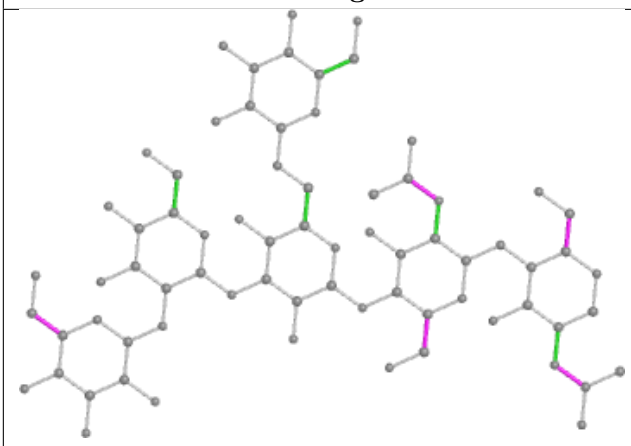

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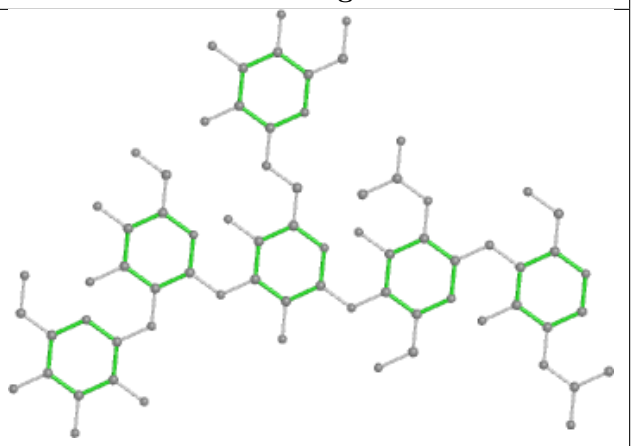
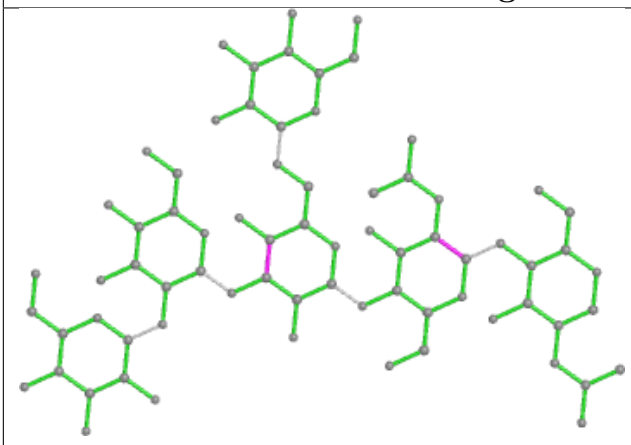


Rings

Oligosaccharide Chain q



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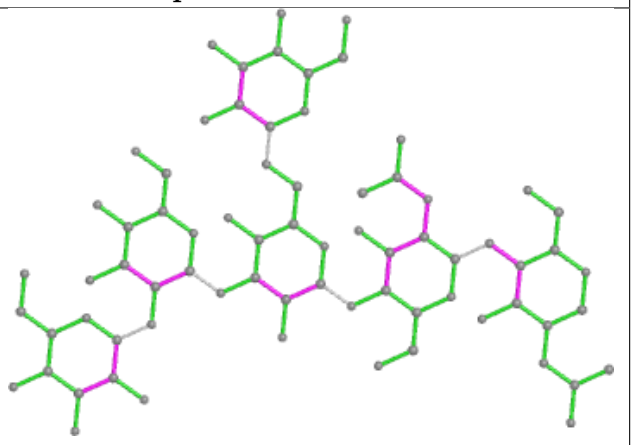

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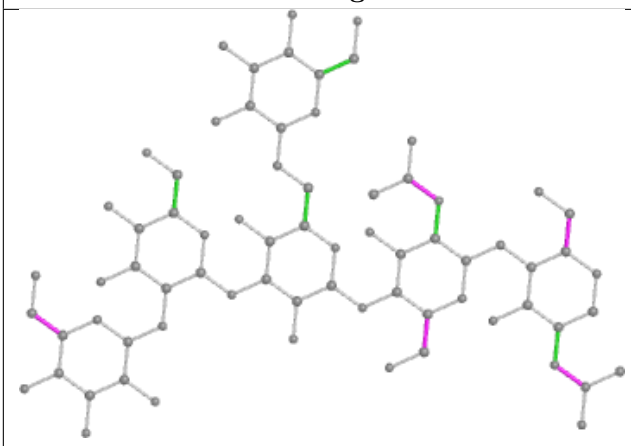

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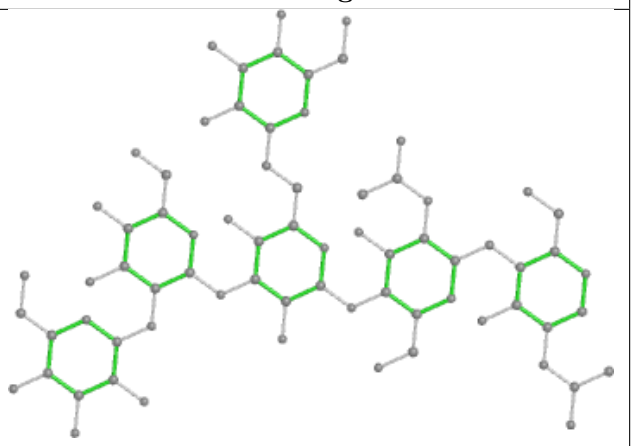
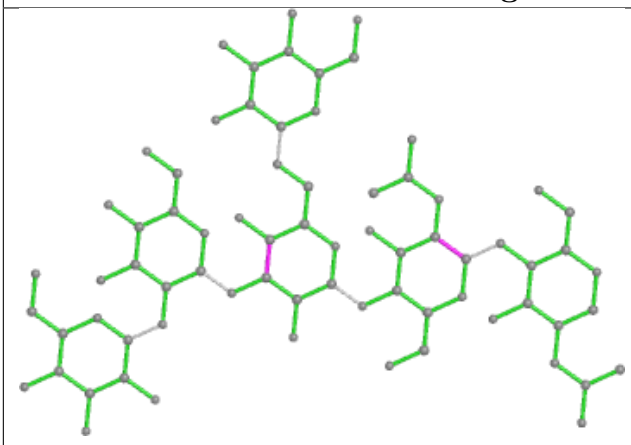


Rings

Oligosaccharide Chain t



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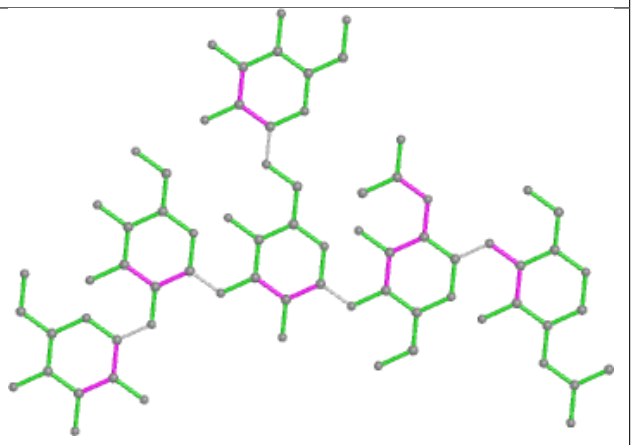

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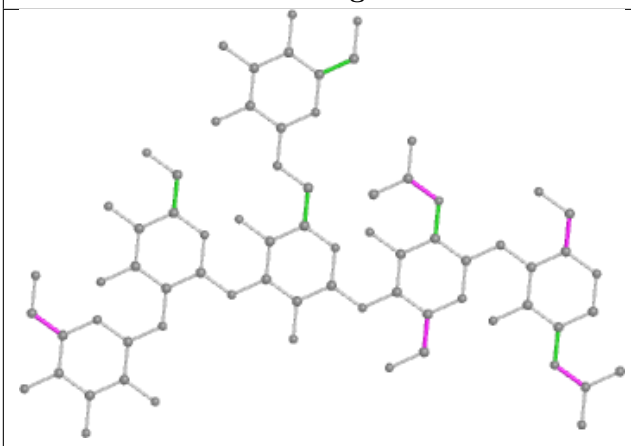

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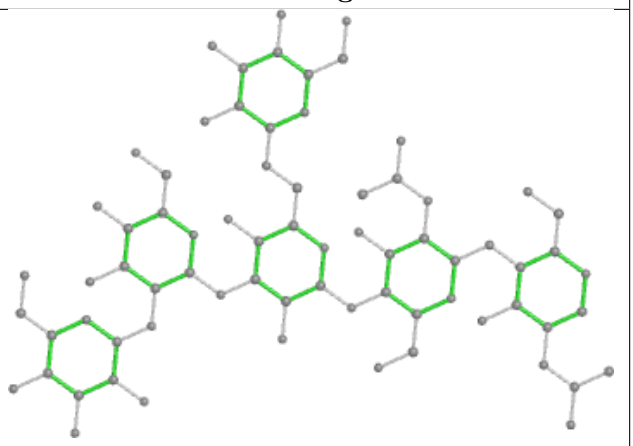
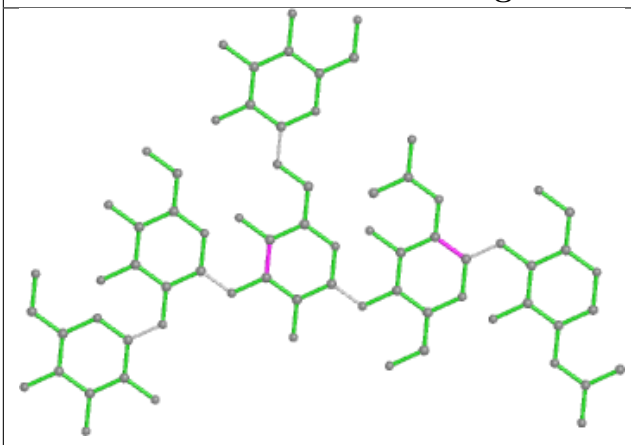


Rings

Oligosaccharide Chain w



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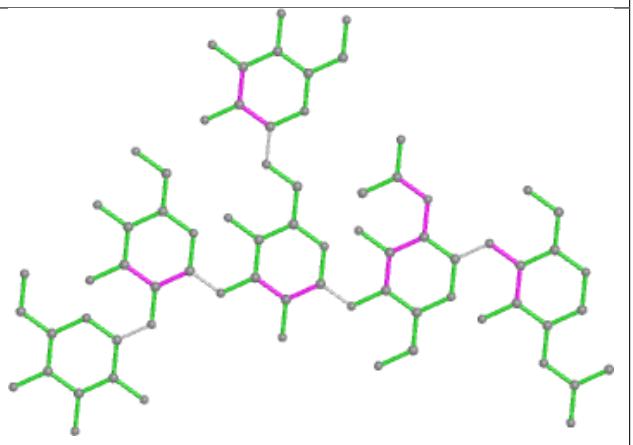

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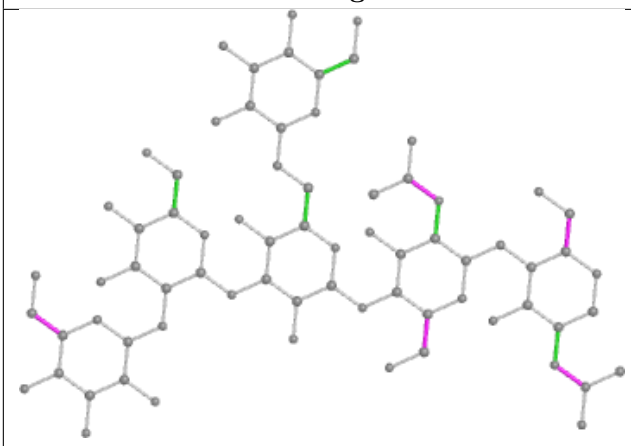

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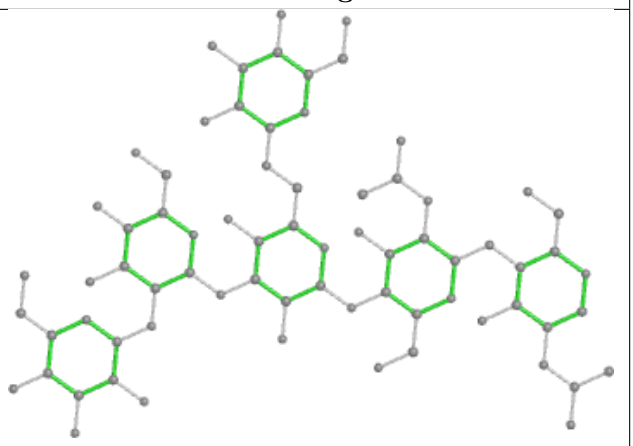
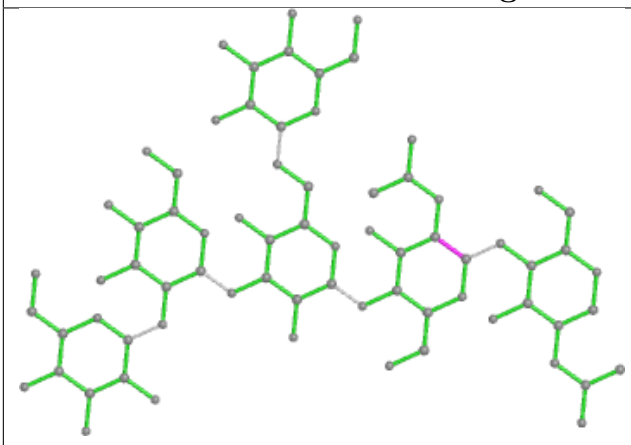


Rings

Oligosaccharide Chain z



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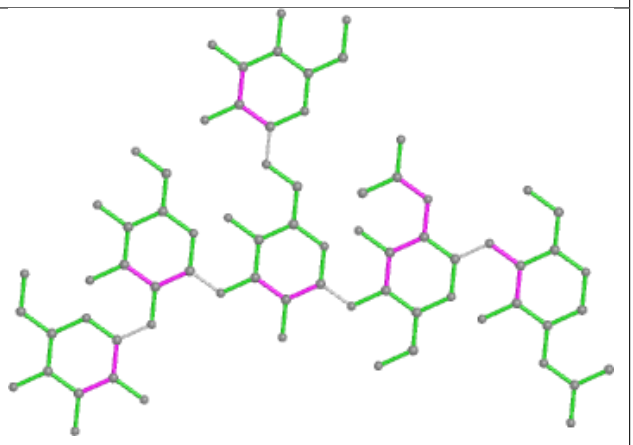
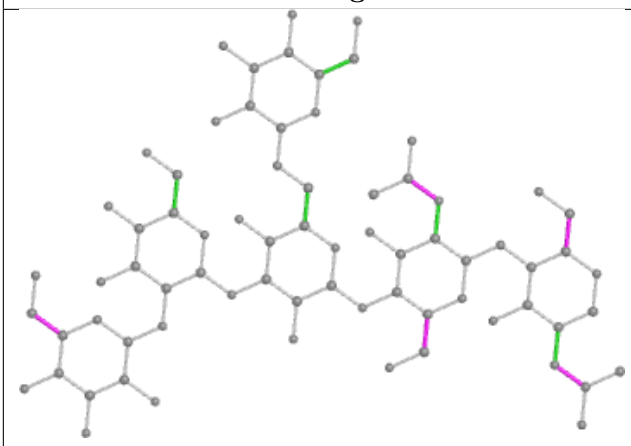


Bond angles



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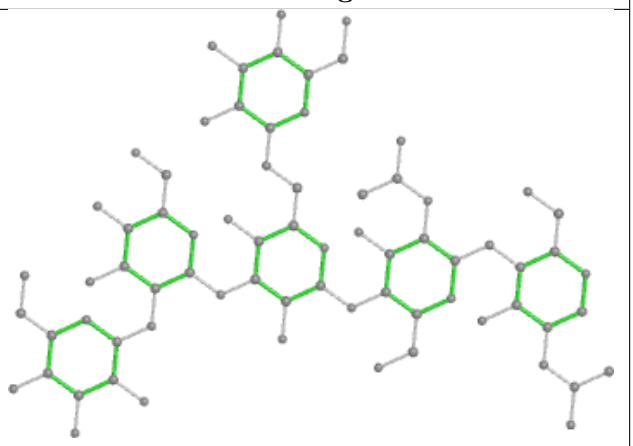
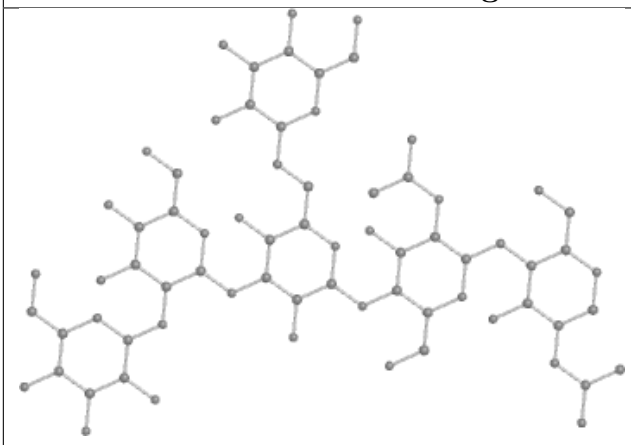


Rings

Oligosaccharide Chain CA



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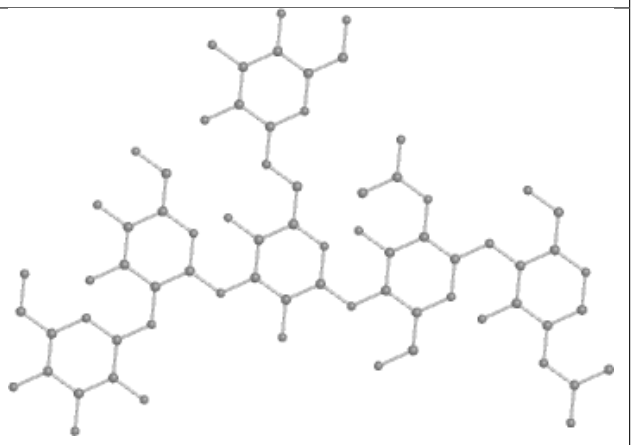

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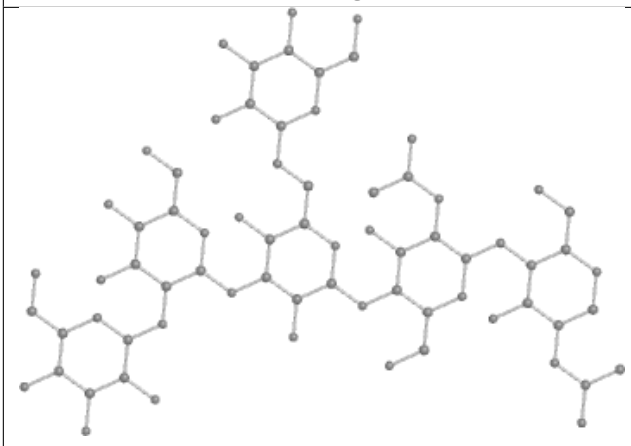

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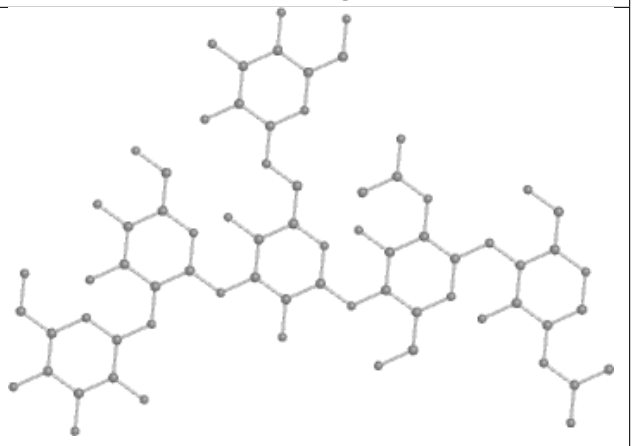
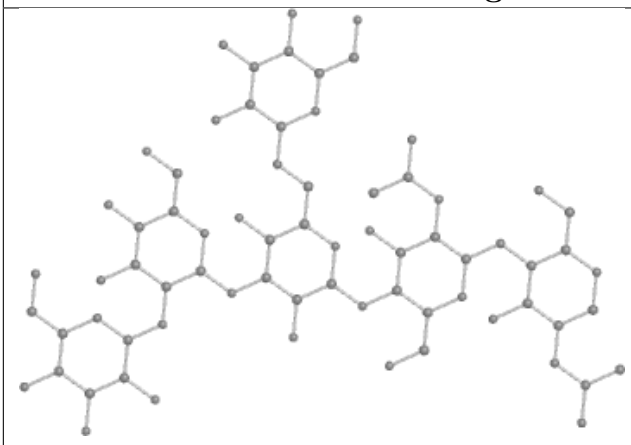


Rings

Oligosaccharide Chain FA



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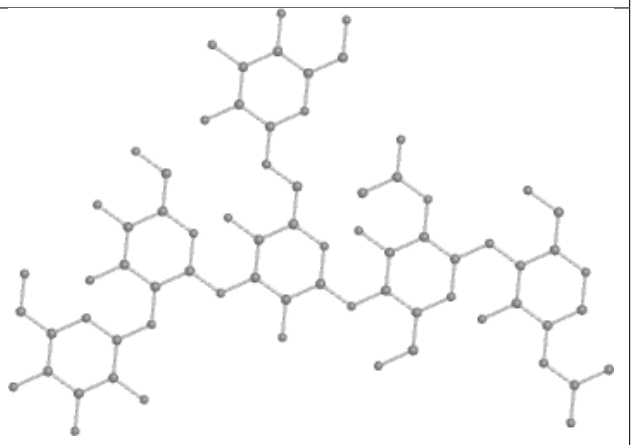

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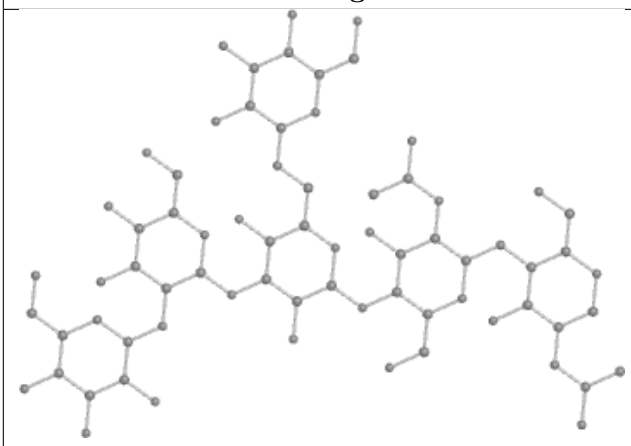

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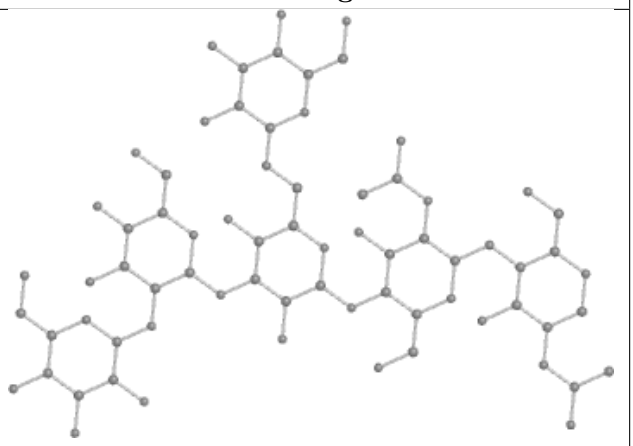
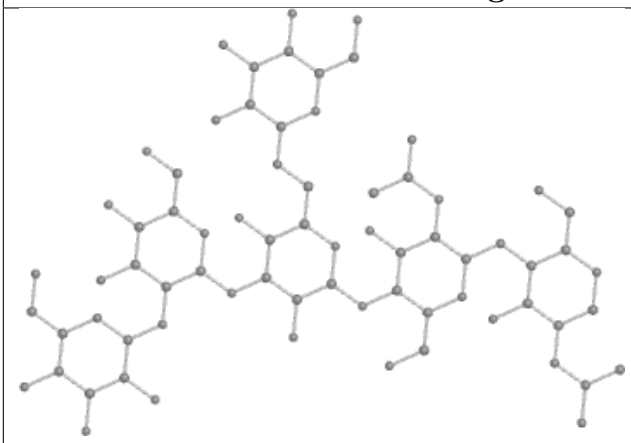


Rings

Oligosaccharide Chain IA



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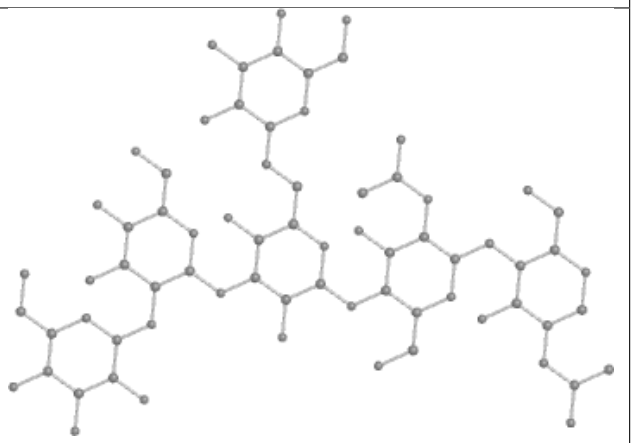
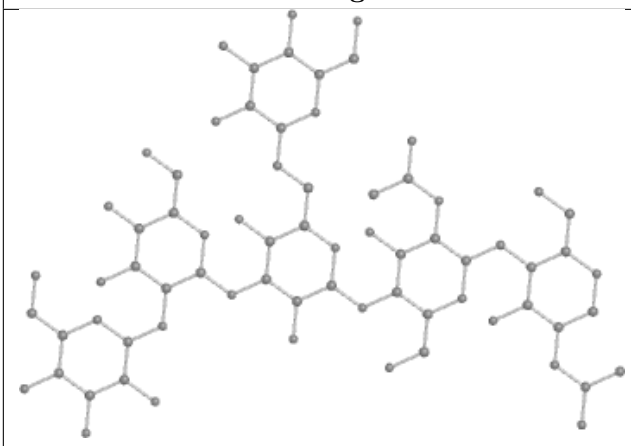


Bond angles



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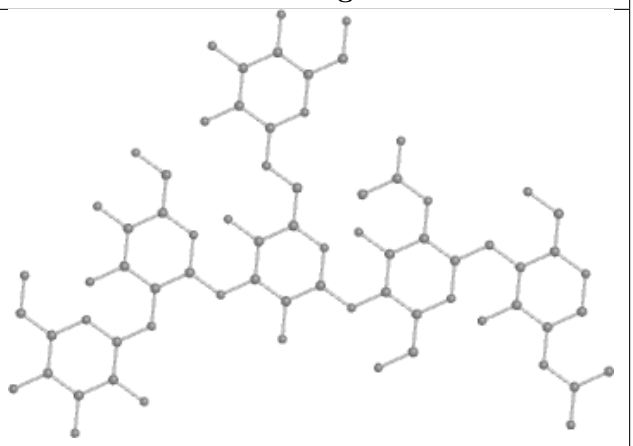
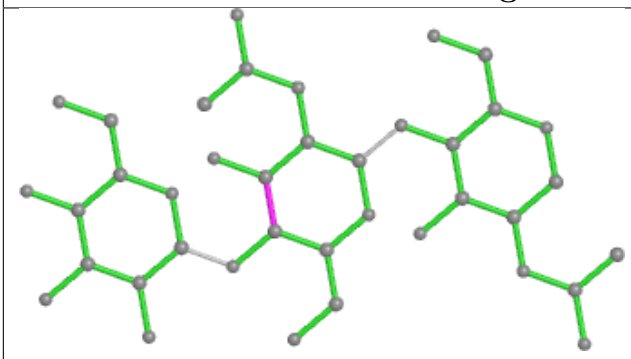


Rings

Oligosaccharide Chain c



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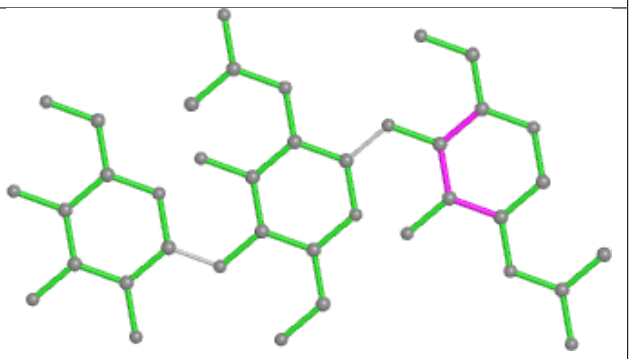

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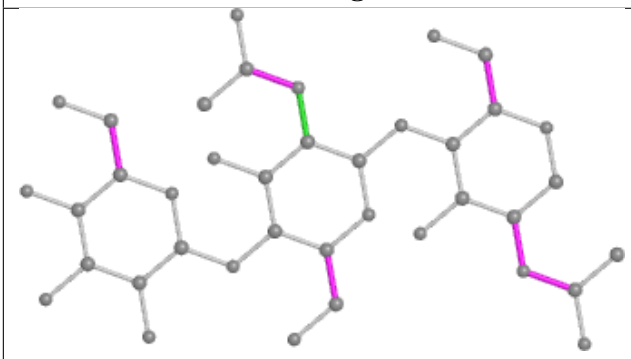

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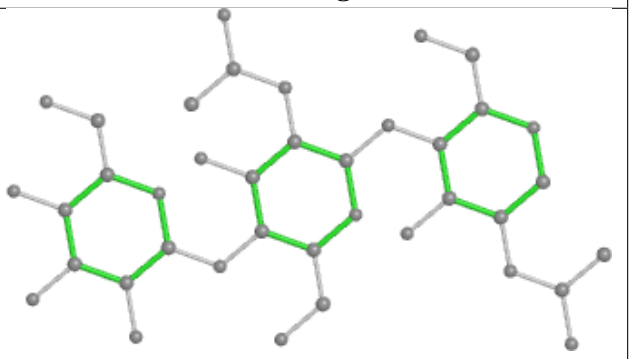
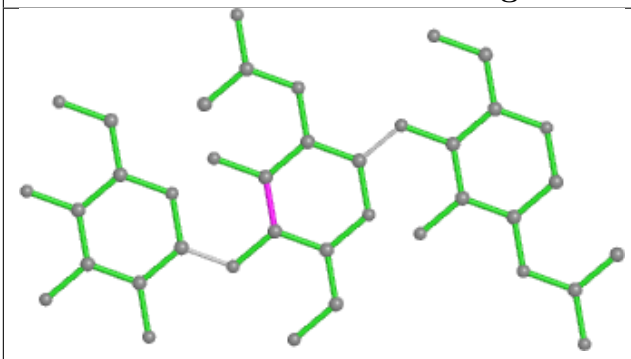
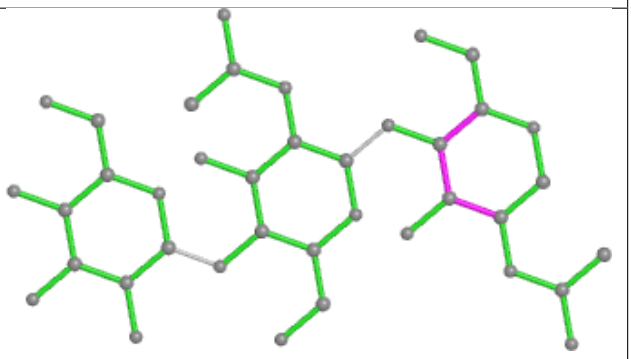


Rings

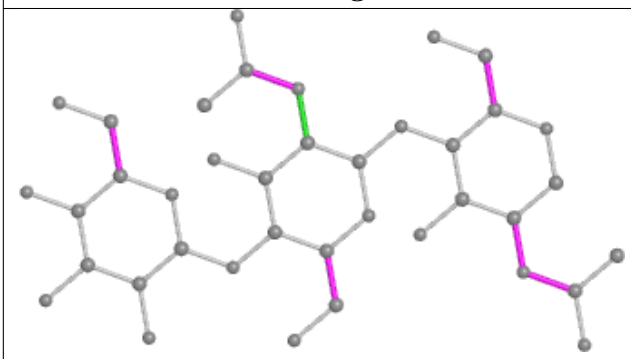
Oligosaccharide Chain f



Bond lengths



Bond angles



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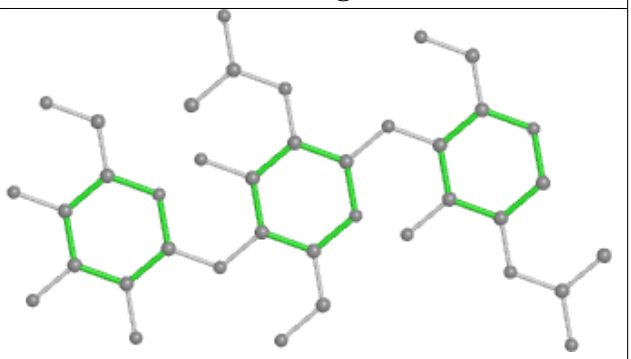
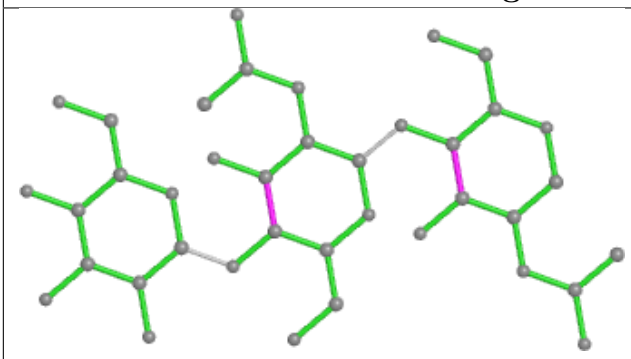
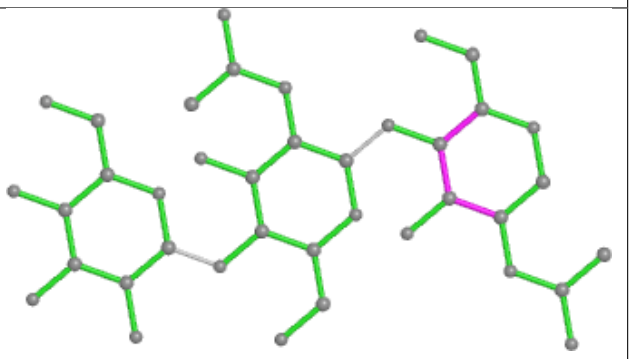


Rings

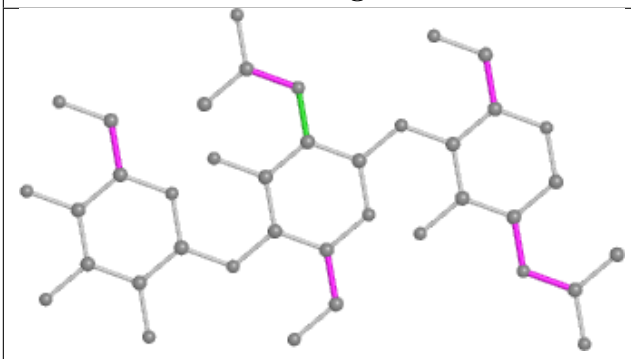
Oligosaccharide Chain i



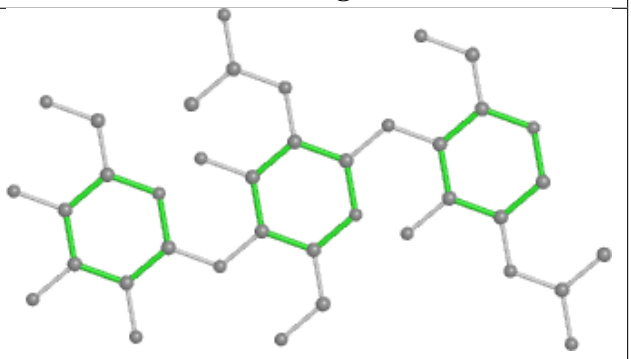
Bond lengths



Bond angles

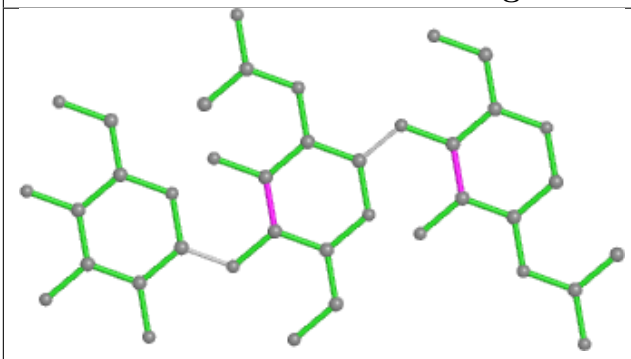


Torsions

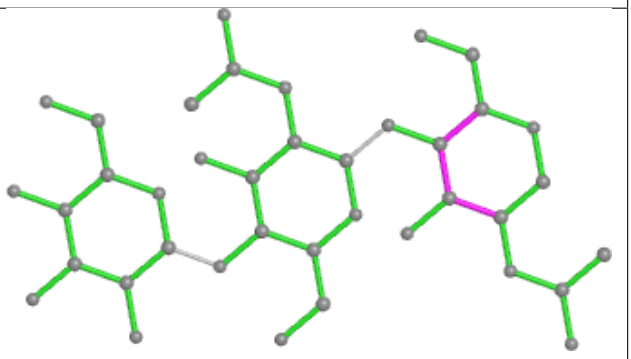


Rings

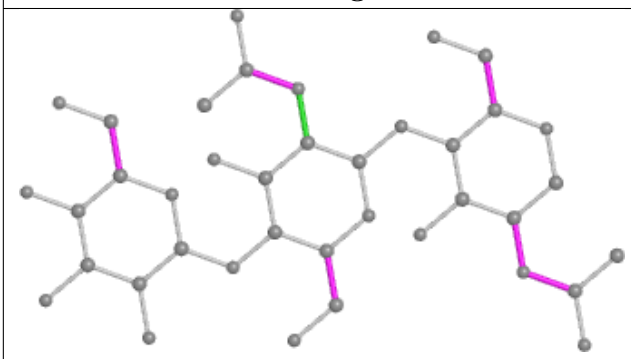
Oligosaccharide Chain l



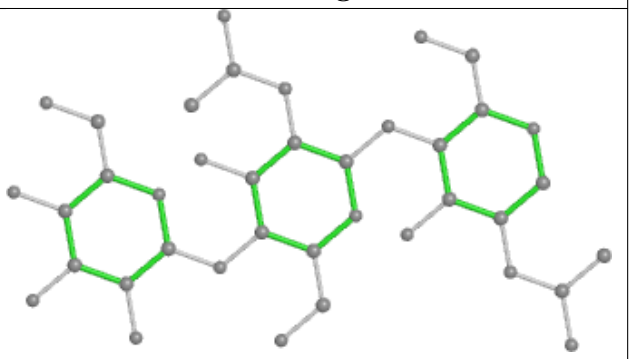
Bond lengths



Bond angles

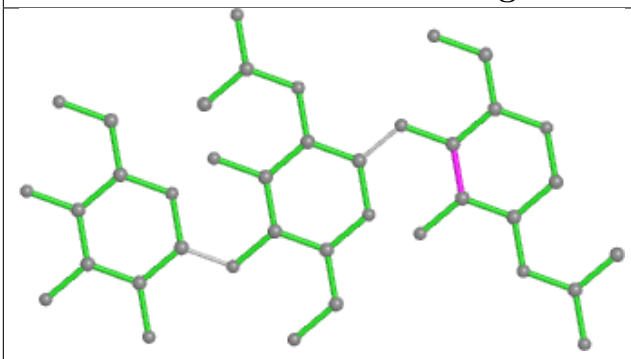


Torsions

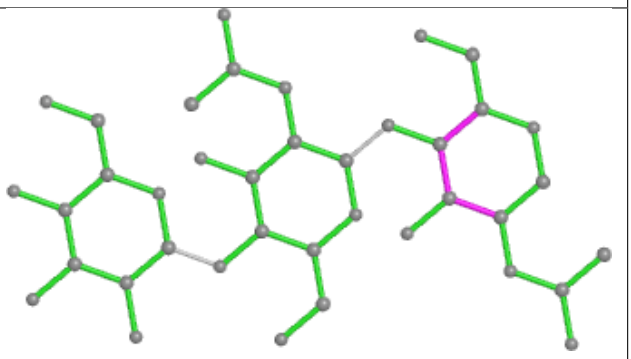


Rings

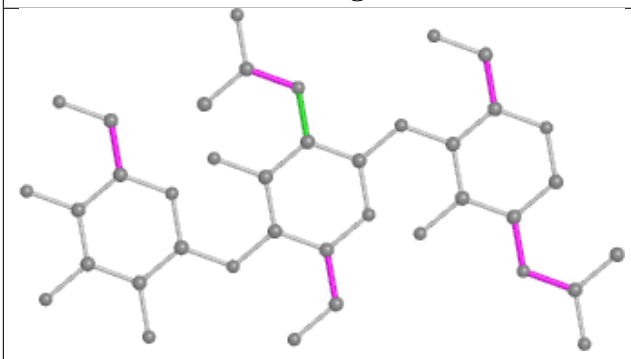
Oligosaccharide Chain o



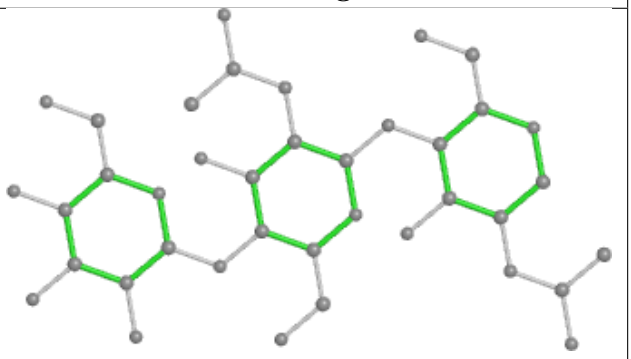
Bond lengths



Bond angles

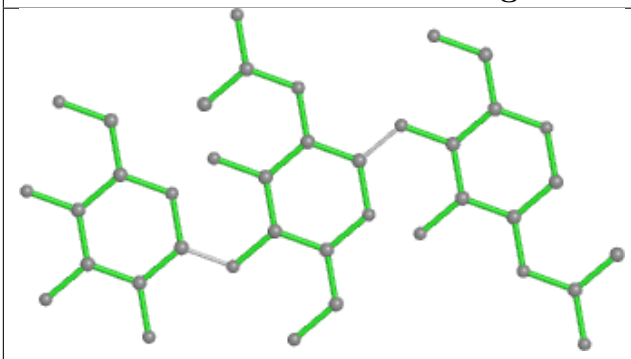


Torsions

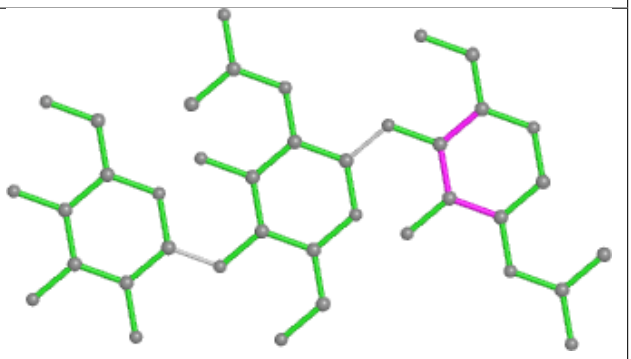


Rings

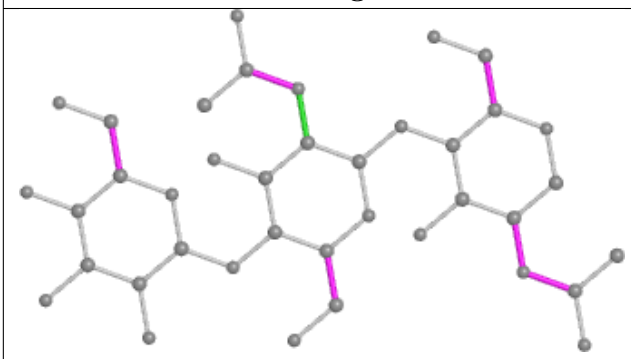
Oligosaccharide Chain r



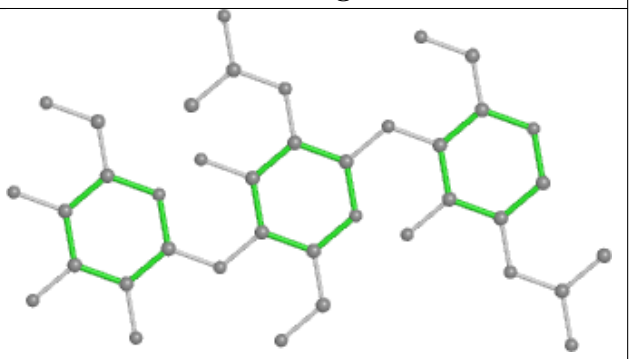
Bond lengths



Bond angles

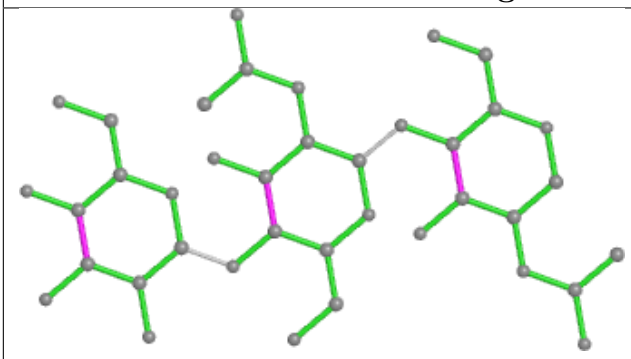


Torsions

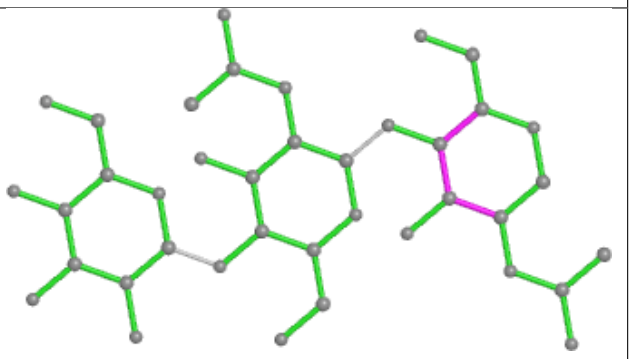


Rings

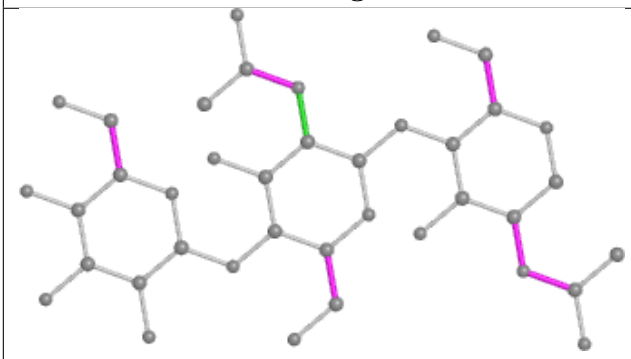
Oligosaccharide Chain u



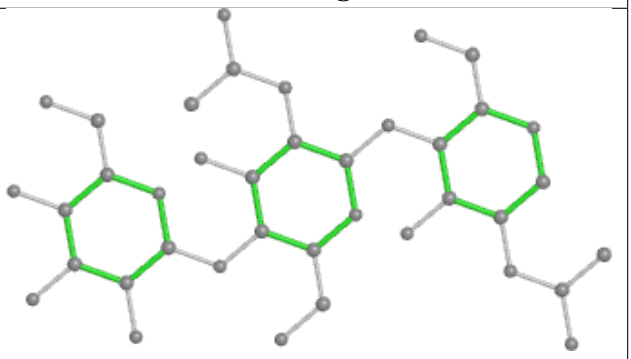
Bond lengths



Bond angles

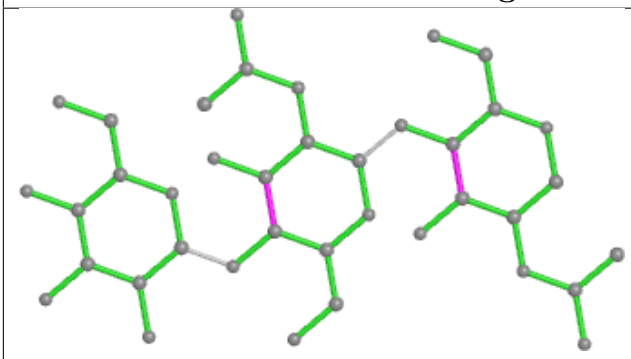


Torsions

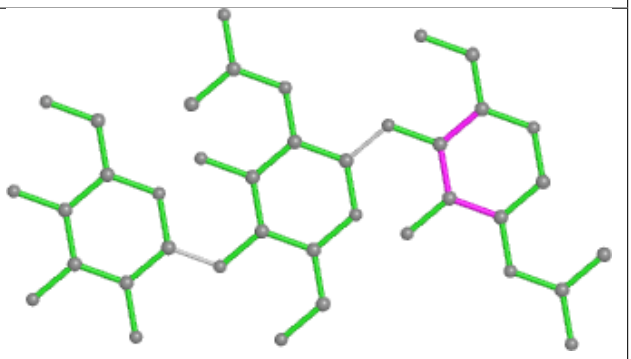


Rings

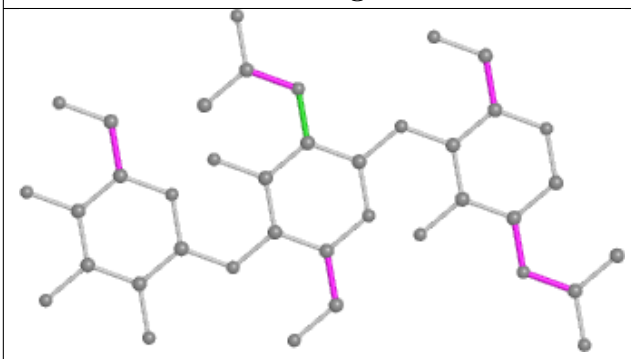
Oligosaccharide Chain x



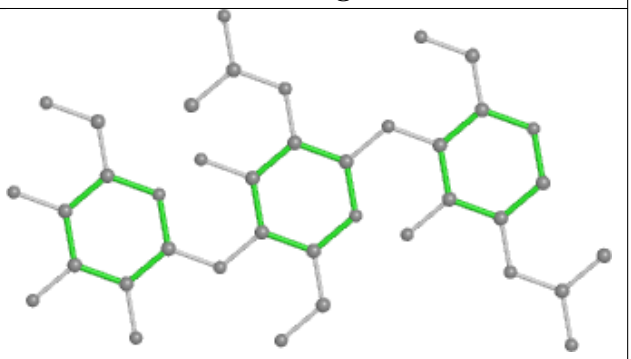
Bond lengths



Bond angles

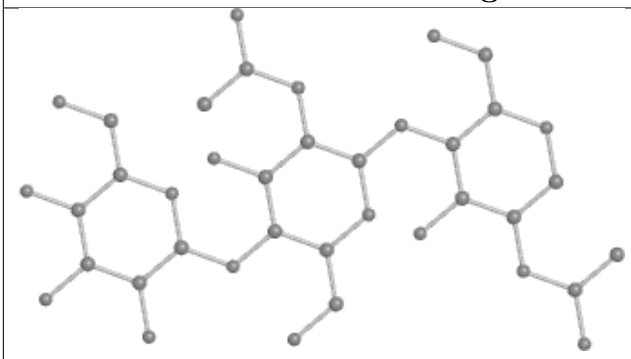


Torsions

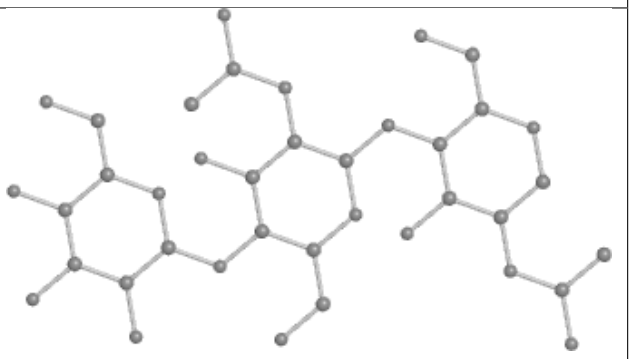


Rings

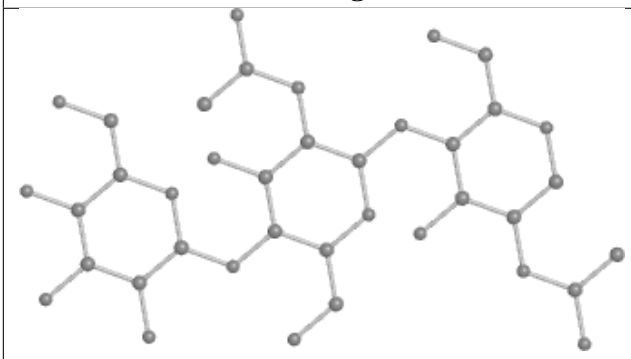
Oligosaccharide Chain AA



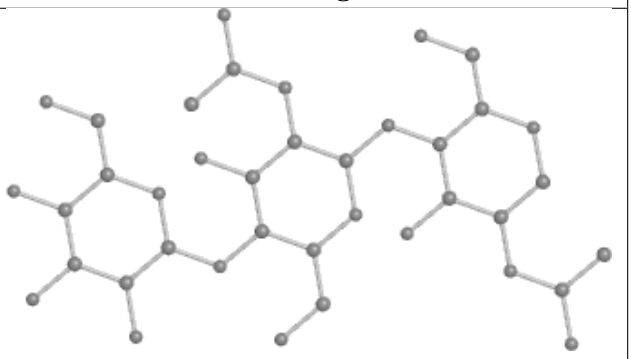
Bond lengths



Bond angles

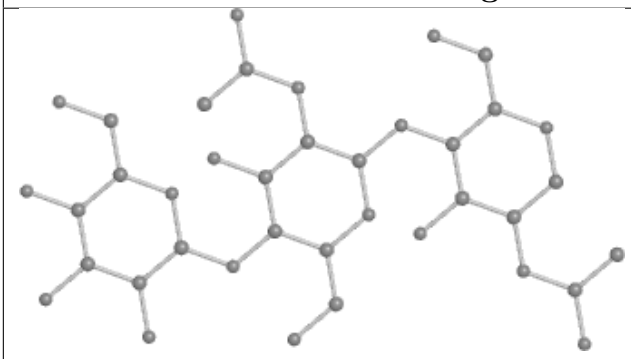


Torsions

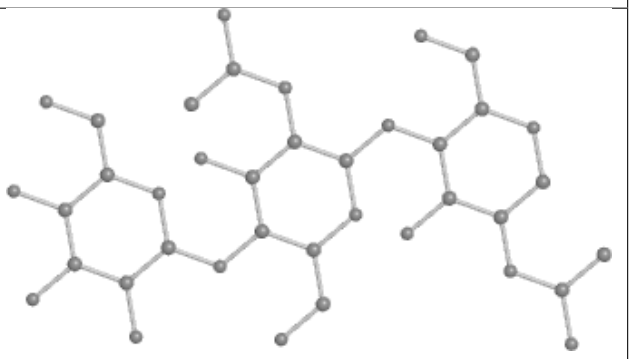


Rings

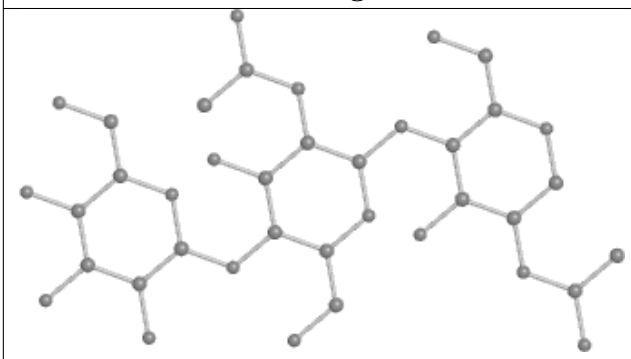
Oligosaccharide Chain DA



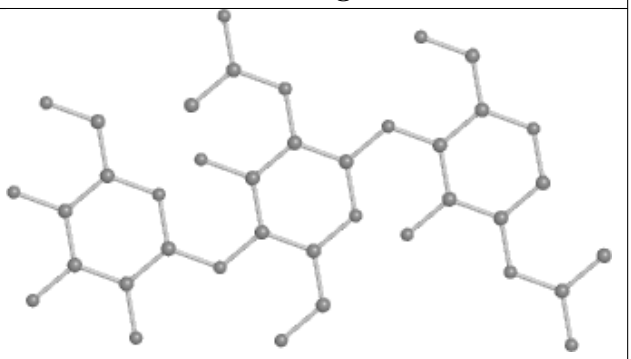
Bond lengths



Bond angles

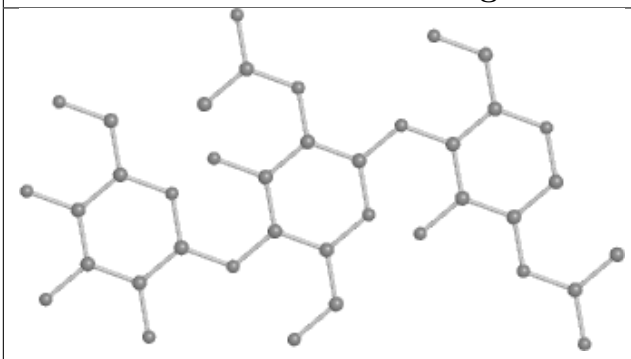


Torsions

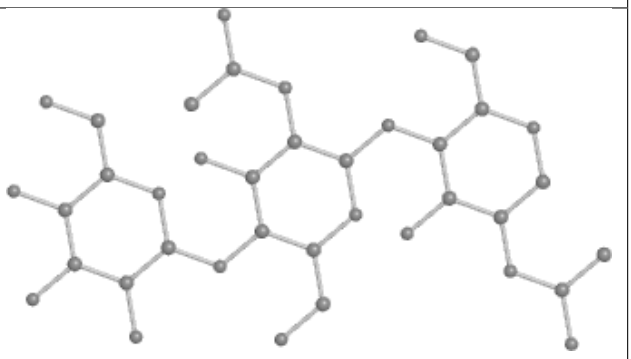


Rings

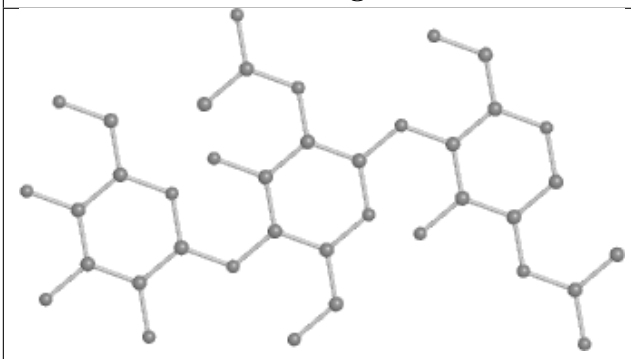
Oligosaccharide Chain GA



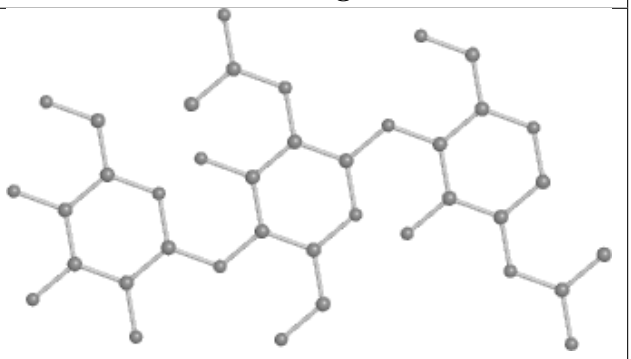
Bond lengths



Bond angles

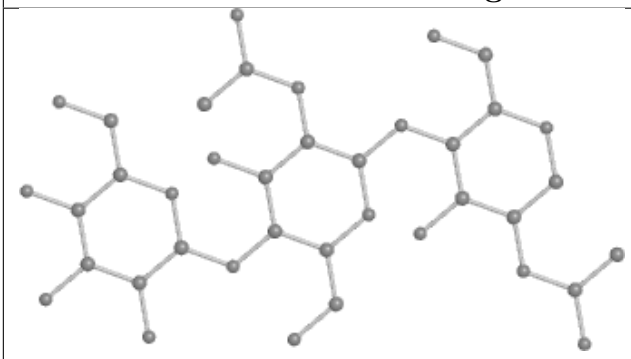


Torsions

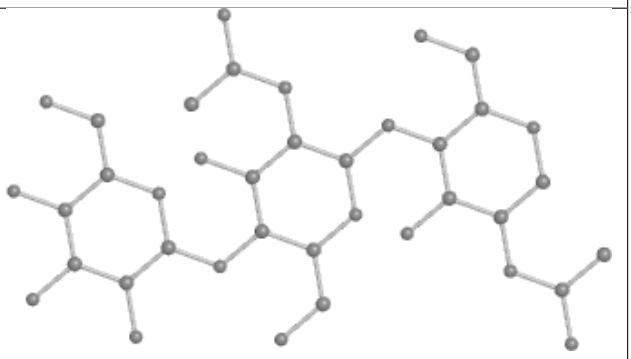


Rings

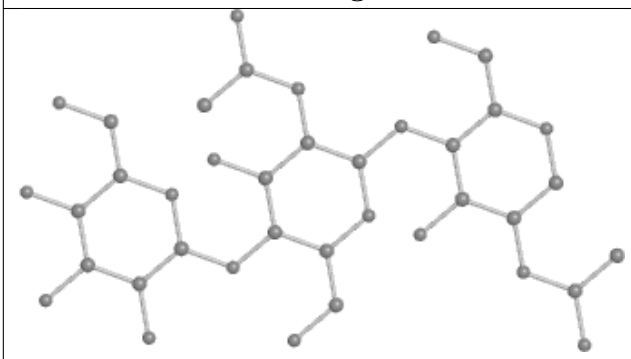
Oligosaccharide Chain JA



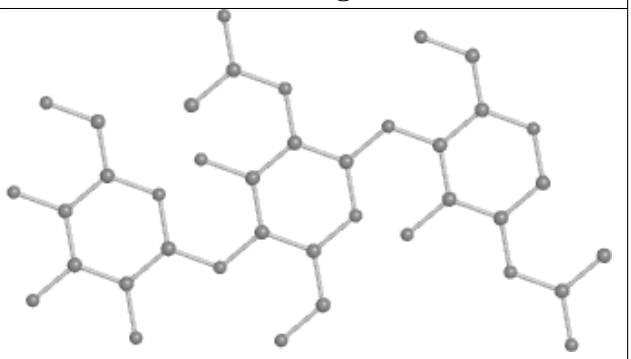
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
7	NAG	C	618	1	14,14,15	0.73	0	17,19,21	0.66	0
7	NAG	C	608	1	14,14,15	0.70	0	17,19,21	0.68	0
7	NAG	J	618	1	14,14,15	0.74	0	17,19,21	0.62	0
7	NAG	B	608	1	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
7	NAG	E	608	1	14,14,15	0.69	0	17,19,21	0.68	0
7	NAG	L	618	1	14,14,15	0.72	0	17,19,21	0.64	0
7	NAG	J	608	1	14,14,15	0.66	0	17,19,21	0.67	0
7	NAG	L	608	1	14,14,15	0.67	0	17,19,21	0.68	1 (5%)
7	NAG	E	618	1	14,14,15	0.72	0	17,19,21	0.64	0
7	NAG	I	618	1	14,14,15	0.74	0	17,19,21	0.65	0
7	NAG	A	618	1	14,14,15	0.72	0	17,19,21	0.66	0
7	NAG	K	618	1	14,14,15	0.75	0	17,19,21	0.64	0
7	NAG	H	618	1	14,14,15	1.15	2 (14%)	17,19,21	1.24	3 (17%)
7	NAG	A	608	1	14,14,15	0.63	0	17,19,21	0.68	0
7	NAG	K	608	1	14,14,15	0.71	0	17,19,21	0.68	0
7	NAG	I	608	1	14,14,15	0.70	0	17,19,21	0.67	0
7	NAG	G	618	1	14,14,15	0.71	0	17,19,21	0.65	0
7	NAG	D	618	1	14,14,15	0.76	1 (7%)	17,19,21	0.65	0
7	NAG	F	618	1	14,14,15	0.75	0	17,19,21	0.63	0
7	NAG	D	608	1	14,14,15	0.79	1 (7%)	17,19,21	0.67	0
7	NAG	B	618	1	14,14,15	0.78	1 (7%)	17,19,21	0.64	0
7	NAG	F	608	1	14,14,15	0.67	0	17,19,21	0.67	0
7	NAG	H	608	1	14,14,15	0.78	1 (7%)	17,19,21	0.68	1 (5%)
7	NAG	G	608	1	14,14,15	0.68	0	17,19,21	0.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	618	1	-	2/6/23/26	0/1/1/1
7	NAG	C	608	1	-	2/6/23/26	0/1/1/1
7	NAG	J	618	1	-	2/6/23/26	0/1/1/1
7	NAG	B	608	1	-	2/6/23/26	0/1/1/1
7	NAG	E	608	1	-	2/6/23/26	0/1/1/1
7	NAG	L	618	1	-	2/6/23/26	0/1/1/1
7	NAG	J	608	1	-	2/6/23/26	0/1/1/1
7	NAG	L	608	1	-	2/6/23/26	0/1/1/1
7	NAG	E	618	1	-	2/6/23/26	0/1/1/1
7	NAG	I	618	1	-	2/6/23/26	0/1/1/1
7	NAG	A	618	1	-	2/6/23/26	0/1/1/1
7	NAG	K	618	1	-	2/6/23/26	0/1/1/1
7	NAG	H	618	1	-	2/6/23/26	0/1/1/1
7	NAG	A	608	1	-	2/6/23/26	0/1/1/1
7	NAG	K	608	1	-	2/6/23/26	0/1/1/1
7	NAG	I	608	1	-	2/6/23/26	0/1/1/1
7	NAG	G	618	1	-	2/6/23/26	0/1/1/1
7	NAG	D	618	1	-	2/6/23/26	0/1/1/1
7	NAG	F	618	1	-	2/6/23/26	0/1/1/1
7	NAG	D	608	1	-	2/6/23/26	0/1/1/1
7	NAG	B	618	1	-	2/6/23/26	0/1/1/1
7	NAG	F	608	1	-	2/6/23/26	0/1/1/1
7	NAG	H	608	1	-	2/6/23/26	0/1/1/1
7	NAG	G	608	1	-	2/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	618	NAG	O5-C5	2.45	1.48	1.43
7	D	608	NAG	C4-C3	2.29	1.58	1.52
7	H	608	NAG	C4-C3	2.26	1.58	1.52
7	B	608	NAG	C4-C3	2.19	1.57	1.52
7	B	618	NAG	C4-C3	2.10	1.57	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	618	NAG	O4-C4-C3	2.63	116.42	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	618	NAG	C3-C4-C5	2.59	114.85	110.24
7	H	618	NAG	C1-O5-C5	2.02	114.93	112.19
7	L	608	NAG	C2-N2-C7	-2.01	120.04	122.90
7	H	608	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	608	NAG	C8-C7-N2-C2
7	A	608	NAG	O7-C7-N2-C2
7	B	608	NAG	C8-C7-N2-C2
7	B	608	NAG	O7-C7-N2-C2
7	C	608	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.

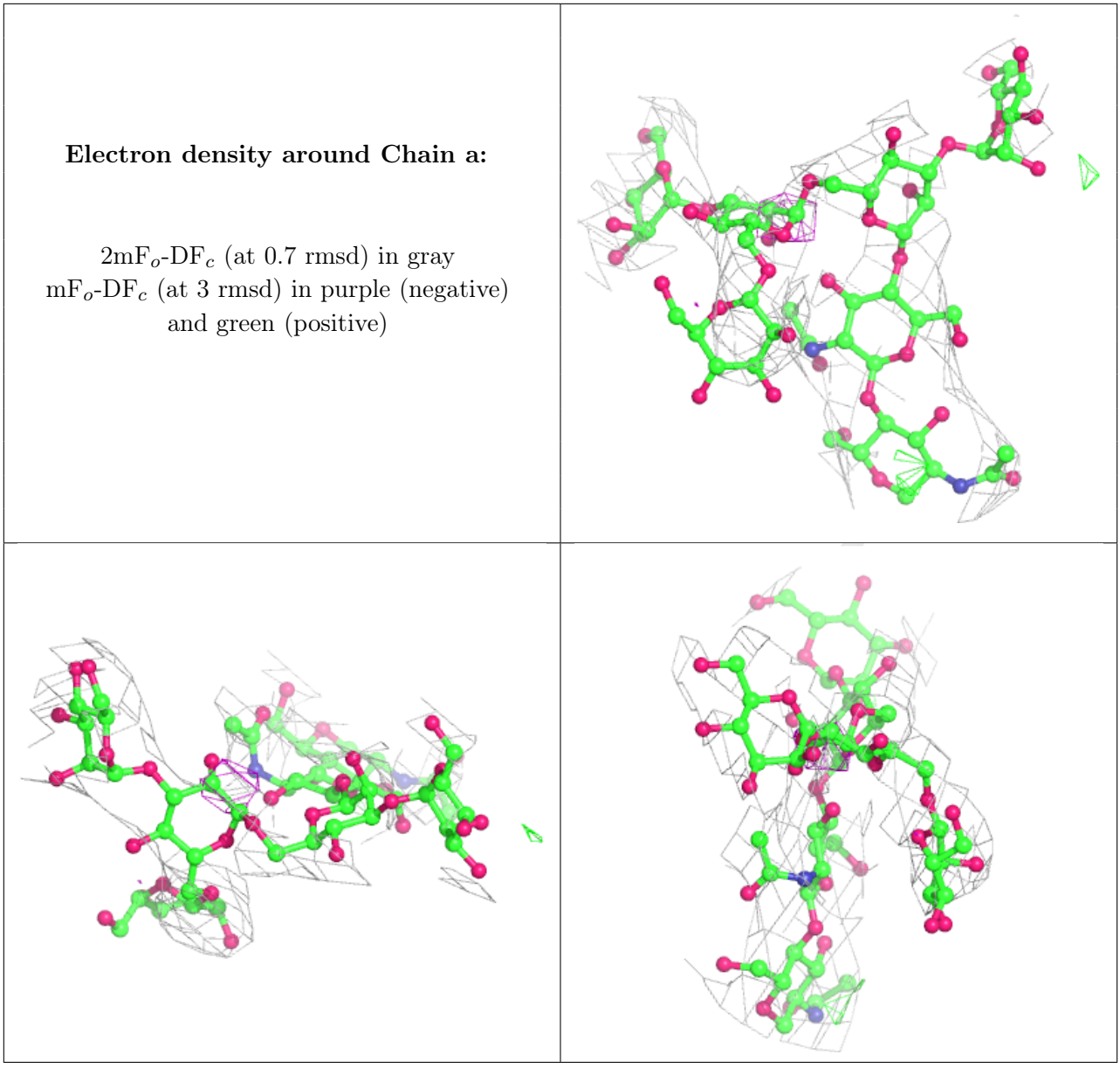
6.3 Carbohydrates

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.

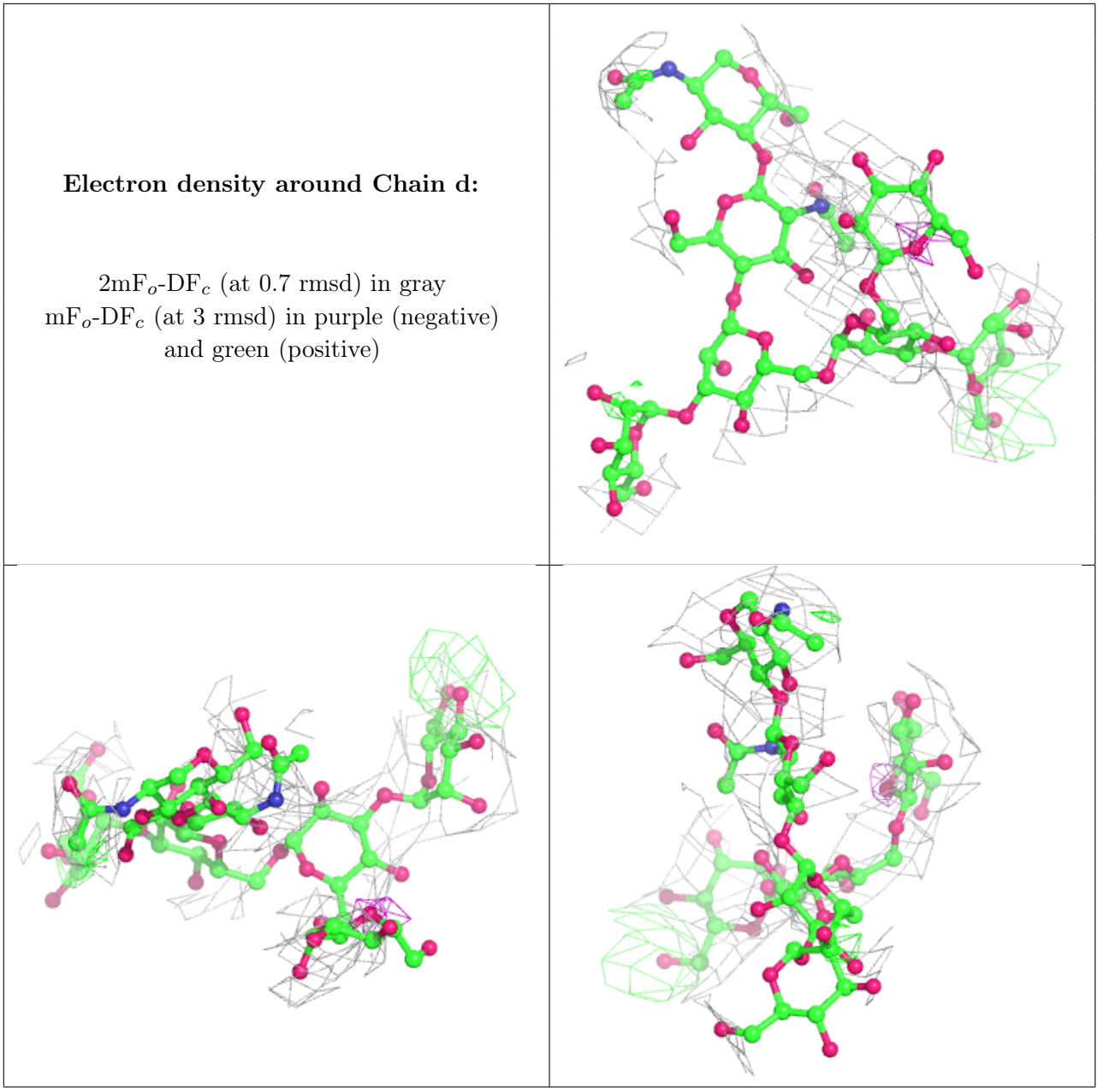
Electron density around Chain a:

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



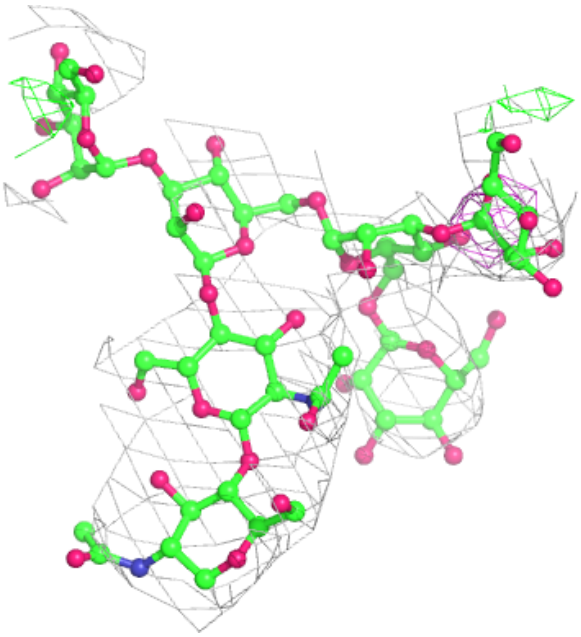
Electron density around Chain d:

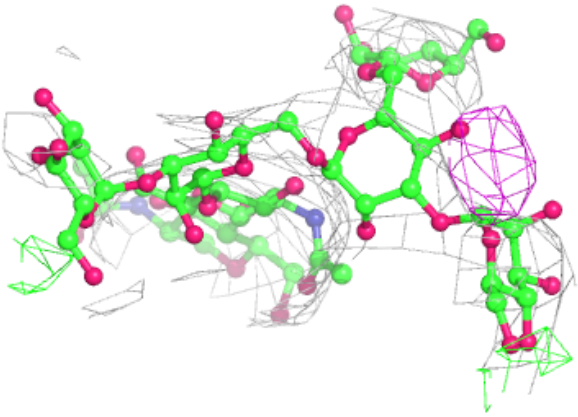
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

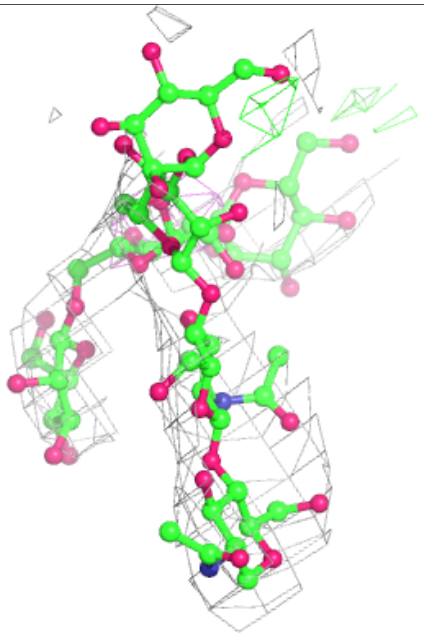


Electron density around Chain g:

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

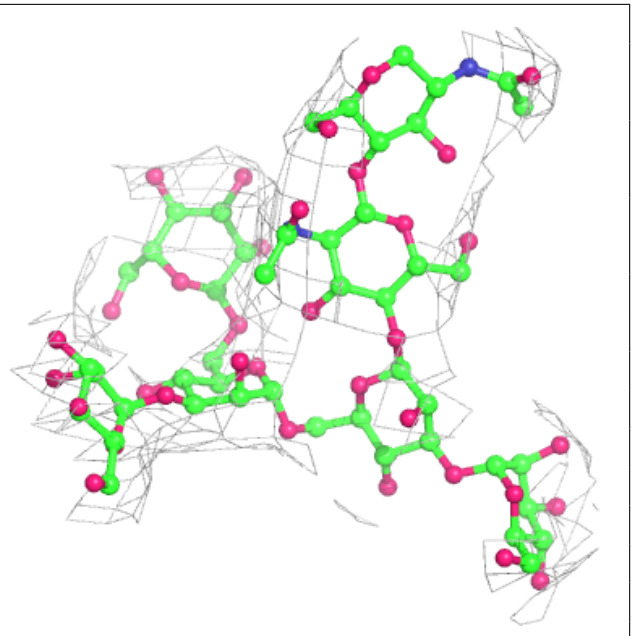


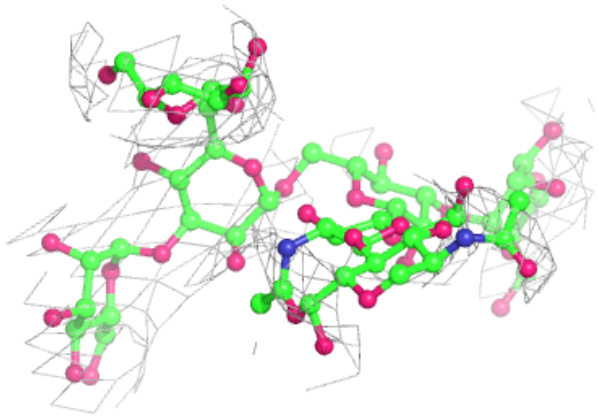


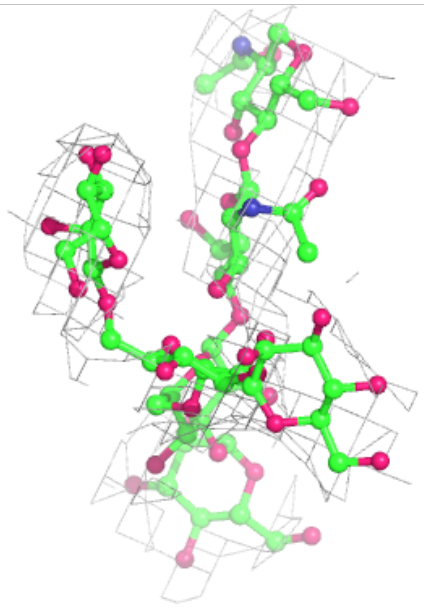


Electron density around Chain j:

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

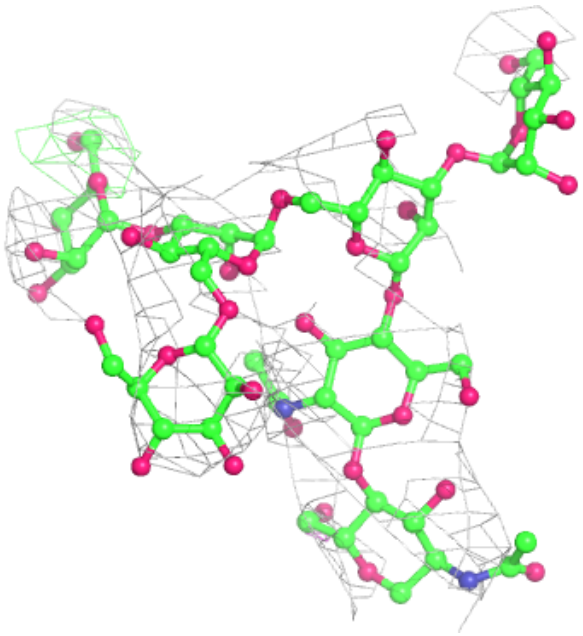


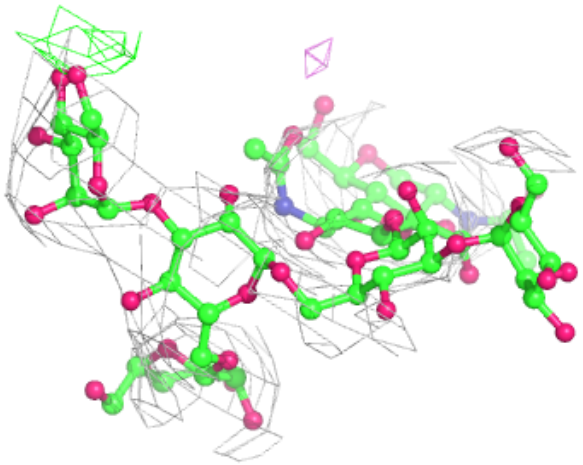


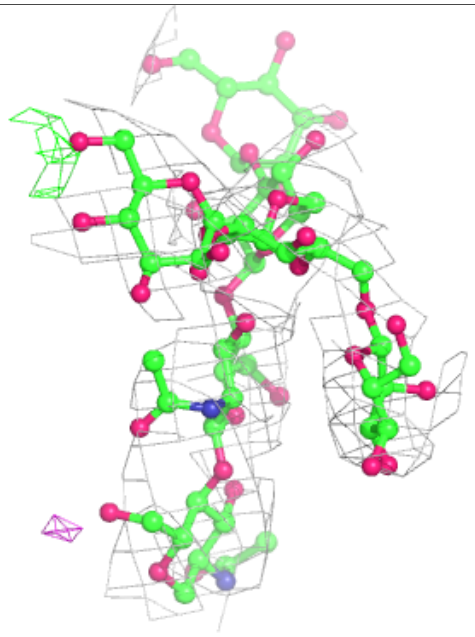


Electron density around Chain m:

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

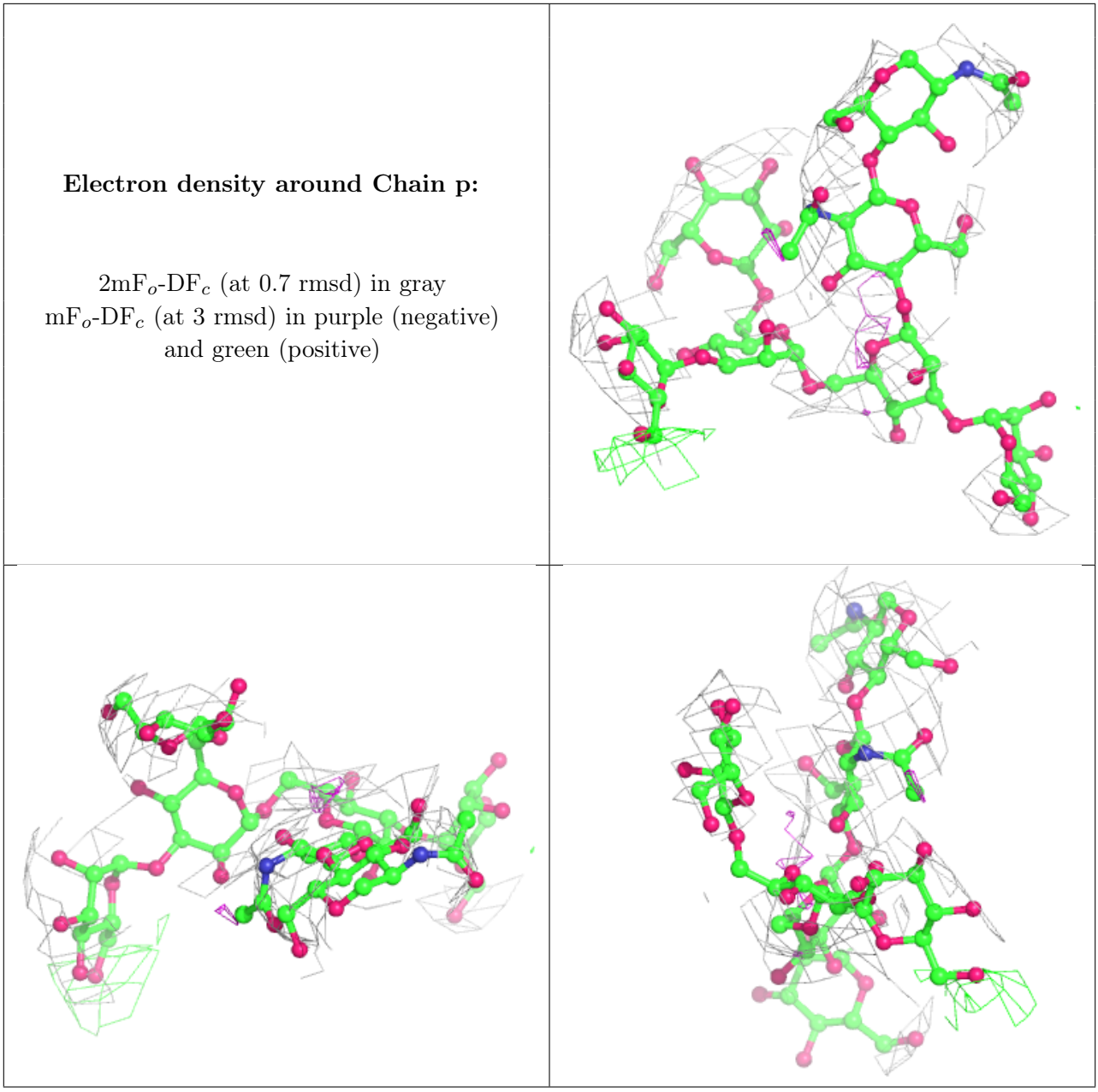






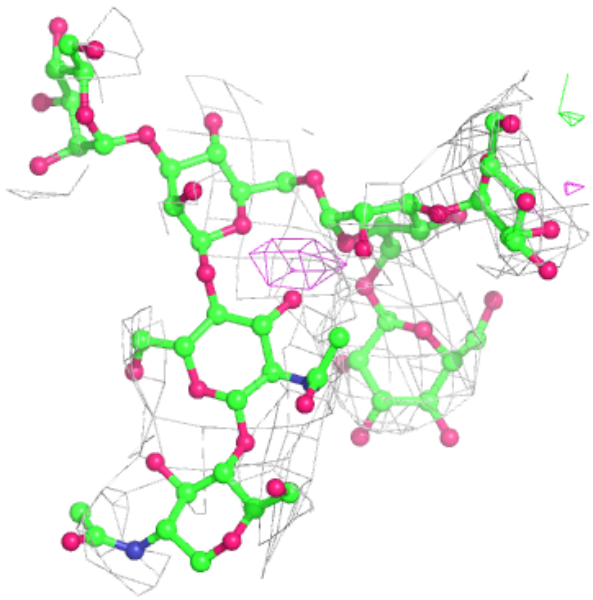
Electron density around Chain p:

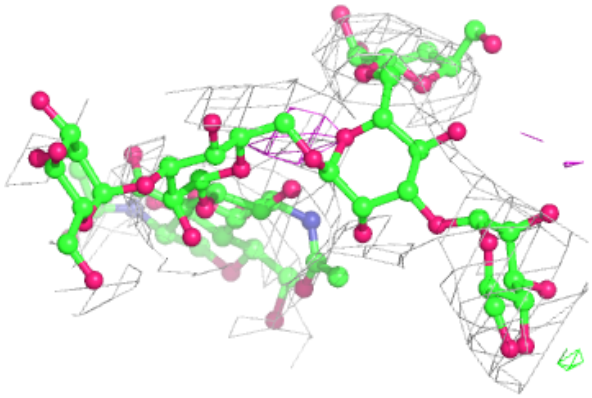
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

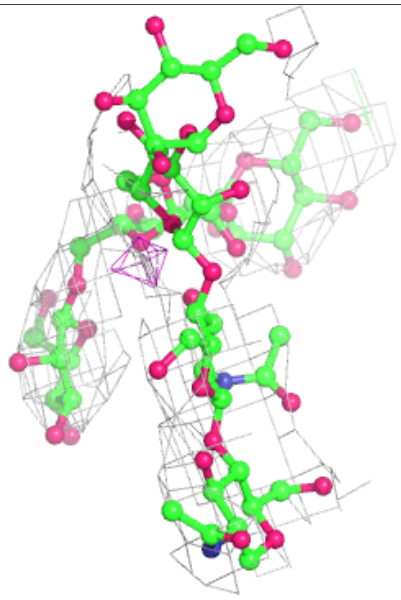


Electron density around Chain s:

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

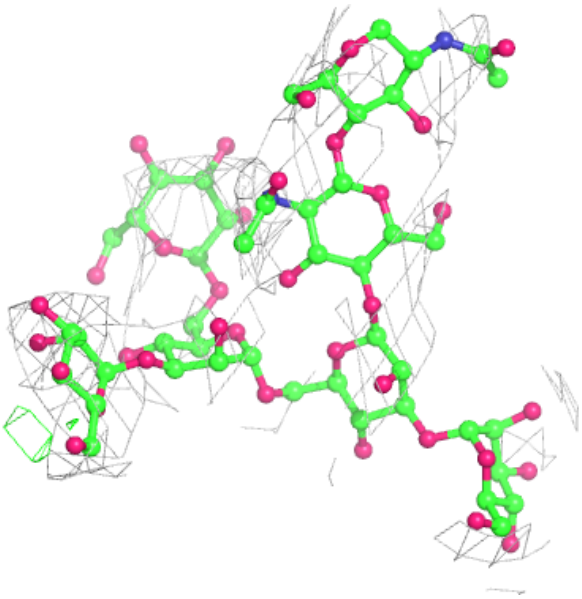


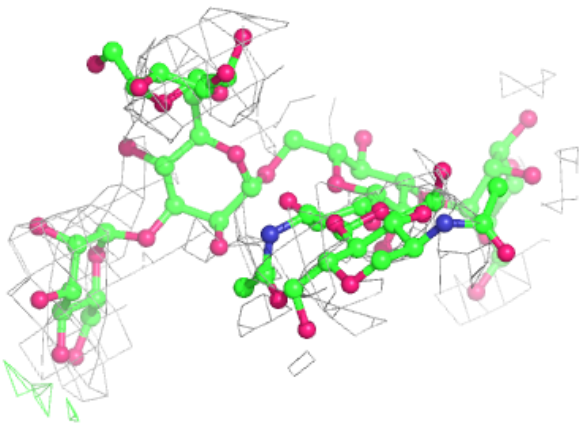


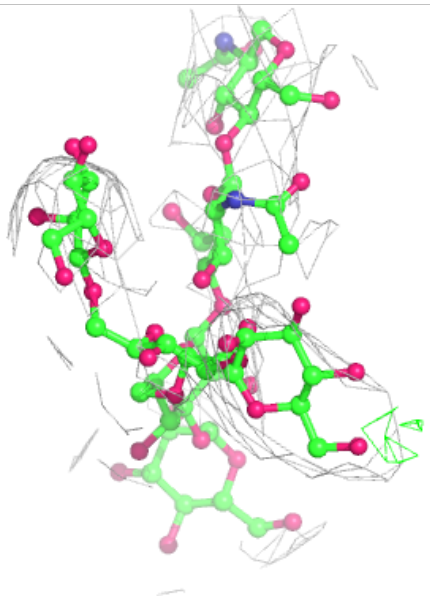


Electron density around Chain v:

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

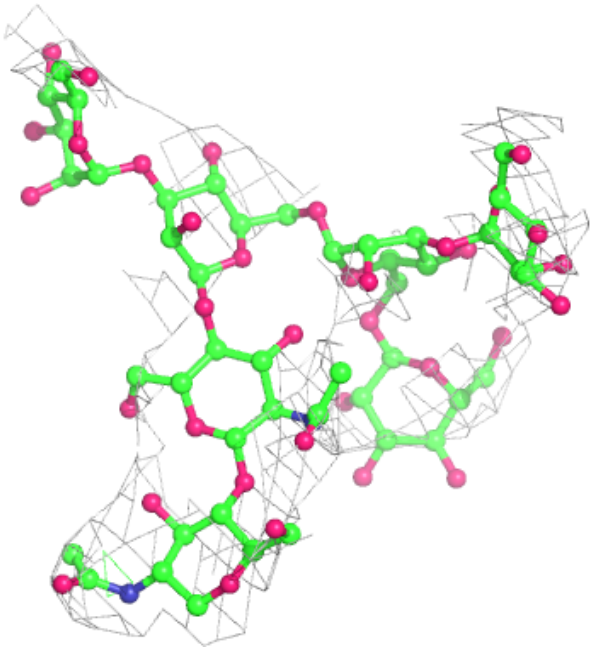


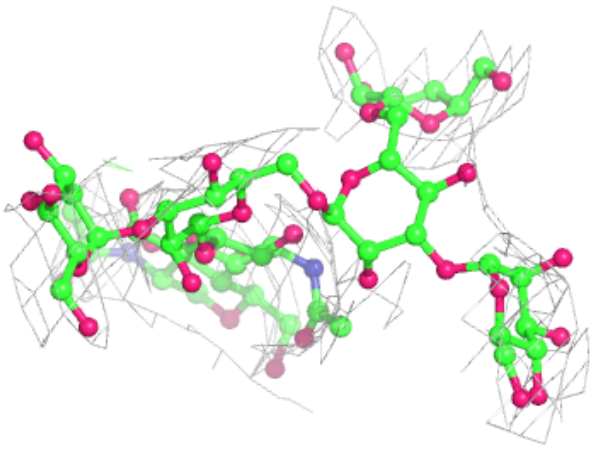


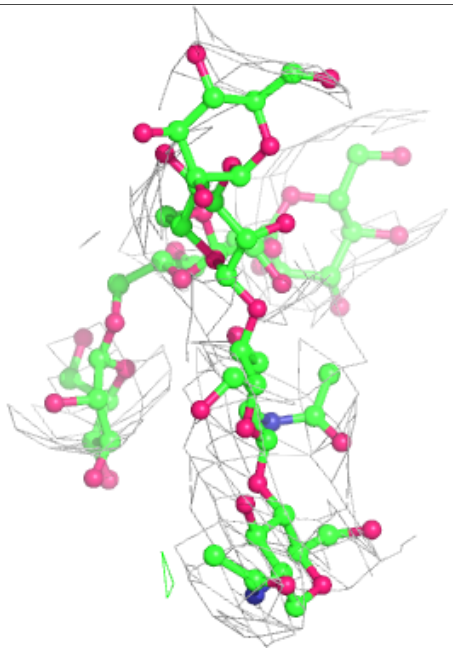


Electron density around Chain y:

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

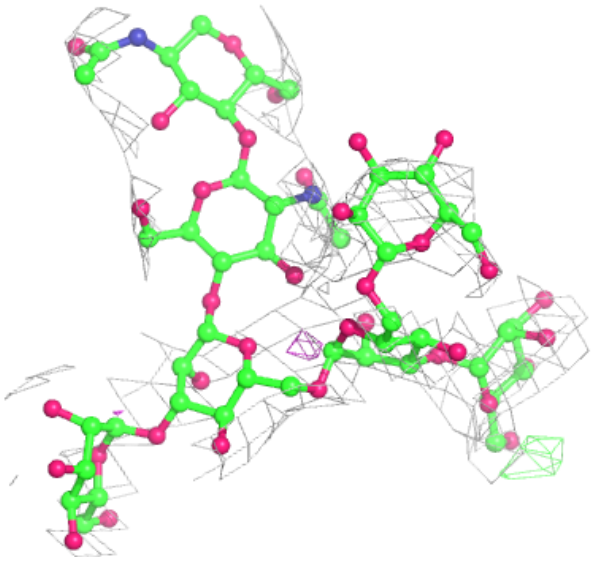


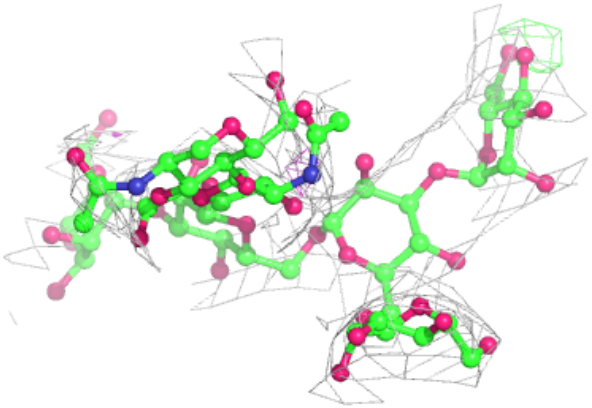


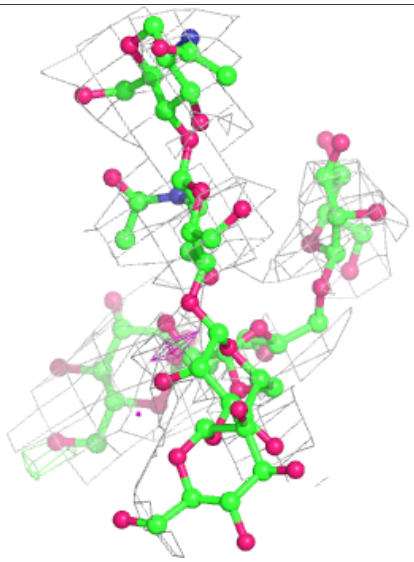


Electron density around Chain BA:

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

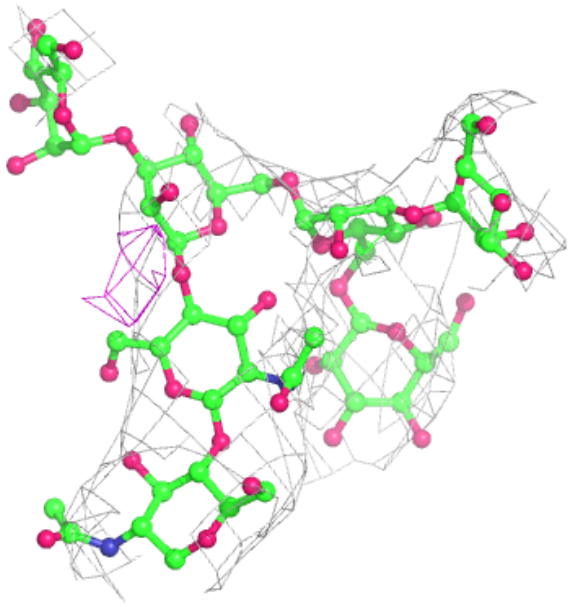


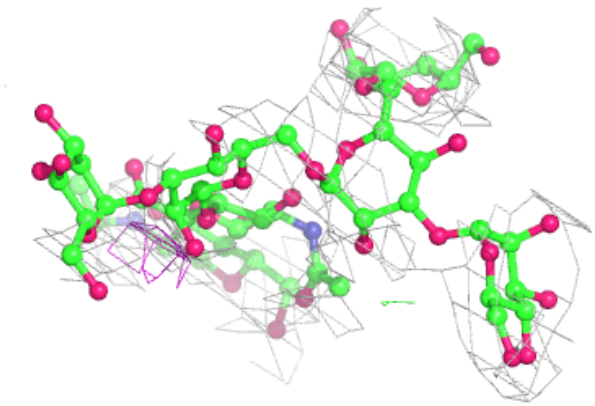


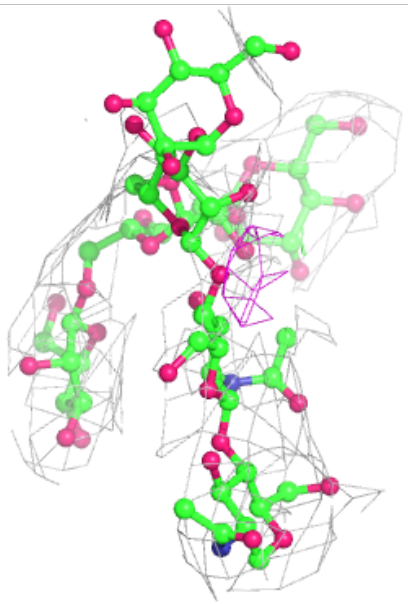


Electron density around Chain EA:

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

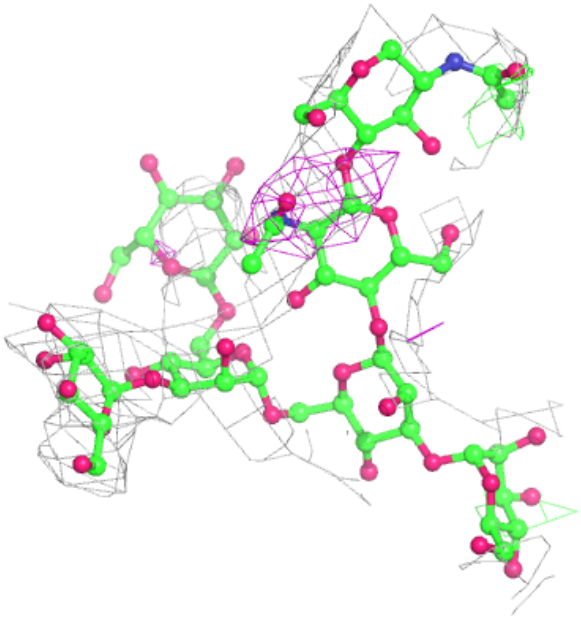


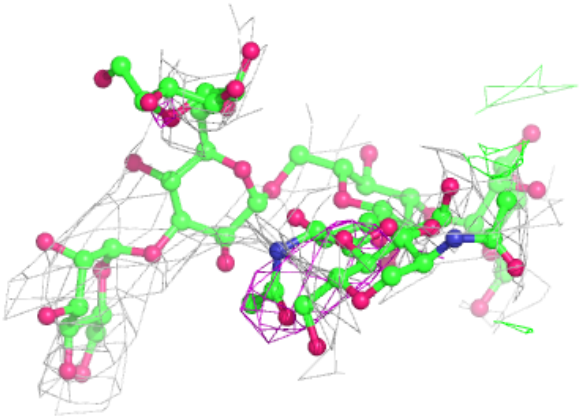


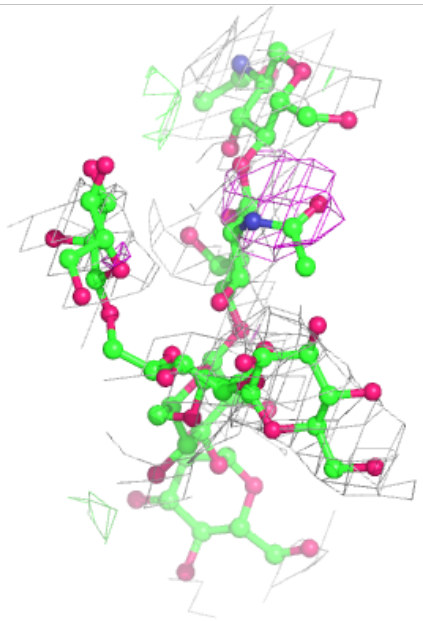


Electron density around Chain HA:

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

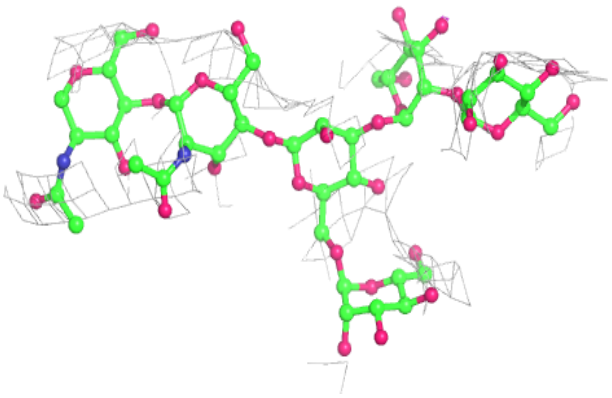


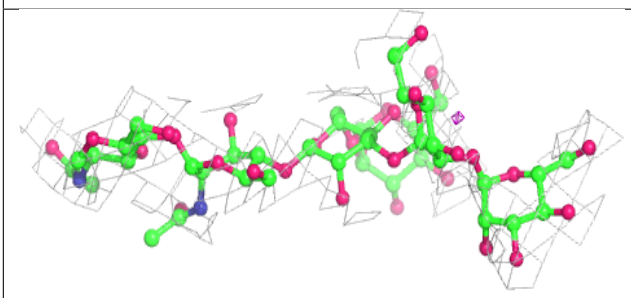


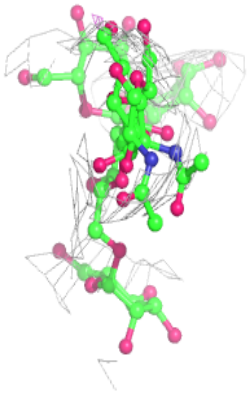


Electron density around Chain b:

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

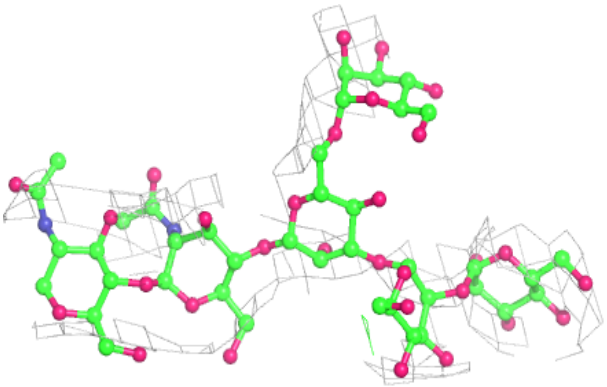


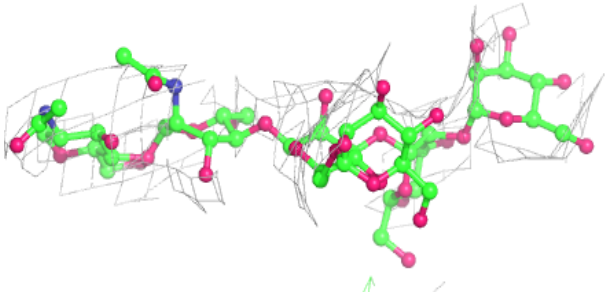


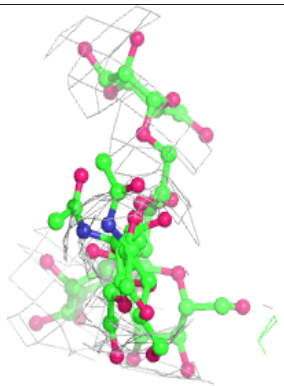


Electron density around Chain e:

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

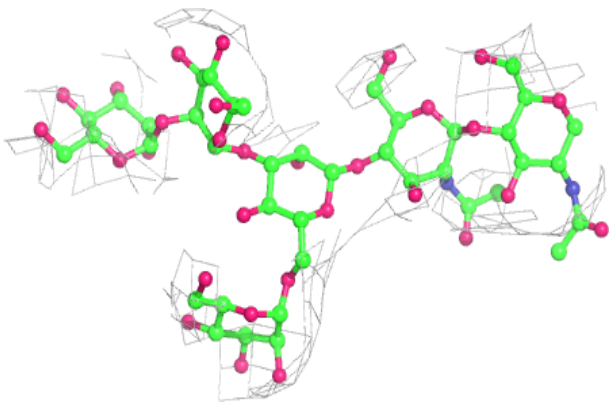


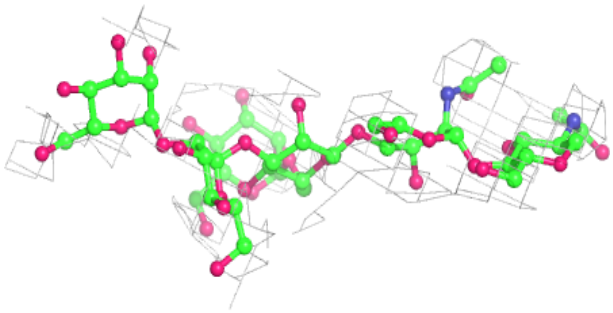


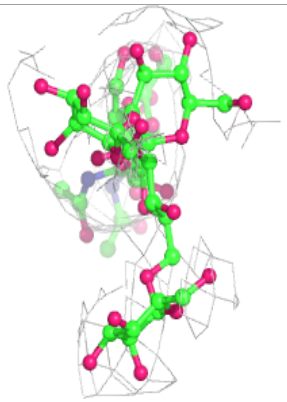


Electron density around Chain h:

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

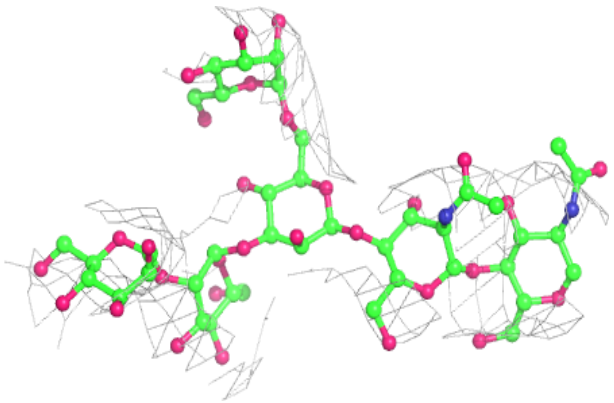


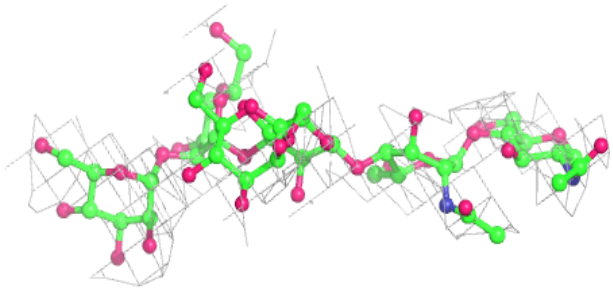


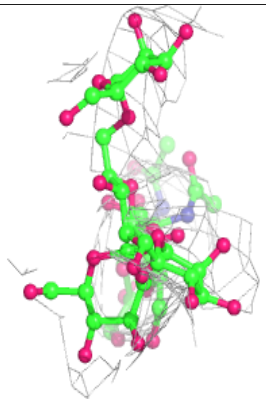


Electron density around Chain k:

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

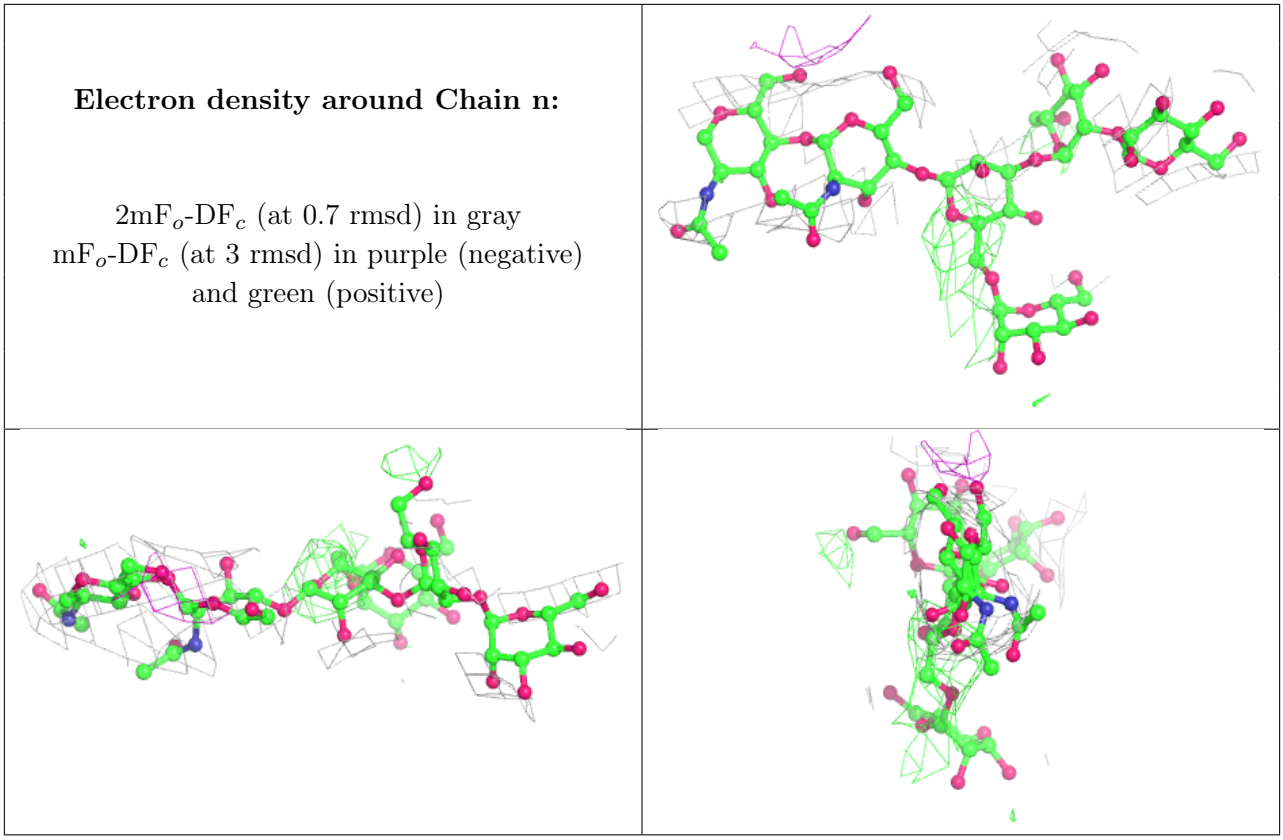






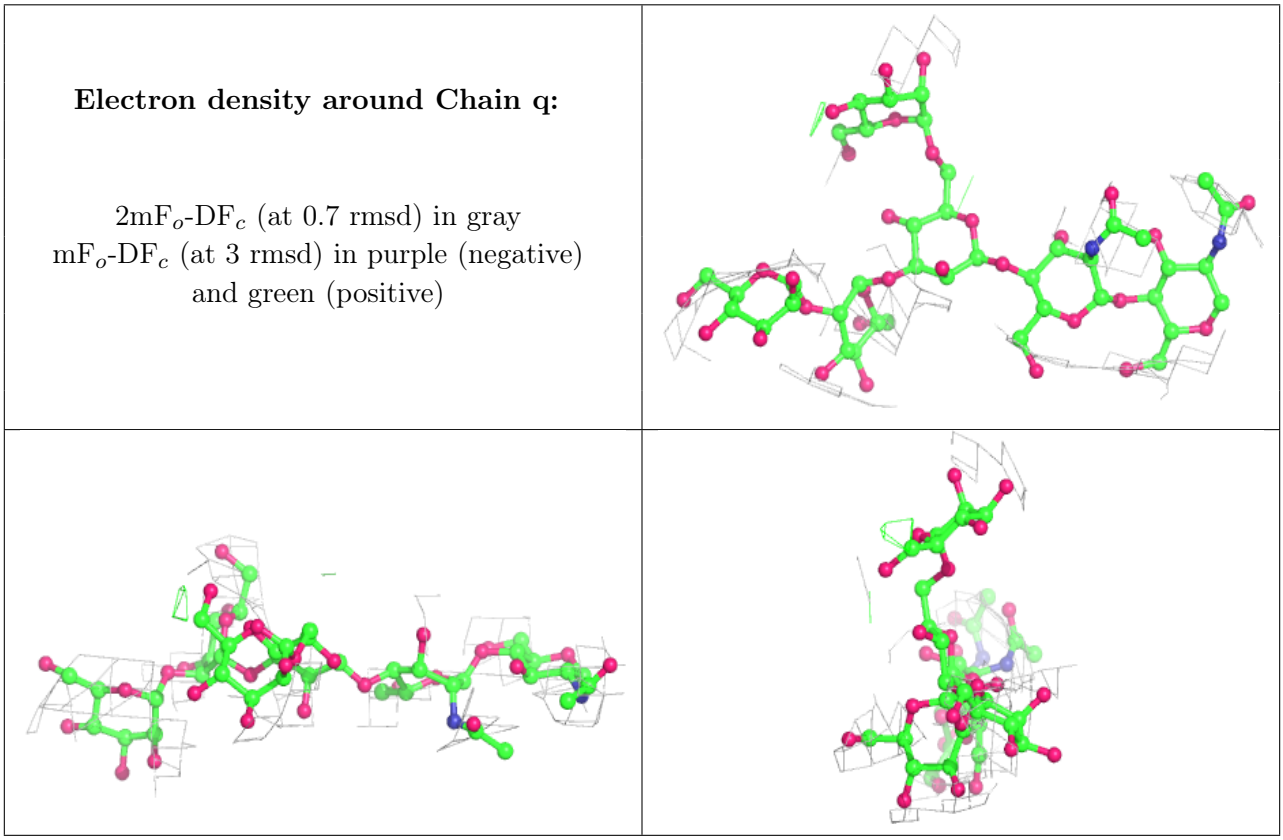
Electron density around Chain n:

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



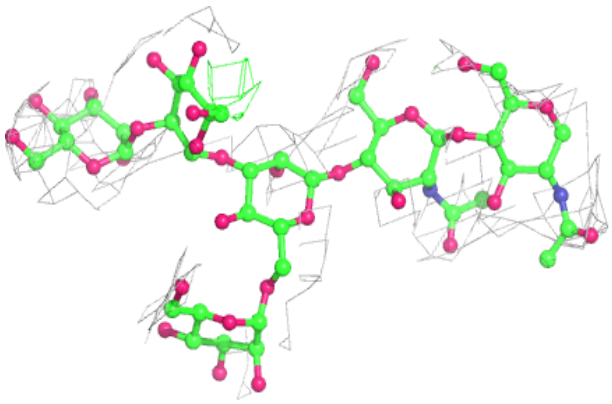
Electron density around Chain q:

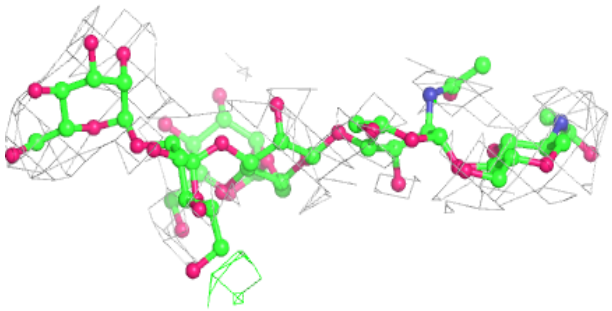
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

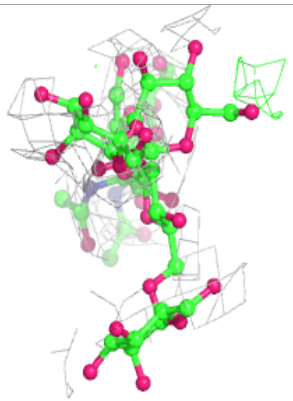


Electron density around Chain t:

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

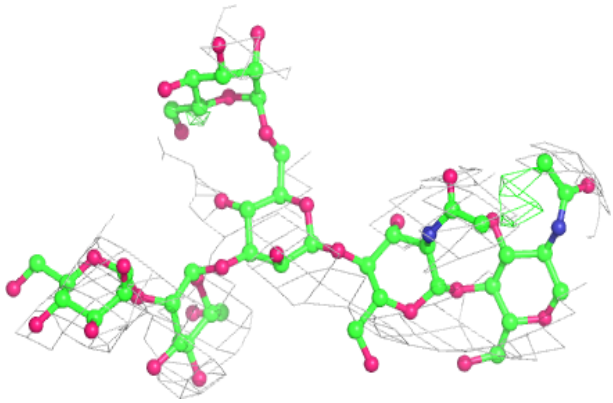


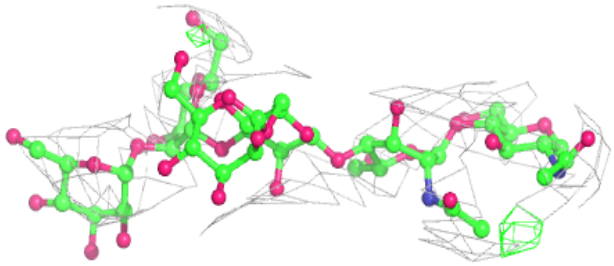


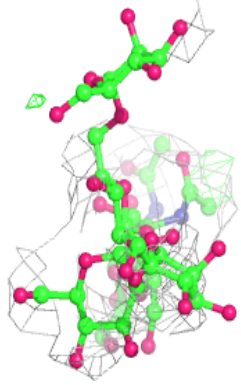


Electron density around Chain w:

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

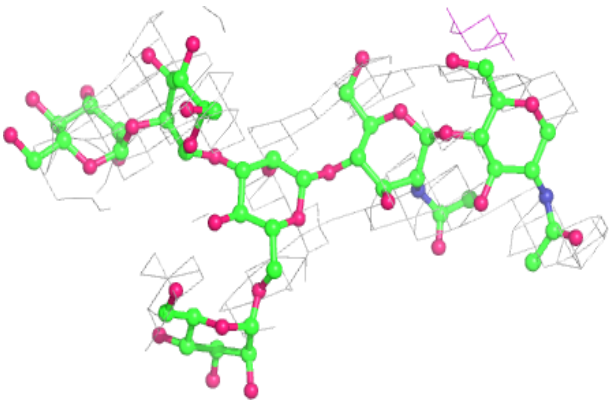


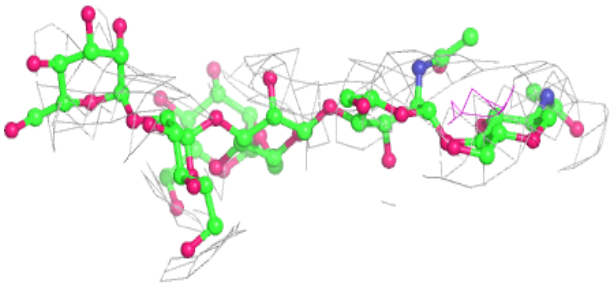


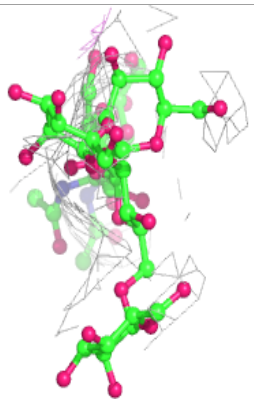


Electron density around Chain z:

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

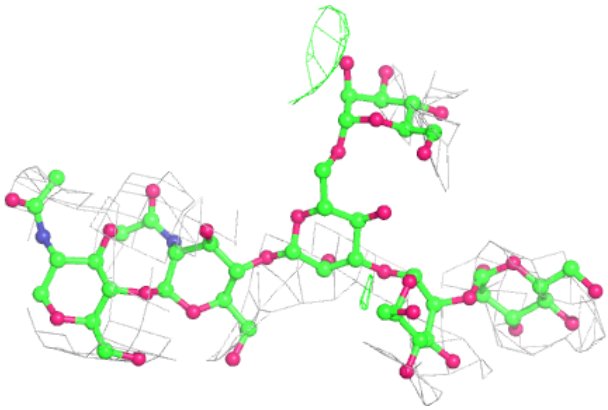


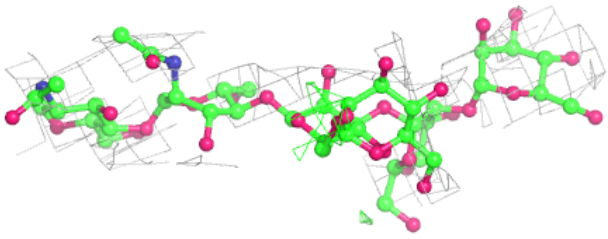


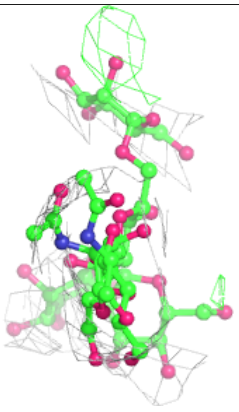


Electron density around Chain CA:

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

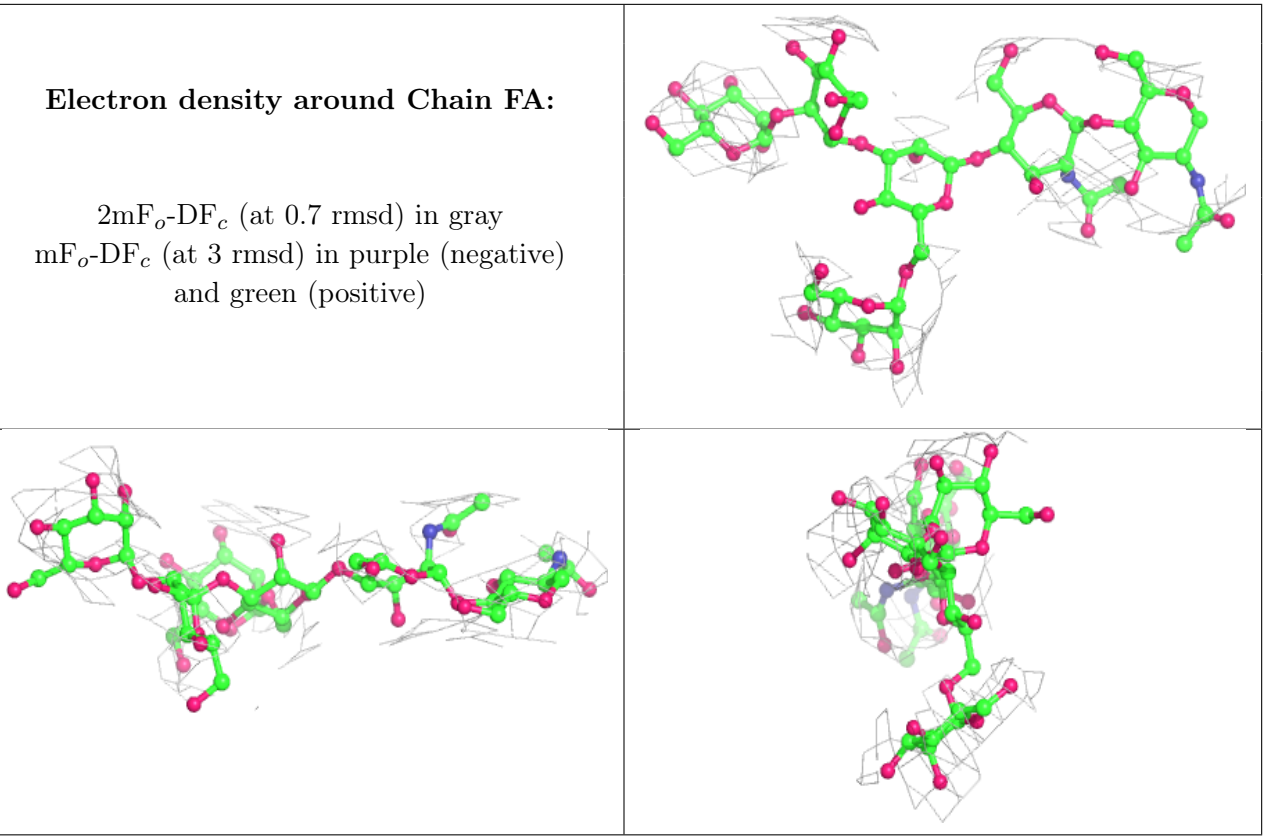






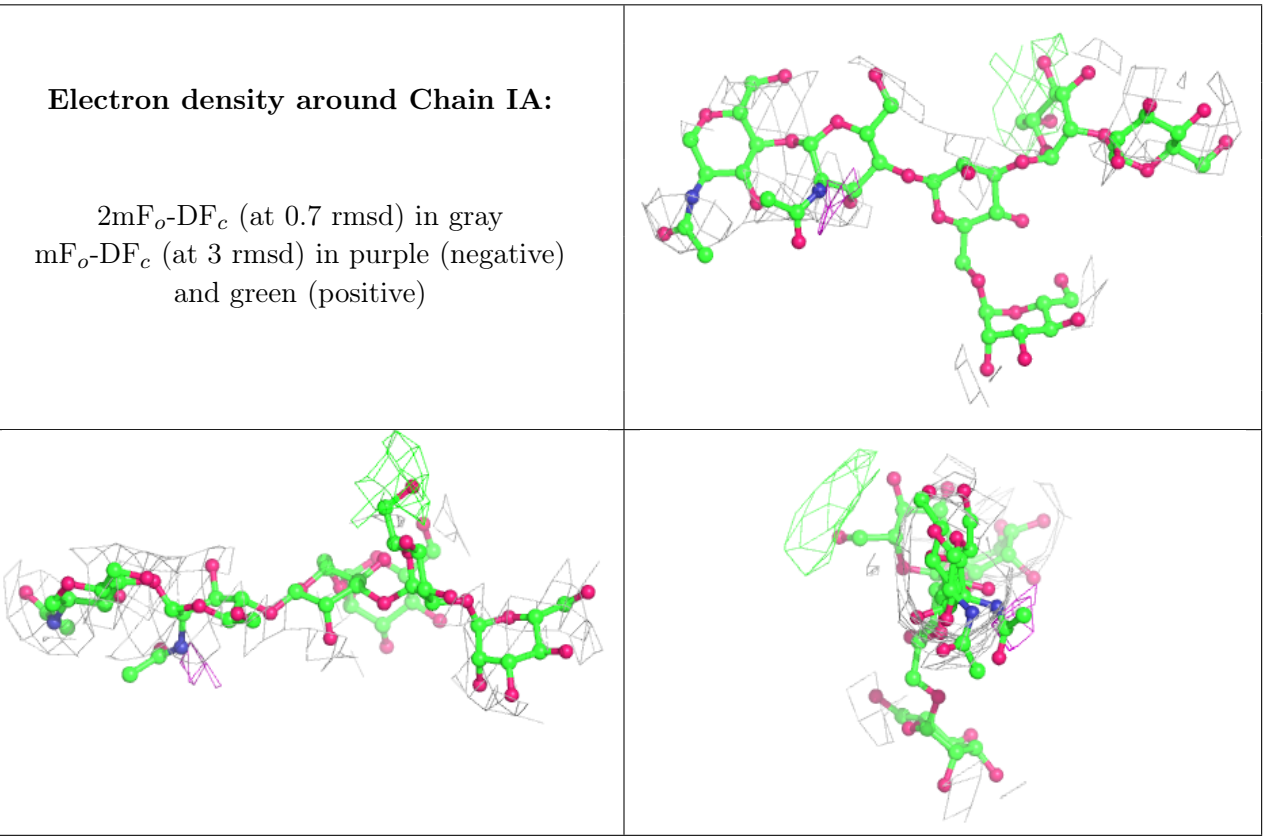
Electron density around Chain FA:

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



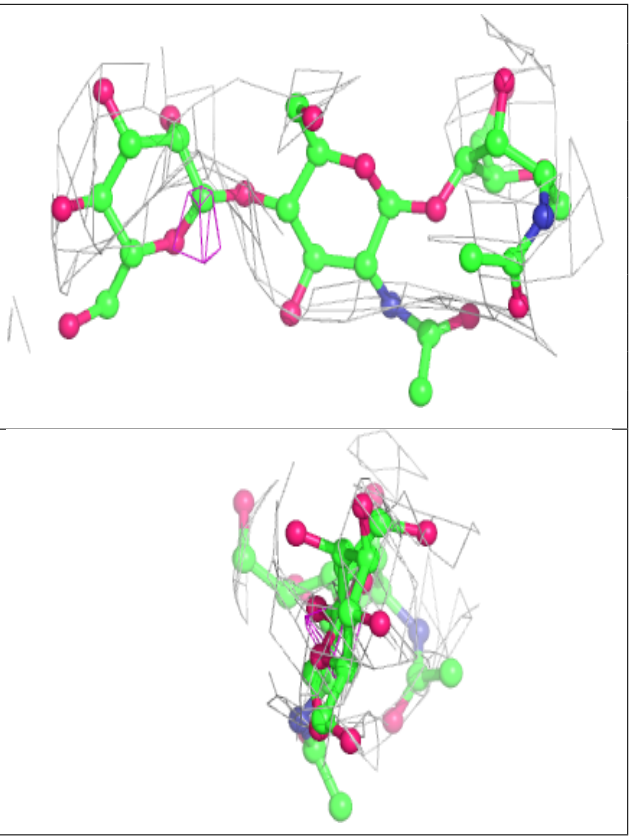
Electron density around Chain IA:

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



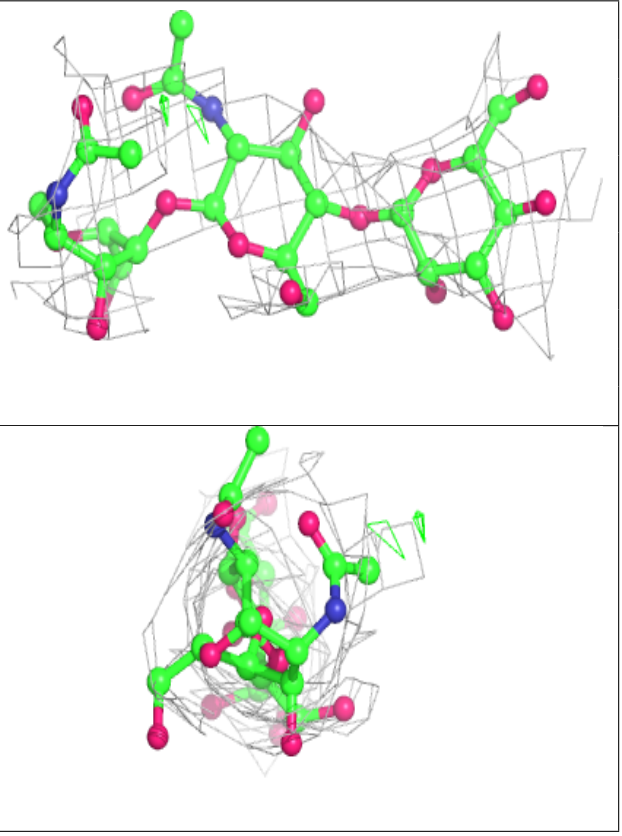
Electron density around Chain c:

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



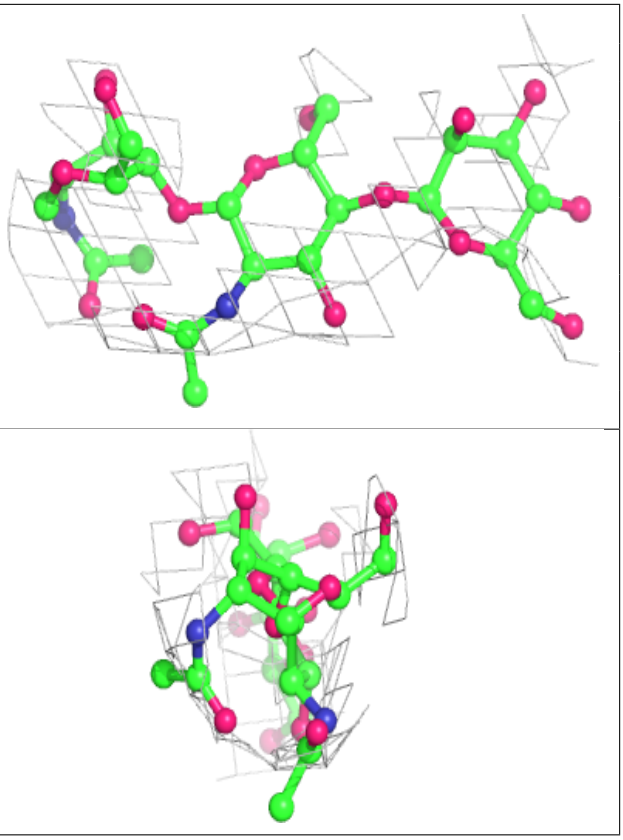
Electron density around Chain f:

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



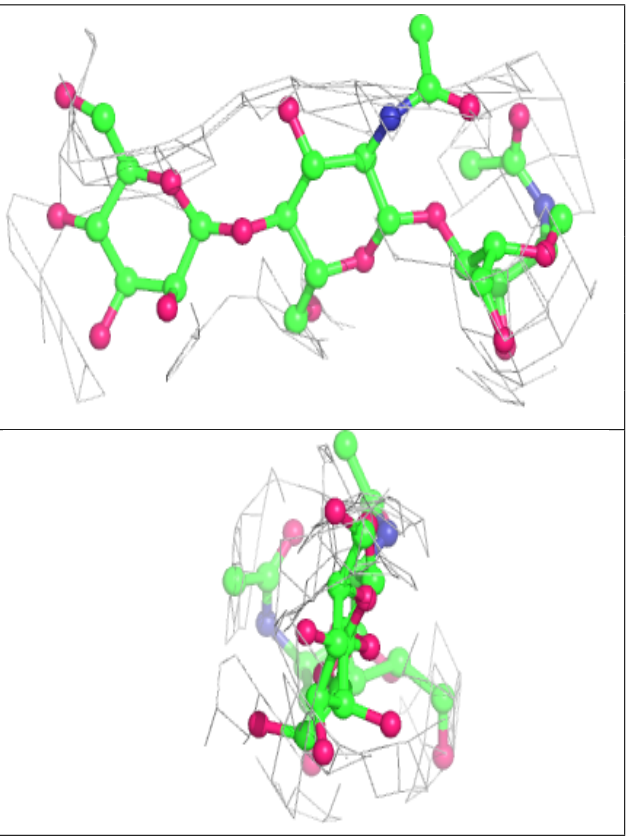
Electron density around Chain i:

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



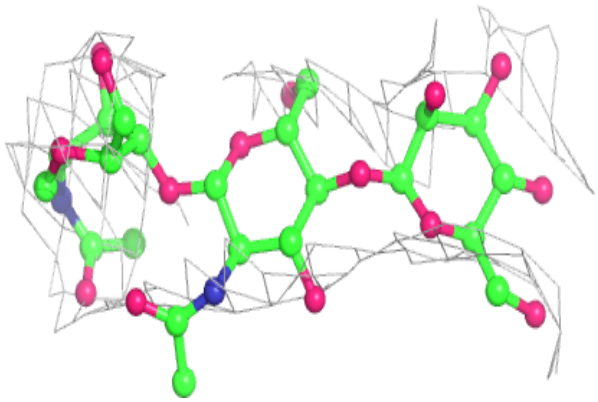
Electron density around Chain l:

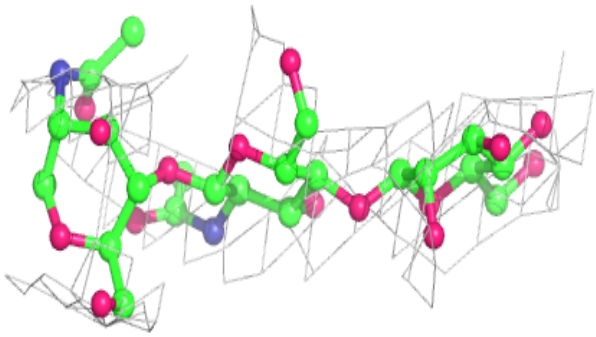
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

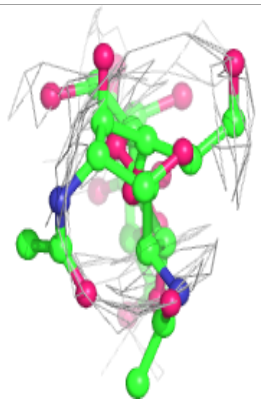


Electron density around Chain o:

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

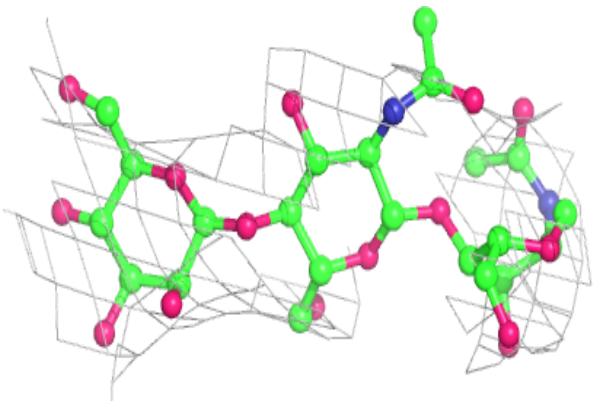


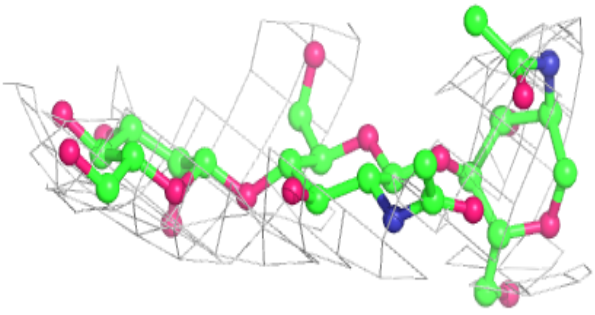


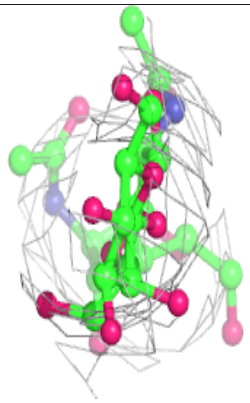


Electron density around Chain r:

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

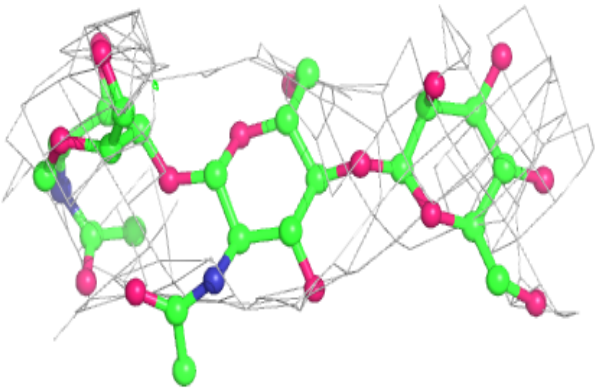


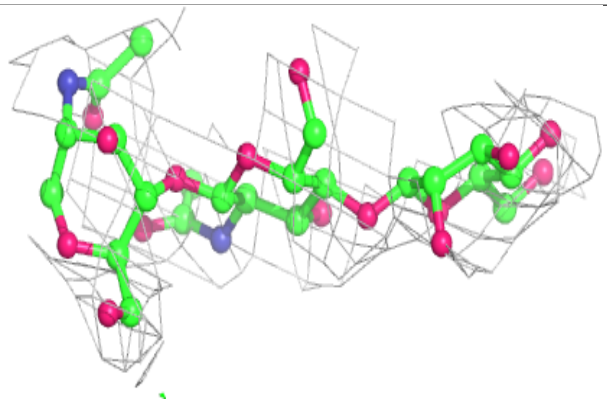


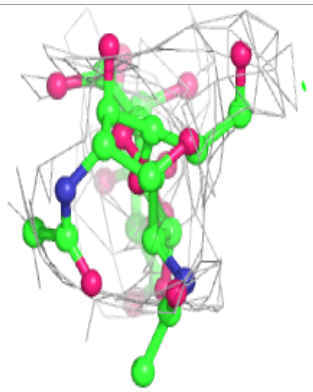


Electron density around Chain u:

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

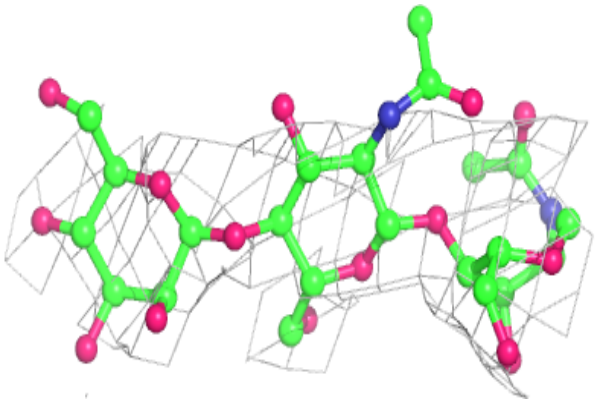


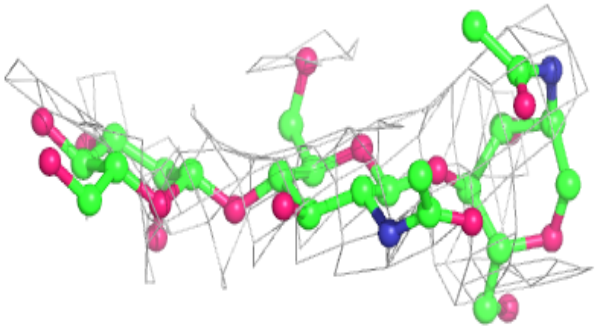


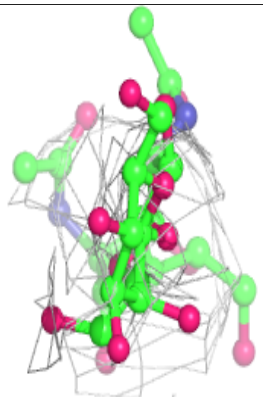


Electron density around Chain x:

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

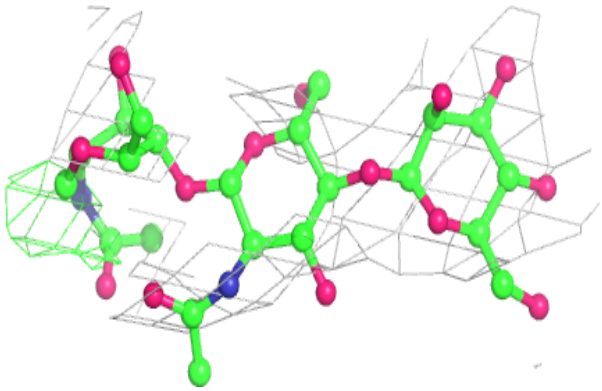


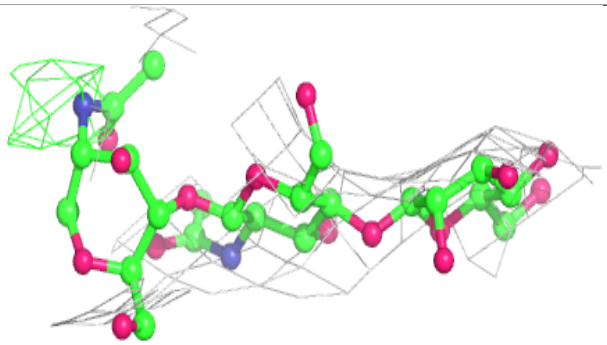


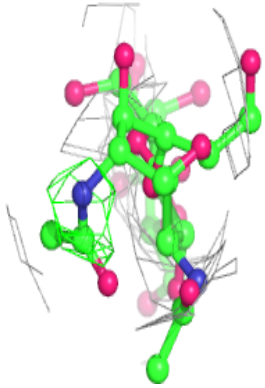


Electron density around Chain AA:

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

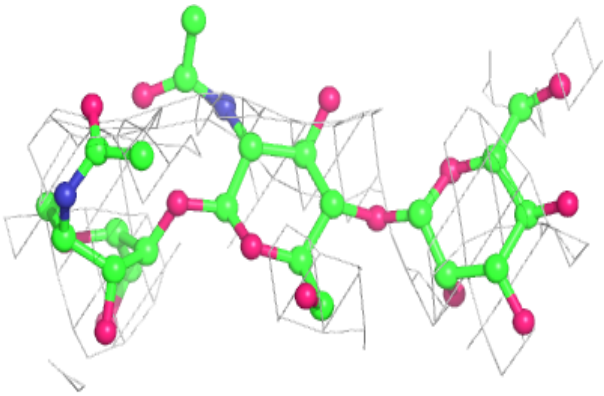


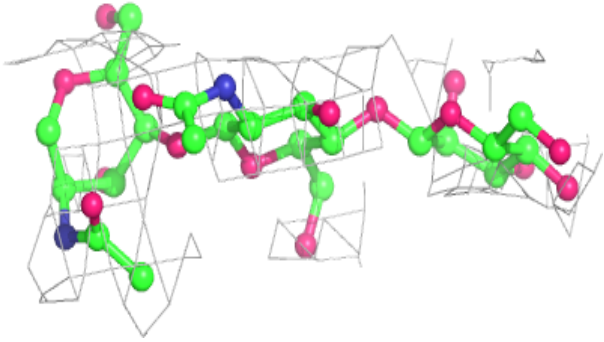


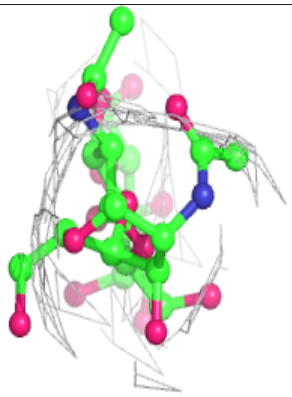


Electron density around Chain DA:

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

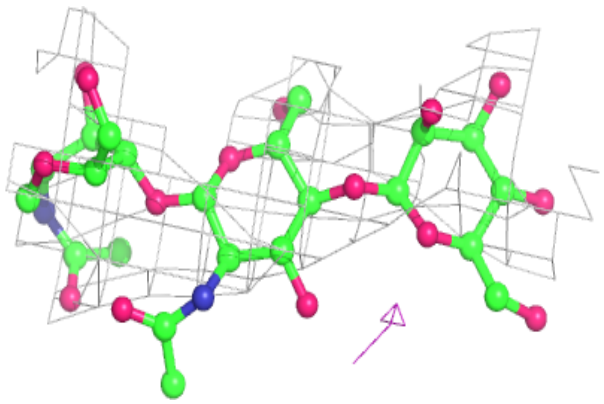


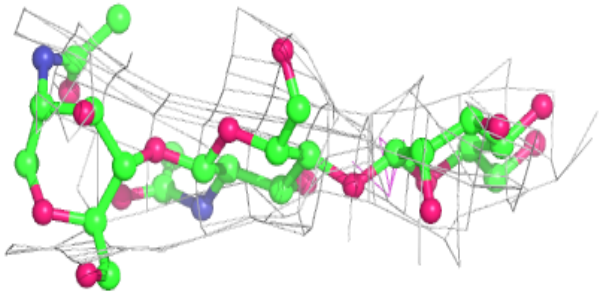


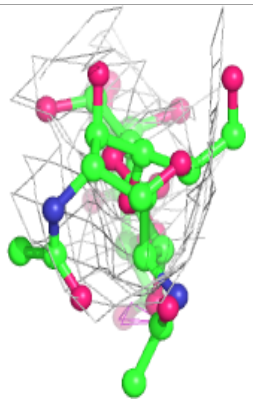


Electron density around Chain GA:

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

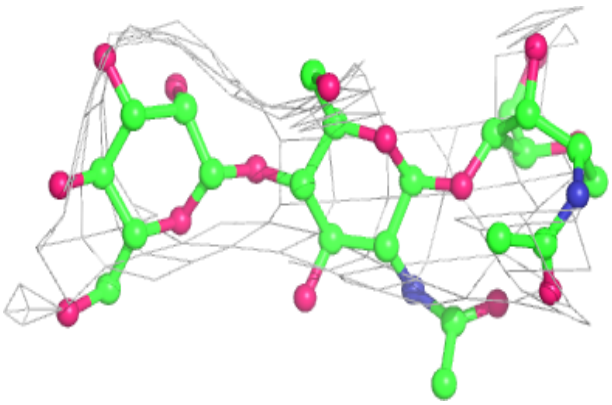


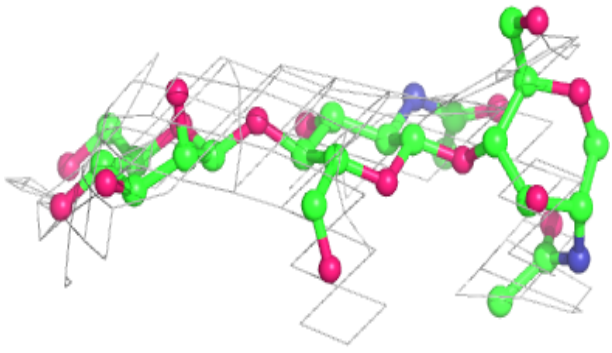


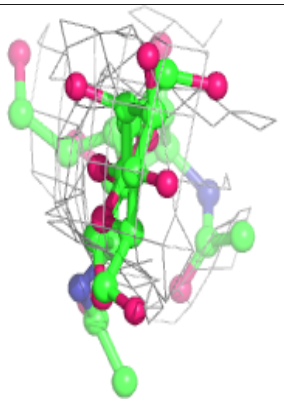


Electron density around Chain JA:

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







6.4 Ligands (i)

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

6.5 Other polymers (i)

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