wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2022 – 10:42 AM EST

PDB ID	:	5WDU
Title	:	HIV-1 Env BG505 SOSIP.664 H72C-H564C trimer in complex with bNAbs PGT122 Fab, 35O22 Fab and NIH45-46 scFv
Authors	:	Julien, J.-P.; Torrents de la Pena, A.; Sanders, R.W.; Wilson, I.A.
Deposited on	:	2017-07-06
Resolution	:	7.00 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:

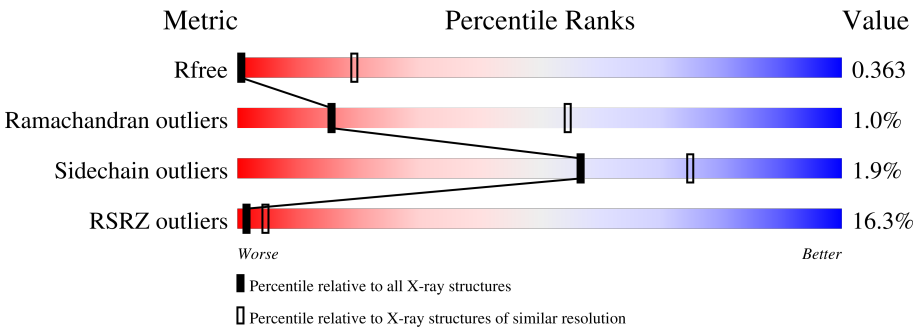
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.00 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	1004 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	471	6% 92% • 5%
1	G	471	3% 92% • 5%
1	Q	471	5% 92% • 5%
2	D	250	16% 86% • 11%
2	O	250	14% 86% • 11%
2	W	250	16% 86% • 11%
3	A	147	2% 82% • 14%

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Mol	Chain	Length	Quality of chain
3	J	147	3% 82% 14%
3	R	147	3% 82% 14%
4	B	210	29% 97%
4	K	210	32% 97%
4	S	210	28% 99%
5	C	232	30% 95%
5	L	232	31% 96%
5	T	232	41% 97%
6	H	242	6% 100%
6	M	242	28% 100%
6	U	242	18% 99%
7	I	213	2% 96%
7	N	213	24% 99%
7	V	213	11% 99%
8	E	5	100%
8	X	5	20% 80%
8	c	5	60% 40%
8	e	5	100%
8	g	5	20% 80%
8	l	5	60% 40%
8	n	5	100%
8	p	5	20% 80%
8	u	5	60% 40%
9	P	3	33% 67%
9	f	3	33% 67%

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Mol	Chain	Length	Quality of chain
9	o	3	33% 67%
10	Y	4	75% 25%
10	h	4	50% 50%
10	q	4	75% 25%
11	Z	7	100%
11	i	7	14% 86%
11	r	7	100%
12	a	6	100%
12	j	6	17% 83%
12	s	6	17% 83%
13	b	2	100%
13	k	2	100%
13	t	2	100%
14	d	8	12% 88%
14	m	8	12% 88%
14	v	8	12% 88%

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
10	NAG	Y	1	-	-	-	X
10	MAN	Y	4	-	-	-	X
10	NAG	h	2	-	-	-	X
10	BMA	h	3	-	-	-	X
10	MAN	h	4	-	-	-	X
11	NAG	Z	2	-	-	-	X
11	BMA	Z	3	-	-	-	X
11	MAN	Z	5	-	-	-	X
11	MAN	Z	6	-	-	-	X
11	MAN	Z	7	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	i	2	-	-	-	X
11	BMA	i	3	-	-	-	X
11	MAN	i	5	-	-	-	X
11	MAN	i	7	-	-	-	X
11	NAG	r	2	-	-	-	X
11	BMA	r	3	-	-	-	X
11	MAN	r	5	-	-	-	X
11	MAN	r	7	-	-	-	X
12	MAN	a	5	-	-	-	X
12	MAN	j	5	-	-	-	X
12	MAN	j	6	-	-	-	X
12	MAN	s	4	-	-	-	X
12	MAN	s	5	-	-	-	X
14	NAG	d	1	-	-	-	X
14	MAN	d	7	-	-	-	X
14	MAN	d	8	-	-	-	X
14	NAG	m	2	-	-	-	X
14	MAN	m	6	-	-	-	X
14	MAN	m	8	-	-	-	X
14	MAN	v	8	-	-	-	X
15	NAG	A	702	-	-	-	X
15	NAG	A	703	-	-	-	X
15	NAG	F	606	-	-	-	X
15	NAG	F	615	-	-	-	X
15	NAG	F	633	-	-	-	X
15	NAG	F	649	-	-	-	X
15	NAG	F	651	-	-	-	X
15	NAG	F	652	-	-	-	X
15	NAG	G	615	-	-	-	X
15	NAG	G	649	-	-	-	X
15	NAG	G	651	-	-	-	X
15	NAG	G	652	-	-	-	X
15	NAG	G	653	-	-	-	X
15	NAG	J	701	-	-	-	X
15	NAG	J	702	-	-	-	X
15	NAG	J	703	-	-	-	X
15	NAG	Q	615	-	-	-	X
15	NAG	Q	633	-	-	-	X
15	NAG	Q	649	-	-	-	X
15	NAG	Q	651	-	-	-	X
15	NAG	Q	652	-	-	-	X
15	NAG	Q	653	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	NAG	R	701	-	-	-	X
15	NAG	R	702	-	-	-	X
15	NAG	R	703	-	-	-	X
2	PCA	D	1	-	-	-	X
2	PCA	W	1	-	-	-	X
8	MAN	E	4	-	-	-	X
8	MAN	X	4	-	-	-	X
8	MAN	c	4	-	-	-	X
8	MAN	c	5	-	-	-	X
8	NAG	e	2	-	-	-	X
8	BMA	e	3	-	-	-	X
8	MAN	e	4	-	-	-	X
8	MAN	e	5	-	-	-	X
8	MAN	g	4	-	-	-	X
8	MAN	g	5	-	-	-	X
8	NAG	l	1	-	-	-	X
8	MAN	l	5	-	-	-	X
8	NAG	n	2	-	-	-	X
8	BMA	n	3	-	-	-	X
8	MAN	n	4	-	-	-	X
8	MAN	n	5	-	-	-	X
8	BMA	p	3	-	-	-	X
8	MAN	p	4	-	-	-	X
8	MAN	p	5	-	-	-	X
9	NAG	P	2	-	-	-	X
9	BMA	P	3	-	-	-	X
9	NAG	f	1	-	-	-	X
9	NAG	f	2	-	-	-	X
9	NAG	o	1	-	-	-	X
9	NAG	o	2	-	-	-	X
9	BMA	o	3	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 41285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	449	3535	2218	624	664	29	0	0	0
1	F	449	3535	2218	624	664	29	0	0	0
1	Q	449	3535	2218	624	664	29	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	72	CYS	HIS	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	460	ALA	SER	conflict	UNP Q2N0S6
G	461	ASN	THR	conflict	UNP Q2N0S6
G	463	THR	SER	conflict	UNP Q2N0S6
G	464	SER	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
F	72	CYS	HIS	conflict	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	460	ALA	SER	conflict	UNP Q2N0S6
F	461	ASN	THR	conflict	UNP Q2N0S6
F	463	THR	SER	conflict	UNP Q2N0S6
F	464	SER	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
Q	72	CYS	HIS	conflict	UNP Q2N0S6
Q	332	ASN	THR	conflict	UNP Q2N0S6
Q	460	ALA	SER	conflict	UNP Q2N0S6
Q	461	ASN	THR	conflict	UNP Q2N0S6
Q	463	THR	SER	conflict	UNP Q2N0S6
Q	464	SER	THR	conflict	UNP Q2N0S6
Q	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called bnAb NIH45-46 scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	223	1761	1107	316	328	10	0	0	0
2	O	222	1753	1102	315	326	10	0	0	0
2	W	223	1761	1107	316	328	10	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	126	1001	633	172	190	6	0	0	0
3	J	126	1001	633	172	190	6	0	0	0
3	R	126	1001	633	172	190	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	CYS	THR	conflict	UNP Q2N0S8
J	605	CYS	THR	conflict	UNP Q2N0S8
R	605	CYS	THR	conflict	UNP Q2N0S8

- Molecule 4 is a protein called bnAb PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	210	1589	998	267	320	4	0	0	0
4	K	210	1589	998	267	320	4	0	0	0
4	S	210	1589	998	267	320	4	0	0	0

- Molecule 5 is a protein called bnAb PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	228	1742	1109	295	333	5	0	0	0
5	L	228	1742	1109	295	333	5	0	0	0
5	T	228	1742	1109	295	333	5	0	0	0

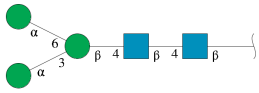
- Molecule 6 is a protein called bnAb 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	242	1832	1165	306	353	8	0	0	0
6	M	242	1832	1165	306	353	8	0	0	0
6	U	242	1832	1165	306	353	8	0	0	0

- Molecule 7 is a protein called bnAb 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	207	1574	989	258	319	8	0	0	0
7	N	213	1615	1012	267	328	8	0	0	0
7	V	213	1615	1012	267	328	8	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	E	5	61	34	2	25	0	0	0
8	X	5	61	34	2	25	0	0	0
8	c	5	61	34	2	25	0	0	0
8	e	5	61	34	2	25	0	0	0
8	g	5	61	34	2	25	0	0	0
8	l	5	61	34	2	25	0	0	0
8	n	5	61	34	2	25	0	0	0

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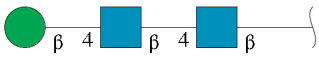
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	p	5	61	34	2	25	0	0	0
8	u	5	61	34	2	25	0	0	0

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

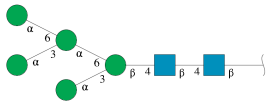


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	P	3	39	22	2	15	0	0	0
9	f	3	39	22	2	15	0	0	0
9	o	3	39	22	2	15	0	0	0

- Molecule 10 is an oligosaccharide called 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.

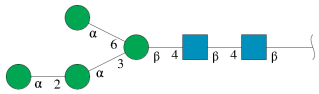
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	Y	4	50	28	2	20	0	0	0
10	h	4	50	28	2	20	0	0	0
10	q	4	50	28	2	20	0	0	0

- Molecule 11 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
			Total	C	N	O			
11	Z	7	83	46	2	35	0	0	0
11	i	7	83	46	2	35	0	0	0
11	r	7	83	46	2	35	0	0	0

- Molecule 12 is an oligosaccharide called 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.

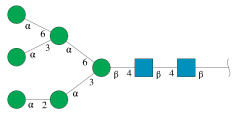


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	a	6	72	40	2	30	0	0	0
12	j	6	72	40	2	30	0	0	0
12	s	6	72	40	2	30	0	0	0

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

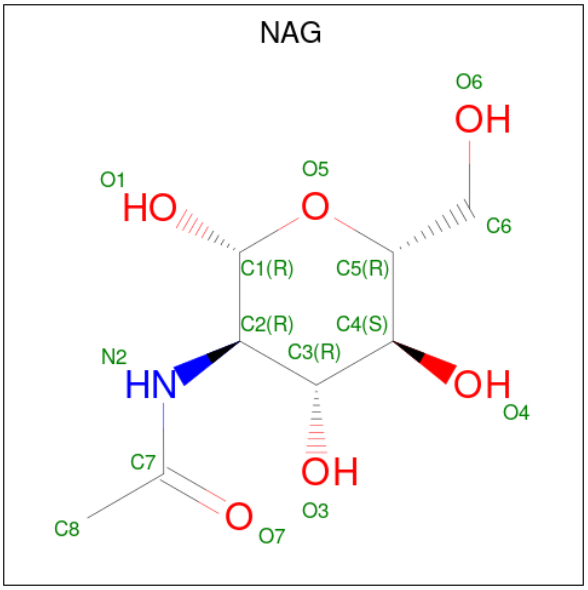
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	b	2	28	16	2	10	0	0	0
13	k	2	28	16	2	10	0	0	0
13	t	2	28	16	2	10	0	0	0

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	d	8	94	52	2	40	0	0	0
14	m	8	94	52	2	40	0	0	0
14	v	8	94	52	2	40	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	G	1	14	8	1	5	0	0
15	G	1	14	8	1	5	0	0
15	G	1	14	8	1	5	0	0
15	G	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	G	1	14	8	1	5	0	0
			Total	C	N	O		
15	G	1	14	8	1	5	0	0
			Total	C	N	O		
15	G	1	14	8	1	5	0	0
			Total	C	N	O		
15	G	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	F	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	Q	1	14	8	1	5	0	0
			Total	C	N	O		
15	A	1	14	8	1	5	0	0

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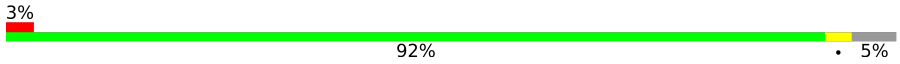
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	A	1	14	8	1	5	0	0
			Total	C	N	O		
15	A	1	14	8	1	5	0	0
			Total	C	N	O		
15	J	1	14	8	1	5	0	0
			Total	C	N	O		
15	J	1	14	8	1	5	0	0
			Total	C	N	O		
15	J	1	14	8	1	5	0	0
			Total	C	N	O		
15	R	1	14	8	1	5	0	0
			Total	C	N	O		
15	R	1	14	8	1	5	0	0
			Total	C	N	O		
15	R	1	14	8	1	5	0	0

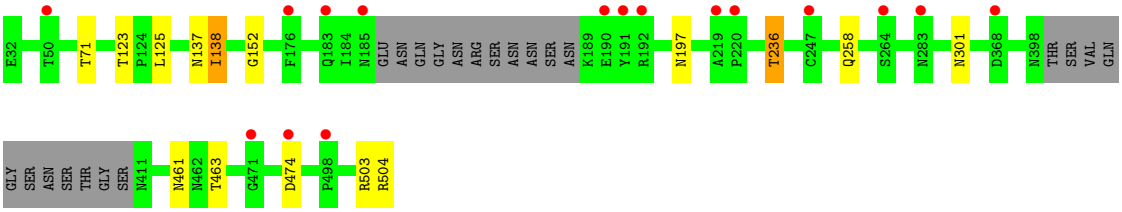
3 Residue-property plots (i)

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

• Molecule 1: Envelope glycoprotein gp160

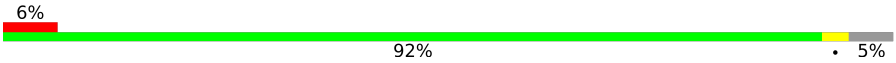
Chain G:

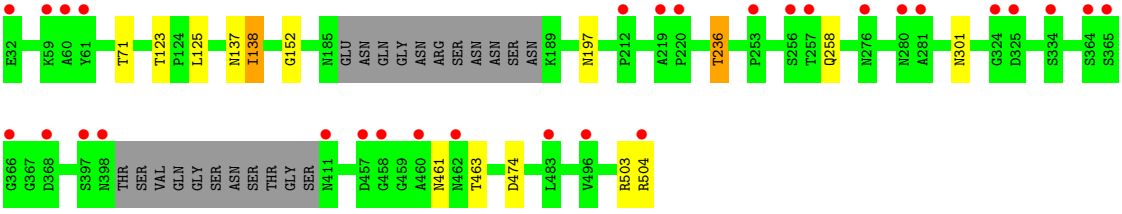




• Molecule 1: Envelope glycoprotein gp160

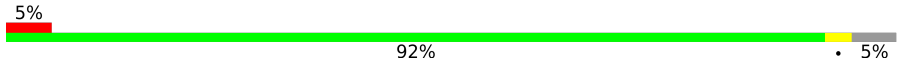
Chain F:

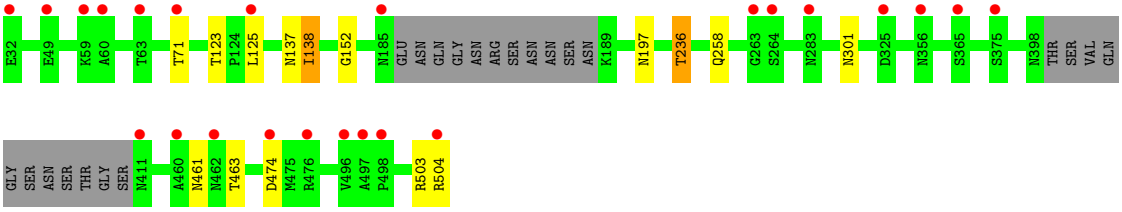




• Molecule 1: Envelope glycoprotein gp160

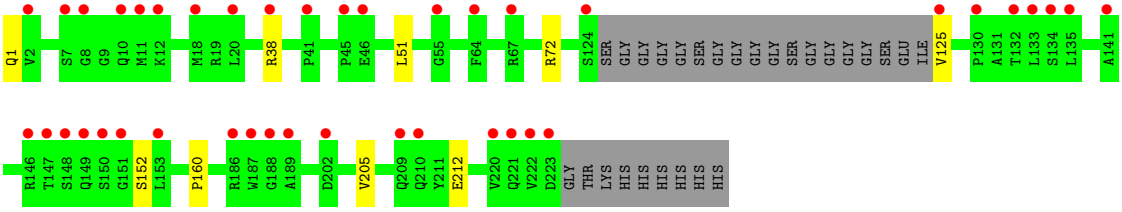
Chain Q:





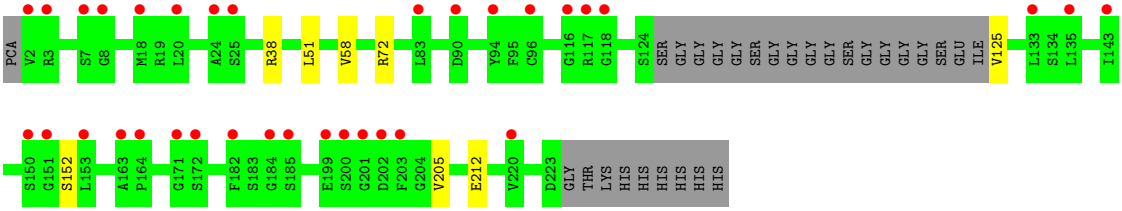
• Molecule 2: bnAb NIH45-46 scFv

Chain D:



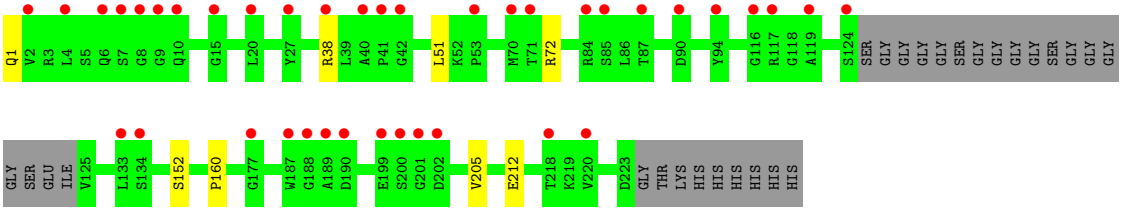
- Molecule 2: bnAb NIH45-46 scFv

Chain O:



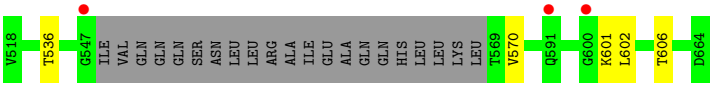
- Molecule 2: bnAb NIH45-46 scFv

Chain W:



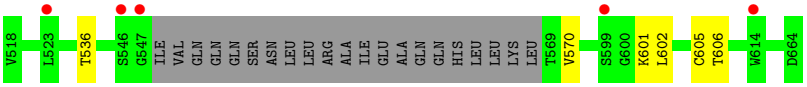
- Molecule 3: Envelope glycoprotein gp160

Chain A:



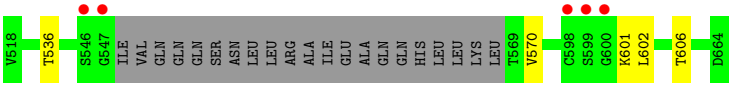
- Molecule 3: Envelope glycoprotein gp160

Chain J:



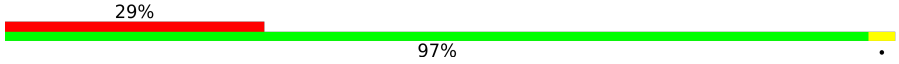
- Molecule 3: Envelope glycoprotein gp160

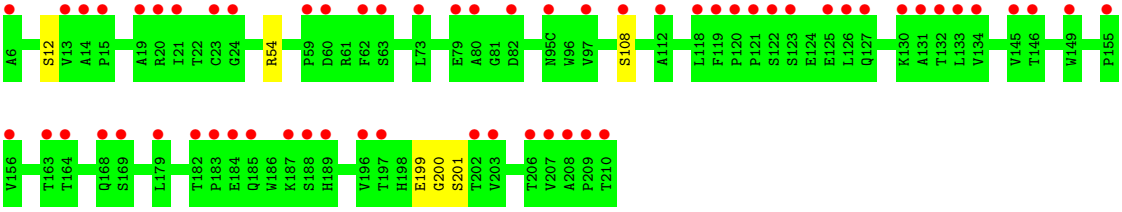
Chain R:



• Molecule 4: bnAb PGT122 Fab light chain

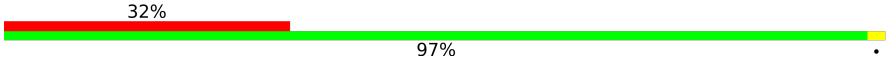
Chain B:

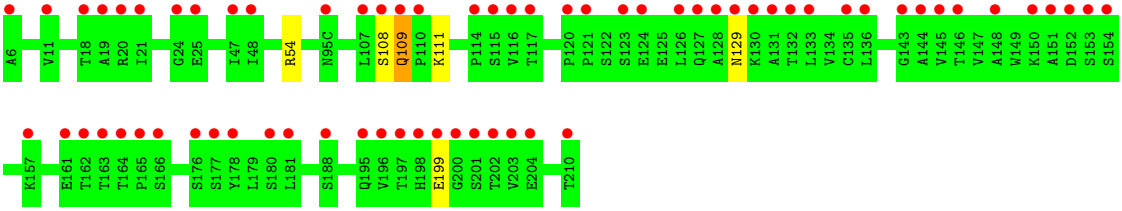




• Molecule 4: bnAb PGT122 Fab light chain

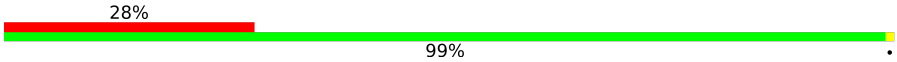
Chain K:

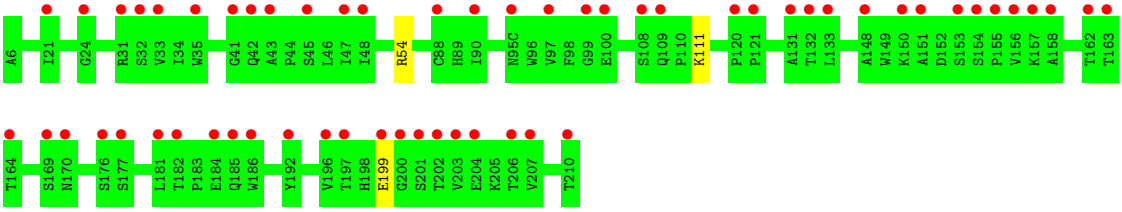




• Molecule 4: bnAb PGT122 Fab light chain

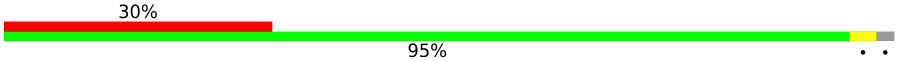
Chain S:

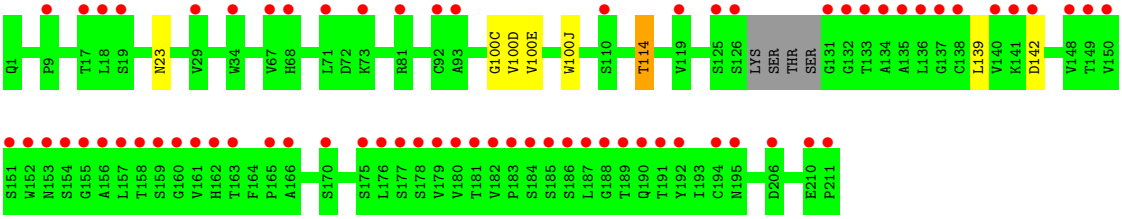




• Molecule 5: bnAb PGT122 Fab heavy chain

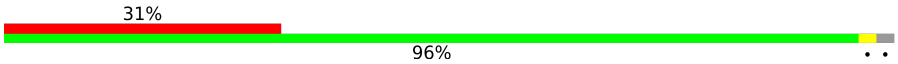
Chain C:

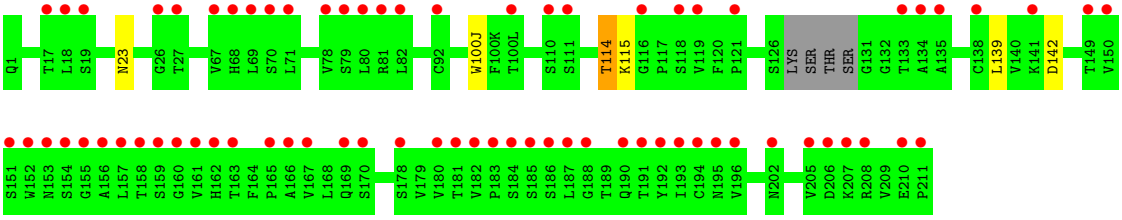




• Molecule 5: bnAb PGT122 Fab heavy chain

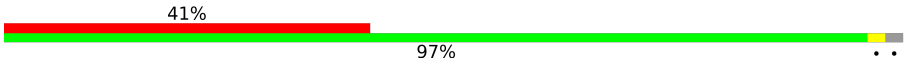
Chain L:

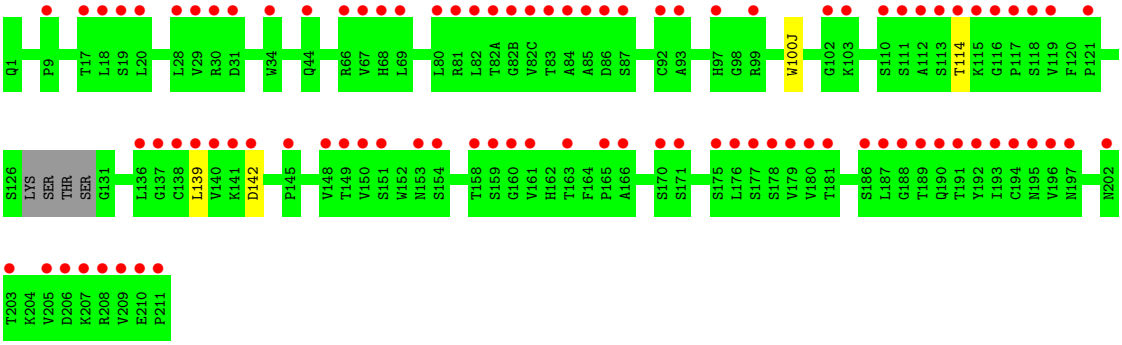




- Molecule 5: bnAb PGT122 Fab heavy chain

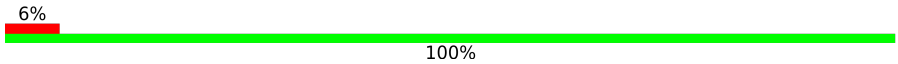
Chain T:

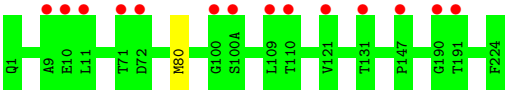




- Molecule 6: bnAb 35O22 Fab heavy chain

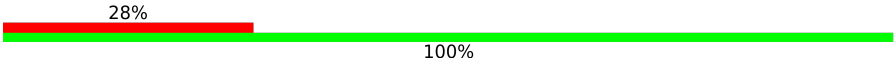
Chain H:

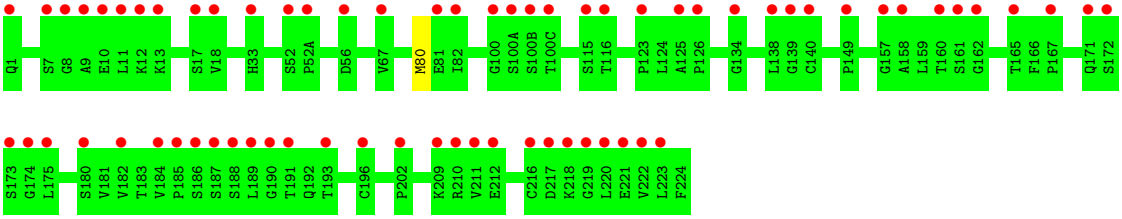




- Molecule 6: bnAb 35O22 Fab heavy chain

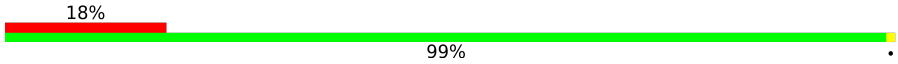
Chain M:

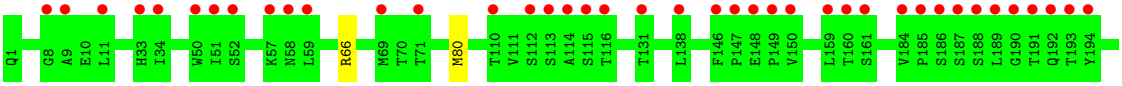




- Molecule 6: bnAb 35O22 Fab heavy chain

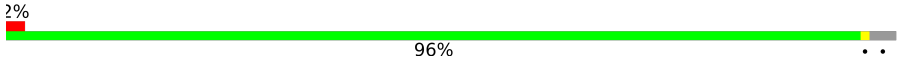
Chain U:

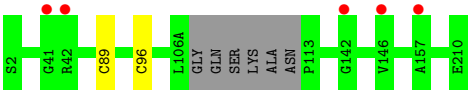




• Molecule 7: bnAb 35O22 Fab light chain

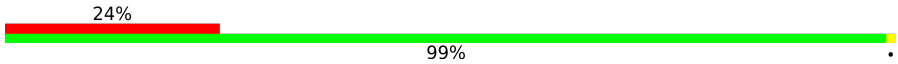
Chain I:

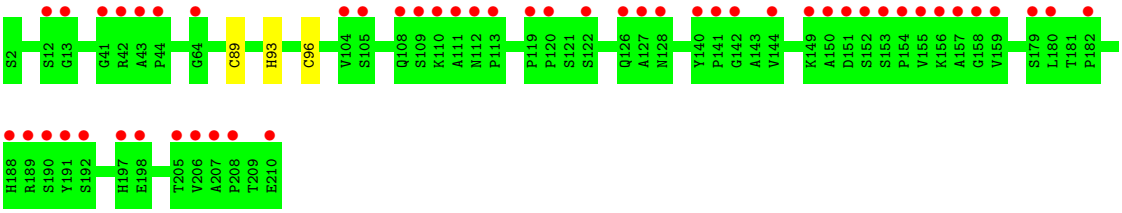




• Molecule 7: bnAb 35O22 Fab light chain

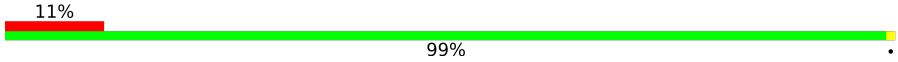
Chain N:

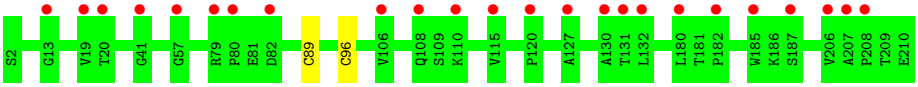




• Molecule 7: bnAb 35O22 Fab light chain

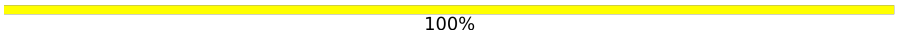
Chain V:





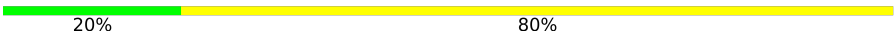
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

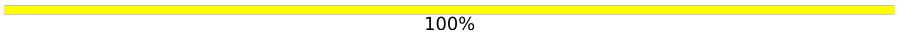
Chain X:



• Molecule 8: 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 c:

• Molecule 8: 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: 

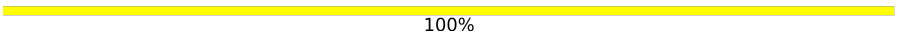
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 8: 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 l:

• Molecule 8: 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 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

• Molecule 8: 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-glucopyra

nose

Chain u:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

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

Chain Y:

• Molecule 10: 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 10: 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 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%

• Molecule 11: 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 i: 14% 86%

• Molecule 11: 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 r: 100%

• Molecule 12: 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 a: 100%

• Molecule 12: 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 j: 17% 83%

• Molecule 12: 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 s: 17% 83%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 100%

NAG1 NAG2

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 100%

NAG1 NAG2

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 100%

NAG1 NAG2

• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 12% 88%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m: 12% 88%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(

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

Chain v:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	361.81Å 215.85Å 176.61Å 90.00° 114.03° 90.00°	Depositor
Resolution (Å)	39.71 – 7.00 39.71 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.71-7.00) 99.9 (39.71-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 7.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.301 , 0.363 0.301 , 0.363	Depositor DCC
R_{free} test set	978 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	277.9	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 387.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	41285	wwPDB-VP
Average B, all atoms (Å^2)	458.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	F	0.27	0/3608	0.51	0/4898
1	G	0.28	0/3608	0.52	0/4898
1	Q	0.27	0/3608	0.51	0/4898
2	D	0.25	0/1800	0.46	0/2439
2	O	0.25	0/1799	0.45	0/2436
2	W	0.25	0/1800	0.46	0/2439
3	A	0.25	0/1019	0.45	0/1382
3	J	0.25	0/1019	0.47	1/1382 (0.1%)
3	R	0.26	0/1019	0.45	0/1382
4	B	0.29	0/1632	0.55	1/2236 (0.0%)
4	K	0.26	0/1632	0.52	1/2236 (0.0%)
4	S	0.26	0/1632	0.48	0/2236
5	C	0.33	0/1789	0.59	1/2443 (0.0%)
5	L	0.26	0/1789	0.49	0/2443
5	T	0.26	0/1789	0.47	0/2443
6	H	0.26	0/1880	0.48	0/2560
6	M	0.25	0/1880	0.48	0/2560
6	U	0.25	0/1880	0.48	0/2560
7	I	0.26	0/1617	0.49	1/2211 (0.0%)
7	N	0.25	0/1659	0.48	1/2269 (0.0%)
7	V	0.25	0/1659	0.47	1/2269 (0.0%)
All	All	0.27	0/40118	0.49	7/54620 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	89	CYS	CA-CB-SG	-6.07	103.08	114.00
7	I	89	CYS	CA-CB-SG	-6.02	103.16	114.00
7	N	89	CYS	CA-CB-SG	-5.79	103.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	605	CYS	CA-CB-SG	-5.37	104.33	114.00
4	K	109	GLN	CB-CA-C	-5.29	99.82	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	443/471 (94%)	392 (88%)	43 (10%)	8 (2%)	8	40
1	G	443/471 (94%)	392 (88%)	43 (10%)	8 (2%)	8	40
1	Q	443/471 (94%)	391 (88%)	44 (10%)	8 (2%)	8	40
2	D	219/250 (88%)	209 (95%)	8 (4%)	2 (1%)	17	57
2	O	218/250 (87%)	208 (95%)	9 (4%)	1 (0%)	29	69
2	W	219/250 (88%)	209 (95%)	8 (4%)	2 (1%)	17	57
3	A	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	9	44
3	J	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	9	44
3	R	122/147 (83%)	107 (88%)	13 (11%)	2 (2%)	9	44
4	B	208/210 (99%)	193 (93%)	13 (6%)	2 (1%)	15	54
4	K	208/210 (99%)	193 (93%)	13 (6%)	2 (1%)	15	54
4	S	208/210 (99%)	192 (92%)	15 (7%)	1 (0%)	29	69
5	C	224/232 (97%)	210 (94%)	10 (4%)	4 (2%)	8	40
5	L	224/232 (97%)	210 (94%)	11 (5%)	3 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	T	224/232 (97%)	210 (94%)	13 (6%)	1 (0%)	34	72
6	H	240/242 (99%)	227 (95%)	13 (5%)	0	100	100
6	M	240/242 (99%)	228 (95%)	12 (5%)	0	100	100
6	U	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34	72
7	I	203/213 (95%)	188 (93%)	15 (7%)	0	100	100
7	N	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
7	V	211/213 (99%)	196 (93%)	15 (7%)	0	100	100
All	All	4992/5295 (94%)	4592 (92%)	351 (7%)	49 (1%)	15	54

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	138	ILE
1	G	197	ASN
1	F	138	ILE
1	F	197	ASN
1	Q	138	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	400/419 (96%)	391 (98%)	9 (2%)	50	70
1	G	400/419 (96%)	391 (98%)	9 (2%)	50	70
1	Q	400/419 (96%)	391 (98%)	9 (2%)	50	70
2	D	184/198 (93%)	178 (97%)	6 (3%)	38	61
2	O	184/198 (93%)	177 (96%)	7 (4%)	33	57
2	W	184/198 (93%)	179 (97%)	5 (3%)	44	65
3	A	108/127 (85%)	105 (97%)	3 (3%)	43	65
3	J	108/127 (85%)	105 (97%)	3 (3%)	43	65
3	R	108/127 (85%)	105 (97%)	3 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	178/178 (100%)	175 (98%)	3 (2%)	60	78
4	K	178/178 (100%)	174 (98%)	4 (2%)	52	71
4	S	178/178 (100%)	176 (99%)	2 (1%)	73	84
5	C	198/202 (98%)	194 (98%)	4 (2%)	55	74
5	L	198/202 (98%)	194 (98%)	4 (2%)	55	74
5	T	198/202 (98%)	195 (98%)	3 (2%)	65	80
6	H	205/205 (100%)	204 (100%)	1 (0%)	88	93
6	M	205/205 (100%)	204 (100%)	1 (0%)	88	93
6	U	205/205 (100%)	204 (100%)	1 (0%)	88	93
7	I	182/186 (98%)	181 (100%)	1 (0%)	88	93
7	N	186/186 (100%)	184 (99%)	2 (1%)	73	84
7	V	186/186 (100%)	185 (100%)	1 (0%)	88	93
All	All	4373/4545 (96%)	4292 (98%)	81 (2%)	57	75

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	536	THR
3	R	536	THR
3	J	606	THR
5	L	100(J)	TRP
4	S	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	616	ASN
4	S	37	GLN
4	S	129	ASN
5	C	198	HIS
5	C	197	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	W	1	2	7,8,9	1.81	1 (14%)	9,10,12	2.15	5 (55%)
2	PCA	D	1	2	7,8,9	1.81	1 (14%)	9,10,12	2.13	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	W	1	2	-	0/0/11/13	0/1/1/1
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	PCA	CD-N	4.68	1.46	1.34
2	W	1	PCA	CD-N	4.66	1.46	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	1	PCA	OE-CD-CG	-3.09	121.37	126.76
2	D	1	PCA	OE-CD-CG	-3.09	121.37	126.76
2	W	1	PCA	CA-N-CD	-2.87	103.74	113.58
2	D	1	PCA	CA-N-CD	-2.84	103.86	113.58
2	W	1	PCA	CB-CA-C	-2.63	109.08	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

135 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	$\#\|Z\| > 2$
8	NAG	E	1	1,8	14,14,15	1.95	1 (7%)	17,19,21	1.48	3 (17%)
8	NAG	E	2	8	14,14,15	2.27	2 (14%)	17,19,21	1.84	3 (17%)
8	BMA	E	3	8	11,11,12	2.80	6 (54%)	15,15,17	2.18	6 (40%)
8	MAN	E	4	8	11,11,12	0.76	0	15,15,17	1.18	2 (13%)
8	MAN	E	5	8	11,11,12	1.71	3 (27%)	15,15,17	3.22	9 (60%)
9	NAG	P	1	1,9	14,14,15	0.88	1 (7%)	17,19,21	0.77	1 (5%)
9	NAG	P	2	9	14,14,15	1.03	1 (7%)	17,19,21	0.66	0
9	BMA	P	3	9	11,11,12	0.74	0	15,15,17	0.77	0
8	NAG	X	1	1,8	14,14,15	2.15	2 (14%)	17,19,21	1.78	3 (17%)
8	NAG	X	2	8	14,14,15	0.69	1 (7%)	17,19,21	0.53	0
8	BMA	X	3	8	11,11,12	0.61	0	15,15,17	0.77	0
8	MAN	X	4	8	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
8	MAN	X	5	8	11,11,12	0.71	0	15,15,17	0.98	1 (6%)
10	NAG	Y	1	1,10	14,14,15	0.38	0	17,19,21	0.59	0
10	NAG	Y	2	10	14,14,15	0.38	0	17,19,21	0.42	0
10	BMA	Y	3	10	11,11,12	0.63	0	15,15,17	0.78	0
10	MAN	Y	4	10	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
11	NAG	Z	1	1,11	14,14,15	1.92	2 (14%)	17,19,21	1.58	3 (17%)
11	NAG	Z	2	11	14,14,15	2.26	2 (14%)	17,19,21	1.90	4 (23%)
11	BMA	Z	3	11	11,11,12	2.45	5 (45%)	15,15,17	2.25	4 (26%)
11	MAN	Z	4	11	11,11,12	1.48	1 (9%)	15,15,17	3.23	7 (46%)
11	MAN	Z	5	11	11,11,12	1.49	2 (18%)	15,15,17	2.93	6 (40%)
11	MAN	Z	6	11	11,11,12	1.38	2 (18%)	15,15,17	3.39	8 (53%)
11	MAN	Z	7	11	11,11,12	2.41	2 (18%)	15,15,17	3.76	6 (40%)
12	NAG	a	1	1,12	14,14,15	0.69	1 (7%)	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	a	2	12	14,14,15	1.87	1 (7%)	17,19,21	1.76	3 (17%)
12	BMA	a	3	12	11,11,12	1.48	3 (27%)	15,15,17	1.29	3 (20%)
12	MAN	a	4	12	11,11,12	1.57	3 (27%)	15,15,17	1.85	3 (20%)
12	MAN	a	5	12	11,11,12	1.39	2 (18%)	15,15,17	1.41	3 (20%)
12	MAN	a	6	12	11,11,12	1.22	1 (9%)	15,15,17	1.82	3 (20%)
13	NAG	b	1	13,1	14,14,15	0.23	0	17,19,21	0.47	0
13	NAG	b	2	13	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	c	1	1,8	14,14,15	0.25	0	17,19,21	0.39	0
8	NAG	c	2	8	14,14,15	0.19	0	17,19,21	0.46	0
8	BMA	c	3	8	11,11,12	0.51	0	15,15,17	0.73	0
8	MAN	c	4	8	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
8	MAN	c	5	8	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
14	NAG	d	1	1,14	14,14,15	0.43	0	17,19,21	1.46	2 (11%)
14	NAG	d	2	14	14,14,15	0.22	0	17,19,21	0.45	0
14	BMA	d	3	14	11,11,12	0.99	1 (9%)	15,15,17	0.99	1 (6%)
14	MAN	d	4	14	11,11,12	1.09	0	15,15,17	2.46	5 (33%)
14	MAN	d	5	14	11,11,12	0.79	0	15,15,17	1.18	2 (13%)
14	MAN	d	6	14	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
14	MAN	d	7	14	11,11,12	0.77	1 (9%)	15,15,17	1.27	2 (13%)
14	MAN	d	8	14	11,11,12	0.76	1 (9%)	15,15,17	1.14	2 (13%)
8	NAG	e	1	1,8	14,14,15	2.74	2 (14%)	17,19,21	1.45	3 (17%)
8	NAG	e	2	8	14,14,15	1.71	2 (14%)	17,19,21	2.11	2 (11%)
8	BMA	e	3	8	11,11,12	2.19	5 (45%)	15,15,17	2.04	7 (46%)
8	MAN	e	4	8	11,11,12	1.21	1 (9%)	15,15,17	1.69	3 (20%)
8	MAN	e	5	8	11,11,12	1.61	4 (36%)	15,15,17	2.36	6 (40%)
9	NAG	f	1	1,9	14,14,15	0.91	1 (7%)	17,19,21	0.76	1 (5%)
9	NAG	f	2	9	14,14,15	1.05	1 (7%)	17,19,21	0.68	0
9	BMA	f	3	9	11,11,12	0.75	0	15,15,17	0.78	0
8	NAG	g	1	1,8	14,14,15	2.13	2 (14%)	17,19,21	1.63	3 (17%)
8	NAG	g	2	8	14,14,15	0.67	1 (7%)	17,19,21	0.55	0
8	BMA	g	3	8	11,11,12	0.61	0	15,15,17	0.76	0
8	MAN	g	4	8	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
8	MAN	g	5	8	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
10	NAG	h	1	1,10	14,14,15	0.69	1 (7%)	17,19,21	0.79	0
10	NAG	h	2	10	14,14,15	0.21	0	17,19,21	0.43	0
10	BMA	h	3	10	11,11,12	0.63	0	15,15,17	0.80	0
10	MAN	h	4	10	11,11,12	0.66	0	15,15,17	1.04	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	i	1	1,11	14,14,15	1.92	2 (14%)	17,19,21	1.69	3 (17%)
11	NAG	i	2	11	14,14,15	2.35	2 (14%)	17,19,21	1.90	4 (23%)
11	BMA	i	3	11	11,11,12	0.23	0	15,15,17	0.72	0
11	MAN	i	4	11	11,11,12	0.86	1 (9%)	15,15,17	1.70	2 (13%)
11	MAN	i	5	11	11,11,12	1.50	2 (18%)	15,15,17	2.90	5 (33%)
11	MAN	i	6	11	11,11,12	1.44	2 (18%)	15,15,17	3.13	7 (46%)
11	MAN	i	7	11	11,11,12	1.07	1 (9%)	15,15,17	2.91	6 (40%)
12	NAG	j	1	1,12	14,14,15	0.16	0	17,19,21	0.57	0
12	NAG	j	2	12	14,14,15	1.22	1 (7%)	17,19,21	1.96	5 (29%)
12	BMA	j	3	12	11,11,12	1.68	3 (27%)	15,15,17	1.41	3 (20%)
12	MAN	j	4	12	11,11,12	1.56	3 (27%)	15,15,17	1.93	3 (20%)
12	MAN	j	5	12	11,11,12	1.31	1 (9%)	15,15,17	1.45	3 (20%)
12	MAN	j	6	12	11,11,12	1.25	2 (18%)	15,15,17	1.89	4 (26%)
13	NAG	k	1	13,1	14,14,15	0.20	0	17,19,21	0.47	0
13	NAG	k	2	13	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	l	1	1,8	14,14,15	0.27	0	17,19,21	0.39	0
8	NAG	l	2	8	14,14,15	0.20	0	17,19,21	0.45	0
8	BMA	l	3	8	11,11,12	0.52	0	15,15,17	0.72	0
8	MAN	l	4	8	11,11,12	0.63	0	15,15,17	1.05	2 (13%)
8	MAN	l	5	8	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
14	NAG	m	1	1,14	14,14,15	0.44	0	17,19,21	1.48	2 (11%)
14	NAG	m	2	14	14,14,15	0.25	0	17,19,21	0.45	0
14	BMA	m	3	14	11,11,12	0.94	1 (9%)	15,15,17	0.99	1 (6%)
14	MAN	m	4	14	11,11,12	1.11	1 (9%)	15,15,17	2.53	5 (33%)
14	MAN	m	5	14	11,11,12	0.69	0	15,15,17	1.13	2 (13%)
14	MAN	m	6	14	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
14	MAN	m	7	14	11,11,12	0.78	1 (9%)	15,15,17	1.28	2 (13%)
14	MAN	m	8	14	11,11,12	0.77	1 (9%)	15,15,17	1.13	2 (13%)
8	NAG	n	1	1,8	14,14,15	1.94	2 (14%)	17,19,21	1.49	3 (17%)
8	NAG	n	2	8	14,14,15	2.66	2 (14%)	17,19,21	1.87	4 (23%)
8	BMA	n	3	8	11,11,12	3.30	6 (54%)	15,15,17	1.90	6 (40%)
8	MAN	n	4	8	11,11,12	0.62	0	15,15,17	1.19	2 (13%)
8	MAN	n	5	8	11,11,12	1.80	4 (36%)	15,15,17	3.26	10 (66%)
9	NAG	o	1	1,9	14,14,15	0.82	1 (7%)	17,19,21	0.79	1 (5%)
9	NAG	o	2	9	14,14,15	1.02	1 (7%)	17,19,21	0.67	0
9	BMA	o	3	9	11,11,12	0.75	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	p	1	1,8	14,14,15	2.16	2 (14%)	17,19,21	1.64	3 (17%)
8	NAG	p	2	8	14,14,15	0.65	1 (7%)	17,19,21	0.55	0
8	BMA	p	3	8	11,11,12	0.60	0	15,15,17	0.77	0
8	MAN	p	4	8	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
8	MAN	p	5	8	11,11,12	0.70	0	15,15,17	0.97	2 (13%)
10	NAG	q	1	1,10	14,14,15	0.50	0	17,19,21	0.66	0
10	NAG	q	2	10	14,14,15	0.28	0	17,19,21	0.50	0
10	BMA	q	3	10	11,11,12	0.64	0	15,15,17	0.80	0
10	MAN	q	4	10	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
11	NAG	r	1	1,11	14,14,15	1.94	2 (14%)	17,19,21	1.72	3 (17%)
11	NAG	r	2	11	14,14,15	2.29	2 (14%)	17,19,21	1.89	4 (23%)
11	BMA	r	3	11	11,11,12	2.22	4 (36%)	15,15,17	2.17	3 (20%)
11	MAN	r	4	11	11,11,12	1.91	3 (27%)	15,15,17	3.30	8 (53%)
11	MAN	r	5	11	11,11,12	1.40	2 (18%)	15,15,17	2.85	6 (40%)
11	MAN	r	6	11	11,11,12	2.20	6 (54%)	15,15,17	3.94	8 (53%)
11	MAN	r	7	11	11,11,12	1.87	4 (36%)	15,15,17	1.64	4 (26%)
12	NAG	s	1	1,12	14,14,15	0.38	0	17,19,21	0.49	0
12	NAG	s	2	12	14,14,15	1.79	1 (7%)	17,19,21	1.82	3 (17%)
12	BMA	s	3	12	11,11,12	1.46	3 (27%)	15,15,17	1.23	3 (20%)
12	MAN	s	4	12	11,11,12	2.82	4 (36%)	15,15,17	2.01	5 (33%)
12	MAN	s	5	12	11,11,12	1.46	2 (18%)	15,15,17	2.52	6 (40%)
12	MAN	s	6	12	11,11,12	1.23	1 (9%)	15,15,17	1.80	3 (20%)
13	NAG	t	1	13,1	14,14,15	0.21	0	17,19,21	0.48	0
13	NAG	t	2	13	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	u	1	1,8	14,14,15	0.28	0	17,19,21	0.41	0
8	NAG	u	2	8	14,14,15	0.21	0	17,19,21	0.45	0
8	BMA	u	3	8	11,11,12	0.53	0	15,15,17	0.74	0
8	MAN	u	4	8	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
8	MAN	u	5	8	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
14	NAG	v	1	1,14	14,14,15	0.60	1 (7%)	17,19,21	1.47	2 (11%)
14	NAG	v	2	14	14,14,15	0.27	0	17,19,21	0.47	0
14	BMA	v	3	14	11,11,12	0.80	0	15,15,17	1.04	1 (6%)
14	MAN	v	4	14	11,11,12	0.75	1 (9%)	15,15,17	1.25	2 (13%)
14	MAN	v	5	14	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
14	MAN	v	6	14	11,11,12	0.92	1 (9%)	15,15,17	1.06	1 (6%)
14	MAN	v	7	14	11,11,12	2.39	5 (45%)	15,15,17	3.83	7 (46%)
14	MAN	v	8	14	11,11,12	0.78	1 (9%)	15,15,17	1.14	2 (13%)

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
8	NAG	E	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	E	2	8	-	1/6/23/26	0/1/1/1
8	BMA	E	3	8	-	1/2/19/22	0/1/1/1
8	MAN	E	4	8	-	0/2/19/22	0/1/1/1
8	MAN	E	5	8	-	0/2/19/22	0/1/1/1
9	NAG	P	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	P	2	9	-	0/6/23/26	0/1/1/1
9	BMA	P	3	9	-	1/2/19/22	0/1/1/1
8	NAG	X	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	1/2/19/22	0/1/1/1
8	MAN	X	5	8	-	0/2/19/22	0/1/1/1
10	NAG	Y	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	1/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
11	NAG	Z	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Z	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Z	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	6	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	7	11	-	0/2/19/22	0/1/1/1
12	NAG	a	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	a	2	12	-	1/6/23/26	0/1/1/1
12	BMA	a	3	12	-	0/2/19/22	0/1/1/1
12	MAN	a	4	12	-	2/2/19/22	0/1/1/1
12	MAN	a	5	12	-	2/2/19/22	0/1/1/1
12	MAN	a	6	12	-	1/2/19/22	0/1/1/1
13	NAG	b	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	b	2	13	-	0/6/23/26	0/1/1/1
8	NAG	c	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
8	MAN	c	4	8	-	0/2/19/22	0/1/1/1
8	MAN	c	5	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	d	1	1,14	-	5/6/23/26	0/1/1/1
14	NAG	d	2	14	-	2/6/23/26	0/1/1/1
14	BMA	d	3	14	-	0/2/19/22	0/1/1/1
14	MAN	d	4	14	-	2/2/19/22	0/1/1/1
14	MAN	d	5	14	-	2/2/19/22	0/1/1/1
14	MAN	d	6	14	-	0/2/19/22	0/1/1/1
14	MAN	d	7	14	-	0/2/19/22	0/1/1/1
14	MAN	d	8	14	-	0/2/19/22	0/1/1/1
8	NAG	e	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
8	MAN	e	4	8	-	1/2/19/22	0/1/1/1
8	MAN	e	5	8	-	0/2/19/22	0/1/1/1
9	NAG	f	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1
9	BMA	f	3	9	-	1/2/19/22	0/1/1/1
8	NAG	g	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	BMA	g	3	8	-	2/2/19/22	0/1/1/1
8	MAN	g	4	8	-	1/2/19/22	0/1/1/1
8	MAN	g	5	8	-	0/2/19/22	0/1/1/1
10	NAG	h	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	h	2	10	-	1/6/23/26	0/1/1/1
10	BMA	h	3	10	-	1/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1
11	NAG	i	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	i	2	11	-	2/6/23/26	0/1/1/1
11	BMA	i	3	11	-	0/2/19/22	0/1/1/1
11	MAN	i	4	11	-	0/2/19/22	0/1/1/1
11	MAN	i	5	11	-	0/2/19/22	0/1/1/1
11	MAN	i	6	11	-	0/2/19/22	0/1/1/1
11	MAN	i	7	11	-	1/2/19/22	0/1/1/1
12	NAG	j	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	j	2	12	-	1/6/23/26	0/1/1/1
12	BMA	j	3	12	-	0/2/19/22	0/1/1/1
12	MAN	j	4	12	-	2/2/19/22	0/1/1/1
12	MAN	j	5	12	-	2/2/19/22	0/1/1/1
12	MAN	j	6	12	-	1/2/19/22	0/1/1/1
13	NAG	k	1	13,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	k	2	13	-	0/6/23/26	0/1/1/1
8	NAG	l	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
8	MAN	l	4	8	-	0/2/19/22	0/1/1/1
8	MAN	l	5	8	-	0/2/19/22	0/1/1/1
14	NAG	m	1	1,14	-	4/6/23/26	0/1/1/1
14	NAG	m	2	14	-	1/6/23/26	0/1/1/1
14	BMA	m	3	14	-	0/2/19/22	0/1/1/1
14	MAN	m	4	14	-	2/2/19/22	0/1/1/1
14	MAN	m	5	14	-	2/2/19/22	0/1/1/1
14	MAN	m	6	14	-	0/2/19/22	0/1/1/1
14	MAN	m	7	14	-	0/2/19/22	0/1/1/1
14	MAN	m	8	14	-	0/2/19/22	0/1/1/1
8	NAG	n	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	n	2	8	-	3/6/23/26	0/1/1/1
8	BMA	n	3	8	-	1/2/19/22	0/1/1/1
8	MAN	n	4	8	-	0/2/19/22	0/1/1/1
8	MAN	n	5	8	-	0/2/19/22	0/1/1/1
9	NAG	o	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	o	2	9	-	0/6/23/26	0/1/1/1
9	BMA	o	3	9	-	1/2/19/22	0/1/1/1
8	NAG	p	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	BMA	p	3	8	-	2/2/19/22	0/1/1/1
8	MAN	p	4	8	-	1/2/19/22	0/1/1/1
8	MAN	p	5	8	-	0/2/19/22	0/1/1/1
10	NAG	q	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	1/6/23/26	0/1/1/1
10	BMA	q	3	10	-	1/2/19/22	0/1/1/1
10	MAN	q	4	10	-	0/2/19/22	0/1/1/1
11	NAG	r	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	r	2	11	-	2/6/23/26	0/1/1/1
11	BMA	r	3	11	-	0/2/19/22	0/1/1/1
11	MAN	r	4	11	-	0/2/19/22	0/1/1/1
11	MAN	r	5	11	-	0/2/19/22	0/1/1/1
11	MAN	r	6	11	-	1/2/19/22	0/1/1/1
11	MAN	r	7	11	-	0/2/19/22	0/1/1/1
12	NAG	s	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	s	2	12	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	s	3	12	-	0/2/19/22	0/1/1/1
12	MAN	s	4	12	-	0/2/19/22	0/1/1/1
12	MAN	s	5	12	-	1/2/19/22	0/1/1/1
12	MAN	s	6	12	-	1/2/19/22	0/1/1/1
13	NAG	t	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	t	2	13	-	0/6/23/26	0/1/1/1
8	NAG	u	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	u	2	8	-	0/6/23/26	0/1/1/1
8	BMA	u	3	8	-	0/2/19/22	0/1/1/1
8	MAN	u	4	8	-	0/2/19/22	0/1/1/1
8	MAN	u	5	8	-	0/2/19/22	0/1/1/1
14	NAG	v	1	1,14	-	3/6/23/26	0/1/1/1
14	NAG	v	2	14	-	2/6/23/26	0/1/1/1
14	BMA	v	3	14	-	0/2/19/22	0/1/1/1
14	MAN	v	4	14	-	2/2/19/22	0/1/1/1
14	MAN	v	5	14	-	2/2/19/22	0/1/1/1
14	MAN	v	6	14	-	0/2/19/22	0/1/1/1
14	MAN	v	7	14	-	0/2/19/22	0/1/1/1
14	MAN	v	8	14	-	0/2/19/22	0/1/1/1

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	1	NAG	O5-C1	-9.72	1.28	1.43
8	n	2	NAG	O5-C1	-9.29	1.28	1.43
11	i	2	NAG	O5-C1	-8.19	1.30	1.43
11	r	2	NAG	O5-C1	-8.02	1.30	1.43
11	Z	2	NAG	O5-C1	-7.87	1.31	1.43

The worst 5 of 313 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	v	7	MAN	O5-C5-C6	-8.66	93.63	107.20
11	r	6	MAN	O5-C1-C2	8.54	123.95	110.77
11	Z	6	MAN	O3-C3-C4	-7.86	92.17	110.35
8	e	2	NAG	C1-O5-C5	7.86	122.84	112.19
11	r	4	MAN	O5-C1-C2	7.40	122.19	110.77

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

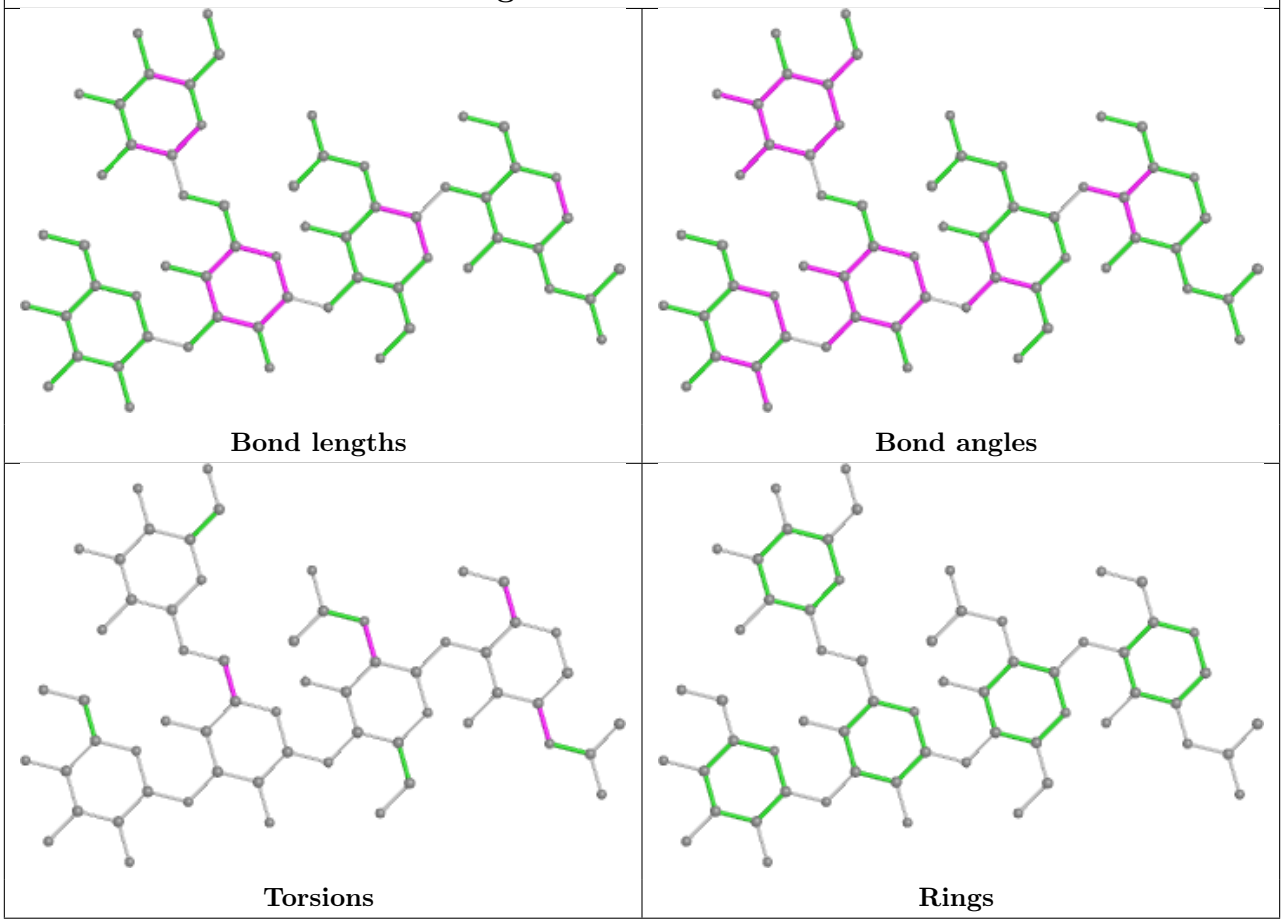
Mol	Chain	Res	Type	Atoms
8	X	3	BMA	C4-C5-C6-O6
8	g	3	BMA	C4-C5-C6-O6
8	p	3	BMA	C4-C5-C6-O6
12	j	1	NAG	C4-C5-C6-O6
11	i	7	MAN	O5-C5-C6-O6

There are no ring outliers.

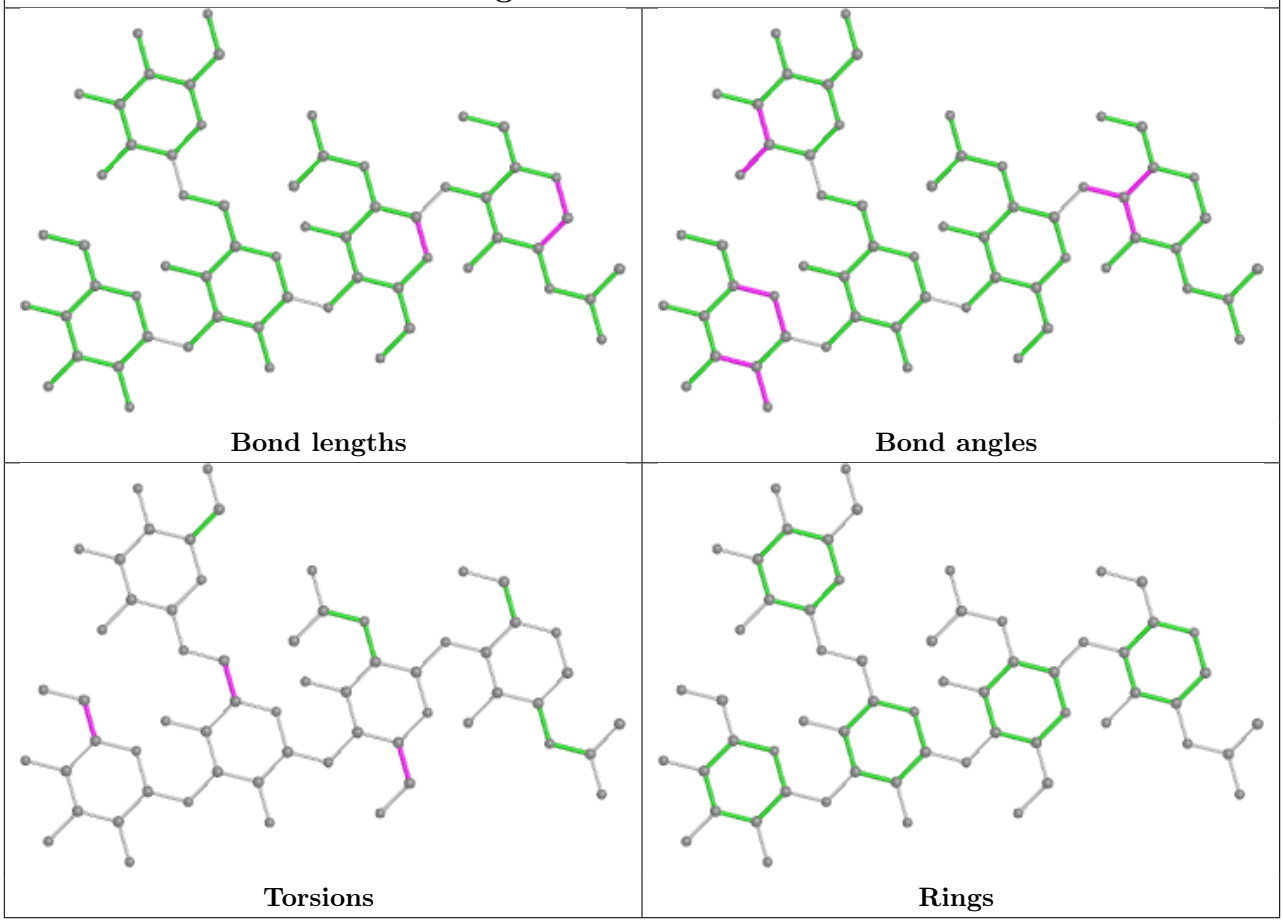
No monomer is involved in short contacts.

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

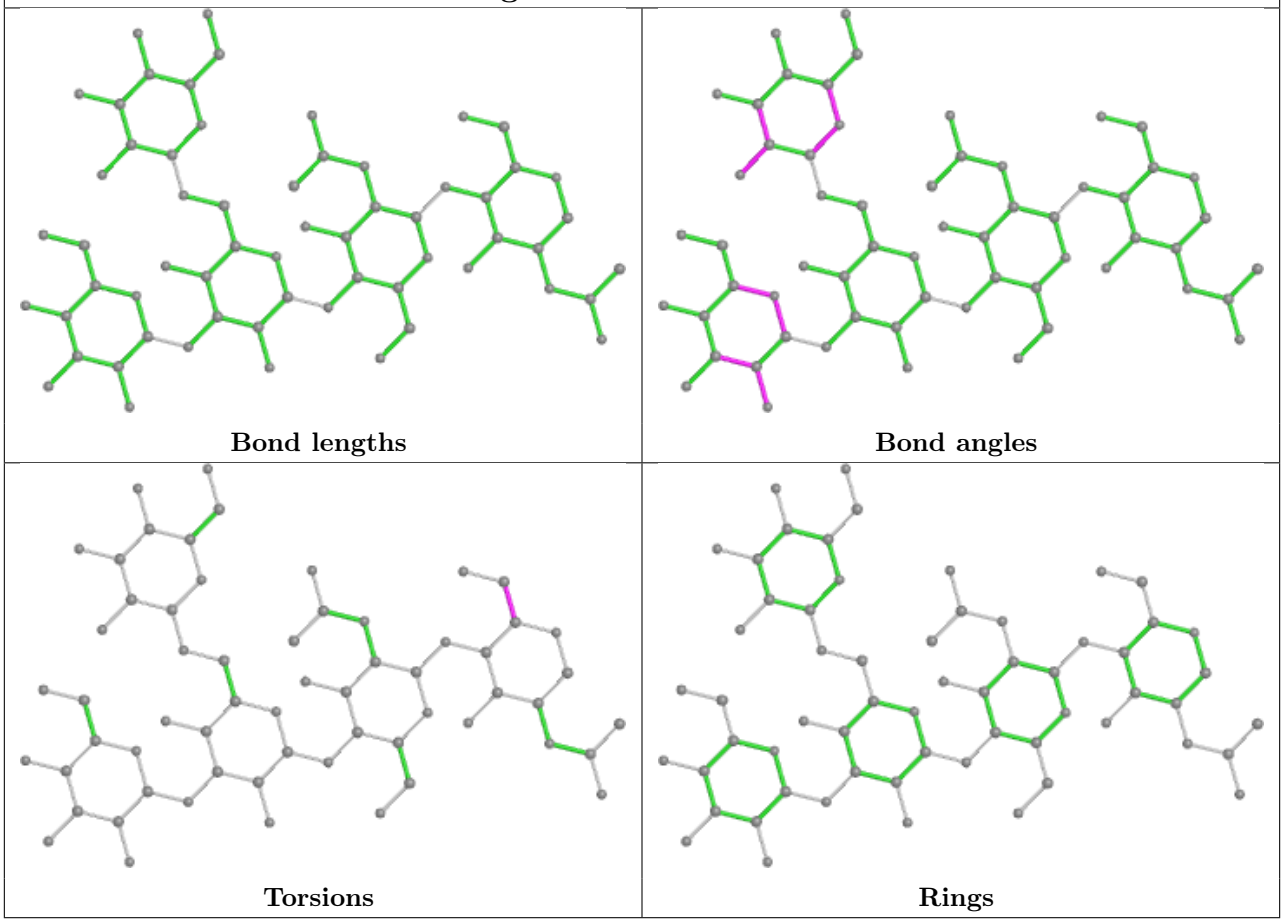
Oligosaccharide Chain E



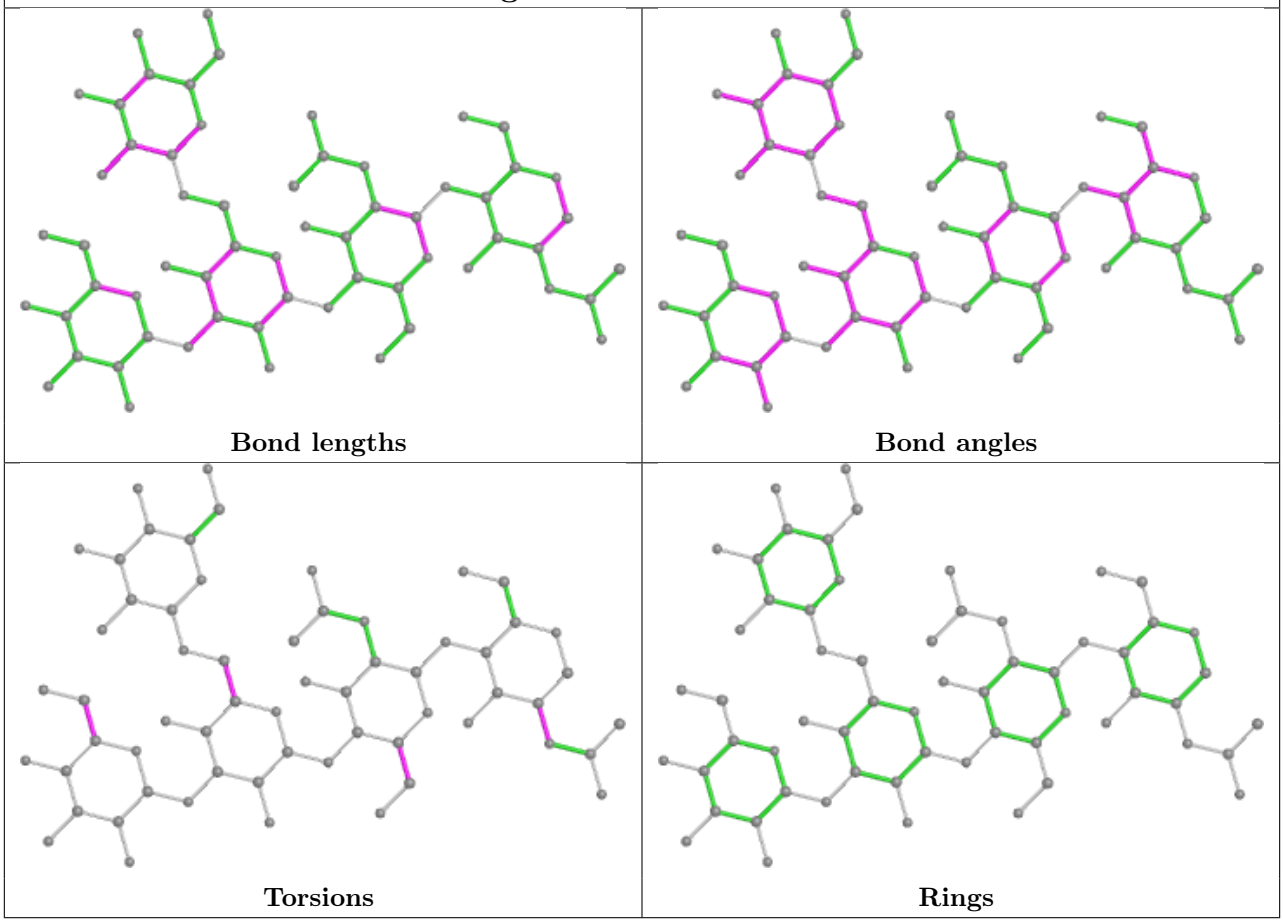
Oligosaccharide Chain X



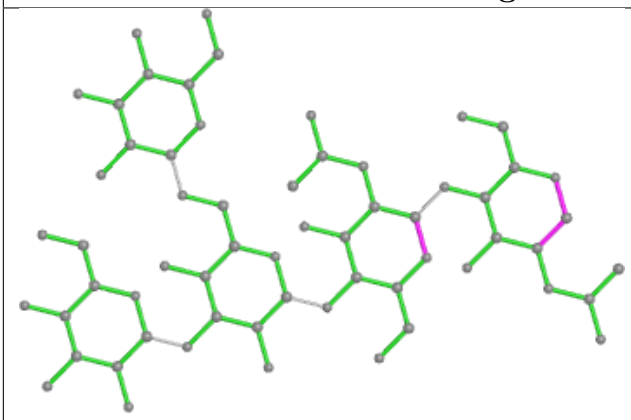
Oligosaccharide Chain c



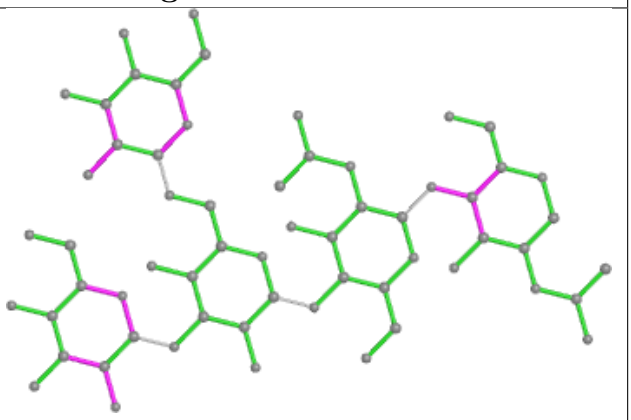
Oligosaccharide Chain e



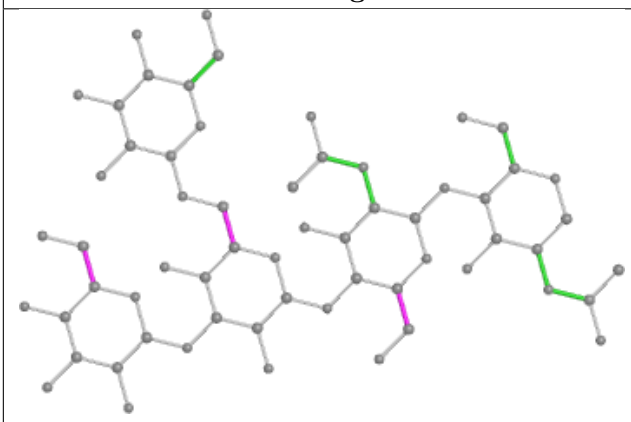
Oligosaccharide Chain g



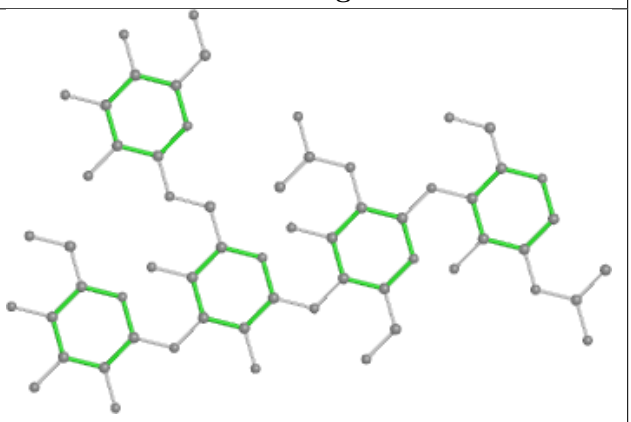
Bond lengths



Bond angles

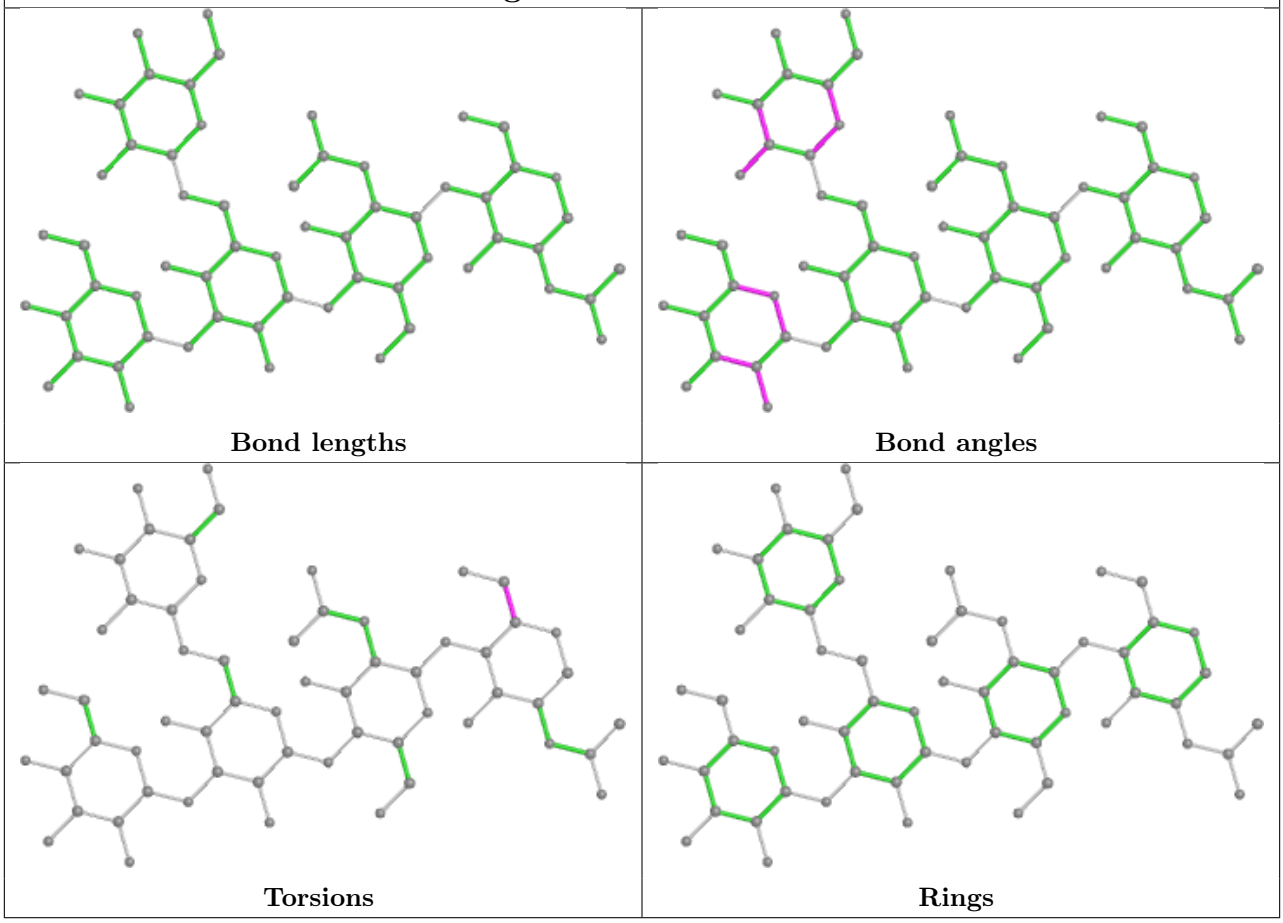


Torsions

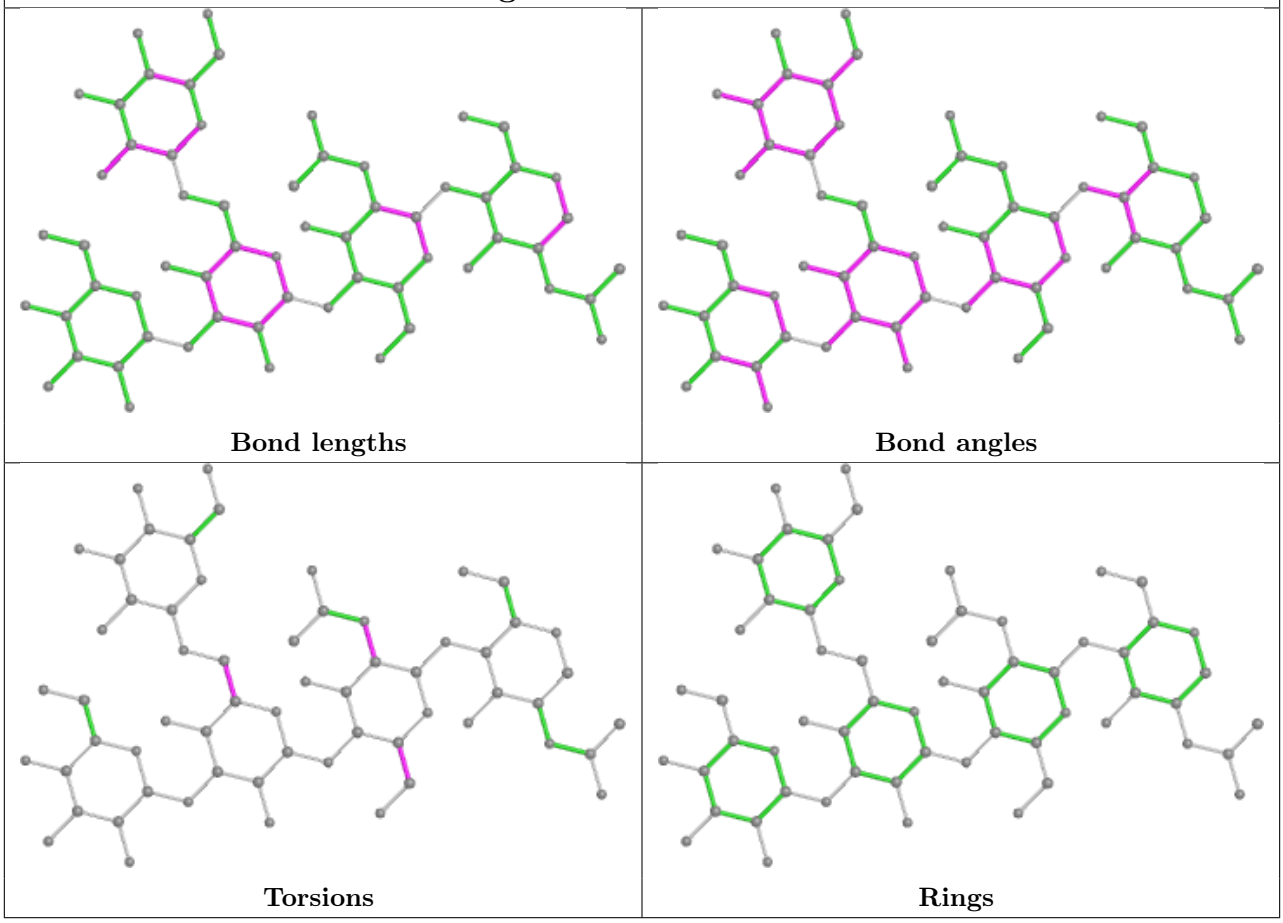


Rings

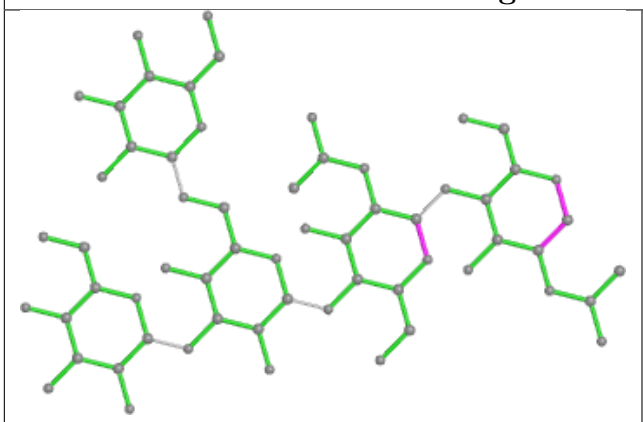
Oligosaccharide Chain l



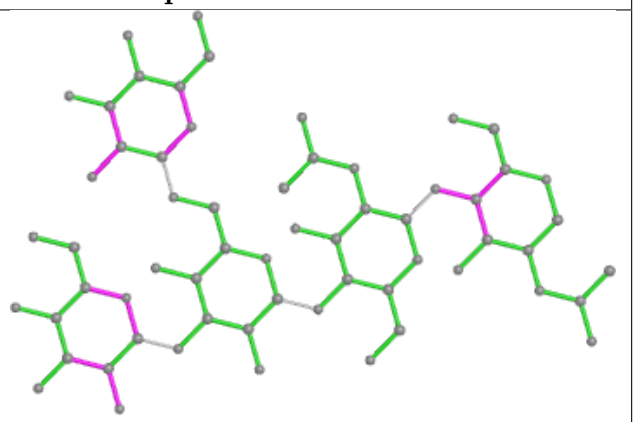
Oligosaccharide Chain n



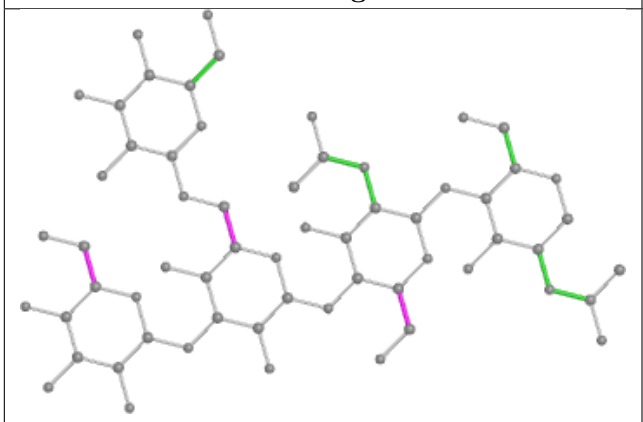
Oligosaccharide Chain p



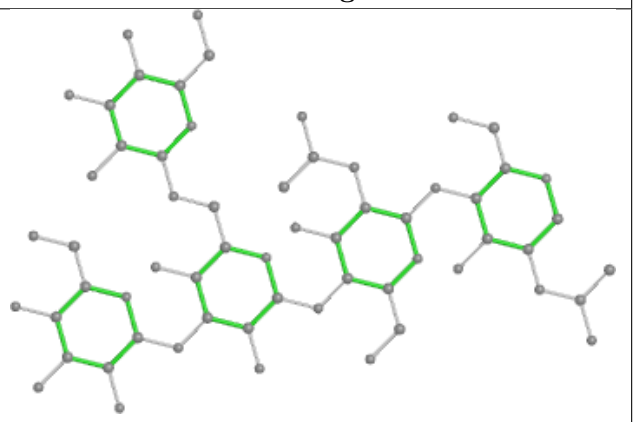
Bond lengths



Bond angles

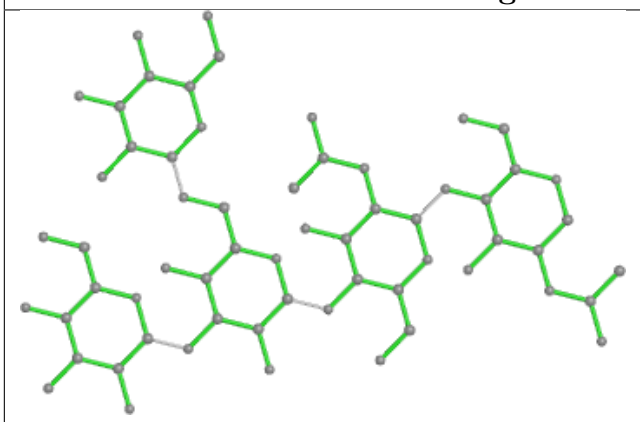


Torsions



Rings

Oligosaccharide Chain u



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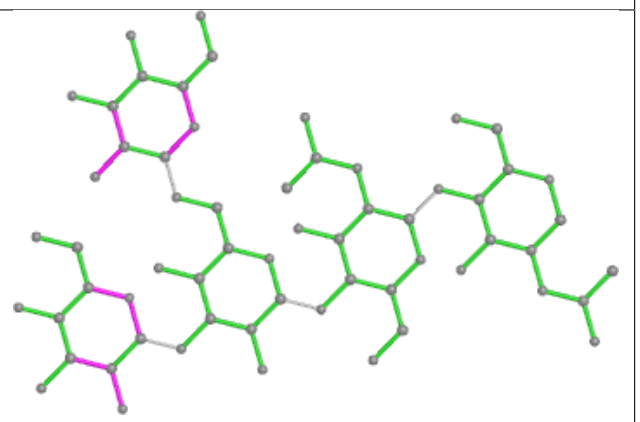
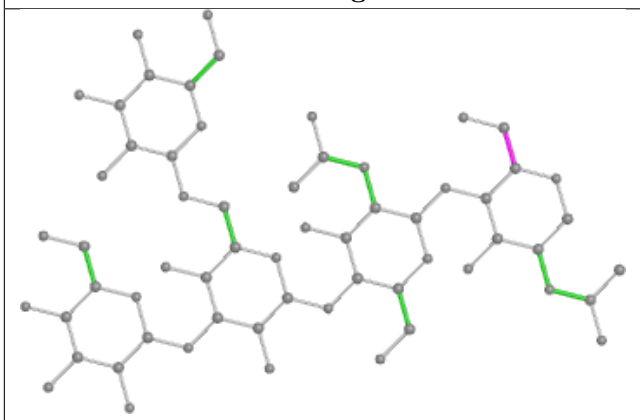
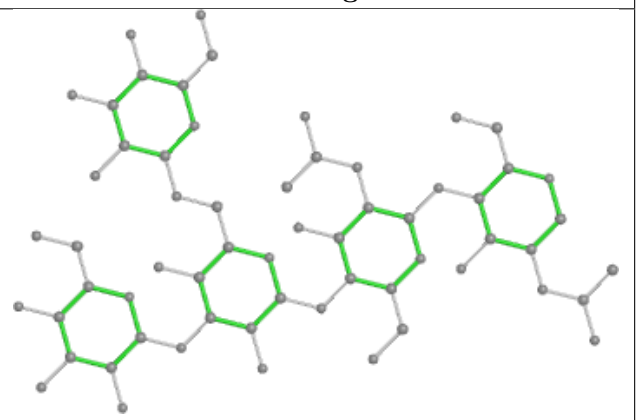


Bond angles

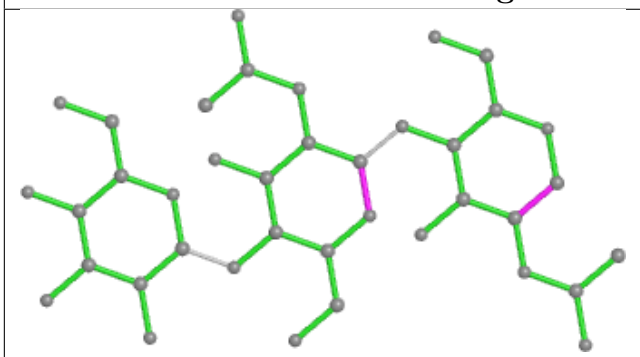


Torsions



Rings

Oligosaccharide Chain P



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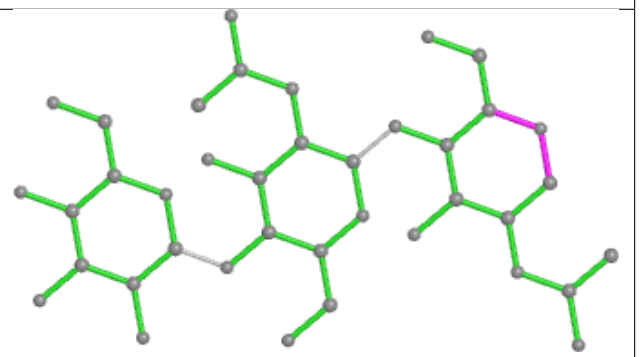
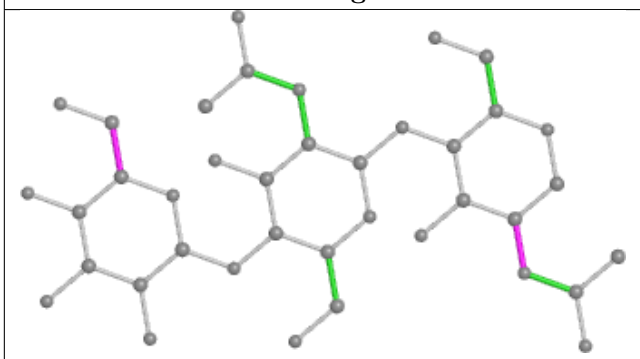


Bond angles



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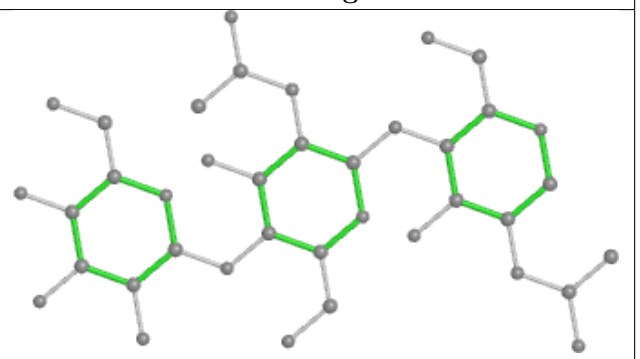
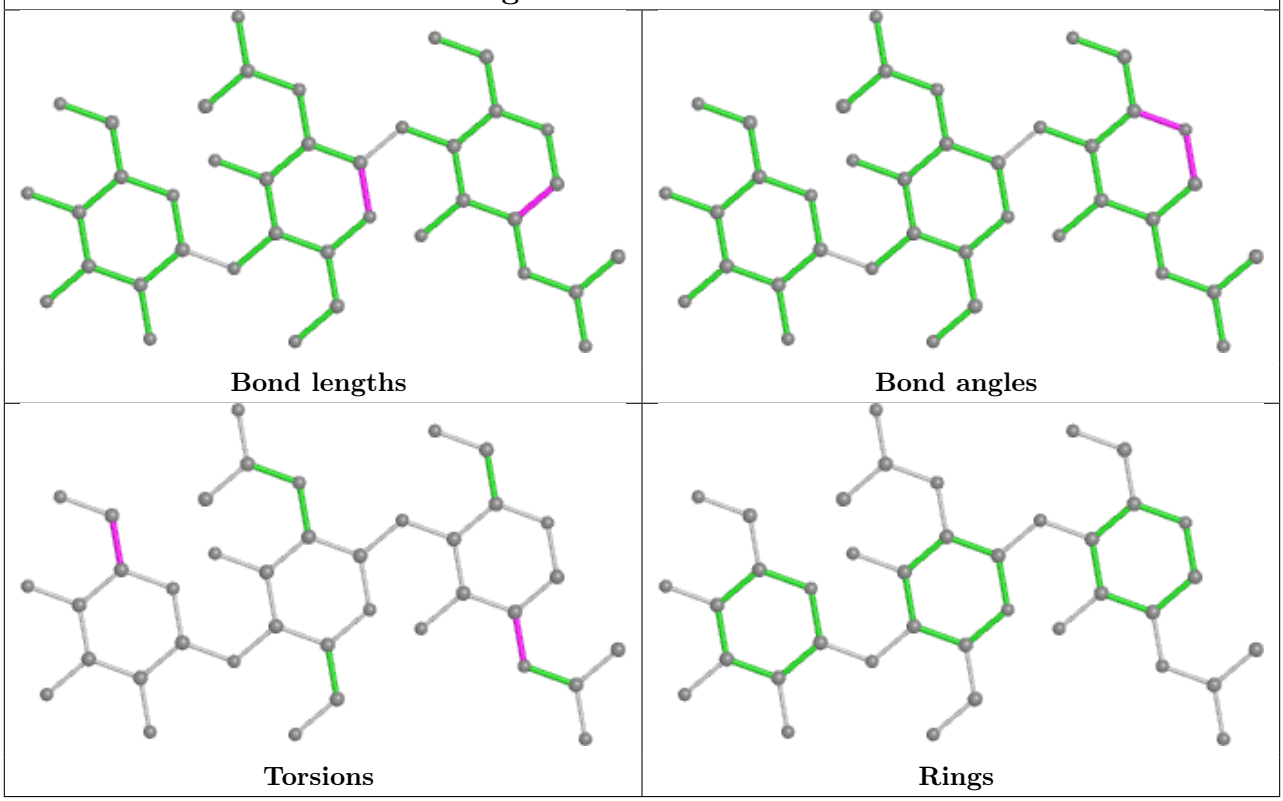
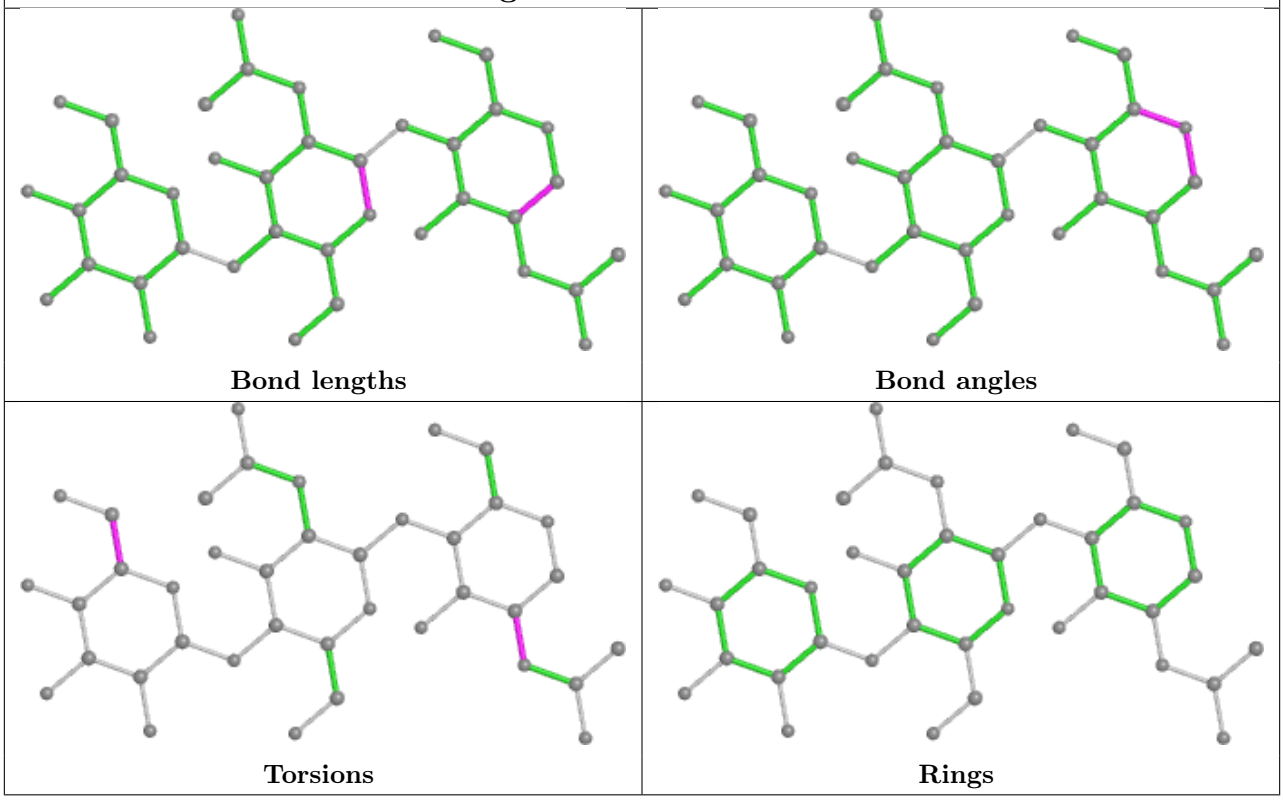


Rings

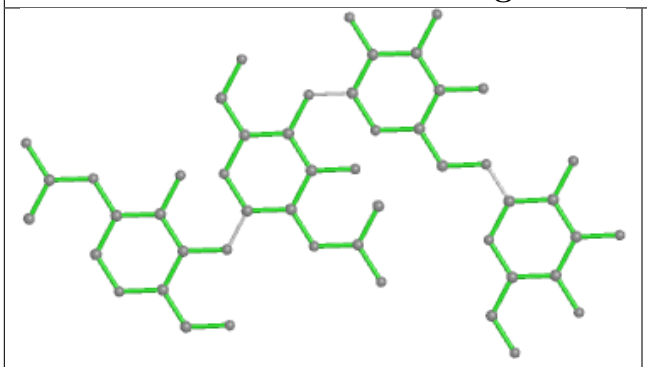
Oligosaccharide Chain f



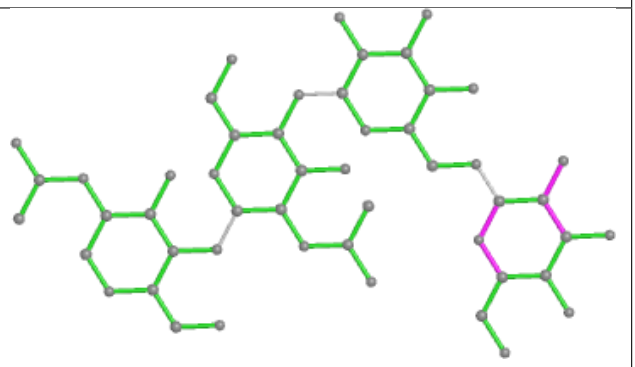
Oligosaccharide Chain o



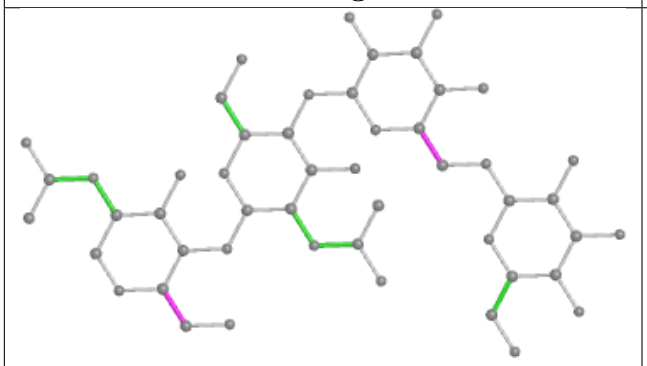
Oligosaccharide Chain Y



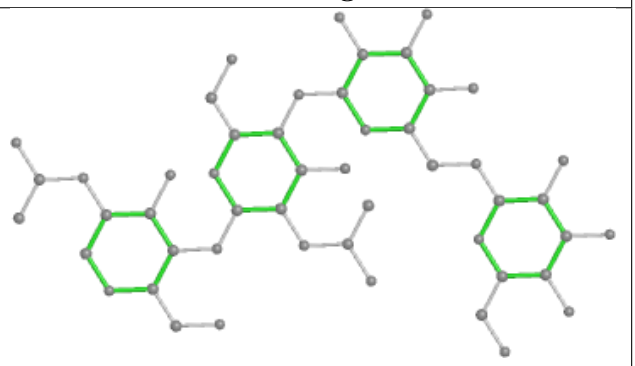
Bond lengths



Bond angles

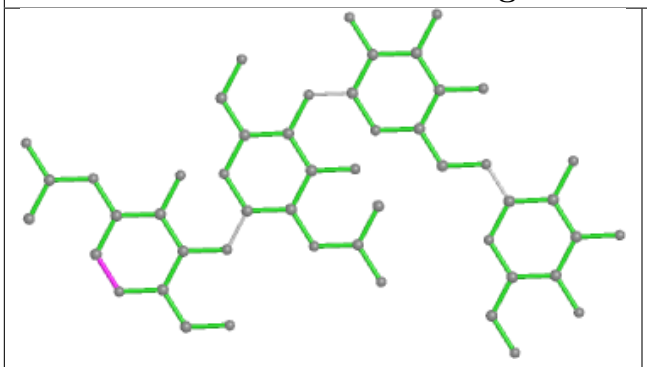


Torsions



Rings

Oligosaccharide Chain h



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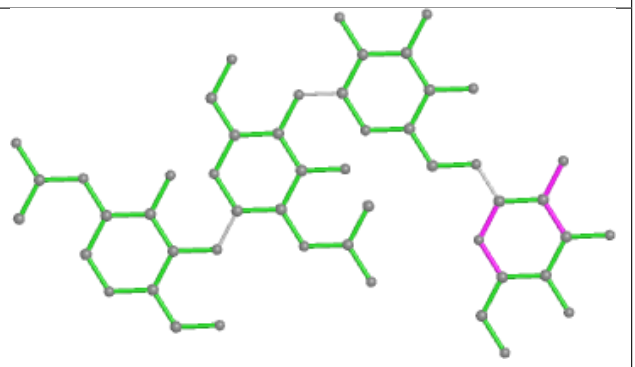
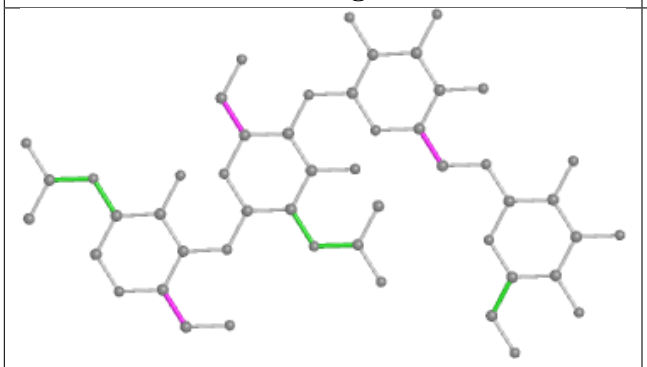


Bond angles



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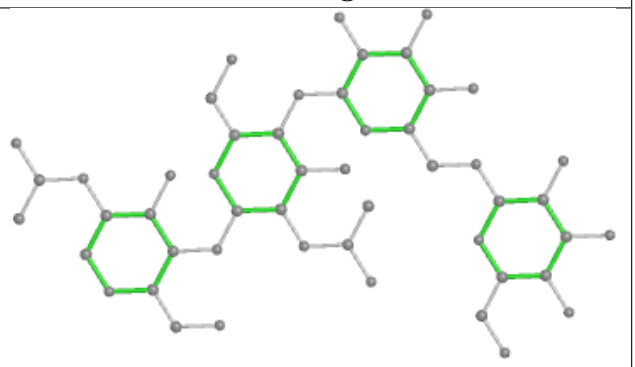
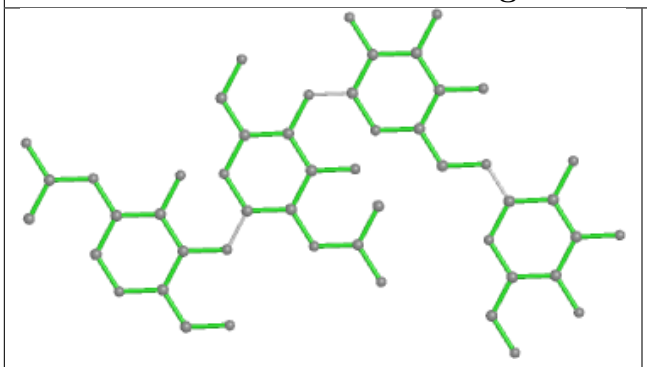


Rings

Oligosaccharide Chain q



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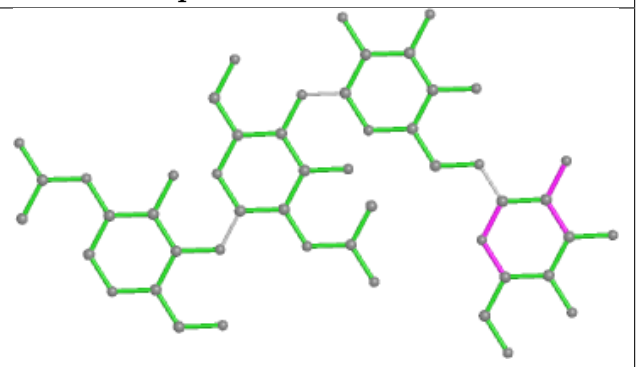
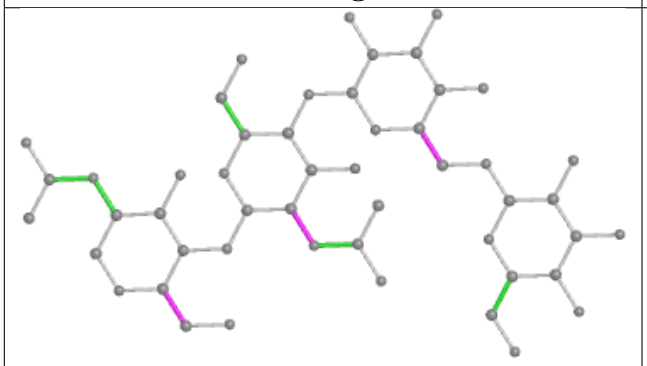
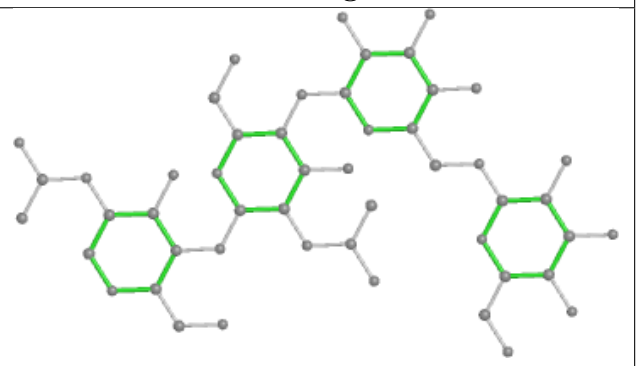


Bond angles

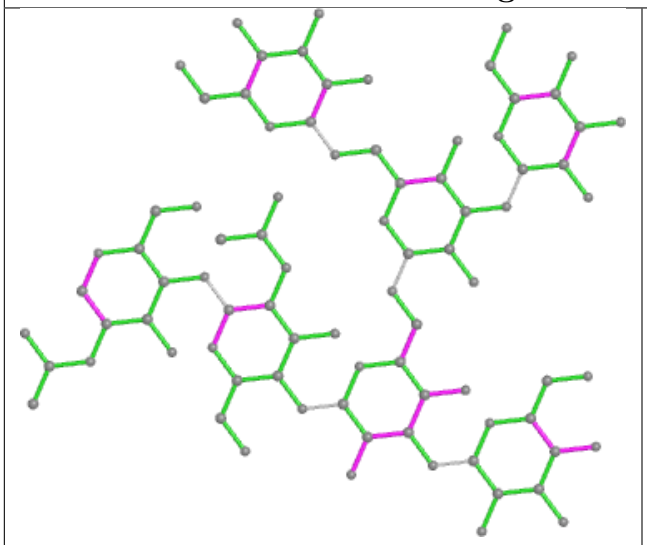


Torsions



Rings

Oligosaccharide Chain Z



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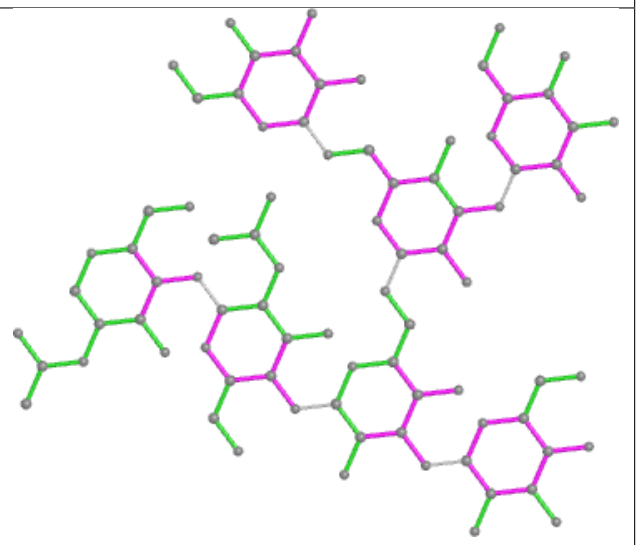
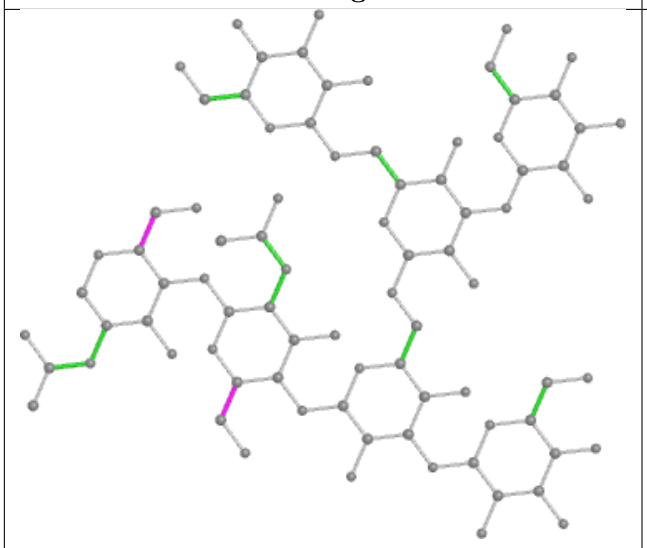


Bond angles



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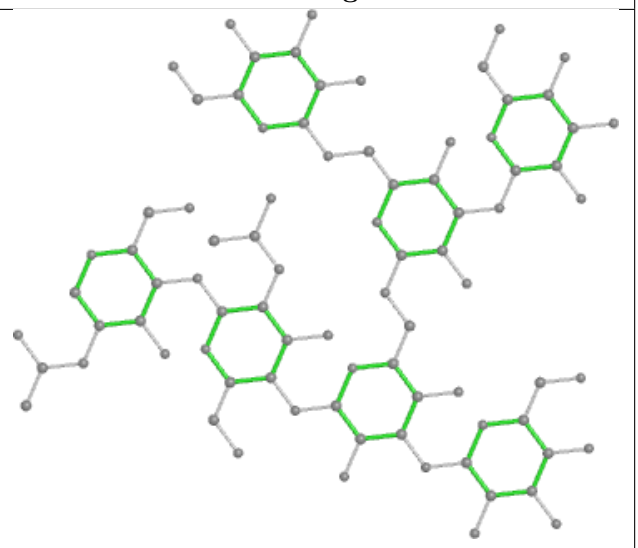
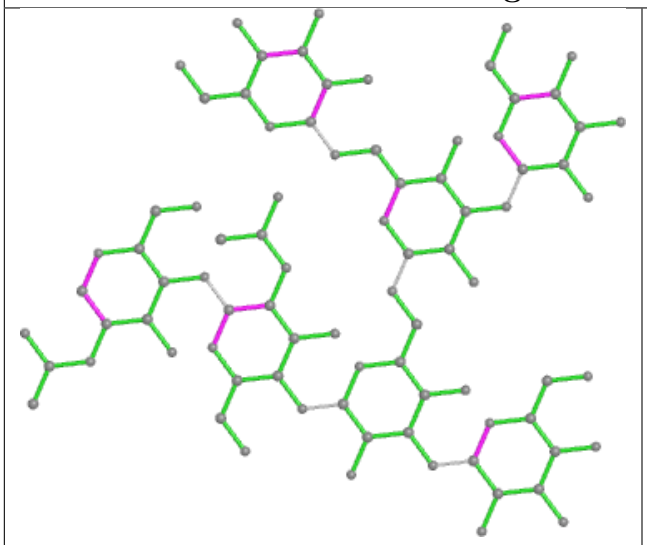


Rings

Oligosaccharide Chain i



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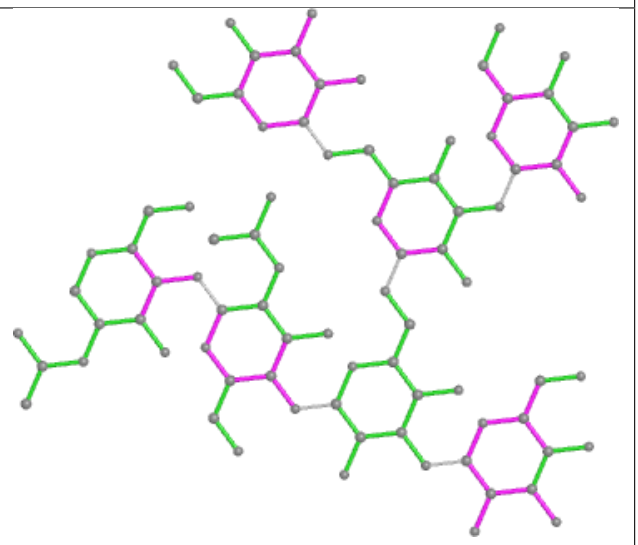
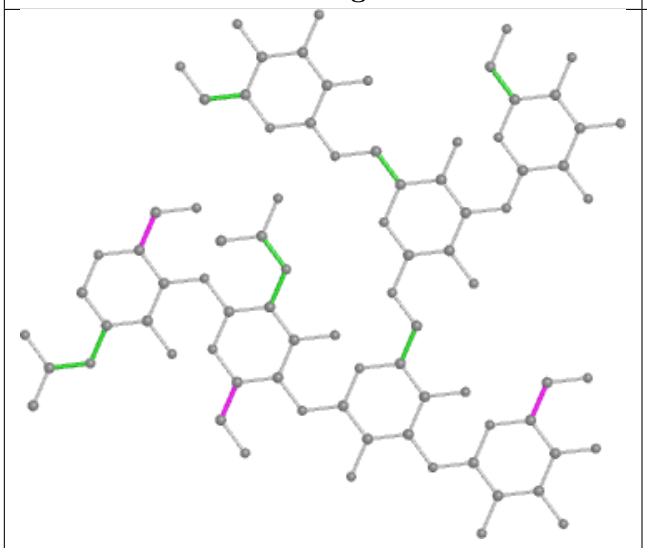


Bond angles



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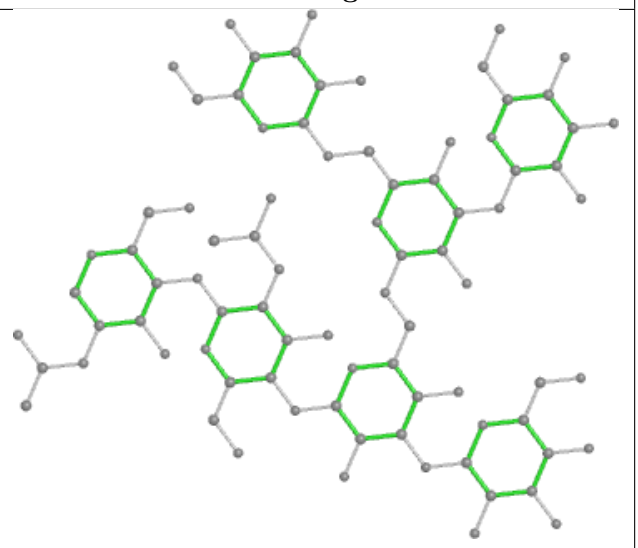
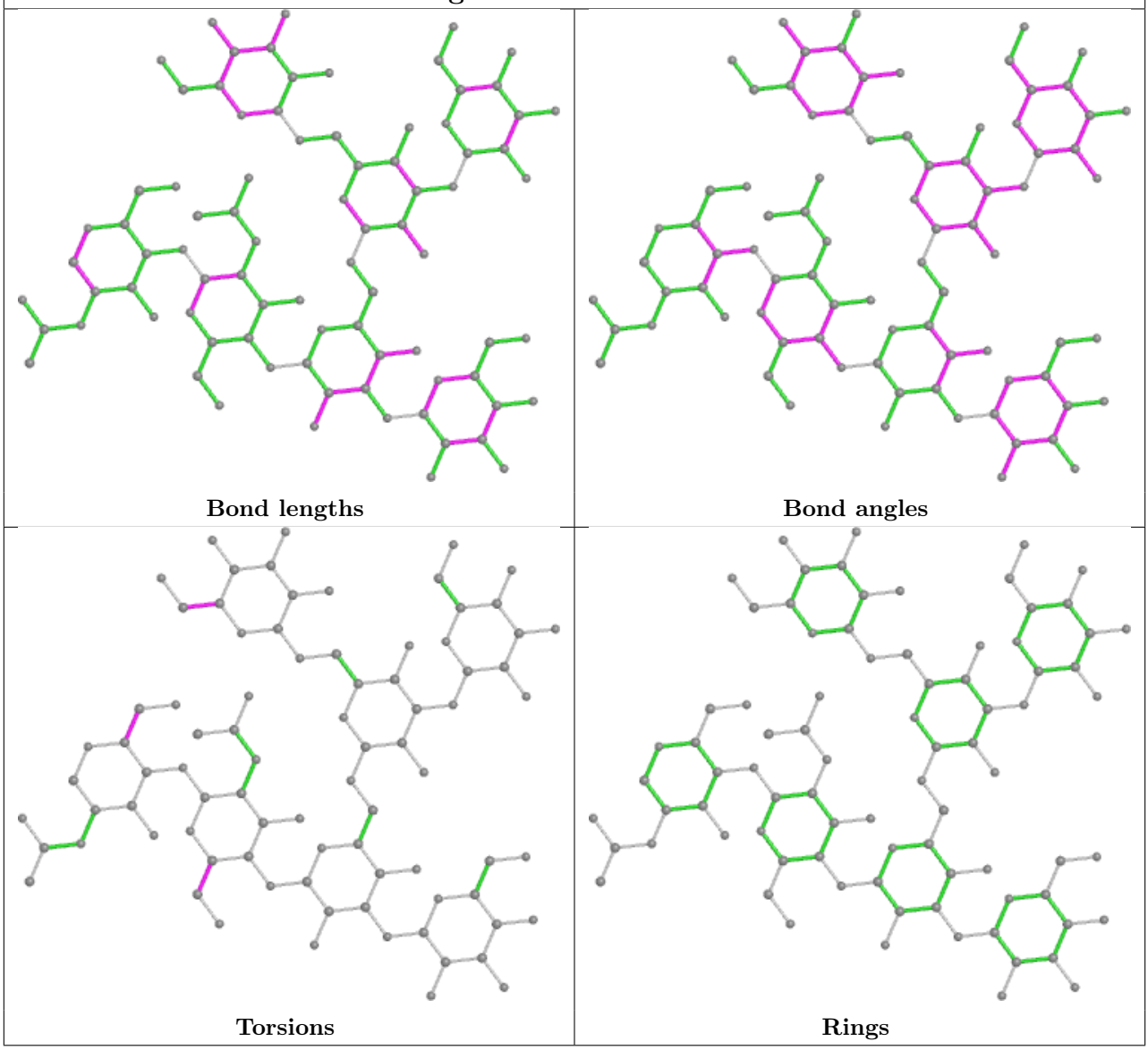
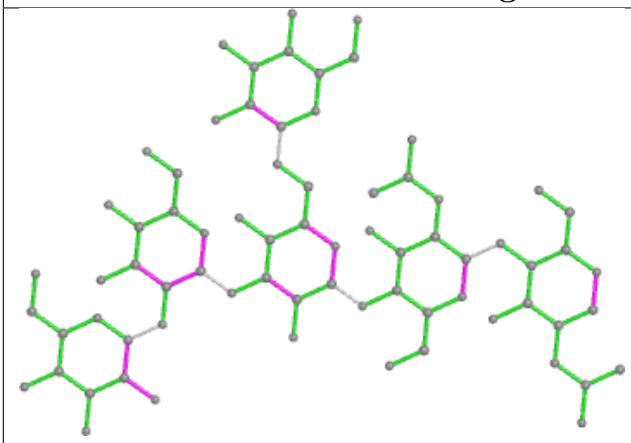


Rings

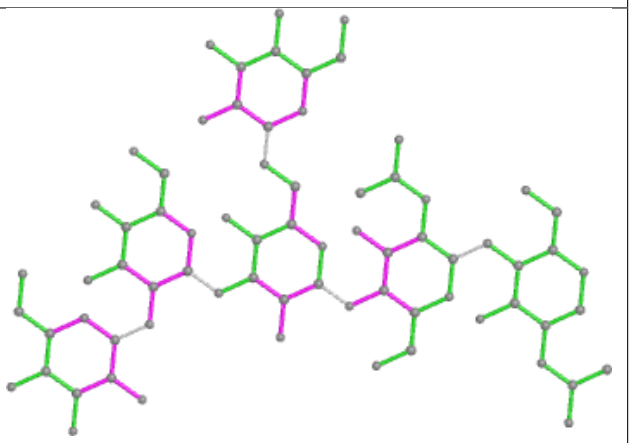
Oligosaccharide Chain r



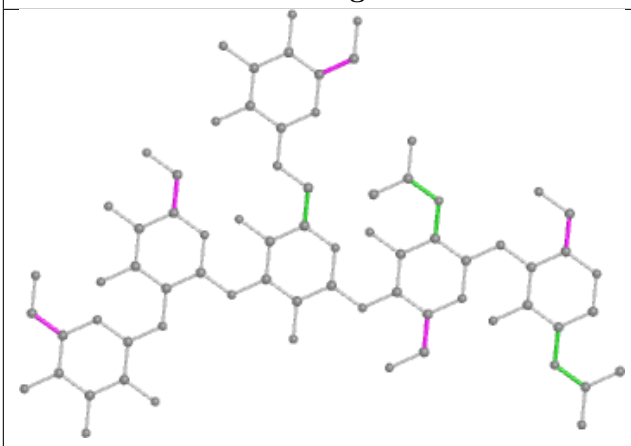
Oligosaccharide Chain a



Bond lengths



Bond angles



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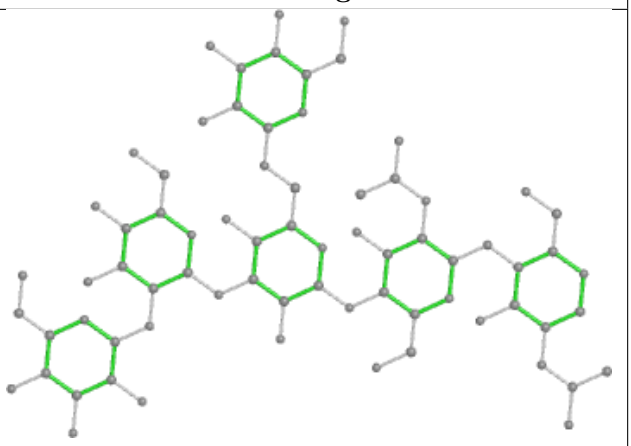
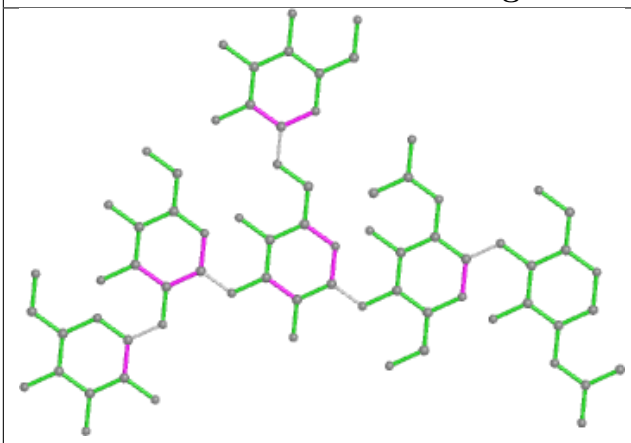


Rings

Oligosaccharide Chain j



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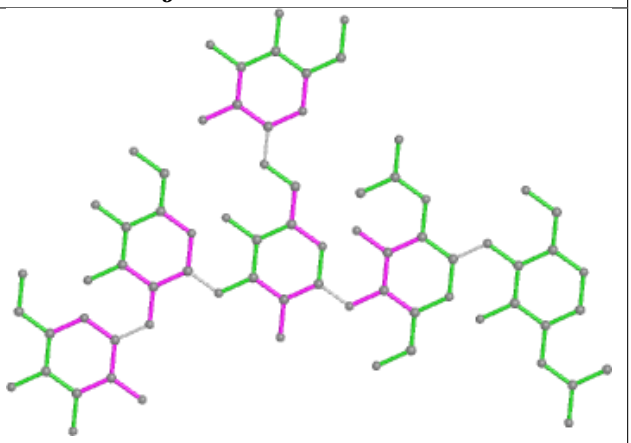
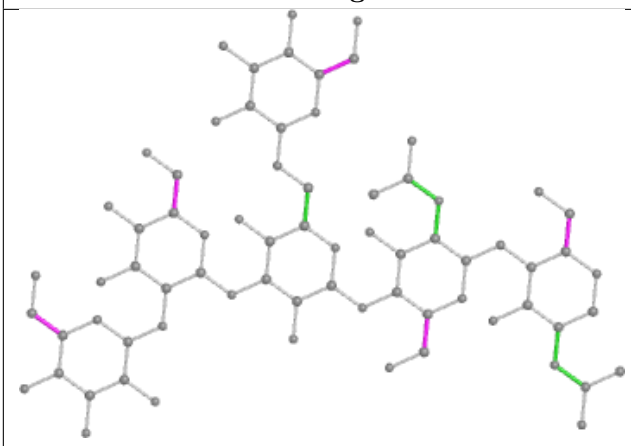


Bond angles



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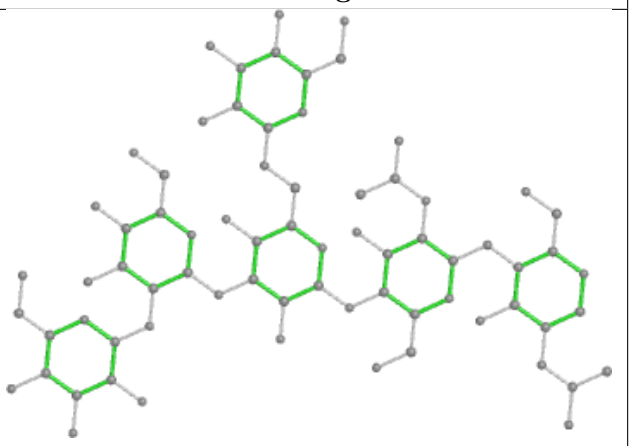
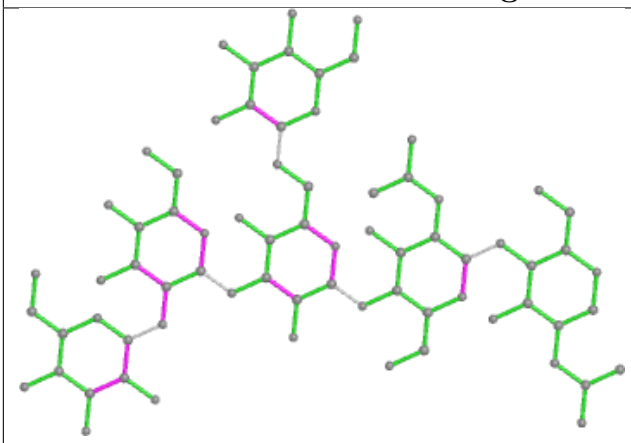


Rings

Oligosaccharide Chain s



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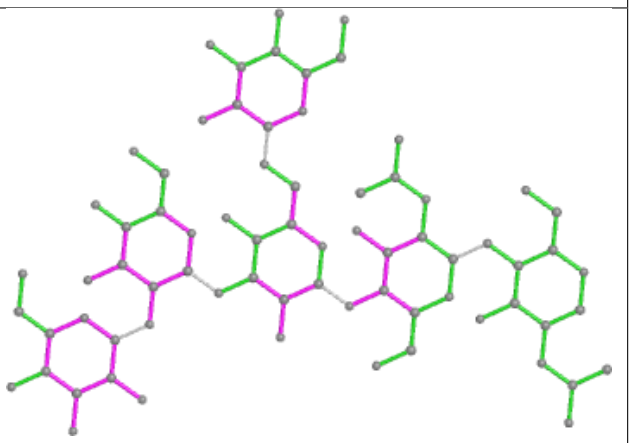
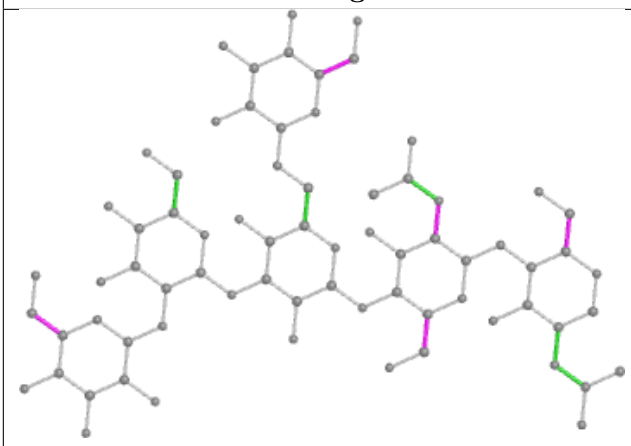
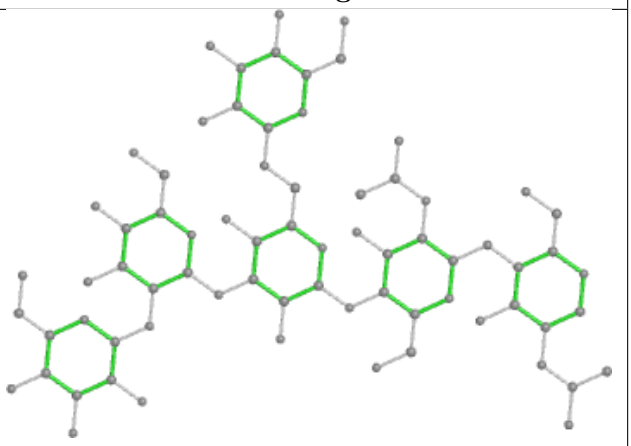


Bond angles

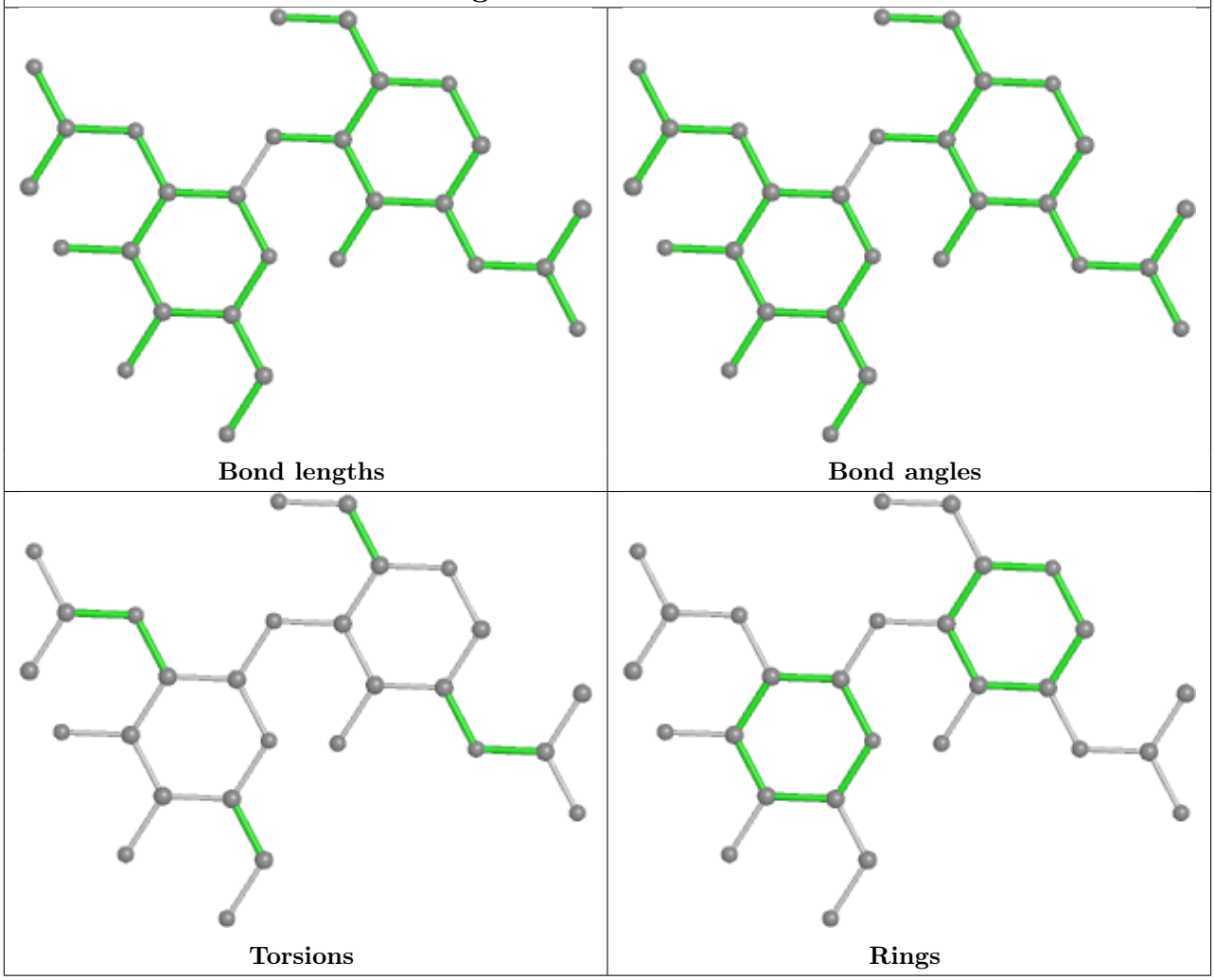


Torsions

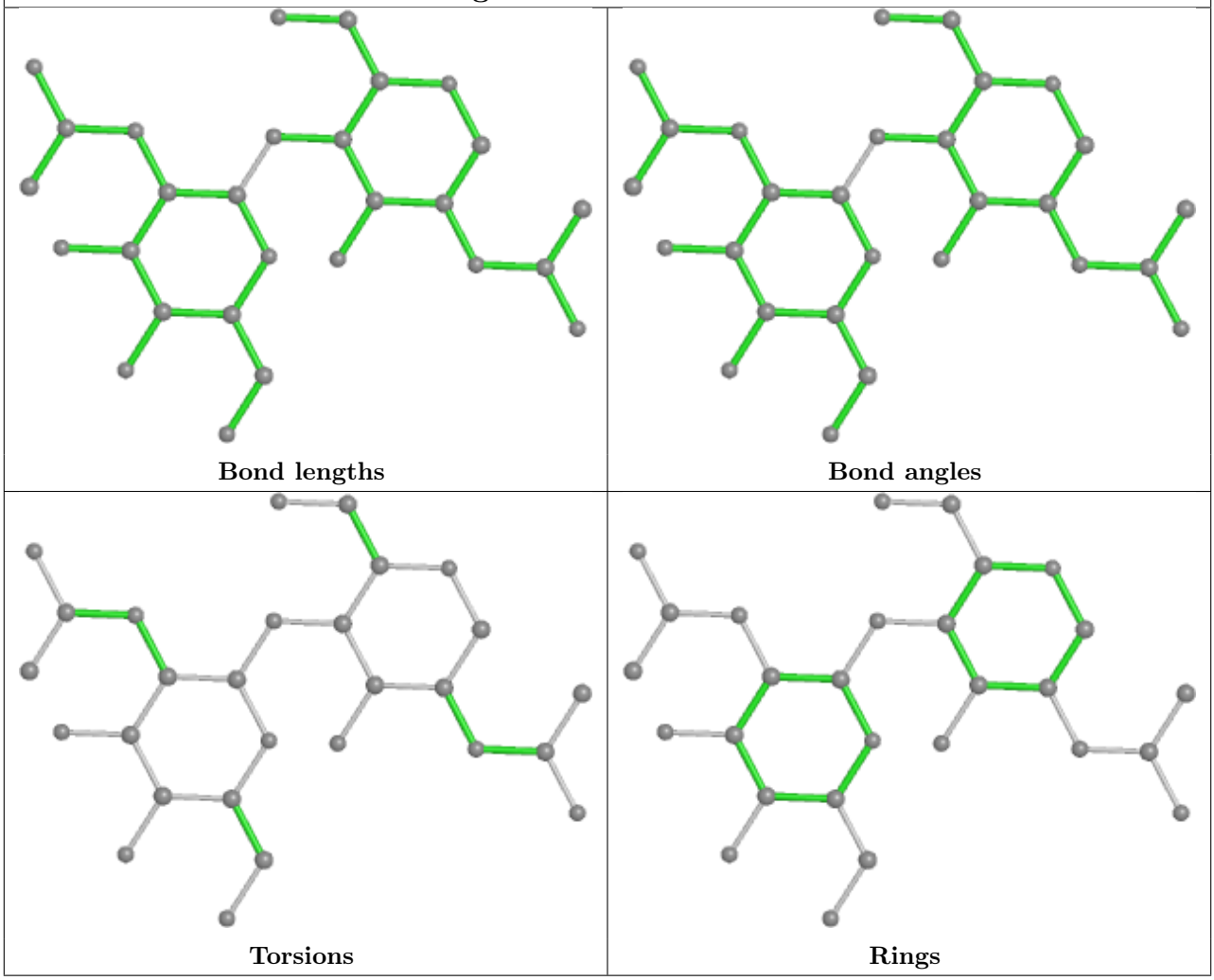


Rings

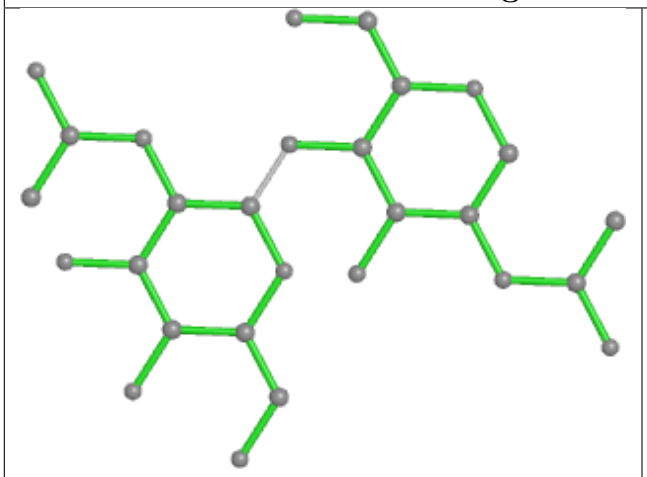
Oligosaccharide Chain b



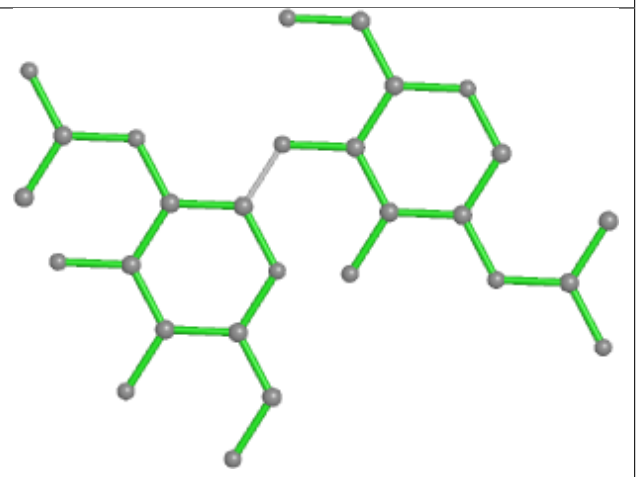
Oligosaccharide Chain k



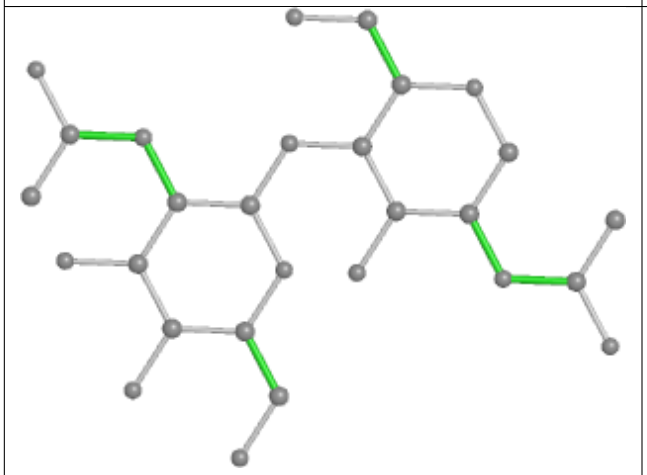
Oligosaccharide Chain t



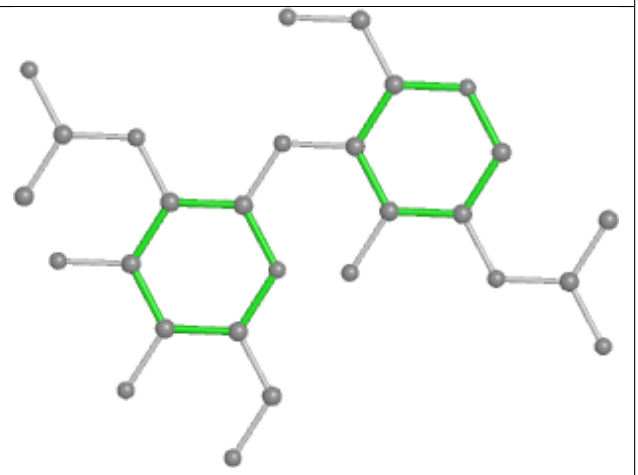
Bond lengths



Bond angles

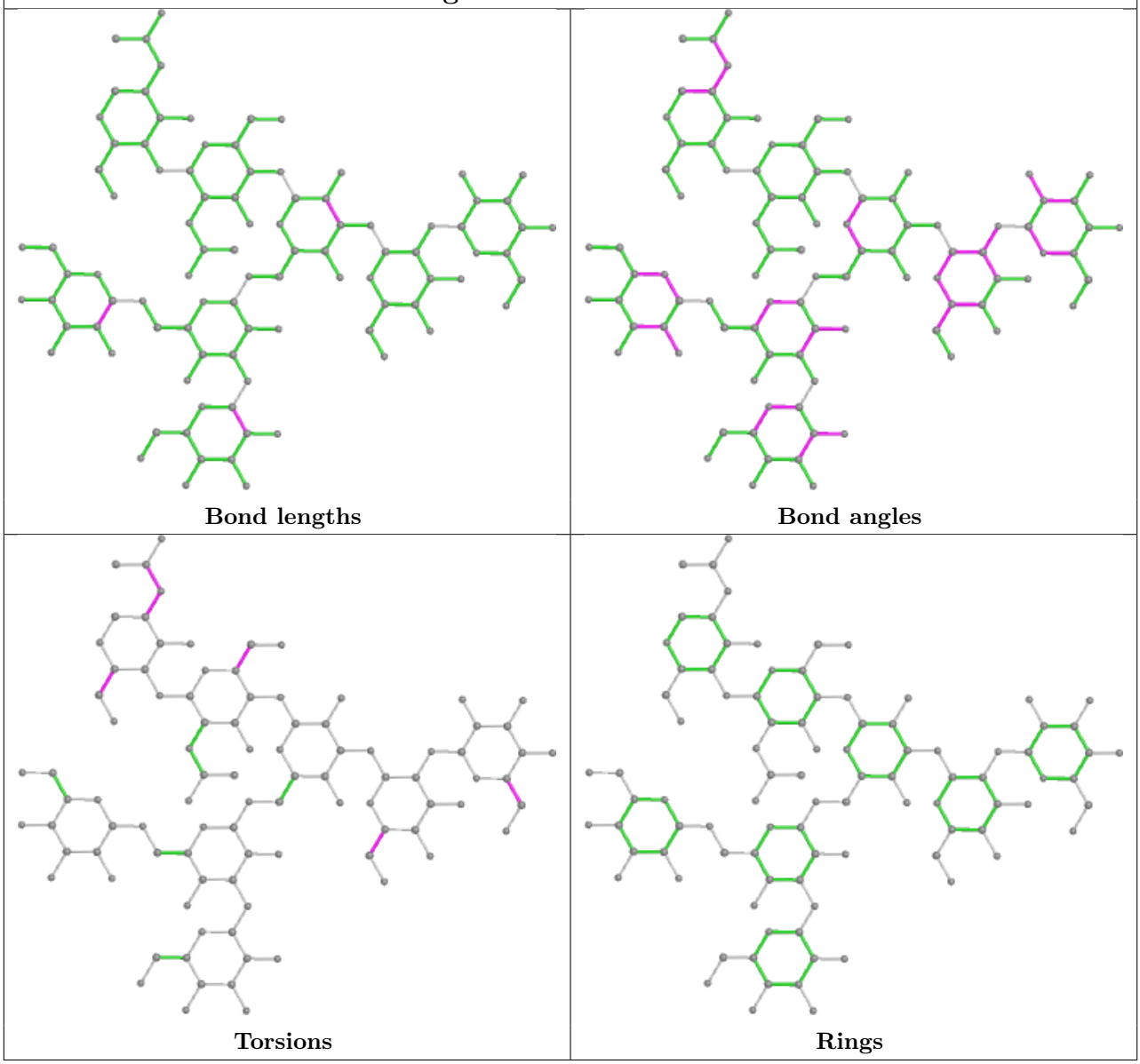


Torsions

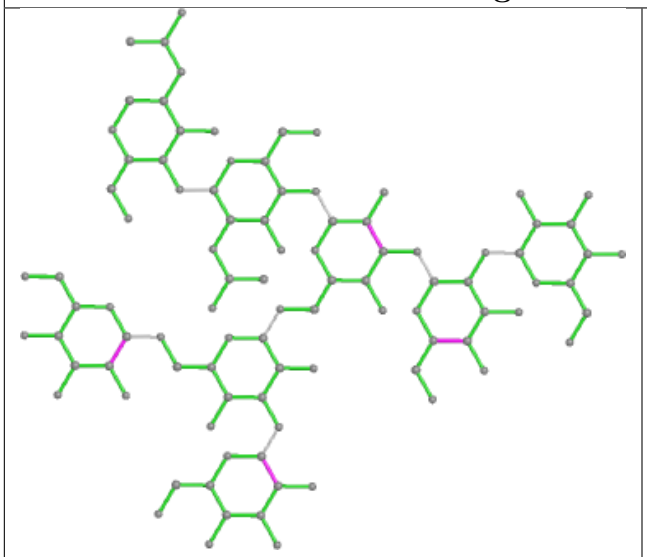


Rings

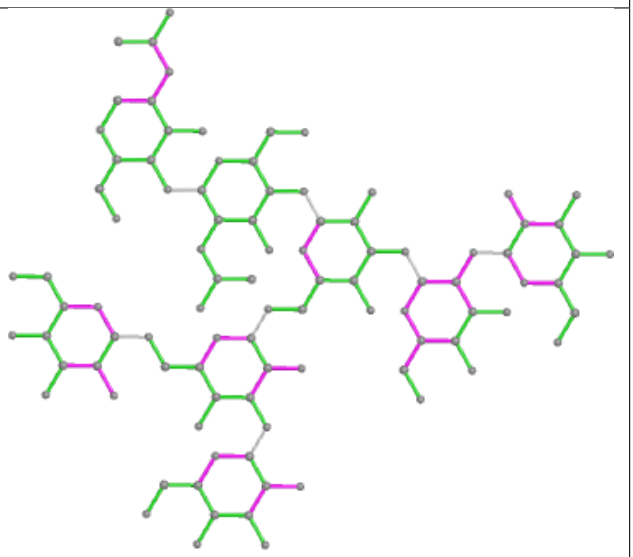
Oligosaccharide Chain d



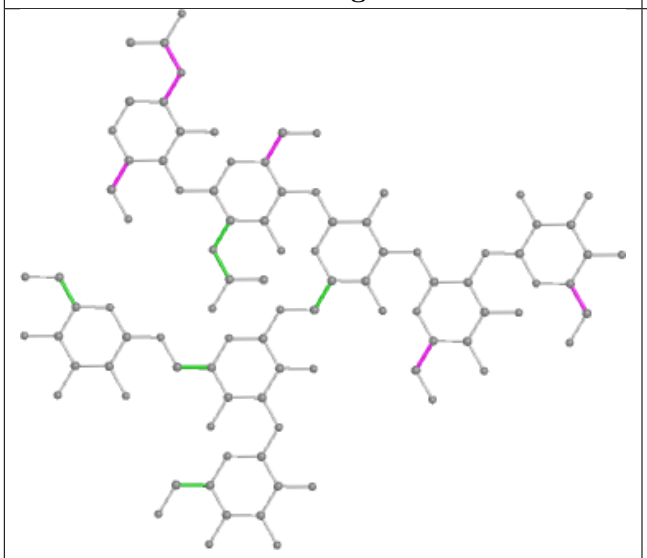
Oligosaccharide Chain m



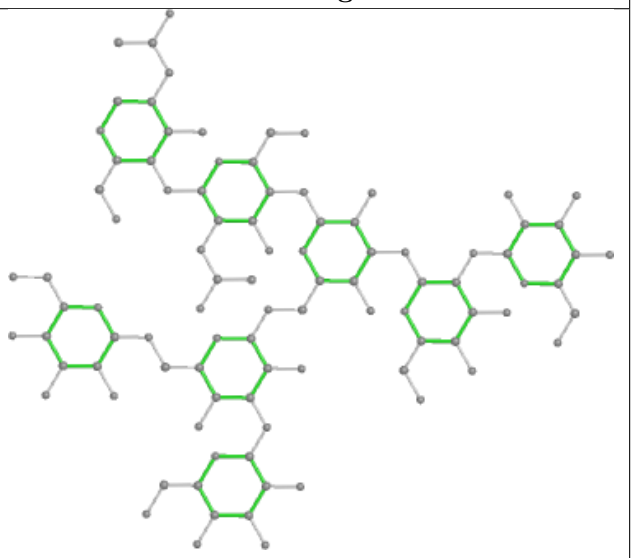
Bond lengths



Bond angles

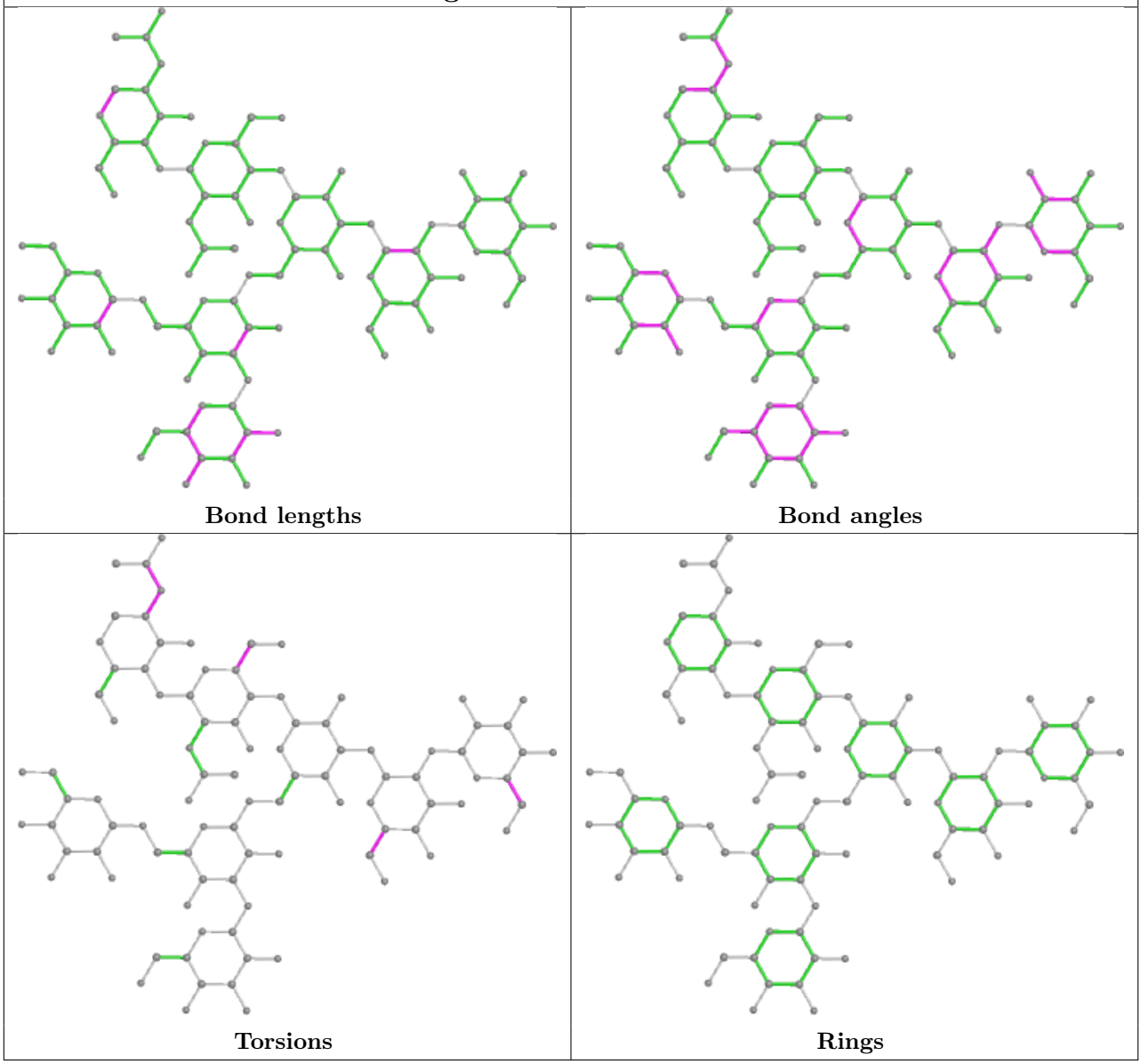


Torsions



Rings

Oligosaccharide Chain v



5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
15	NAG	A	702	3	14,14,15	0.66	1 (7%)	17,19,21	0.54	0
15	NAG	Q	606	1	14,14,15	0.41	0	17,19,21	0.55	0
15	NAG	G	652	1	14,14,15	0.18	0	17,19,21	0.33	0
15	NAG	Q	615	1	14,14,15	0.19	0	17,19,21	0.47	0
15	NAG	F	652	1	14,14,15	0.19	0	17,19,21	0.35	0
15	NAG	G	653	1	14,14,15	0.47	0	17,19,21	0.49	0
15	NAG	G	606	1	14,14,15	0.44	0	17,19,21	0.54	0
15	NAG	R	701	3	14,14,15	0.79	1 (7%)	17,19,21	0.54	0
15	NAG	F	651	1	14,14,15	0.22	0	17,19,21	0.36	0
15	NAG	Q	649	1	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
15	NAG	Q	653	1	14,14,15	1.10	1 (7%)	17,19,21	0.74	1 (5%)
15	NAG	Q	633	1	14,14,15	0.21	0	17,19,21	0.40	0
15	NAG	F	649	1	14,14,15	1.67	3 (21%)	17,19,21	2.38	8 (47%)
15	NAG	Q	650	1	14,14,15	0.25	0	17,19,21	0.54	0
15	NAG	F	606	1	14,14,15	0.42	0	17,19,21	0.54	0
15	NAG	F	633	1	14,14,15	0.22	0	17,19,21	0.38	0
15	NAG	F	615	1	14,14,15	0.17	0	17,19,21	0.47	0
15	NAG	G	615	1	14,14,15	0.94	2 (14%)	17,19,21	0.88	1 (5%)
15	NAG	F	650	1	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
15	NAG	G	649	1	14,14,15	1.79	2 (14%)	17,19,21	2.32	8 (47%)
15	NAG	G	651	1	14,14,15	0.34	0	17,19,21	0.50	0
15	NAG	G	650	1	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
15	NAG	A	701	3	14,14,15	0.66	1 (7%)	17,19,21	0.57	0
15	NAG	F	653	1	14,14,15	0.82	1 (7%)	17,19,21	0.58	0
15	NAG	Q	651	1	14,14,15	2.08	1 (7%)	17,19,21	2.09	6 (35%)
15	NAG	G	633	1	14,14,15	0.24	0	17,19,21	0.38	0
15	NAG	R	702	3	14,14,15	0.77	1 (7%)	17,19,21	0.60	0
15	NAG	J	702	3	14,14,15	0.91	1 (7%)	17,19,21	0.57	0
15	NAG	A	703	3	14,14,15	0.62	0	17,19,21	0.83	0
15	NAG	R	703	3	14,14,15	0.65	0	17,19,21	0.81	0
15	NAG	J	703	3	14,14,15	0.69	1 (7%)	17,19,21	0.83	0
15	NAG	J	701	3	14,14,15	0.65	1 (7%)	17,19,21	0.60	0
15	NAG	Q	652	1	14,14,15	0.18	0	17,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	702	3	-	0/6/23/26	0/1/1/1
15	NAG	Q	606	1	-	1/6/23/26	0/1/1/1
15	NAG	G	652	1	-	4/6/23/26	0/1/1/1
15	NAG	Q	615	1	-	4/6/23/26	0/1/1/1
15	NAG	F	652	1	-	4/6/23/26	0/1/1/1
15	NAG	G	653	1	-	2/6/23/26	0/1/1/1
15	NAG	G	606	1	-	1/6/23/26	0/1/1/1
15	NAG	R	701	3	-	2/6/23/26	0/1/1/1
15	NAG	F	651	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	649	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	653	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	633	1	-	0/6/23/26	0/1/1/1
15	NAG	F	649	1	-	1/6/23/26	0/1/1/1
15	NAG	Q	650	1	-	0/6/23/26	0/1/1/1
15	NAG	F	606	1	-	1/6/23/26	0/1/1/1
15	NAG	F	633	1	-	0/6/23/26	0/1/1/1
15	NAG	F	615	1	-	4/6/23/26	0/1/1/1
15	NAG	G	615	1	-	3/6/23/26	0/1/1/1
15	NAG	F	650	1	-	0/6/23/26	0/1/1/1
15	NAG	G	649	1	-	1/6/23/26	0/1/1/1
15	NAG	G	651	1	-	0/6/23/26	0/1/1/1
15	NAG	G	650	1	-	0/6/23/26	0/1/1/1
15	NAG	A	701	3	-	0/6/23/26	0/1/1/1
15	NAG	F	653	1	-	0/6/23/26	0/1/1/1
15	NAG	Q	651	1	-	0/6/23/26	0/1/1/1
15	NAG	G	633	1	-	0/6/23/26	0/1/1/1
15	NAG	R	702	3	-	0/6/23/26	0/1/1/1
15	NAG	J	702	3	-	0/6/23/26	0/1/1/1
15	NAG	A	703	3	-	0/6/23/26	0/1/1/1
15	NAG	R	703	3	-	0/6/23/26	0/1/1/1
15	NAG	J	703	3	-	0/6/23/26	0/1/1/1
15	NAG	J	701	3	-	2/6/23/26	0/1/1/1
15	NAG	Q	652	1	-	4/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	651	NAG	O5-C1	-7.20	1.32	1.43
15	G	649	NAG	O5-C1	-5.53	1.34	1.43
15	F	649	NAG	O5-C1	-4.83	1.36	1.43
15	Q	653	NAG	O5-C1	-3.59	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	702	NAG	O5-C1	-3.07	1.38	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	649	NAG	C3-C4-C5	4.73	118.67	110.24
15	G	649	NAG	C3-C4-C5	4.44	118.16	110.24
15	G	649	NAG	O4-C4-C5	4.07	119.41	109.30
15	Q	651	NAG	O4-C4-C5	4.03	119.31	109.30
15	F	649	NAG	O4-C4-C5	4.01	119.25	109.30

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	615	NAG	O5-C5-C6-O6
15	Q	615	NAG	O5-C5-C6-O6
15	G	653	NAG	C4-C5-C6-O6
15	G	615	NAG	O5-C5-C6-O6
15	G	652	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	F	449/471 (95%)	0.43	30 (6%)	17	18	261, 419, 512, 568	0
1	G	449/471 (95%)	0.35	16 (3%)	42	38	251, 420, 504, 599	0
1	Q	449/471 (95%)	0.43	24 (5%)	26	26	240, 430, 527, 617	0
2	D	222/250 (88%)	1.03	41 (18%)	1	4	303, 478, 541, 600	0
2	O	222/250 (88%)	0.92	34 (15%)	2	5	285, 453, 530, 563	0
2	W	222/250 (88%)	1.01	39 (17%)	1	4	292, 497, 603, 637	0
3	A	126/147 (85%)	0.07	3 (2%)	59	52	241, 374, 496, 610	0
3	J	126/147 (85%)	0.18	5 (3%)	38	34	245, 378, 467, 584	0
3	R	126/147 (85%)	0.28	5 (3%)	38	34	209, 367, 476, 681	0
4	B	210/210 (100%)	1.34	61 (29%)	0	2	274, 470, 717, 766	0
4	K	210/210 (100%)	1.66	67 (31%)	0	2	308, 556, 766, 872	0
4	S	210/210 (100%)	1.51	58 (27%)	0	2	316, 507, 686, 716	0
5	C	228/232 (98%)	1.73	70 (30%)	0	2	328, 474, 737, 788	0
5	L	228/232 (98%)	1.51	72 (31%)	0	2	311, 467, 818, 919	0
5	T	228/232 (98%)	2.14	94 (41%)	0	1	367, 548, 770, 828	0
6	H	242/242 (100%)	0.37	14 (5%)	23	23	214, 360, 510, 653	0
6	M	242/242 (100%)	1.37	68 (28%)	0	2	272, 501, 677, 748	0
6	U	242/242 (100%)	0.94	43 (17%)	1	4	214, 438, 635, 673	0
7	I	207/213 (97%)	0.32	5 (2%)	59	52	139, 326, 450, 512	0
7	N	213/213 (100%)	1.17	51 (23%)	0	2	209, 470, 714, 764	0
7	V	213/213 (100%)	0.69	24 (11%)	5	9	175, 400, 572, 618	0
All	All	5064/5295 (95%)	0.90	824 (16%)	1	4	139, 441, 705, 919	0

The worst 5 of 824 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	178	SER	14.5
4	K	201	SER	13.9
4	K	200	GLY	11.9
5	C	185	SER	10.1
4	K	165	PRO	9.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PCA	W	1	8/9	0.51	0.94	355,368,480,481	0
2	PCA	D	1	8/9	0.56	0.90	434,443,508,513	0

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BMA	o	3	11/12	0.00	1.08	641,642,644,644	0
14	MAN	m	8	11/12	0.02	0.92	506,514,524,533	0
11	MAN	Z	6	11/12	0.06	0.58	708,709,711,711	0
11	MAN	r	7	11/12	0.22	0.89	620,620,620,620	0
11	MAN	Z	7	11/12	0.28	0.84	488,488,488,488	0
8	MAN	p	4	11/12	0.34	0.59	563,590,602,606	0
11	BMA	r	3	11/12	0.34	0.46	549,550,550,551	0
9	BMA	P	3	11/12	0.35	0.78	536,538,539,539	0
8	MAN	g	5	11/12	0.36	0.54	526,544,561,562	0
12	MAN	s	5	11/12	0.38	0.72	589,589,589,589	0
8	MAN	X	5	11/12	0.43	0.33	510,528,545,546	0
8	MAN	e	5	11/12	0.45	0.57	555,558,560,561	0
11	BMA	Z	3	11/12	0.45	0.43	541,543,545,545	0
8	MAN	n	4	11/12	0.49	0.56	422,422,423,424	0
14	MAN	v	8	11/12	0.49	0.62	480,486,493,502	0
11	BMA	i	3	11/12	0.50	0.62	485,487,490,492	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BMA	e	3	11/12	0.50	0.66	558,559,560,562	0
8	MAN	p	5	11/12	0.51	0.59	546,563,582,583	0
10	MAN	h	4	11/12	0.52	0.57	519,522,525,526	0
10	BMA	h	3	11/12	0.54	0.50	437,440,442,443	0
8	MAN	l	5	11/12	0.55	0.61	622,623,625,625	0
8	MAN	e	4	11/12	0.56	0.53	508,509,512,512	0
9	NAG	P	2	14/15	0.57	0.43	511,513,515,517	0
8	BMA	p	3	11/12	0.57	0.54	527,544,557,575	0
8	BMA	n	3	11/12	0.58	0.52	470,471,471,471	0
8	MAN	g	4	11/12	0.58	0.52	637,667,676,683	0
10	MAN	q	4	11/12	0.58	0.36	526,527,528,529	0
8	BMA	g	3	11/12	0.59	0.36	626,642,653,670	0
8	MAN	c	5	11/12	0.59	0.50	540,543,547,549	0
8	NAG	e	2	14/15	0.60	0.66	499,504,507,509	0
10	MAN	Y	4	11/12	0.60	0.61	580,581,582,583	0
11	NAG	i	2	14/15	0.60	0.51	501,506,509,511	0
12	MAN	j	6	11/12	0.61	0.89	507,511,517,517	0
12	MAN	j	5	11/12	0.61	0.61	453,467,469,470	0
8	MAN	n	5	11/12	0.62	0.43	457,458,458,459	0
14	MAN	m	6	11/12	0.63	0.53	469,477,482,485	0
8	BMA	c	3	11/12	0.65	0.35	512,514,518,519	0
11	MAN	r	5	11/12	0.65	0.66	605,605,606,607	0
9	NAG	f	2	14/15	0.65	0.47	485,488,490,491	0
14	MAN	d	8	11/12	0.66	0.49	390,393,399,407	0
8	MAN	X	4	11/12	0.66	0.51	521,546,562,562	0
8	MAN	E	4	11/12	0.66	0.54	400,402,404,404	0
10	NAG	Y	1	14/15	0.66	0.45	401,402,404,405	0
9	NAG	f	1	14/15	0.67	0.57	473,478,482,482	0
9	NAG	o	2	14/15	0.68	0.50	620,622,625,626	0
8	NAG	l	1	14/15	0.68	0.50	477,479,481,483	0
8	MAN	c	4	11/12	0.69	0.52	502,506,510,511	0
11	MAN	i	7	11/12	0.69	0.67	448,448,448,448	0
14	NAG	d	1	14/15	0.70	0.47	456,462,468,471	0
11	MAN	i	4	11/12	0.71	0.31	489,492,496,496	0
12	MAN	a	5	11/12	0.71	0.41	502,517,520,521	0
11	MAN	r	4	11/12	0.71	0.30	576,577,579,579	0
10	NAG	h	2	14/15	0.71	0.44	419,421,424,425	0
11	MAN	r	6	11/12	0.71	0.28	454,455,456,457	0
8	NAG	n	1	14/15	0.72	0.36	426,428,429,430	0
11	MAN	Z	4	11/12	0.72	0.36	613,615,616,616	0
11	NAG	r	2	14/15	0.73	0.44	509,510,511,511	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	BMA	q	3	11/12	0.73	0.35	489,490,491,492	0
11	NAG	Z	2	14/15	0.73	0.40	470,472,474,476	0
11	MAN	i	5	11/12	0.74	0.50	507,509,513,514	0
8	MAN	l	4	11/12	0.74	0.38	512,515,515,517	0
14	MAN	v	6	11/12	0.74	0.25	481,485,491,492	0
14	NAG	m	2	14/15	0.74	0.46	427,437,446,456	0
9	NAG	o	1	14/15	0.75	0.41	542,543,544,545	0
11	NAG	i	1	14/15	0.75	0.40	417,419,420,421	0
11	MAN	Z	5	11/12	0.76	0.55	582,584,585,586	0
12	MAN	s	6	11/12	0.77	0.40	440,445,450,450	0
14	MAN	d	7	11/12	0.77	0.75	499,503,504,506	0
8	BMA	l	3	11/12	0.78	0.23	537,539,542,542	0
14	MAN	v	4	11/12	0.78	0.38	452,458,471,472	0
12	MAN	s	4	11/12	0.78	0.46	567,567,567,567	0
8	NAG	n	2	14/15	0.78	0.56	492,493,494,495	0
14	BMA	m	3	11/12	0.79	0.36	470,474,482,483	0
8	BMA	X	3	11/12	0.79	0.23	526,543,558,577	0
14	NAG	m	1	14/15	0.80	0.38	426,430,436,438	0
9	NAG	P	1	14/15	0.80	0.32	529,532,535,535	0
14	MAN	v	5	11/12	0.80	0.37	454,458,461,462	0
11	MAN	i	6	11/12	0.80	0.23	438,440,445,447	0
10	BMA	Y	3	11/12	0.80	0.46	467,469,470,471	0
11	NAG	r	1	14/15	0.81	0.34	388,390,392,393	0
8	NAG	l	2	14/15	0.81	0.29	461,463,465,465	0
8	NAG	g	2	14/15	0.81	0.33	531,555,576,580	0
12	NAG	j	1	14/15	0.81	0.58	433,439,447,461	0
14	NAG	d	2	14/15	0.81	0.54	452,460,471,473	0
12	BMA	j	3	11/12	0.81	0.29	407,417,420,424	0
8	BMA	u	3	11/12	0.81	0.19	480,480,481,481	0
10	NAG	Y	2	14/15	0.81	0.47	426,430,433,434	0
14	BMA	v	3	11/12	0.82	0.40	445,449,459,463	0
14	MAN	d	6	11/12	0.82	0.58	465,467,473,475	0
13	NAG	t	2	14/15	0.82	0.33	521,522,522,523	0
8	NAG	p	2	14/15	0.82	0.53	465,488,513,516	0
13	NAG	t	1	14/15	0.82	0.24	446,447,448,449	0
12	MAN	a	4	11/12	0.83	0.32	479,498,500,501	0
14	BMA	d	3	11/12	0.83	0.48	471,476,486,491	0
10	NAG	q	1	14/15	0.83	0.34	404,407,410,412	0
8	BMA	E	3	11/12	0.84	0.37	434,435,439,440	0
12	BMA	a	3	11/12	0.84	0.27	418,427,431,437	0
8	MAN	u	4	11/12	0.84	0.37	558,559,560,561	0
10	NAG	h	1	14/15	0.84	0.40	345,348,350,351	0

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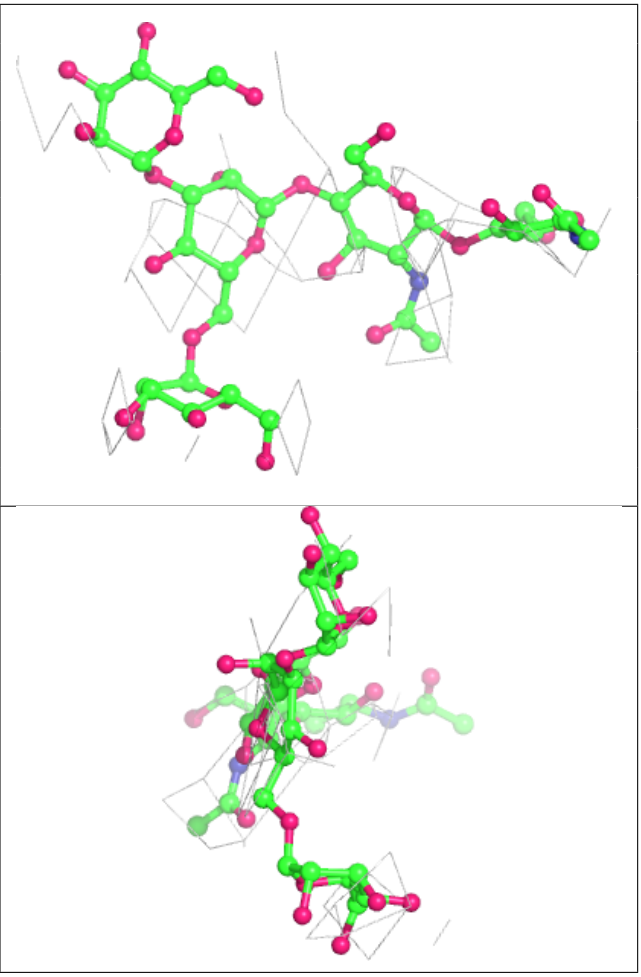
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MAN	a	6	11/12	0.84	0.42	408,413,418,418	0
8	NAG	X	2	14/15	0.84	0.26	418,443,465,472	0
8	NAG	c	2	14/15	0.85	0.25	410,416,420,420	0
14	MAN	v	7	11/12	0.85	0.28	455,460,462,463	0
14	MAN	m	7	11/12	0.85	0.62	425,428,432,433	0
8	MAN	E	5	11/12	0.86	0.51	482,484,485,485	0
11	NAG	Z	1	14/15	0.86	0.31	401,403,404,404	0
8	NAG	g	1	14/15	0.86	0.27	414,418,440,441	0
13	NAG	b	1	14/15	0.86	0.19	374,378,381,382	0
13	NAG	k	1	14/15	0.86	0.23	367,370,375,376	0
12	MAN	j	4	11/12	0.87	0.65	469,484,487,488	0
9	BMA	f	3	11/12	0.87	0.27	435,438,442,444	0
8	NAG	X	1	14/15	0.87	0.27	395,399,426,427	0
12	NAG	s	1	14/15	0.87	0.36	420,425,434,447	0
12	BMA	s	3	11/12	0.87	0.25	508,516,520,524	0
12	NAG	j	2	14/15	0.88	0.43	366,376,381,387	0
12	NAG	a	2	14/15	0.88	0.28	366,377,383,390	0
8	NAG	E	1	14/15	0.88	0.26	366,367,368,369	0
12	NAG	a	1	14/15	0.88	0.36	324,331,339,351	0
14	MAN	m	5	11/12	0.89	0.18	384,389,393,393	0
10	NAG	q	2	14/15	0.89	0.27	485,487,489,489	0
8	MAN	u	5	11/12	0.89	0.24	435,435,438,438	0
14	MAN	d	4	11/12	0.89	0.24	410,421,430,432	0
14	NAG	v	1	14/15	0.89	0.23	374,381,388,390	0
14	NAG	v	2	14/15	0.89	0.31	432,437,446,450	0
8	NAG	p	1	14/15	0.90	0.28	364,371,393,395	0
8	NAG	e	1	14/15	0.90	0.28	444,448,454,455	0
8	NAG	E	2	14/15	0.90	0.23	430,433,437,437	0
13	NAG	k	2	14/15	0.91	0.23	416,421,426,426	0
14	MAN	d	5	11/12	0.91	0.24	392,395,397,399	0
13	NAG	b	2	14/15	0.91	0.33	398,401,404,406	0
8	NAG	u	2	14/15	0.91	0.18	352,353,354,354	0
8	NAG	c	1	14/15	0.92	0.23	348,350,351,353	0
8	NAG	u	1	14/15	0.93	0.21	345,347,349,350	0
14	MAN	m	4	11/12	0.93	0.17	400,403,419,420	0
12	NAG	s	2	14/15	0.94	0.25	434,446,451,458	0

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

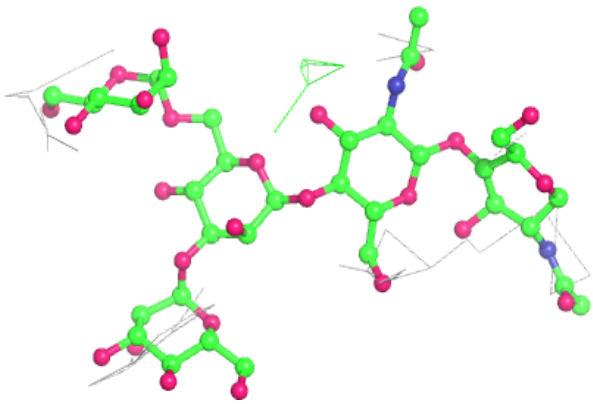
Electron density around Chain E:

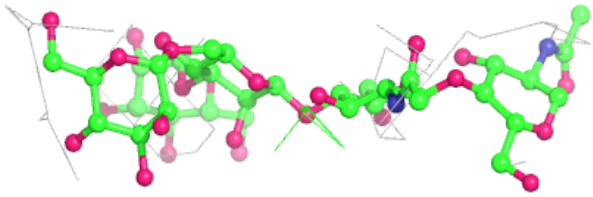
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

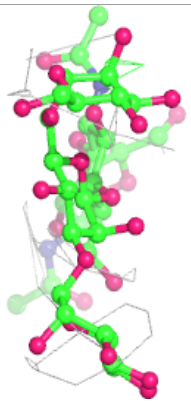


Electron density around Chain X:

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

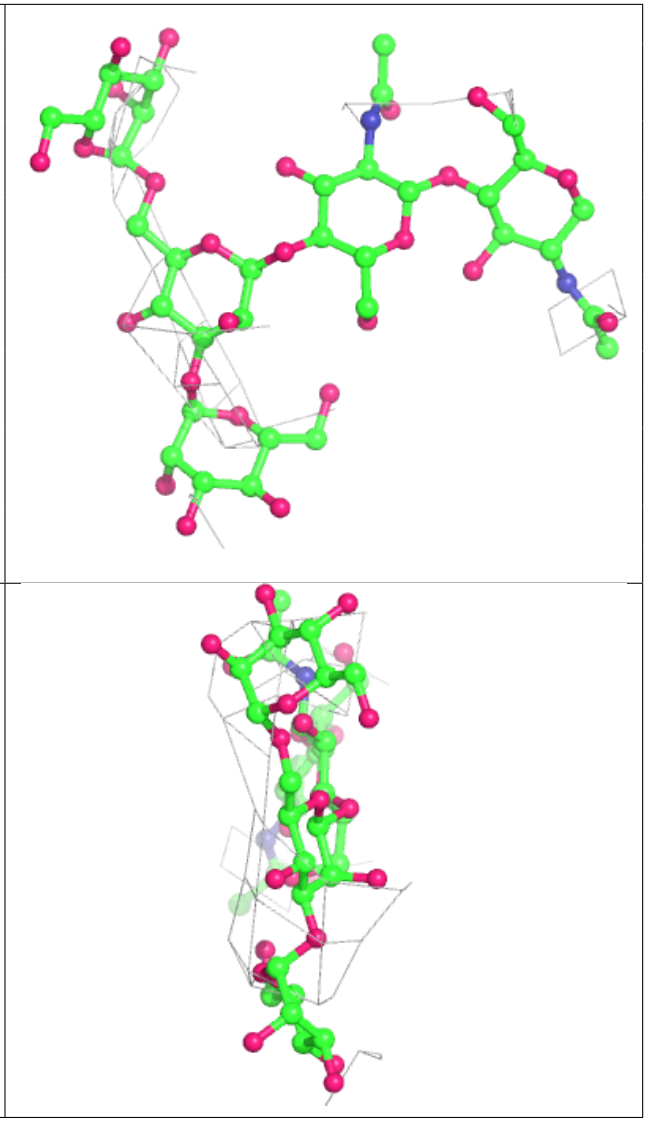






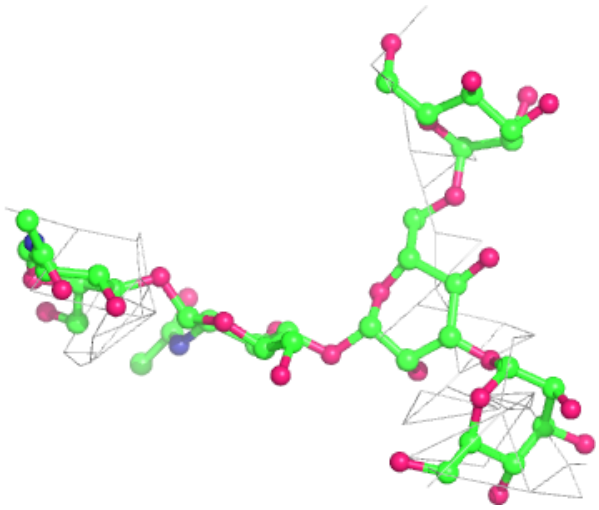
Electron density around Chain c:

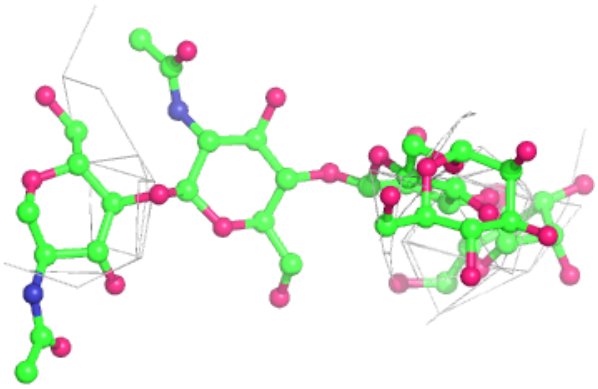
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

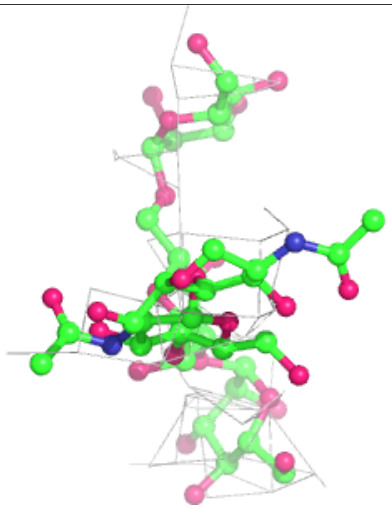


Electron density around Chain e:

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

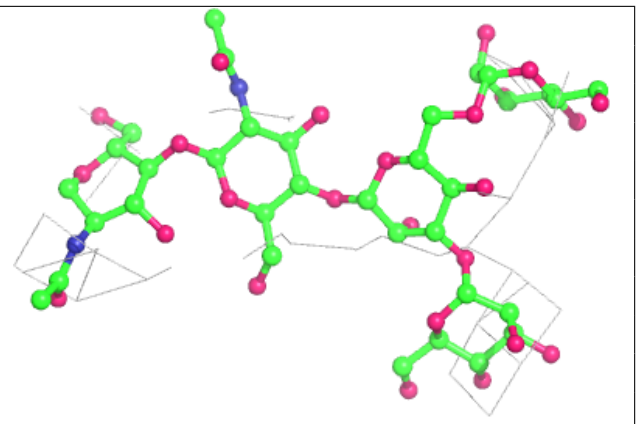


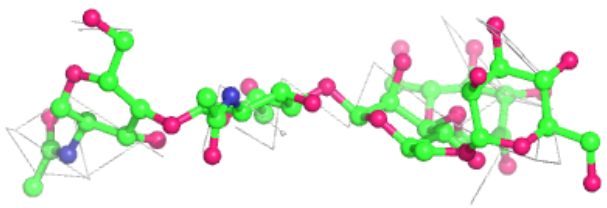


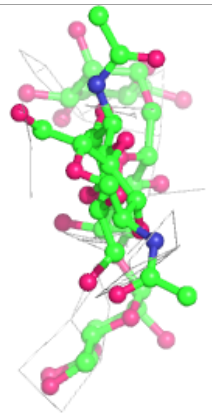


Electron density around Chain g:

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

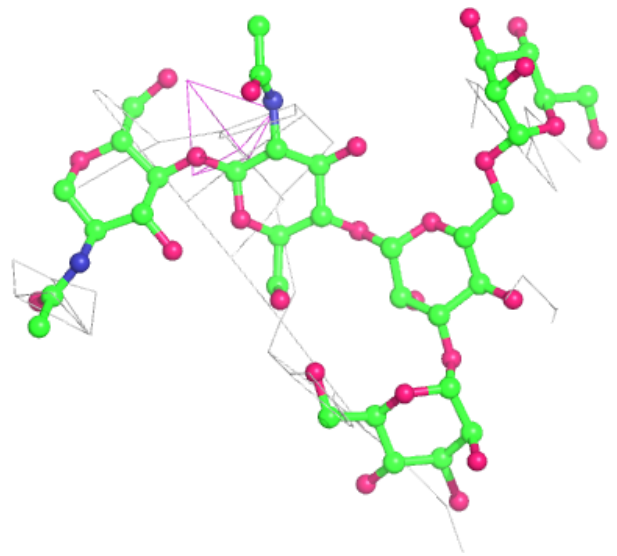


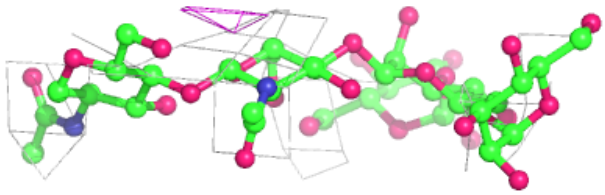


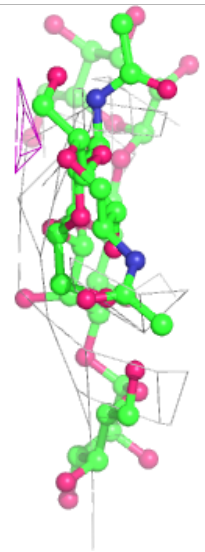


Electron density around Chain l:

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

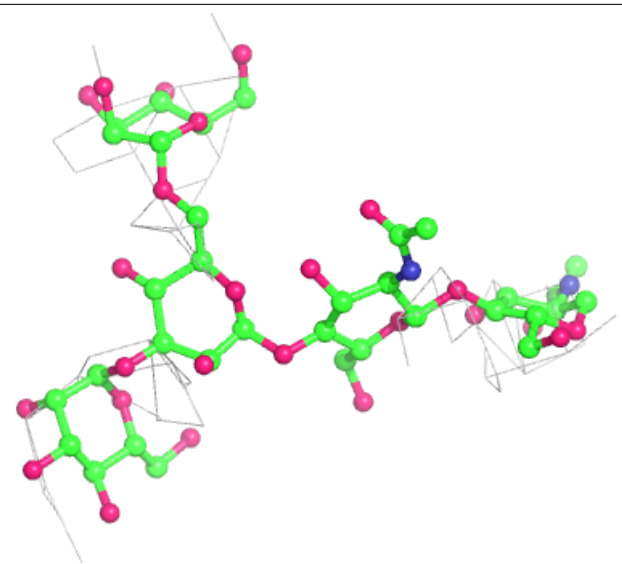


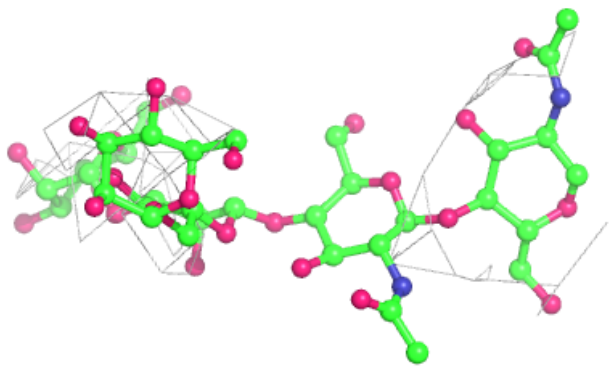


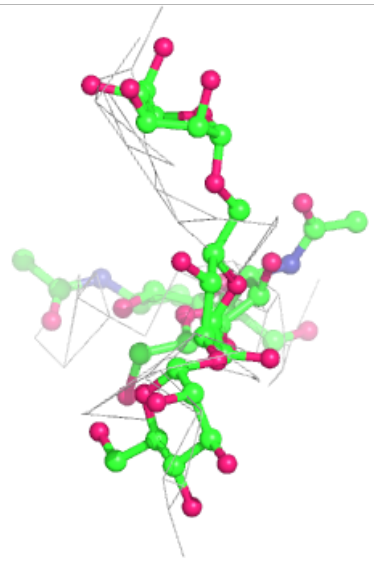


Electron density around Chain n:

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

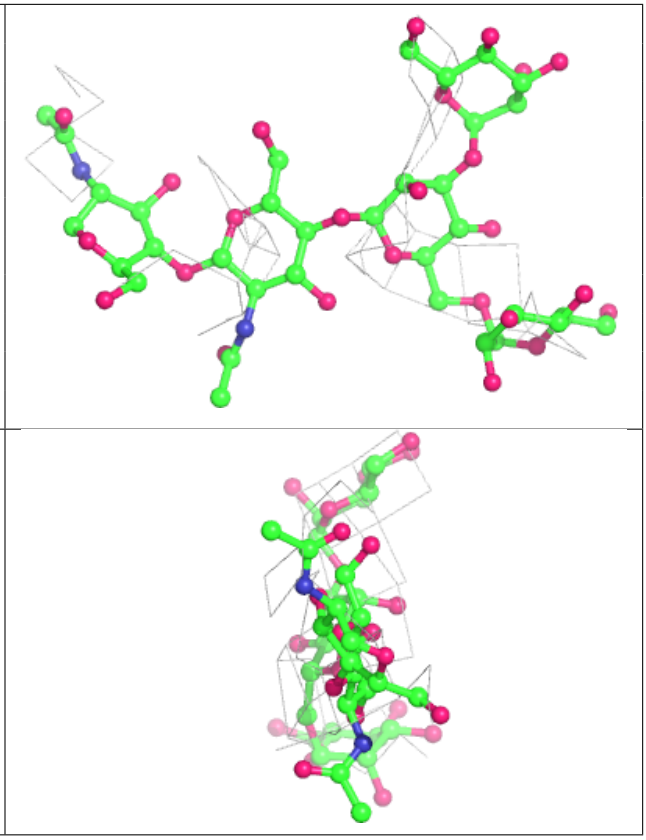


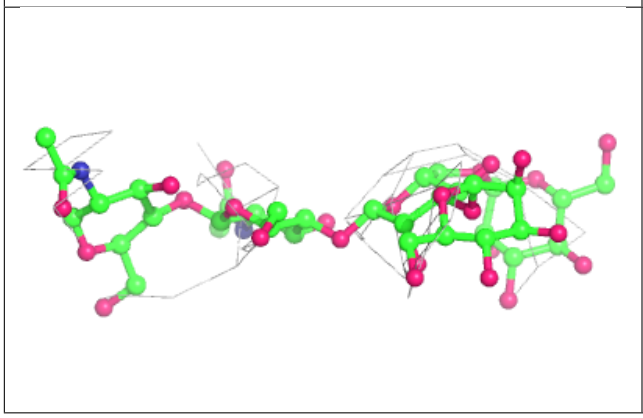




Electron density around Chain p:

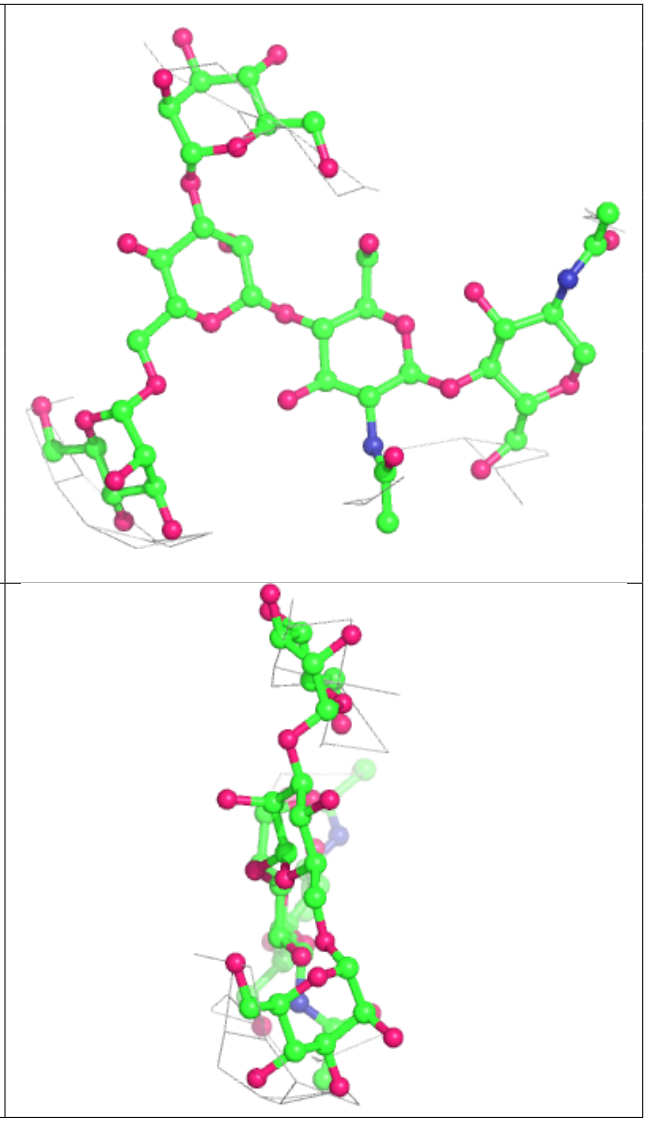
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





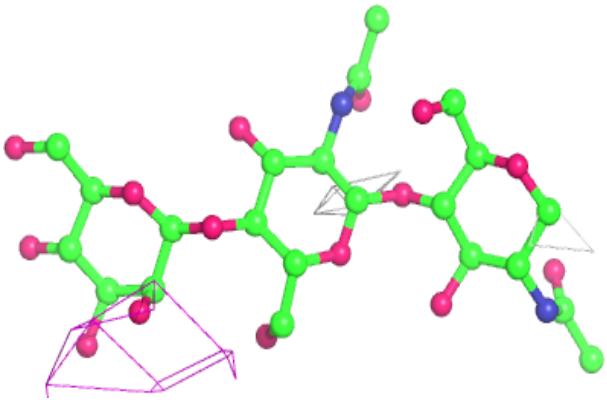
Electron density around Chain u:

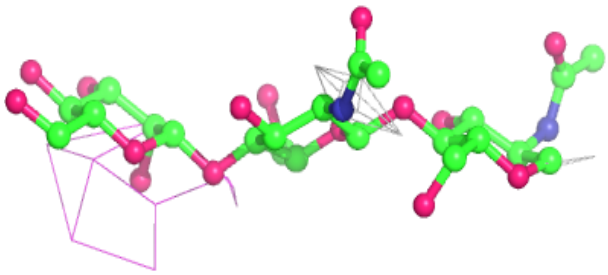
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

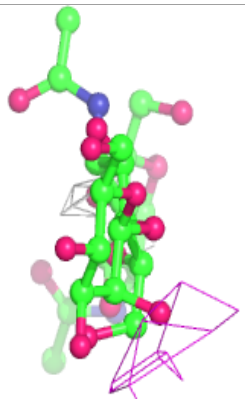


Electron density around Chain P:

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

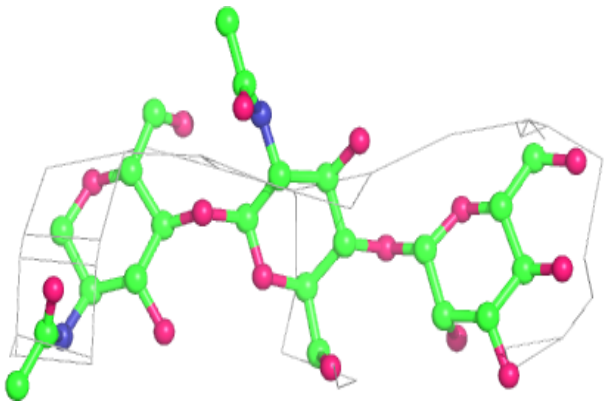


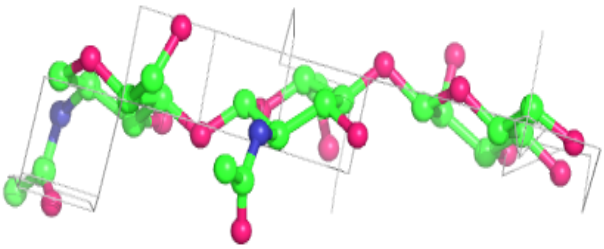


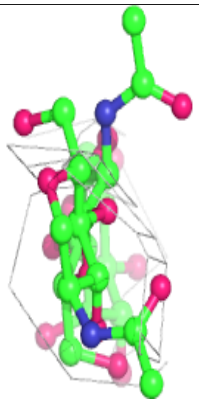


Electron density around Chain f:

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

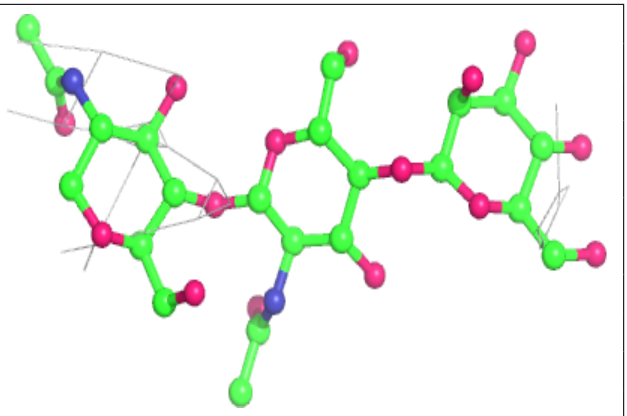


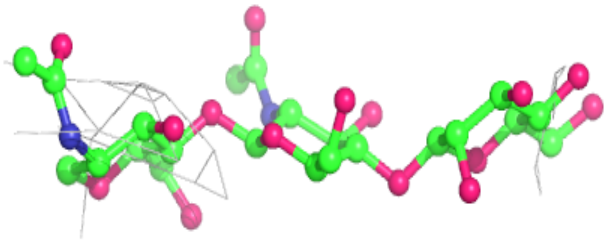


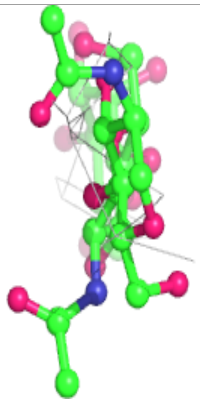


Electron density around Chain o:

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

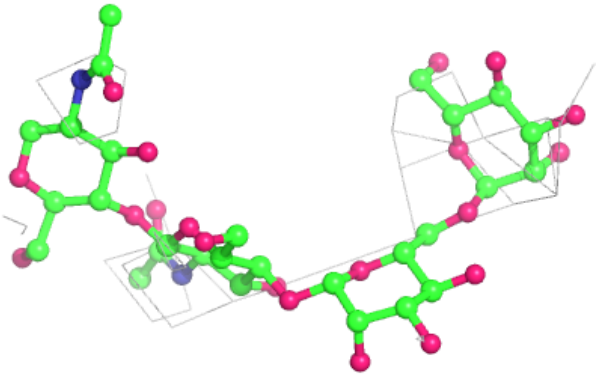


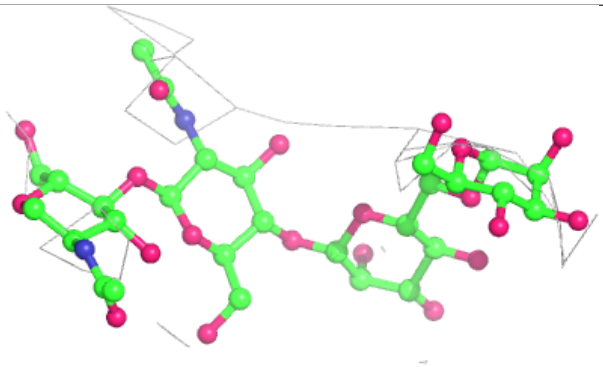


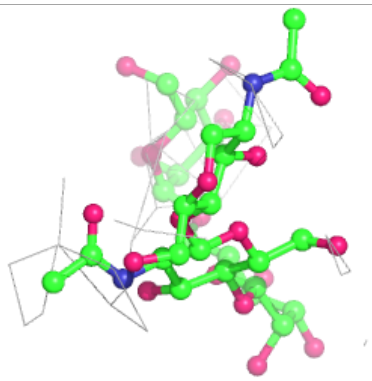


Electron density around Chain Y:

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

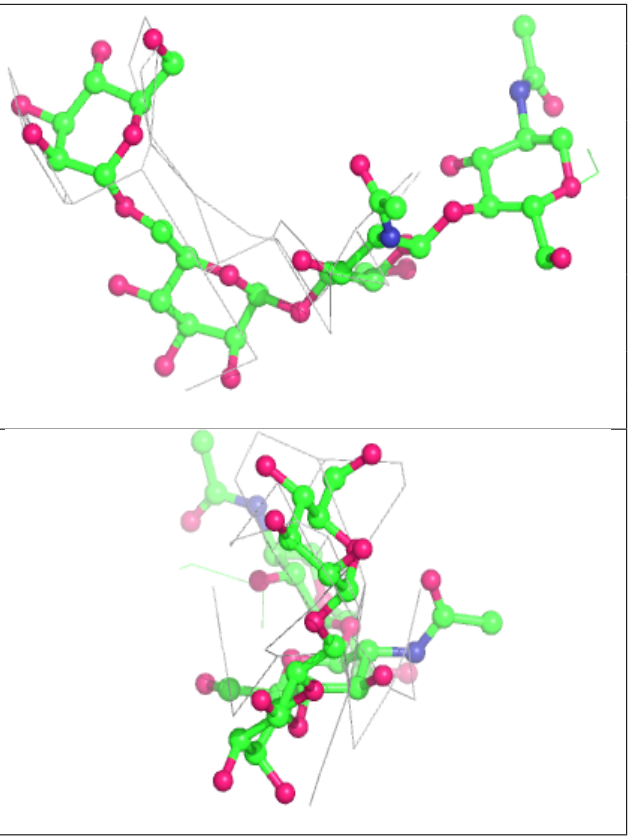






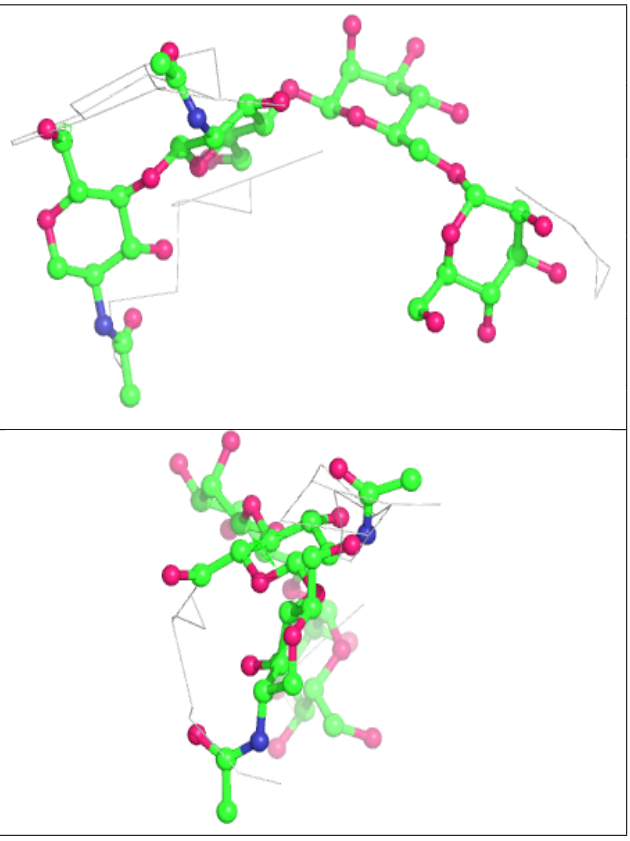
Electron density around Chain h:

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



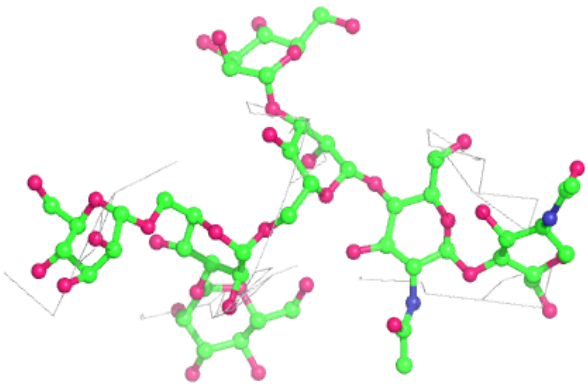
Electron density around Chain q:

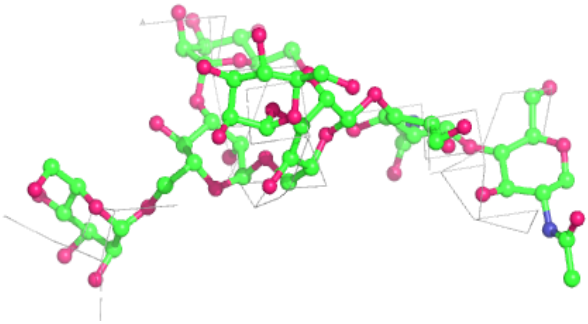
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

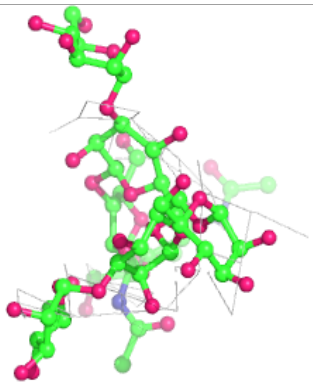


Electron density around Chain Z:

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

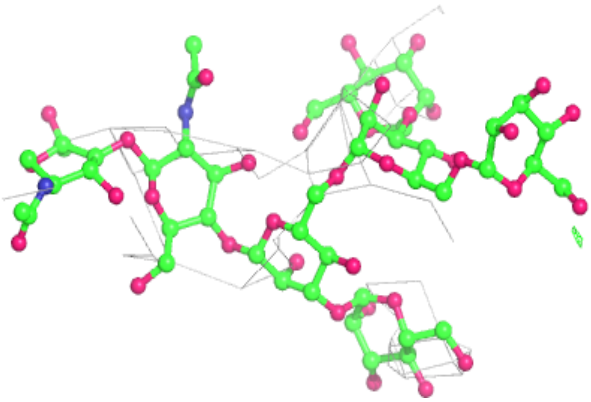


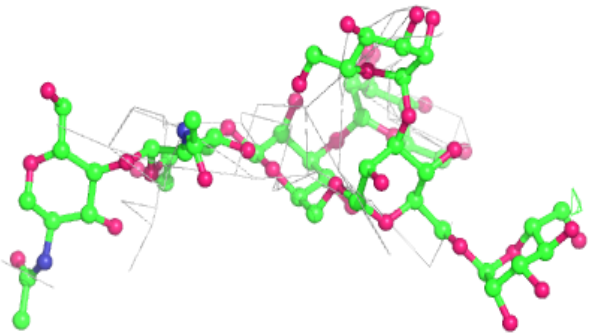


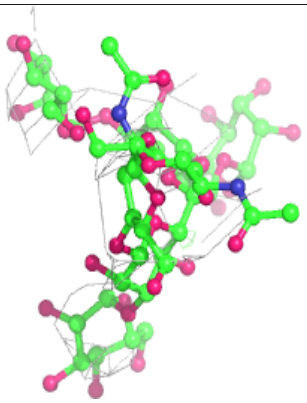


Electron density around Chain i:

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

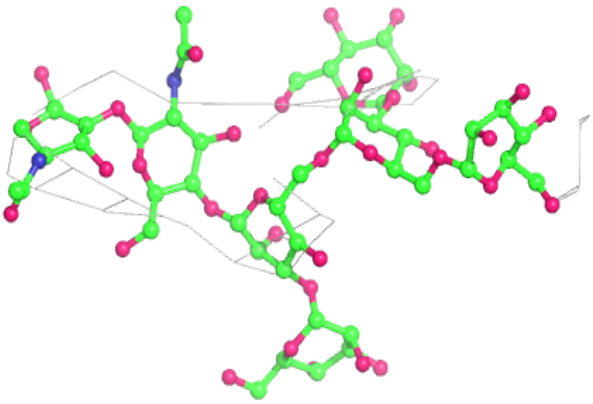


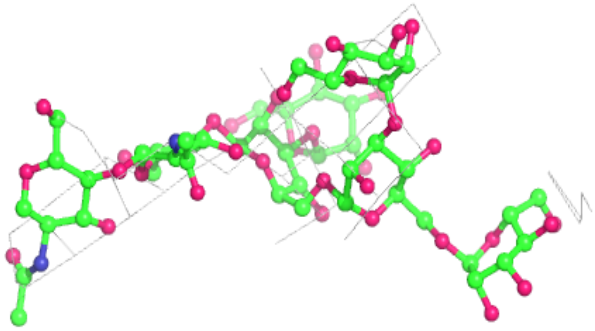


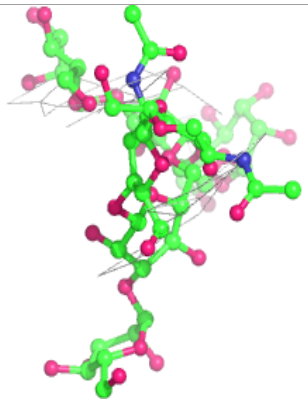


Electron density around Chain r:

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

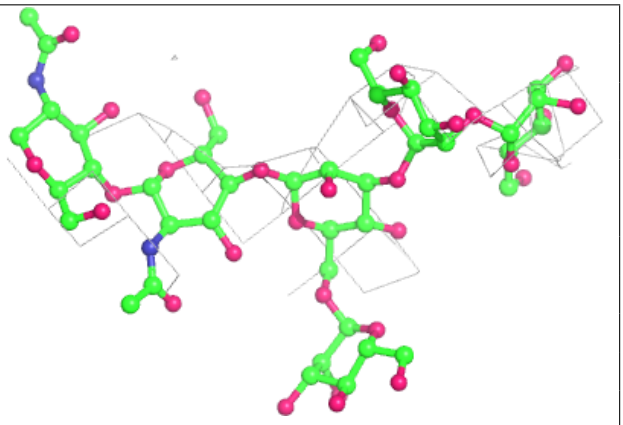


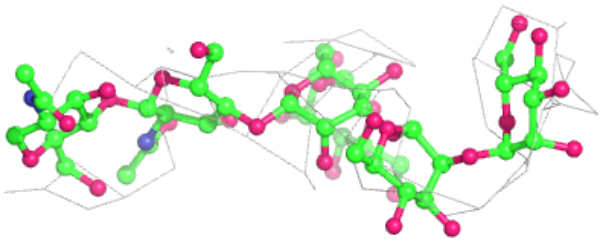


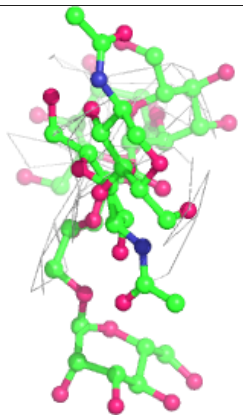


Electron density around Chain a:

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

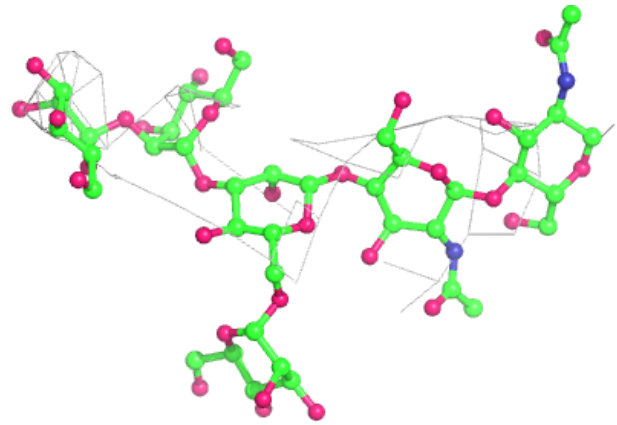


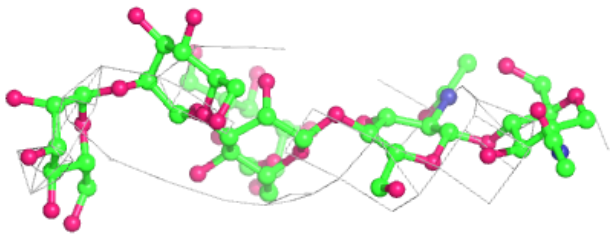


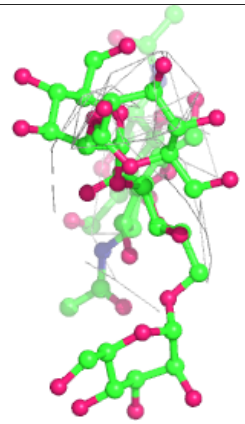


Electron density around Chain j:

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

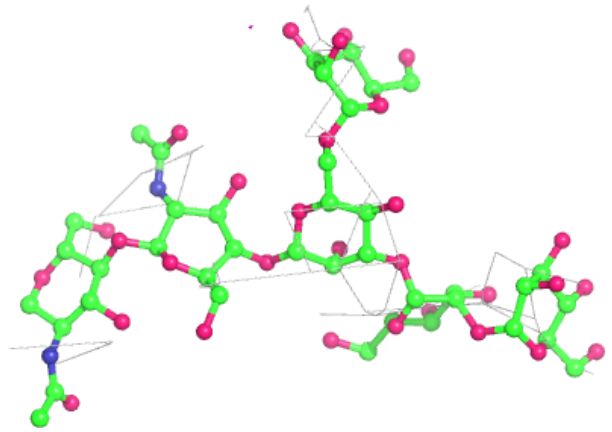


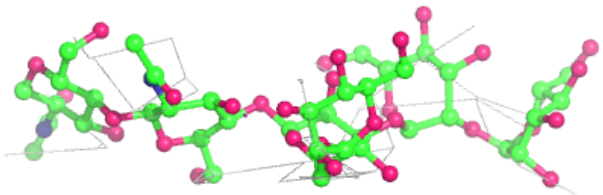


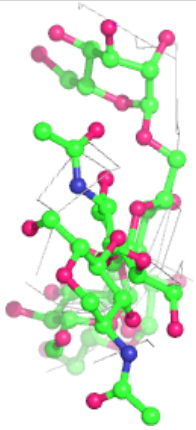


Electron density around Chain s:

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

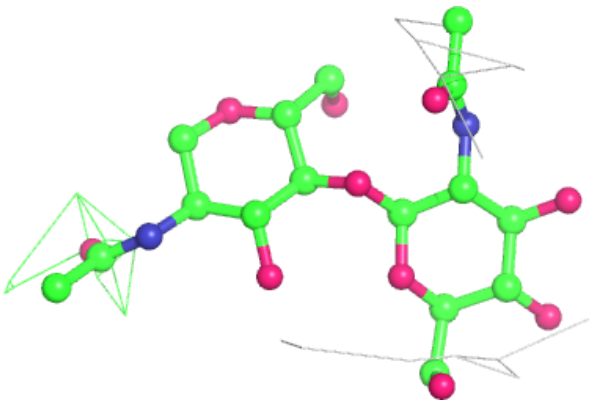


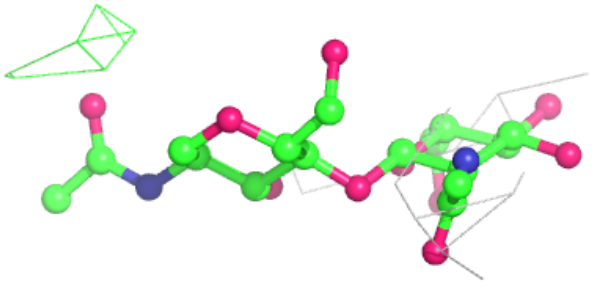


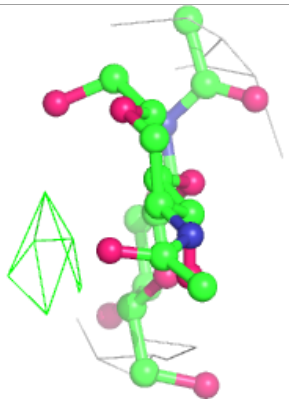


Electron density around Chain b:

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

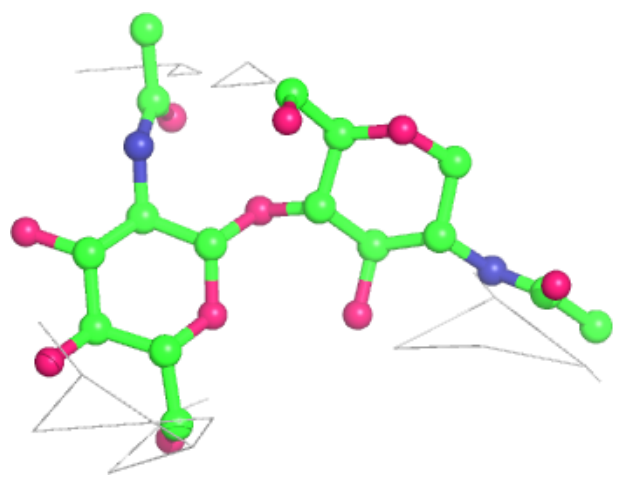


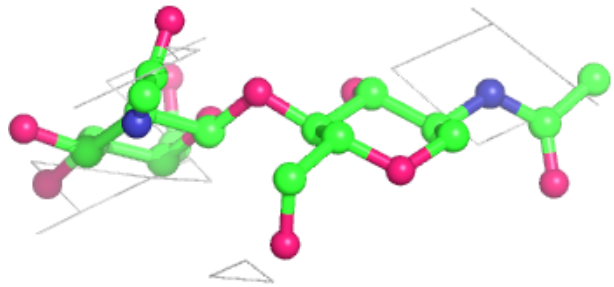


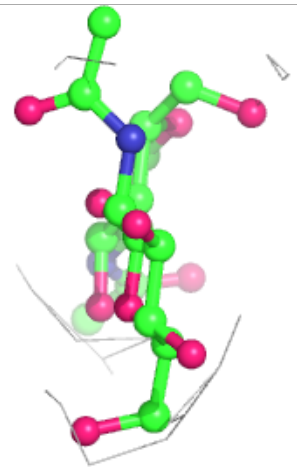


Electron density around Chain k:

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

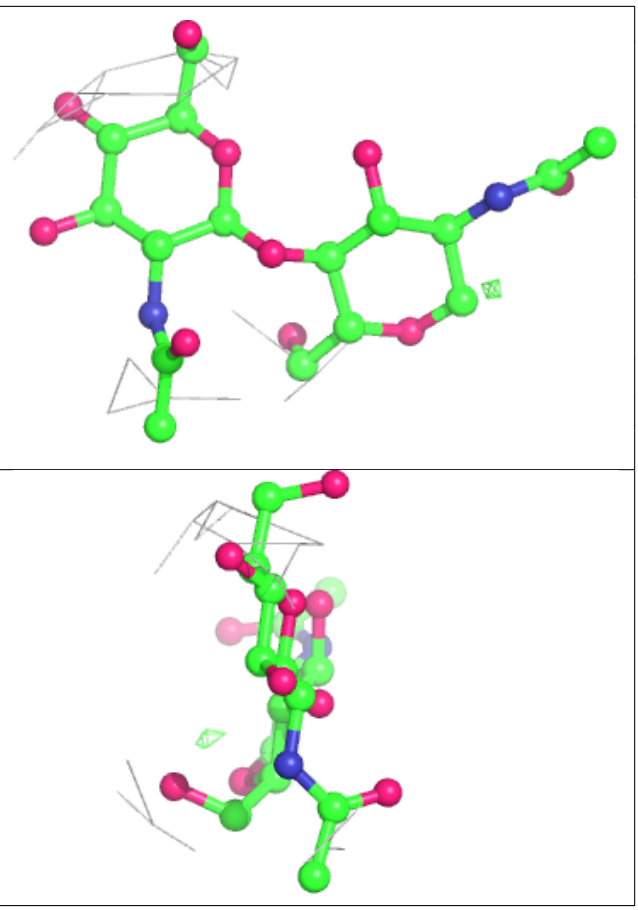


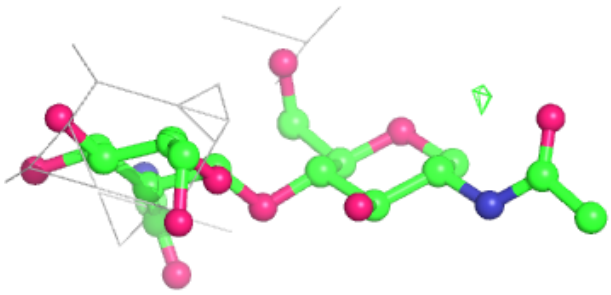




Electron density around Chain t:

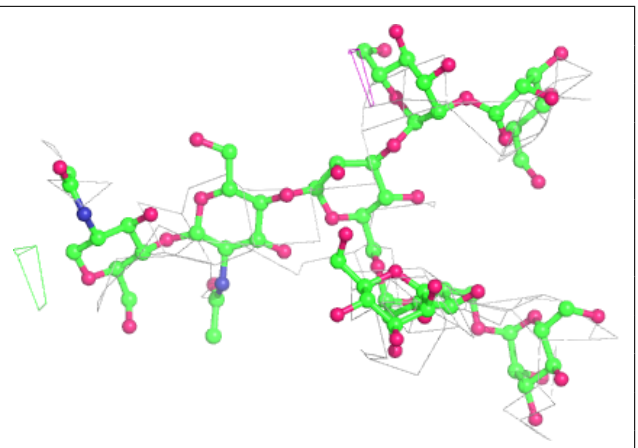
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

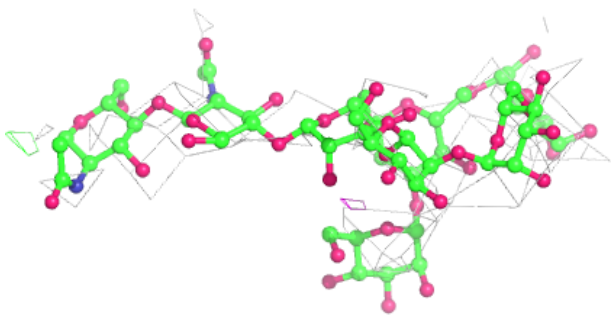


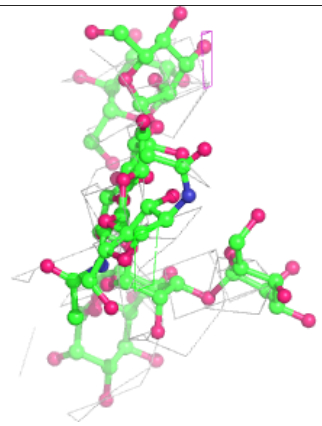


Electron density around Chain d:

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

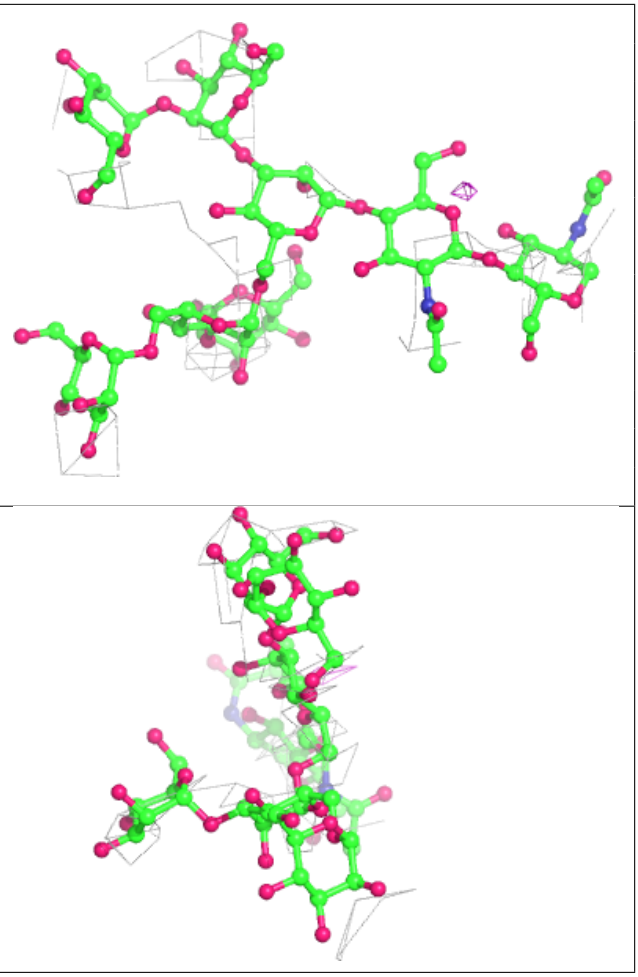






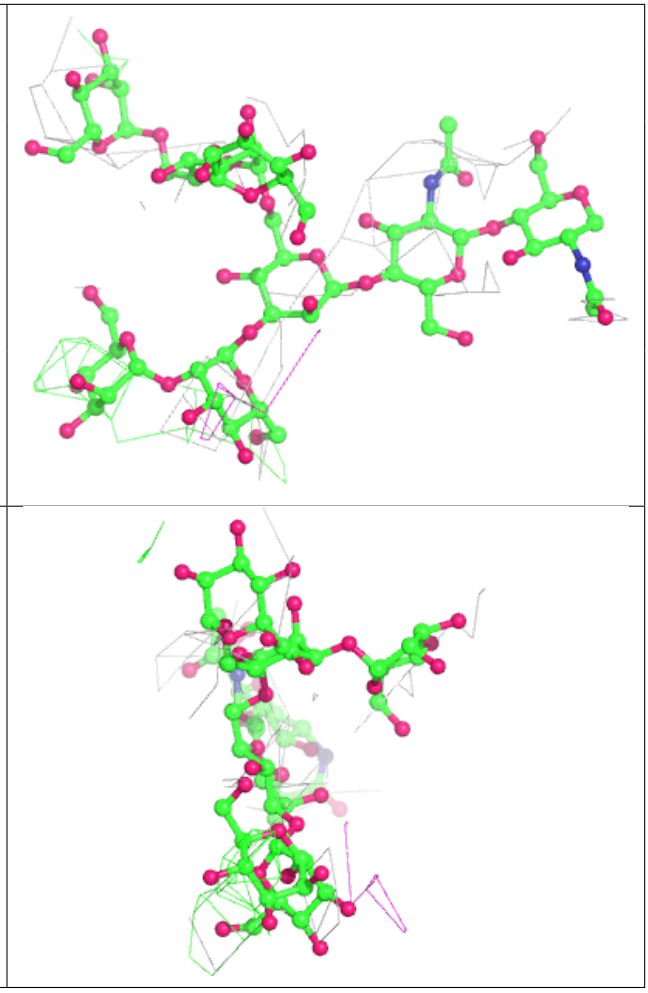
Electron density around Chain m:

$2mF_o$-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 v:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	NAG	G	649	14/15	0.36	0.71	491,493,495,496	0
15	NAG	Q	615	14/15	0.46	0.77	499,500,501,502	0
15	NAG	Q	649	14/15	0.48	0.76	505,508,510,511	0
15	NAG	F	615	14/15	0.49	0.65	506,511,514,515	0
15	NAG	R	701	14/15	0.57	0.62	448,450,452,452	0
15	NAG	F	651	14/15	0.58	0.60	425,429,432,434	0
15	NAG	Q	651	14/15	0.59	0.82	446,448,449,449	0
15	NAG	Q	652	14/15	0.60	0.58	410,411,411,411	0
15	NAG	G	653	14/15	0.61	0.46	431,431,431,431	0
15	NAG	R	703	14/15	0.63	0.54	390,390,390,390	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	NAG	G	651	14/15	0.66	0.54	448,451,453,454	0
15	NAG	J	703	14/15	0.66	0.48	511,511,511,511	0
15	NAG	F	652	14/15	0.67	0.49	405,407,410,411	0
15	NAG	Q	633	14/15	0.67	0.46	517,518,519,519	0
15	NAG	G	606	14/15	0.68	0.27	449,452,455,456	0
15	NAG	F	649	14/15	0.68	0.53	468,470,474,474	0
15	NAG	F	606	14/15	0.68	0.42	460,464,467,468	0
15	NAG	G	615	14/15	0.69	0.43	429,431,432,434	0
15	NAG	J	701	14/15	0.71	0.64	503,510,514,514	0
15	NAG	G	633	14/15	0.73	0.37	475,477,480,480	0
15	NAG	J	702	14/15	0.74	0.64	480,482,485,487	0
15	NAG	A	702	14/15	0.74	0.41	410,413,414,415	0
15	NAG	F	633	14/15	0.75	0.48	511,516,521,523	0
15	NAG	Q	653	14/15	0.76	0.46	441,441,441,441	0
15	NAG	G	652	14/15	0.78	0.43	302,308,311,311	0
15	NAG	A	703	14/15	0.79	0.56	461,461,461,461	0
15	NAG	R	702	14/15	0.80	0.52	479,481,484,484	0
15	NAG	F	653	14/15	0.81	0.50	399,399,399,399	0
15	NAG	Q	606	14/15	0.82	0.29	474,477,479,480	0
15	NAG	A	701	14/15	0.89	0.56	406,407,409,409	0
15	NAG	F	650	14/15	0.90	0.32	345,348,352,354	0
15	NAG	Q	650	14/15	0.91	0.43	351,352,354,354	0
15	NAG	G	650	14/15	0.92	0.22	347,349,352,353	0

6.5 Other polymers (i)

There are no such residues in this entry.