Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2024 – 10:15 AM EDT

PDB ID	:	8TGO
Title	:	Crystal structure of the BG505 triple tandem trimer gp140 HIV-1 Env in complex with PGT124 and 35O22
Authors	:	Xian, Y.; Yuan, M.; Wilson, I.A.
Deposited on	:	2023-07-12
Resolution	:	5.75 Å(reported)

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

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

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

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

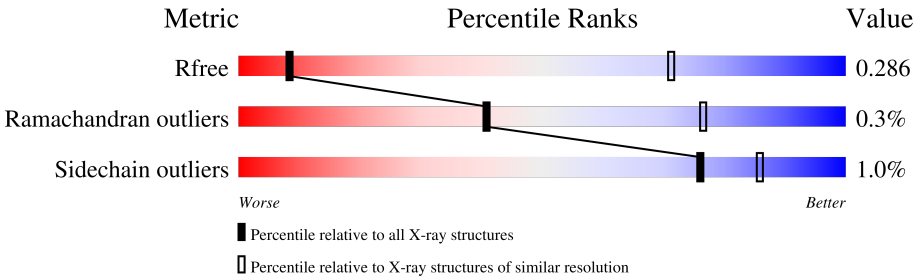
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.75 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	1007 (7.66-3.86)
Ramachandran outliers	138981	1002 (7.60-3.86)
Sidechain outliers	138945	1005 (7.70-3.82)

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

Mol	Chain	Length	Quality of chain
1	B	164	75% 25%
1	H	164	73% . 26%
1	a	164	74% . 25%
2	D	286	80% . 17%
2	L	286	79% . 17%
2	b	286	80% . 17%
3	C	214	96% . .
3	P	214	97% . .

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Mol	Chain	Length	Quality of chain
3	c	214	97%
4	G	490	89% 10%
4	R	490	89% 10%
4	e	490	89% 10%
5	O	235	55% 45%
5	S	235	97%
5	f	235	97%
6	A	5	40% 60%
7	F	2	100%
7	K	2	100%
7	M	2	100%
7	T	2	100%
7	U	2	100%
7	W	2	100%
7	X	2	100%
7	g	2	100%
7	h	2	100%
7	j	2	100%
7	l	2	100%
7	o	2	100%
7	p	2	100%
7	r	2	100%
8	I	3	100%
8	J	3	100%
8	Y	3	100%

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Mol	Chain	Length	Quality of chain
8	Z	3	100%
8	m	3	100%
8	n	3	100%
9	N	10	10% 90%
9	i	10	10% 90%
9	q	10	10% 90%
10	V	4	50% 50%
10	k	4	75% 25%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29645 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 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	123	Total	C	N	O	S	0	0	0
			967	609	167	185	6			
1	H	122	Total	C	N	O	S	0	0	0
			963	607	166	184	6			
1	a	123	Total	C	N	O	S	0	0	0
			967	609	167	185	6			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
B	665	GLY	-	expression tag	UNP Q2N0S6
B	666	SER	-	expression tag	UNP Q2N0S6
B	667	GLY	-	expression tag	UNP Q2N0S6
B	668	GLY	-	expression tag	UNP Q2N0S6
B	669	SER	-	expression tag	UNP Q2N0S6
B	670	GLY	-	expression tag	UNP Q2N0S6
B	671	GLY	-	expression tag	UNP Q2N0S6
B	672	SER	-	expression tag	UNP Q2N0S6
B	673	GLY	-	expression tag	UNP Q2N0S6
B	674	SER	-	expression tag	UNP Q2N0S6
B	675	GLY	-	expression tag	UNP Q2N0S6
H	519	SER	PHE	conflict	UNP Q2N0S6
H	559	PRO	ILE	conflict	UNP Q2N0S6
H	568	ASP	LEU	conflict	UNP Q2N0S6
H	570	HIS	VAL	conflict	UNP Q2N0S6
H	585	HIS	ARG	conflict	UNP Q2N0S6
H	605	CYS	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	665	GLY	-	expression tag	UNP Q2N0S6
H	666	SER	-	expression tag	UNP Q2N0S6
H	667	GLY	-	expression tag	UNP Q2N0S6
H	668	GLY	-	expression tag	UNP Q2N0S6
H	669	SER	-	expression tag	UNP Q2N0S6
H	670	GLY	-	expression tag	UNP Q2N0S6
H	671	GLY	-	expression tag	UNP Q2N0S6
H	672	SER	-	expression tag	UNP Q2N0S6
H	673	GLY	-	expression tag	UNP Q2N0S6
H	674	SER	-	expression tag	UNP Q2N0S6
H	675	GLY	-	expression tag	UNP Q2N0S6
a	519	SER	PHE	conflict	UNP Q2N0S6
a	559	PRO	ILE	conflict	UNP Q2N0S6
a	568	ASP	LEU	conflict	UNP Q2N0S6
a	570	HIS	VAL	conflict	UNP Q2N0S6
a	585	HIS	ARG	conflict	UNP Q2N0S6
a	605	CYS	THR	conflict	UNP Q2N0S6
a	665	GLY	-	expression tag	UNP Q2N0S6
a	666	SER	-	expression tag	UNP Q2N0S6
a	667	GLY	-	expression tag	UNP Q2N0S6
a	668	GLY	-	expression tag	UNP Q2N0S6
a	669	SER	-	expression tag	UNP Q2N0S6
a	670	GLY	-	expression tag	UNP Q2N0S6
a	671	GLY	-	expression tag	UNP Q2N0S6
a	672	SER	-	expression tag	UNP Q2N0S6
a	673	GLY	-	expression tag	UNP Q2N0S6
a	674	SER	-	expression tag	UNP Q2N0S6
a	675	GLY	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	236	Total	C	N	O	S	0	0	0
			1820	1148	305	356	11			
2	L	236	Total	C	N	O	S	0	0	0
			1820	1148	305	356	11			
2	b	236	Total	C	N	O	S	0	0	0
			1820	1148	305	356	11			

- Molecule 3 is a protein called PGT124 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	208	Total	C	N	O	S	0	0	0
			1580	997	268	310	5			
3	P	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	c	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	439	Total	C	N	O	S	0	0	0
			3473	2190	610	646	27			
4	R	439	Total	C	N	O	S	0	0	0
			3473	2190	610	646	27			
4	e	439	Total	C	N	O	S	0	0	0
			3473	2190	610	646	27			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	64	LYS	GLU	conflict	UNP Q2N0S6
G	106	GLU	THR	conflict	UNP Q2N0S6
G	271	ILE	MET	conflict	UNP Q2N0S6
G	288	LEU	PHE	conflict	UNP Q2N0S6
G	304	VAL	ARG	conflict	UNP Q2N0S6
G	316	TRP	ALA	conflict	UNP Q2N0S6
G	319	TYR	ALA	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	500	LYS	ARG	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	508	GLY	-	expression tag	UNP Q2N0S6
G	509	GLY	-	expression tag	UNP Q2N0S6
G	510	SER	-	expression tag	UNP Q2N0S6
G	511	GLY	-	expression tag	UNP Q2N0S6
G	512	GLY	-	expression tag	UNP Q2N0S6
G	513	GLY	-	expression tag	UNP Q2N0S6
G	514	GLY	-	expression tag	UNP Q2N0S6
G	515	SER	-	expression tag	UNP Q2N0S6
G	516	GLY	-	expression tag	UNP Q2N0S6
G	517	GLY	-	expression tag	UNP Q2N0S6
G	518	GLY	-	expression tag	UNP Q2N0S6
G	519	GLY	-	expression tag	UNP Q2N0S6
G	520	SER	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	521	GLY	-	expression tag	UNP Q2N0S6
G	522	GLY	-	expression tag	UNP Q2N0S6
R	64	LYS	GLU	conflict	UNP Q2N0S6
R	106	GLU	THR	conflict	UNP Q2N0S6
R	271	ILE	MET	conflict	UNP Q2N0S6
R	288	LEU	PHE	conflict	UNP Q2N0S6
R	304	VAL	ARG	conflict	UNP Q2N0S6
R	316	TRP	ALA	conflict	UNP Q2N0S6
R	319	TYR	ALA	conflict	UNP Q2N0S6
R	332	ASN	THR	conflict	UNP Q2N0S6
R	500	LYS	ARG	conflict	UNP Q2N0S6
R	501	CYS	ALA	conflict	UNP Q2N0S6
R	508	GLY	-	expression tag	UNP Q2N0S6
R	509	GLY	-	expression tag	UNP Q2N0S6
R	510	SER	-	expression tag	UNP Q2N0S6
R	511	GLY	-	expression tag	UNP Q2N0S6
R	512	GLY	-	expression tag	UNP Q2N0S6
R	513	GLY	-	expression tag	UNP Q2N0S6
R	514	GLY	-	expression tag	UNP Q2N0S6
R	515	SER	-	expression tag	UNP Q2N0S6
R	516	GLY	-	expression tag	UNP Q2N0S6
R	517	GLY	-	expression tag	UNP Q2N0S6
R	518	GLY	-	expression tag	UNP Q2N0S6
R	519	GLY	-	expression tag	UNP Q2N0S6
R	520	SER	-	expression tag	UNP Q2N0S6
R	521	GLY	-	expression tag	UNP Q2N0S6
R	522	GLY	-	expression tag	UNP Q2N0S6
e	64	LYS	GLU	conflict	UNP Q2N0S6
e	106	GLU	THR	conflict	UNP Q2N0S6
e	271	ILE	MET	conflict	UNP Q2N0S6
e	288	LEU	PHE	conflict	UNP Q2N0S6
e	304	VAL	ARG	conflict	UNP Q2N0S6
e	316	TRP	ALA	conflict	UNP Q2N0S6
e	319	TYR	ALA	conflict	UNP Q2N0S6
e	332	ASN	THR	conflict	UNP Q2N0S6
e	500	LYS	ARG	conflict	UNP Q2N0S6
e	501	CYS	ALA	conflict	UNP Q2N0S6
e	508	GLY	-	expression tag	UNP Q2N0S6
e	509	GLY	-	expression tag	UNP Q2N0S6
e	510	SER	-	expression tag	UNP Q2N0S6
e	511	GLY	-	expression tag	UNP Q2N0S6
e	512	GLY	-	expression tag	UNP Q2N0S6

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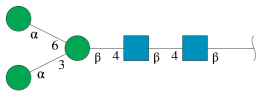
Chain	Residue	Modelled	Actual	Comment	Reference
e	513	GLY	-	expression tag	UNP Q2N0S6
e	514	GLY	-	expression tag	UNP Q2N0S6
e	515	SER	-	expression tag	UNP Q2N0S6
e	516	GLY	-	expression tag	UNP Q2N0S6
e	517	GLY	-	expression tag	UNP Q2N0S6
e	518	GLY	-	expression tag	UNP Q2N0S6
e	519	GLY	-	expression tag	UNP Q2N0S6
e	520	SER	-	expression tag	UNP Q2N0S6
e	521	GLY	-	expression tag	UNP Q2N0S6
e	522	GLY	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called PGT124 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	O	130	Total	C	N	O	S	0	0	0
			1030	655	175	197	3			
5	S	230	Total	C	N	O	S	0	0	0
			1750	1109	292	344	5			
5	f	230	Total	C	N	O	S	0	0	0
			1750	1109	292	344	5			

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

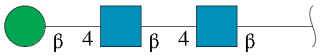


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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
7	F	2	Total C N O 28 16 2 10	0	0	0
7	K	2	Total C N O 28 16 2 10	0	0	0
7	M	2	Total C N O 28 16 2 10	0	0	0
7	T	2	Total C N O 28 16 2 10	0	0	0
7	U	2	Total C N O 28 16 2 10	0	0	0
7	W	2	Total C N O 28 16 2 10	0	0	0
7	X	2	Total C N O 28 16 2 10	0	0	0
7	g	2	Total C N O 28 16 2 10	0	0	0
7	h	2	Total C N O 28 16 2 10	0	0	0
7	j	2	Total C N O 28 16 2 10	0	0	0
7	l	2	Total C N O 28 16 2 10	0	0	0
7	o	2	Total C N O 28 16 2 10	0	0	0
7	p	2	Total C N O 28 16 2 10	0	0	0
7	r	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 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
8	I	3	Total C N O 39 22 2 15	0	0	0
8	J	3	Total C N O 39 22 2 15	0	0	0
8	Y	3	Total C N O 39 22 2 15	0	0	0

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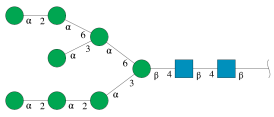
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	Z	3	Total C N O 39 22 2 15	0	0	0
8	m	3	Total C N O 39 22 2 15	0	0	0
8	n	3	Total C N O 39 22 2 15	0	0	0

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

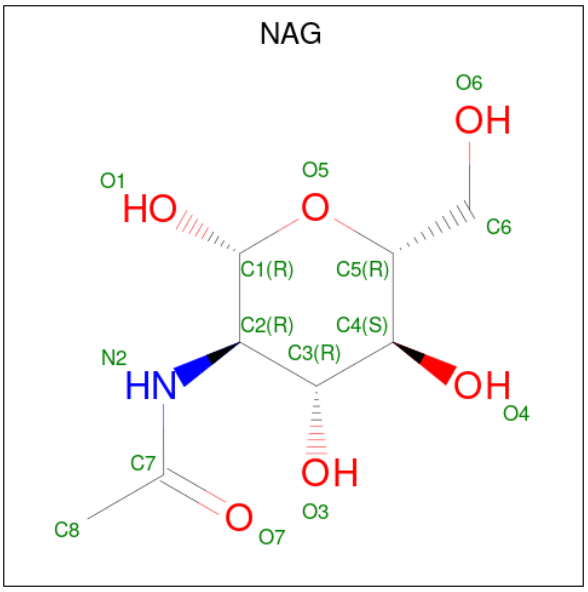


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	N	10	Total C N O 116 64 2 50	0	0	0
9	i	10	Total C N O 116 64 2 50	0	0	0
9	q	10	Total C N O 116 64 2 50	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	V	4	Total C N O 50 28 2 20	0	0	0
10	k	4	Total C N O 50 28 2 20	0	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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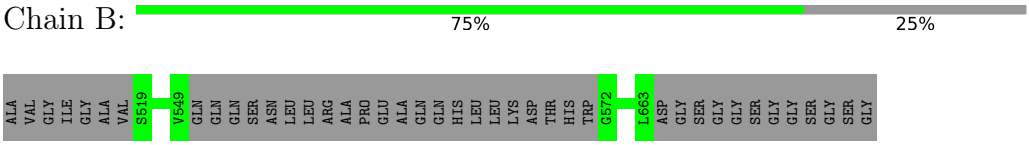
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	R	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	a	1	Total C N O 14 8 1 5	0	0
11	a	1	Total C N O 14 8 1 5	0	0
11	a	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 14 8 1 5	0	0
11	e	1	Total C N O 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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

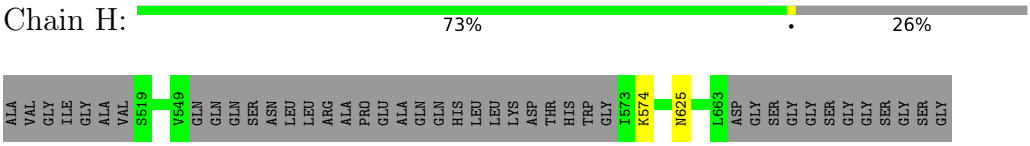
- Molecule 1: Envelope glycoprotein gp41

Chain B:



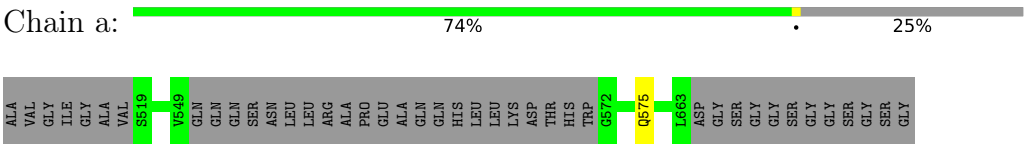
- Molecule 1: Envelope glycoprotein gp41

Chain H:



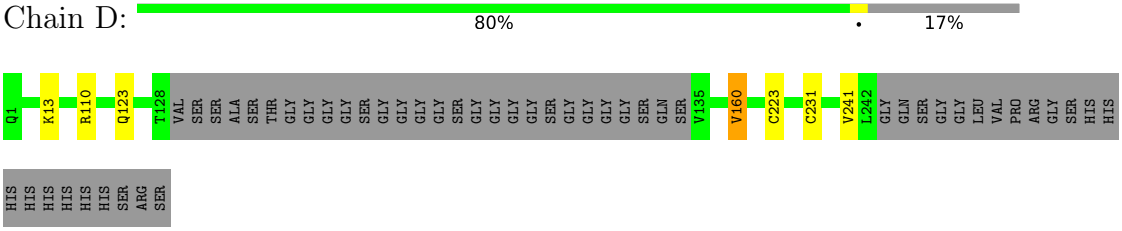
- Molecule 1: Envelope glycoprotein gp41

Chain a:



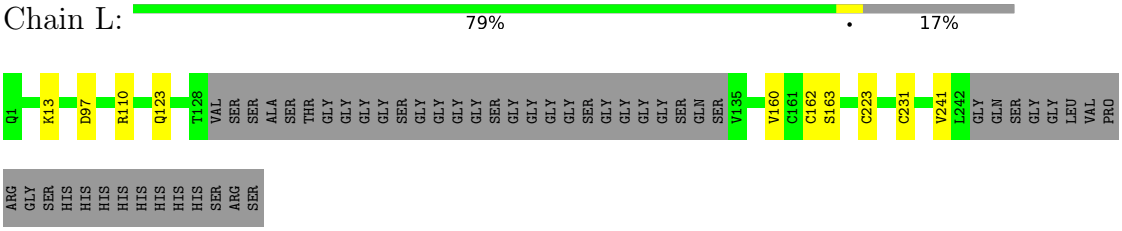
- Molecule 2: 35O22 scFv

Chain D:



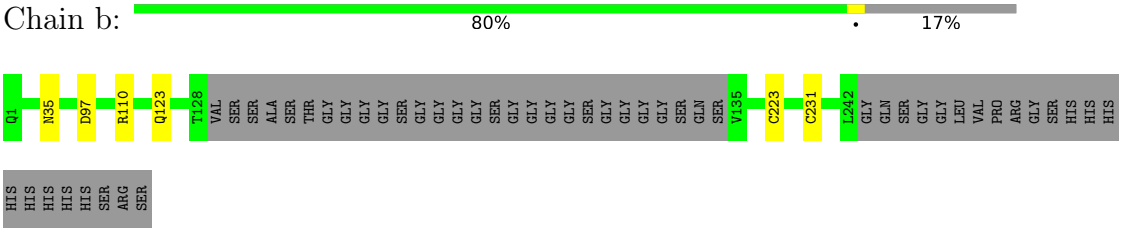
- Molecule 2: 35O22 scFv

Chain L:



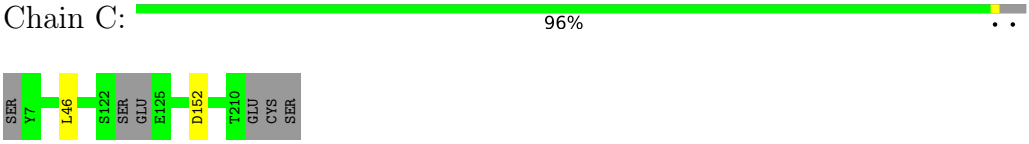
• Molecule 2: 35O22 scFv

Chain b:



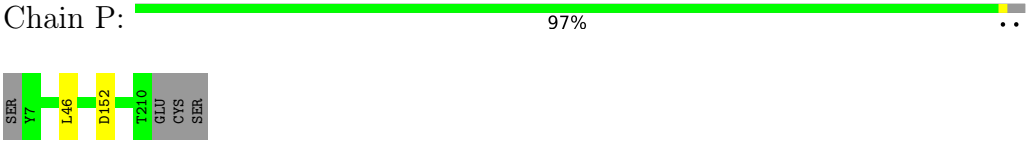
• Molecule 3: PGT124 light chain

Chain C:



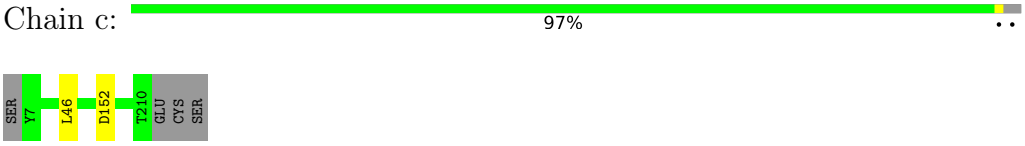
• Molecule 3: PGT124 light chain

Chain P:



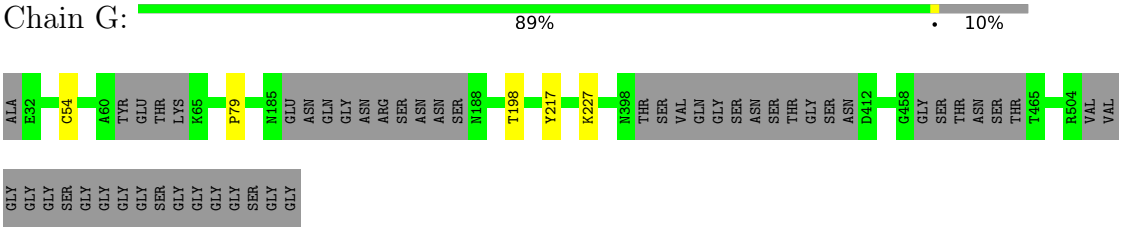
• Molecule 3: PGT124 light chain

Chain c:



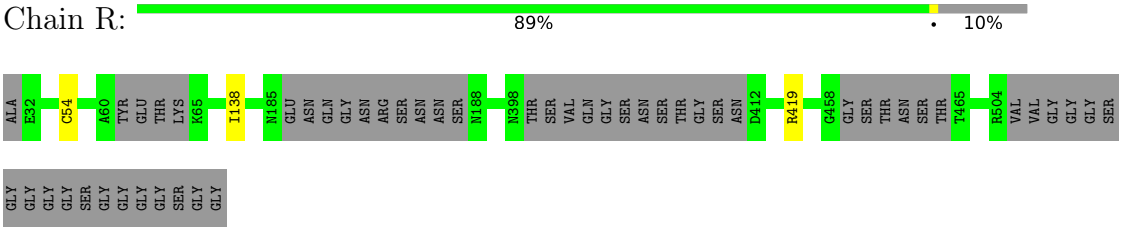
• Molecule 4: Envelope glycoprotein gp120

Chain G:



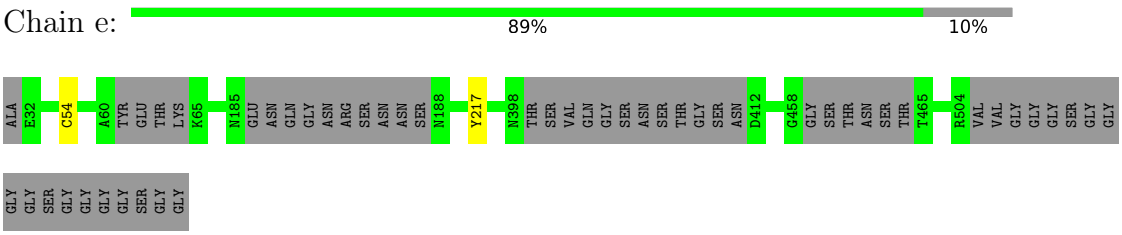
• Molecule 4: Envelope glycoprotein gp120

Chain R:



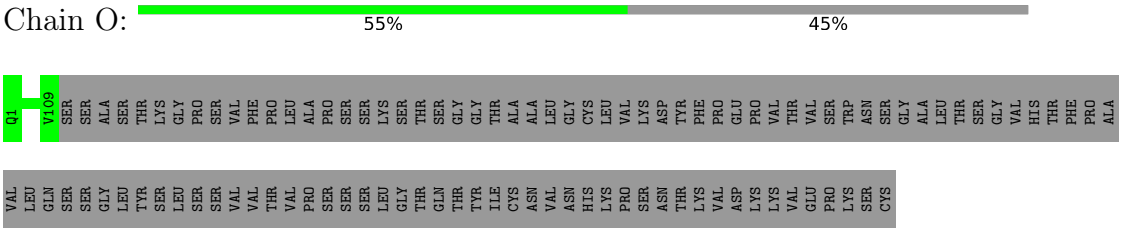
• Molecule 4: Envelope glycoprotein gp120

Chain e:



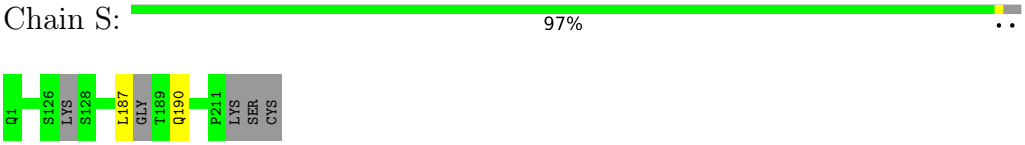
• Molecule 5: PGT124 heavy chain

Chain O:



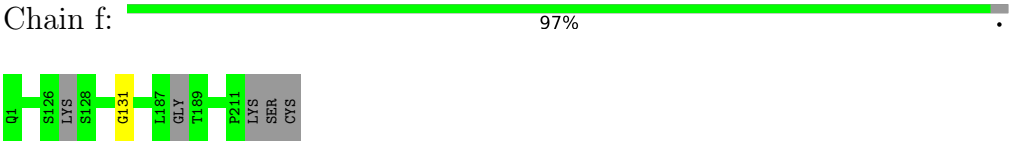
• Molecule 5: PGT124 heavy chain

Chain S:



• Molecule 5: PGT124 heavy chain

Chain f:

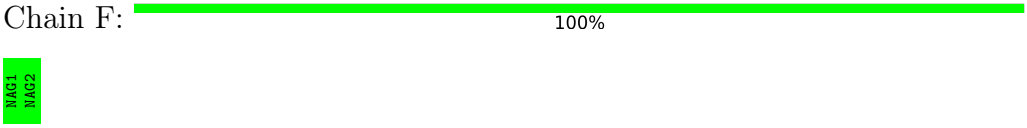


• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

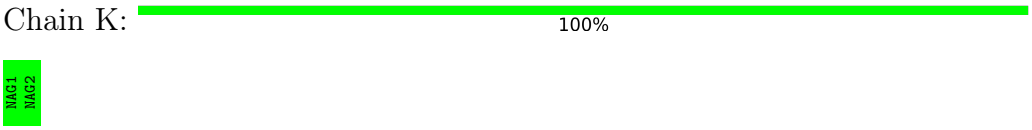
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



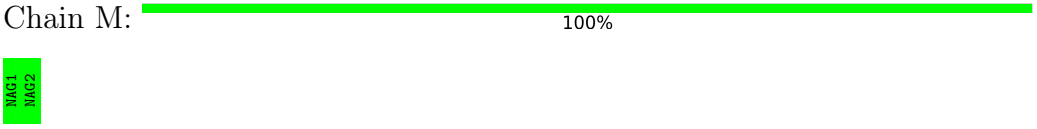
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



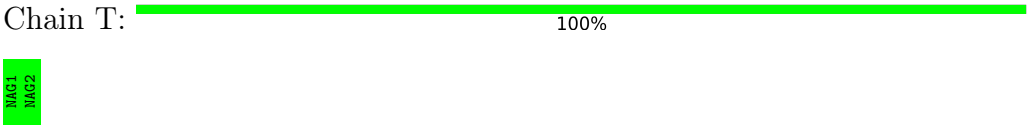
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



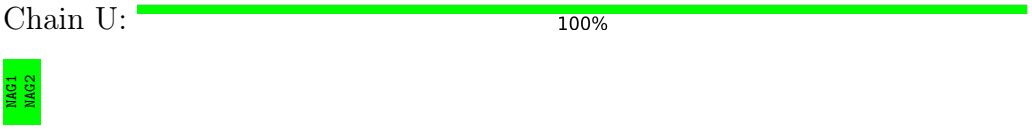
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



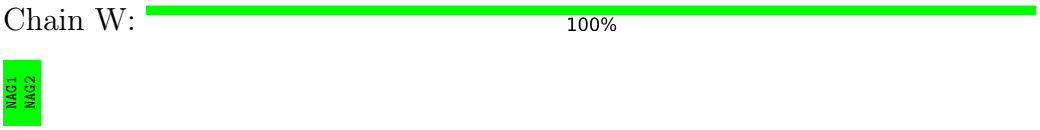
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



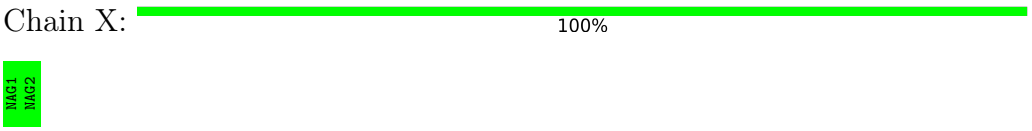
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain X:

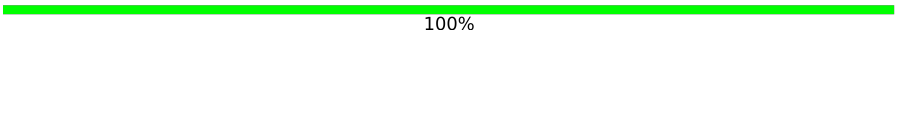


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

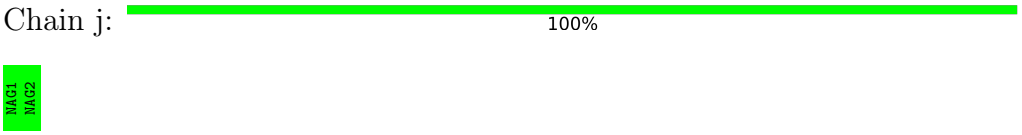
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



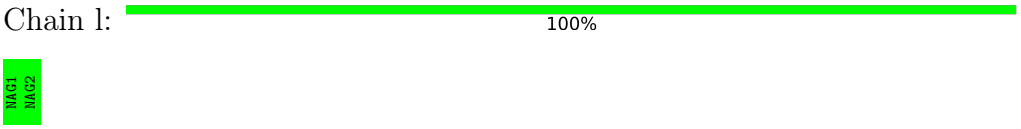
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



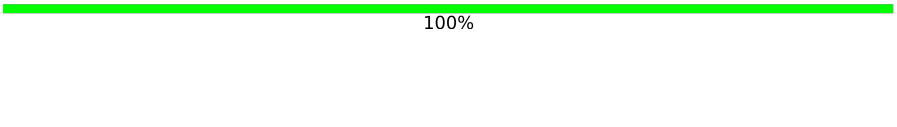
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



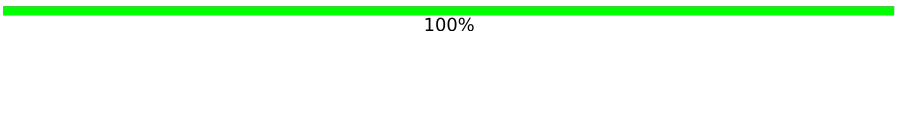
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



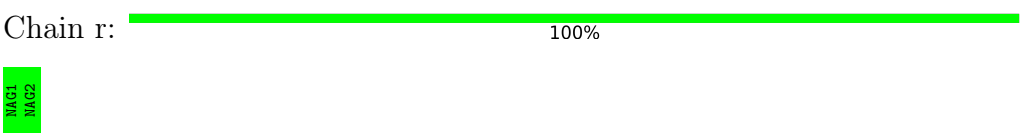
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



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

Chain r:

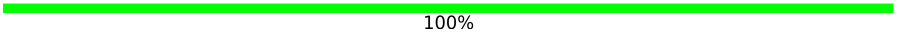


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



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

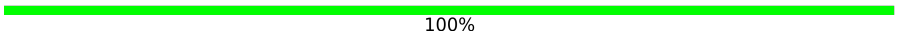
Chain Y:

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

Chain Z:

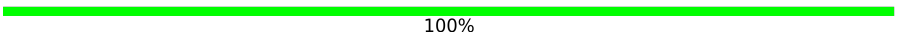
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain n:

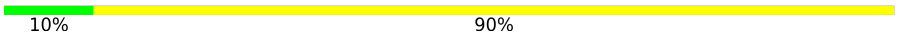


• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

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

Chain i:



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

Chain q:

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

Chain V:

• Molecule 10: 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 k:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	357.59Å 212.04Å 207.71Å 90.00° 125.07° 90.00°	Depositor
Resolution (Å)	41.08 – 5.75 41.08 – 5.75	Depositor EDS
% Data completeness (in resolution range)	92.3 (41.08-5.75) 92.3 (41.08-5.75)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 5.72Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.242 , 0.292 0.239 , 0.286	Depositor DCC
R_{free} test set	1551 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å^2)	213.2	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 414.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.039 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.047 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.034 for -h-k-l,l,k 0.049 for -h+k-l,-l,-k 0.035 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.030 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.048 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.035 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.327 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.327 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.038 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	29645	wwPDB-VP
Average B, all atoms (Å^2)	359.0	wwPDB-VP

[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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.24	0/983	0.44	0/1332
1	H	0.23	0/979	0.45	0/1327
1	a	0.24	0/983	0.45	0/1332
2	D	0.27	0/1871	0.51	0/2552
2	L	0.28	0/1871	0.52	0/2552
2	b	0.25	0/1871	0.51	0/2552
3	C	0.25	0/1622	0.50	1/2215 (0.0%)
3	P	0.25	0/1638	0.51	1/2238 (0.0%)
3	c	0.25	0/1638	0.50	1/2238 (0.0%)
4	G	0.26	0/3546	0.52	0/4813
4	R	0.25	0/3546	0.51	0/4813
4	e	0.25	0/3546	0.50	0/4813
5	O	0.25	0/1055	0.52	0/1436
5	S	0.28	0/1792	0.52	0/2445
5	f	0.26	0/1792	0.52	0/2445
All	All	0.26	0/28733	0.50	3/39103 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	46	LEU	CA-CB-CG	5.67	128.34	115.30
3	c	46	LEU	CA-CB-CG	5.63	128.26	115.30
3	C	46	LEU	CA-CB-CG	5.36	127.63	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	119/164 (73%)	114 (96%)	5 (4%)	0	100	100
1	H	118/164 (72%)	112 (95%)	6 (5%)	0	100	100
1	a	119/164 (73%)	113 (95%)	6 (5%)	0	100	100
2	D	232/286 (81%)	213 (92%)	17 (7%)	2 (1%)	17	56
2	L	232/286 (81%)	210 (90%)	18 (8%)	4 (2%)	9	42
2	b	232/286 (81%)	214 (92%)	18 (8%)	0	100	100
3	C	204/214 (95%)	193 (95%)	10 (5%)	1 (0%)	29	69
3	P	208/214 (97%)	197 (95%)	10 (5%)	1 (0%)	29	69
3	c	208/214 (97%)	197 (95%)	10 (5%)	1 (0%)	29	69
4	G	429/490 (88%)	405 (94%)	23 (5%)	1 (0%)	47	81
4	R	429/490 (88%)	405 (94%)	23 (5%)	1 (0%)	47	81
4	e	429/490 (88%)	405 (94%)	24 (6%)	0	100	100
5	O	128/235 (54%)	124 (97%)	4 (3%)	0	100	100
5	S	224/235 (95%)	216 (96%)	8 (4%)	0	100	100
5	f	224/235 (95%)	215 (96%)	8 (4%)	1 (0%)	34	72
All	All	3535/4167 (85%)	3333 (94%)	190 (5%)	12 (0%)	41	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	160	VAL
2	L	241	VAL
2	D	241	VAL

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Mol	Chain	Res	Type
3	C	152	ASP
2	L	162	CYS
2	L	163	SER
3	P	152	ASP
3	c	152	ASP
4	R	138	ILE
5	f	131	GLY
2	D	160	VAL
4	G	79	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	105/133 (79%)	105 (100%)	0	100	100
1	H	105/133 (79%)	103 (98%)	2 (2%)	57	75
1	a	105/133 (79%)	104 (99%)	1 (1%)	76	86
2	D	202/231 (87%)	196 (97%)	6 (3%)	41	63
2	L	202/231 (87%)	196 (97%)	6 (3%)	41	63
2	b	202/231 (87%)	196 (97%)	6 (3%)	41	63
3	C	174/180 (97%)	174 (100%)	0	100	100
3	P	176/180 (98%)	176 (100%)	0	100	100
3	c	176/180 (98%)	176 (100%)	0	100	100
4	G	394/427 (92%)	390 (99%)	4 (1%)	76	86
4	R	394/427 (92%)	392 (100%)	2 (0%)	88	93
4	e	394/427 (92%)	392 (100%)	2 (0%)	88	93
5	O	112/203 (55%)	112 (100%)	0	100	100
5	S	199/203 (98%)	197 (99%)	2 (1%)	76	86
5	f	199/203 (98%)	199 (100%)	0	100	100
All	All	3139/3522 (89%)	3108 (99%)	31 (1%)	76	86

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	13	LYS
2	D	110	ARG
2	D	123	GLN
2	D	160	VAL
2	D	223	CYS
2	D	231	CYS
4	G	54	CYS
4	G	198	THR
4	G	217	TYR
4	G	227	LYS
1	H	574	LYS
1	H	625	ASN
2	L	13	LYS
2	L	97	ASP
2	L	110	ARG
2	L	123	GLN
2	L	223	CYS
2	L	231	CYS
4	R	54	CYS
4	R	419	ARG
5	S	187	LEU
5	S	190	GLN
1	a	575	GLN
2	b	35	ASN
2	b	97	ASP
2	b	110	ARG
2	b	123	GLN
2	b	223	CYS
2	b	231	CYS
4	e	54	CYS
4	e	217	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	P	170	ASN
4	R	105	HIS
4	e	105	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

89 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	1	6,4	14,14,15	0.29	0	17,19,21	0.33	0
6	NAG	A	2	6	14,14,15	0.47	0	17,19,21	0.51	0
6	BMA	A	3	6	11,11,12	1.00	1 (9%)	15,15,17	0.95	1 (6%)
6	MAN	A	4	6	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
6	MAN	A	5	6	11,11,12	0.92	1 (9%)	15,15,17	1.47	3 (20%)
7	NAG	F	1	2,7	14,14,15	0.17	0	17,19,21	0.40	0
7	NAG	F	2	7	14,14,15	0.29	0	17,19,21	0.55	0
8	NAG	I	1	8,4	14,14,15	0.26	0	17,19,21	0.45	0
8	NAG	I	2	8	14,14,15	0.24	0	17,19,21	0.41	0
8	BMA	I	3	8	11,11,12	0.67	0	15,15,17	0.74	0
8	NAG	J	1	8,4	14,14,15	0.27	0	17,19,21	0.48	0
8	NAG	J	2	8	14,14,15	0.20	0	17,19,21	0.42	0
8	BMA	J	3	8	11,11,12	0.66	0	15,15,17	0.78	0
7	NAG	K	1	4,7	14,14,15	0.27	0	17,19,21	0.44	0
7	NAG	K	2	7	14,14,15	0.20	0	17,19,21	0.45	0
7	NAG	M	1	4,7	14,14,15	0.22	0	17,19,21	0.40	0
7	NAG	M	2	7	14,14,15	0.23	0	17,19,21	0.50	0
9	NAG	N	1	9,4	14,14,15	0.73	1 (7%)	17,19,21	1.40	2 (11%)
9	MAN	N	10	9	11,11,12	0.94	0	15,15,17	1.17	2 (13%)
9	NAG	N	2	9	14,14,15	0.24	0	17,19,21	0.41	0
9	BMA	N	3	9	11,11,12	1.04	0	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	N	4	9	11,11,12	1.06	1 (9%)	15,15,17	1.35	2 (13%)
9	MAN	N	5	9	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
9	MAN	N	6	9	11,11,12	0.78	0	15,15,17	0.98	2 (13%)
9	MAN	N	7	9	11,11,12	0.80	0	15,15,17	1.01	2 (13%)
9	MAN	N	8	9	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
9	MAN	N	9	9	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
7	NAG	T	1	4,7	14,14,15	0.25	0	17,19,21	0.53	0
7	NAG	T	2	7	14,14,15	0.34	0	17,19,21	0.41	0
7	NAG	U	1	4,7	14,14,15	0.21	0	17,19,21	0.48	0
7	NAG	U	2	7	14,14,15	0.26	0	17,19,21	0.45	0
10	NAG	V	1	10,4	14,14,15	0.30	0	17,19,21	0.33	0
10	NAG	V	2	10	14,14,15	0.52	0	17,19,21	0.60	0
10	BMA	V	3	10	11,11,12	0.93	1 (9%)	15,15,17	1.03	1 (6%)
10	MAN	V	4	10	11,11,12	0.70	0	15,15,17	2.78	4 (26%)
7	NAG	W	1	4,7	14,14,15	0.30	0	17,19,21	0.59	0
7	NAG	W	2	7	14,14,15	0.47	0	17,19,21	0.58	0
7	NAG	X	1	2,7	14,14,15	0.22	0	17,19,21	0.40	0
7	NAG	X	2	7	14,14,15	0.29	0	17,19,21	0.55	0
8	NAG	Y	1	8,4	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	Y	2	8	14,14,15	0.23	0	17,19,21	0.43	0
8	BMA	Y	3	8	11,11,12	0.63	0	15,15,17	0.75	0
8	NAG	Z	1	8,4	14,14,15	0.27	0	17,19,21	0.49	0
8	NAG	Z	2	8	14,14,15	0.31	0	17,19,21	0.43	0
8	BMA	Z	3	8	11,11,12	0.68	0	15,15,17	0.80	0
7	NAG	g	1	4,7	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	g	2	7	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	h	1	4,7	14,14,15	0.21	0	17,19,21	0.39	0
7	NAG	h	2	7	14,14,15	0.23	0	17,19,21	0.49	0
9	NAG	i	1	9,4	14,14,15	0.72	1 (7%)	17,19,21	1.40	2 (11%)
9	MAN	i	10	9	11,11,12	0.89	0	15,15,17	1.15	1 (6%)
9	NAG	i	2	9	14,14,15	0.25	0	17,19,21	0.41	0
9	BMA	i	3	9	11,11,12	1.15	1 (9%)	15,15,17	1.02	1 (6%)
9	MAN	i	4	9	11,11,12	1.07	1 (9%)	15,15,17	1.37	2 (13%)
9	MAN	i	5	9	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
9	MAN	i	6	9	11,11,12	0.78	0	15,15,17	0.97	2 (13%)
9	MAN	i	7	9	11,11,12	0.82	0	15,15,17	1.00	2 (13%)
9	MAN	i	8	9	11,11,12	0.71	0	15,15,17	1.13	2 (13%)
9	MAN	i	9	9	11,11,12	0.71	0	15,15,17	1.23	2 (13%)
7	NAG	j	1	4,7	14,14,15	0.22	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	j	2	7	14,14,15	0.27	0	17,19,21	0.40	0
10	NAG	k	1	10,4	14,14,15	0.43	0	17,19,21	0.36	0
10	NAG	k	2	10	14,14,15	0.31	0	17,19,21	0.58	0
10	BMA	k	3	10	11,11,12	0.68	0	15,15,17	0.76	0
10	MAN	k	4	10	11,11,12	0.76	0	15,15,17	1.57	4 (26%)
7	NAG	l	1	2,7	14,14,15	0.23	0	17,19,21	0.41	0
7	NAG	l	2	7	14,14,15	0.27	0	17,19,21	0.54	0
8	NAG	m	1	8	14,14,15	0.20	0	17,19,21	0.45	0
8	NAG	m	2	8	14,14,15	0.27	0	17,19,21	0.40	0
8	BMA	m	3	8	11,11,12	0.64	0	15,15,17	0.73	0
8	NAG	n	1	8,4	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	n	2	8	14,14,15	0.24	0	17,19,21	0.42	0
8	BMA	n	3	8	11,11,12	0.63	0	15,15,17	0.76	0
7	NAG	o	1	4,7	14,14,15	0.29	0	17,19,21	0.48	0
7	NAG	o	2	7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	p	1	4,7	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	p	2	7	14,14,15	0.20	0	17,19,21	0.50	0
9	NAG	q	1	9,4	14,14,15	0.72	1 (7%)	17,19,21	1.43	2 (11%)
9	MAN	q	10	9	11,11,12	0.90	0	15,15,17	1.15	1 (6%)
9	NAG	q	2	9	14,14,15	0.25	0	17,19,21	0.38	0
9	BMA	q	3	9	11,11,12	0.97	0	15,15,17	0.98	1 (6%)
9	MAN	q	4	9	11,11,12	1.08	1 (9%)	15,15,17	1.36	4 (26%)
9	MAN	q	5	9	11,11,12	0.74	0	15,15,17	1.19	2 (13%)
9	MAN	q	6	9	11,11,12	0.79	0	15,15,17	0.98	2 (13%)
9	MAN	q	7	9	11,11,12	0.73	0	15,15,17	1.02	2 (13%)
9	MAN	q	8	9	11,11,12	0.74	0	15,15,17	1.06	1 (6%)
9	MAN	q	9	9	11,11,12	0.77	0	15,15,17	1.30	2 (13%)
7	NAG	r	1	4,7	14,14,15	0.22	0	17,19,21	0.47	0
7	NAG	r	2	7	14,14,15	0.34	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	A	2	6	-	2/6/23/26	0/1/1/1
6	BMA	A	3	6	-	2/2/19/22	0/1/1/1
6	MAN	A	4	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	5	6	-	2/2/19/22	1/1/1/1
7	NAG	F	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
8	NAG	I	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	BMA	J	3	8	-	1/2/19/22	0/1/1/1
7	NAG	K	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	NAG	M	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	1/6/23/26	0/1/1/1
9	NAG	N	1	9,4	-	5/6/23/26	0/1/1/1
9	MAN	N	10	9	-	0/2/19/22	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	BMA	N	3	9	-	0/2/19/22	0/1/1/1
9	MAN	N	4	9	-	0/2/19/22	0/1/1/1
9	MAN	N	5	9	-	2/2/19/22	0/1/1/1
9	MAN	N	6	9	-	0/2/19/22	0/1/1/1
9	MAN	N	7	9	-	0/2/19/22	0/1/1/1
9	MAN	N	8	9	-	0/2/19/22	0/1/1/1
9	MAN	N	9	9	-	0/2/19/22	0/1/1/1
7	NAG	T	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	NAG	U	1	4,7	-	1/6/23/26	0/1/1/1
7	NAG	U	2	7	-	1/6/23/26	0/1/1/1
10	NAG	V	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
10	MAN	V	4	10	-	0/2/19/22	0/1/1/1
7	NAG	W	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
8	NAG	Y	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	8,4	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	q	5	9	-	2/2/19/22	0/1/1/1
9	MAN	q	6	9	-	0/2/19/22	0/1/1/1
9	MAN	q	7	9	-	0/2/19/22	0/1/1/1
9	MAN	q	8	9	-	0/2/19/22	0/1/1/1
9	MAN	q	9	9	-	0/2/19/22	0/1/1/1
7	NAG	r	1	4,7	-	0/6/23/26	0/1/1/1
7	NAG	r	2	7	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	4	MAN	C1-C2	3.10	1.59	1.52
9	i	4	MAN	C1-C2	3.10	1.59	1.52
9	q	4	MAN	C1-C2	2.96	1.58	1.52
9	N	1	NAG	O5-C1	-2.59	1.39	1.43
9	q	1	NAG	O5-C1	-2.56	1.39	1.43
9	i	1	NAG	O5-C1	-2.56	1.39	1.43
9	i	3	BMA	O5-C1	-2.39	1.39	1.43
10	V	3	BMA	C4-C3	2.17	1.57	1.52
6	A	3	BMA	C1-C2	2.14	1.57	1.52
6	A	5	MAN	C1-C2	2.07	1.56	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	V	4	MAN	C1-O5-C5	8.41	123.59	112.19
10	V	4	MAN	O5-C1-C2	4.85	118.26	110.77
9	q	1	NAG	C2-N2-C7	4.46	129.25	122.90
9	N	1	NAG	C2-N2-C7	4.40	129.16	122.90
9	i	1	NAG	C2-N2-C7	4.38	129.14	122.90
9	q	9	MAN	C1-O5-C5	4.12	117.77	112.19
9	N	9	MAN	C1-O5-C5	3.77	117.30	112.19
10	k	4	MAN	C1-O5-C5	3.71	117.22	112.19
9	i	9	MAN	C1-O5-C5	3.65	117.14	112.19
6	A	5	MAN	C1-O5-C5	3.50	116.93	112.19
10	V	4	MAN	C1-C2-C3	3.31	113.74	109.67
9	q	5	MAN	O2-C2-C3	-3.22	103.69	110.14
9	q	8	MAN	C1-O5-C5	3.09	116.38	112.19
9	N	8	MAN	C1-O5-C5	3.08	116.37	112.19
9	i	8	MAN	C1-O5-C5	2.98	116.23	112.19
9	i	5	MAN	O2-C2-C3	-2.93	104.26	110.14
9	N	4	MAN	C1-O5-C5	2.92	116.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	5	MAN	O2-C2-C3	-2.81	104.50	110.14
9	i	4	MAN	C1-O5-C5	2.81	116.00	112.19
9	q	4	MAN	C1-O5-C5	2.68	115.83	112.19
9	q	5	MAN	C1-O5-C5	2.66	115.80	112.19
6	A	4	MAN	C1-O5-C5	2.58	115.69	112.19
9	N	5	MAN	C1-O5-C5	2.55	115.64	112.19
10	V	3	BMA	O3-C3-C4	2.53	116.20	110.35
9	i	5	MAN	C1-O5-C5	2.51	115.60	112.19
9	i	3	BMA	C1-C2-C3	2.49	112.73	109.67
10	V	4	MAN	O2-C2-C3	-2.47	105.20	110.14
9	q	3	BMA	C1-C2-C3	2.41	112.62	109.67
9	i	10	MAN	O2-C2-C3	-2.38	105.38	110.14
6	A	3	BMA	O3-C3-C2	2.37	114.54	109.99
9	q	10	MAN	O2-C2-C3	-2.35	105.43	110.14
9	N	10	MAN	O2-C2-C3	-2.34	105.44	110.14
10	k	4	MAN	O5-C5-C6	-2.34	103.54	107.20
10	k	4	MAN	O5-C1-C2	2.34	114.38	110.77
9	N	6	MAN	C1-O5-C5	2.30	115.31	112.19
9	N	1	NAG	C1-C2-N2	2.29	114.40	110.49
9	i	1	NAG	C1-C2-N2	2.28	114.39	110.49
6	A	5	MAN	O5-C5-C6	2.27	110.77	107.20
9	q	7	MAN	C1-O5-C5	2.27	115.26	112.19
9	q	6	MAN	C1-O5-C5	2.26	115.25	112.19
9	q	1	NAG	C1-C2-N2	2.24	114.32	110.49
9	N	3	BMA	C1-C2-C3	2.23	112.41	109.67
10	k	4	MAN	O2-C2-C3	-2.22	105.68	110.14
9	N	7	MAN	O2-C2-C3	-2.21	105.71	110.14
6	A	4	MAN	O2-C2-C3	-2.20	105.73	110.14
9	i	4	MAN	C1-C2-C3	2.20	112.37	109.67
9	i	6	MAN	C1-O5-C5	2.19	115.16	112.19
9	N	6	MAN	O2-C2-C3	-2.19	105.76	110.14
9	i	9	MAN	O2-C2-C3	-2.18	105.76	110.14
9	i	6	MAN	O2-C2-C3	-2.18	105.77	110.14
9	q	7	MAN	O2-C2-C3	-2.18	105.78	110.14
9	q	6	MAN	O2-C2-C3	-2.18	105.78	110.14
9	N	9	MAN	O2-C2-C3	-2.17	105.80	110.14
9	q	9	MAN	O2-C2-C3	-2.17	105.80	110.14
9	q	4	MAN	O2-C2-C1	2.16	113.57	109.15
9	N	8	MAN	O3-C3-C2	2.14	114.10	109.99
9	N	7	MAN	C1-O5-C5	2.14	115.09	112.19
9	i	7	MAN	O2-C2-C3	-2.10	105.93	110.14
9	i	7	MAN	C1-O5-C5	2.09	115.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	4	MAN	C1-C2-C3	2.07	112.21	109.67
6	A	5	MAN	O2-C2-C3	-2.06	106.01	110.14
9	q	4	MAN	O5-C1-C2	2.05	113.94	110.77
9	N	10	MAN	C1-O5-C5	2.04	114.96	112.19
9	q	4	MAN	C1-C2-C3	2.04	112.17	109.67
9	i	8	MAN	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	NAG	O5-C5-C6-O6
6	A	3	BMA	O5-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
6	A	5	MAN	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
10	V	2	NAG	C4-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
8	n	1	NAG	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
9	q	2	NAG	O5-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
8	J	1	NAG	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
6	A	3	BMA	C4-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
6	A	5	MAN	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
8	n	1	NAG	C4-C5-C6-O6
9	q	2	NAG	C4-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
9	N	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	q	5	MAN	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
9	i	5	MAN	C4-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
8	m	1	NAG	C8-C7-N2-C2
8	m	1	NAG	O7-C7-N2-C2
9	N	1	NAG	C8-C7-N2-C2
9	N	1	NAG	O7-C7-N2-C2
9	i	1	NAG	C8-C7-N2-C2
9	i	1	NAG	O7-C7-N2-C2
9	q	1	NAG	C8-C7-N2-C2
9	q	1	NAG	O7-C7-N2-C2
7	X	1	NAG	O5-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
8	J	2	NAG	C4-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
6	A	2	NAG	O5-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
9	N	5	MAN	O5-C5-C6-O6
9	i	5	MAN	O5-C5-C6-O6
9	q	5	MAN	O5-C5-C6-O6
7	F	1	NAG	O5-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
8	Z	3	BMA	O5-C5-C6-O6
8	n	3	BMA	O5-C5-C6-O6
6	A	4	MAN	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
10	k	4	MAN	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
9	i	1	NAG	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
8	J	3	BMA	O5-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	I	1	NAG	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
9	i	1	NAG	O5-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
6	A	2	NAG	C4-C5-C6-O6
10	V	1	NAG	O5-C5-C6-O6
7	F	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	l	2	NAG	C3-C2-N2-C7
10	k	2	NAG	C3-C2-N2-C7
7	j	1	NAG	O5-C5-C6-O6
10	k	1	NAG	O5-C5-C6-O6
9	N	1	NAG	C3-C2-N2-C7
9	i	1	NAG	C3-C2-N2-C7
9	q	1	NAG	C3-C2-N2-C7
8	m	2	NAG	C4-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
9	q	1	NAG	C4-C5-C6-O6

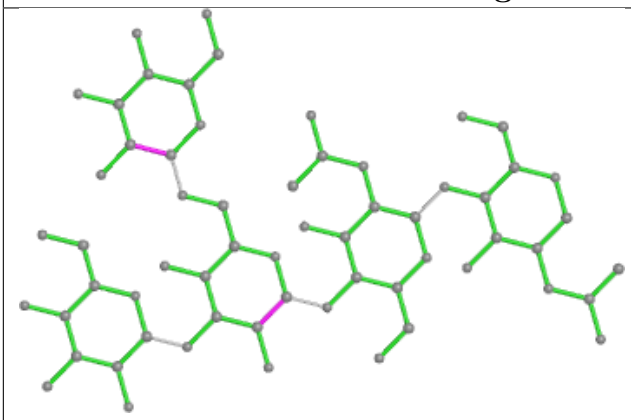
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5	MAN	C1-C2-C3-C4-C5-O5

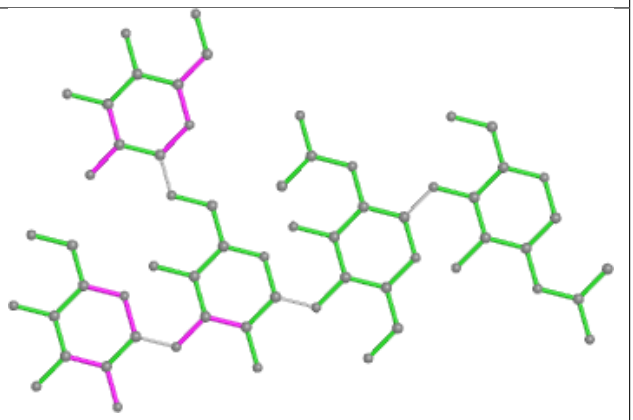
No monomer is involved in short contacts.

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

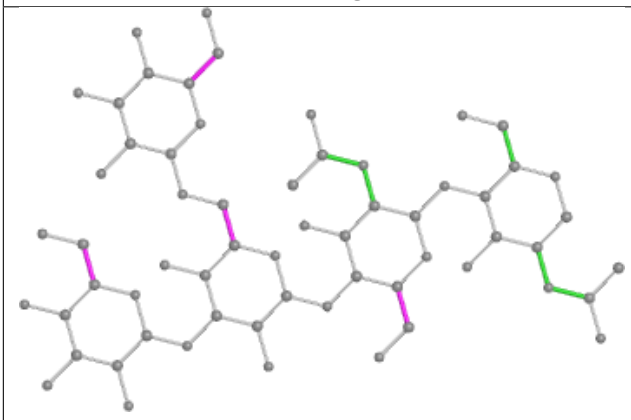
Oligosaccharide Chain A



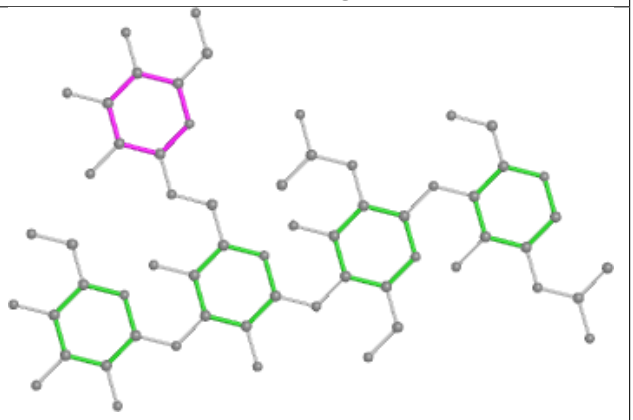
Bond lengths



Bond angles

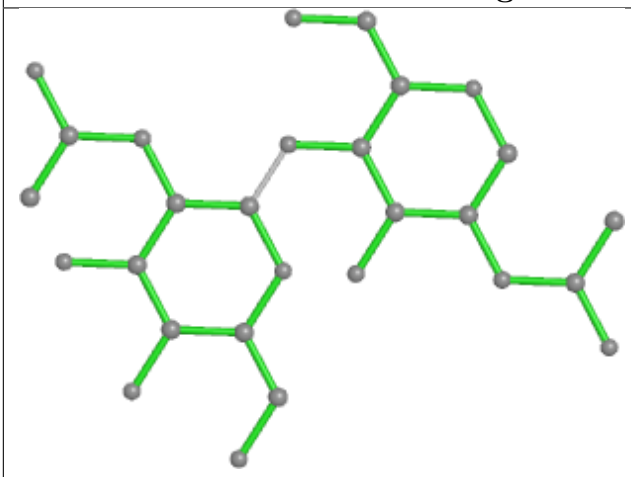


Torsions

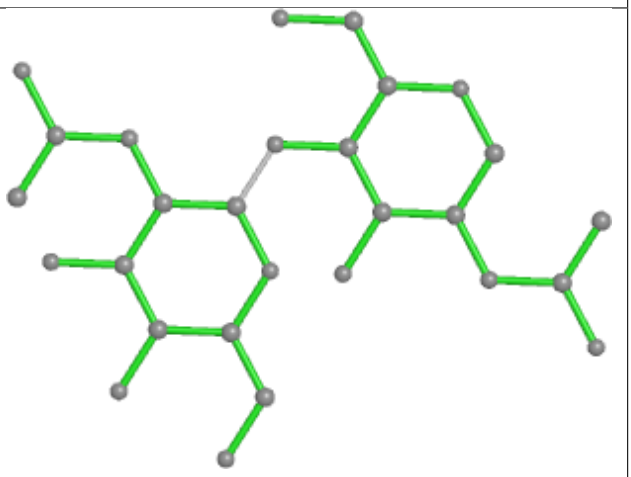


Rings

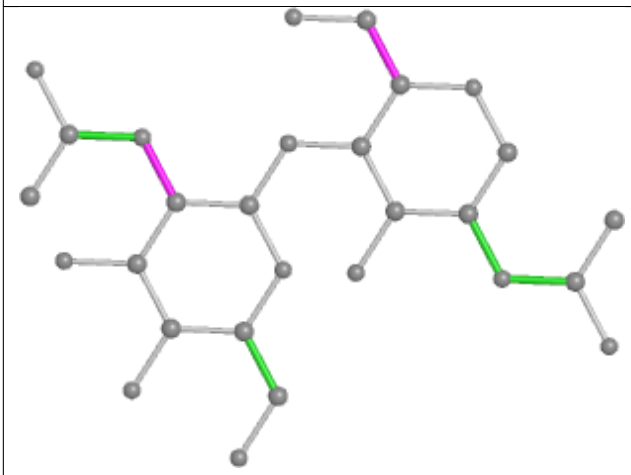
Oligosaccharide Chain F



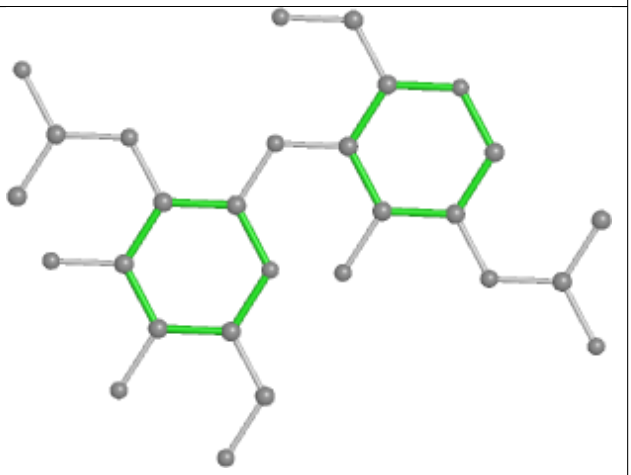
Bond lengths



Bond angles

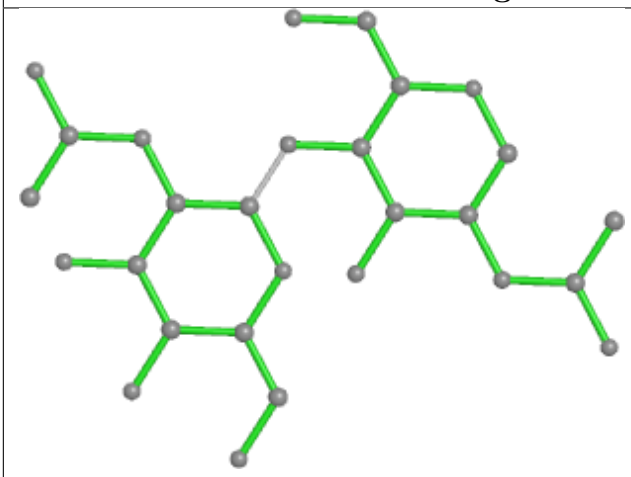


Torsions

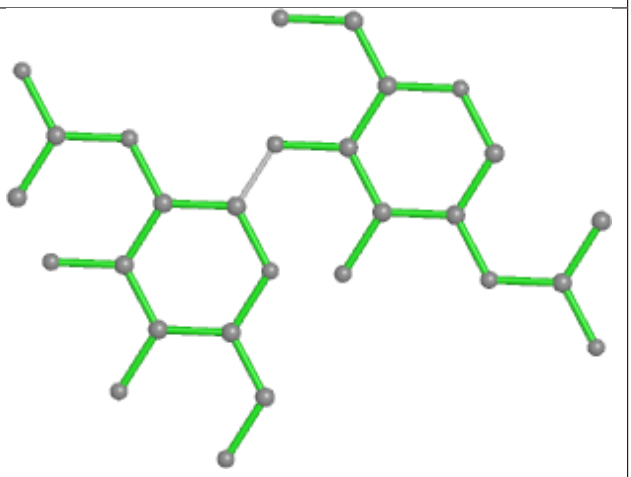


Rings

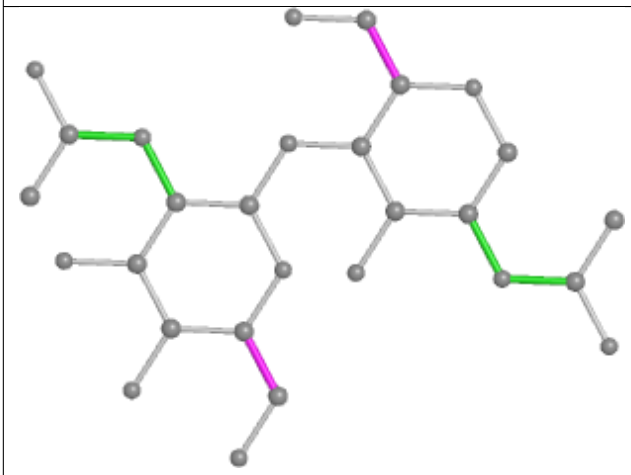
Oligosaccharide Chain K



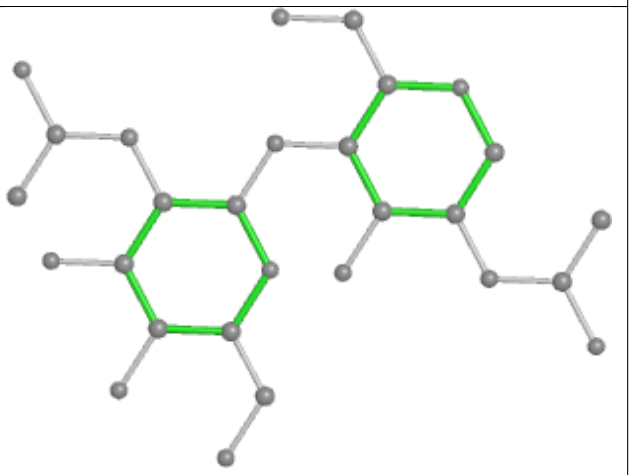
Bond lengths



Bond angles

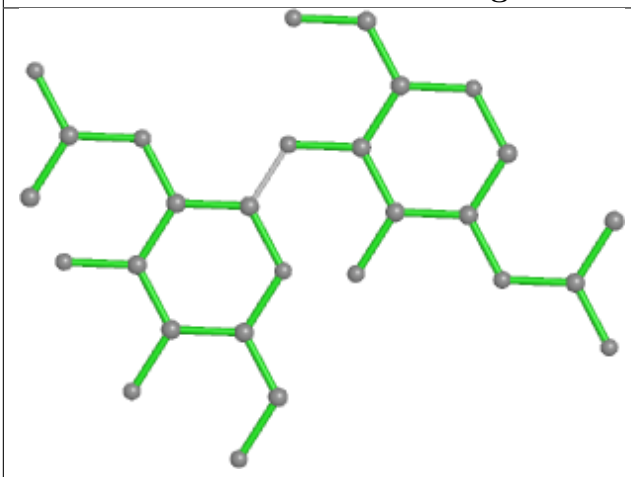


Torsions

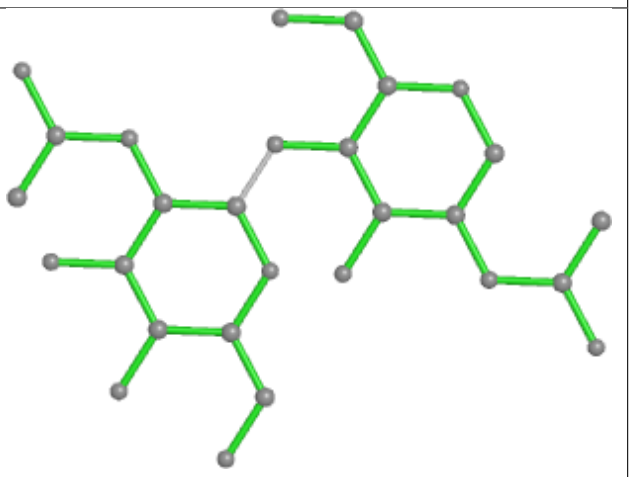


Rings

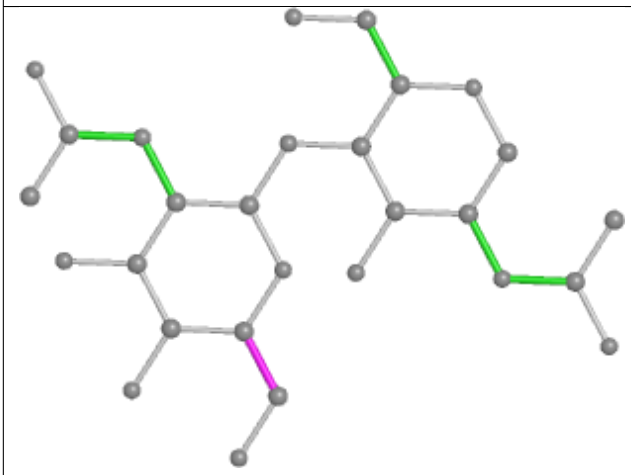
Oligosaccharide Chain M



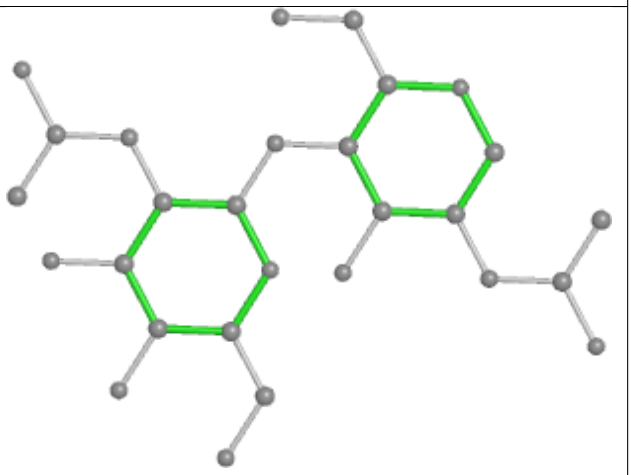
Bond lengths



Bond angles

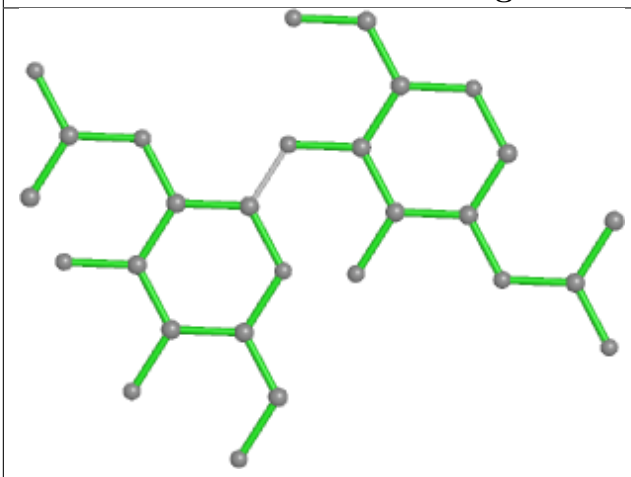


Torsions

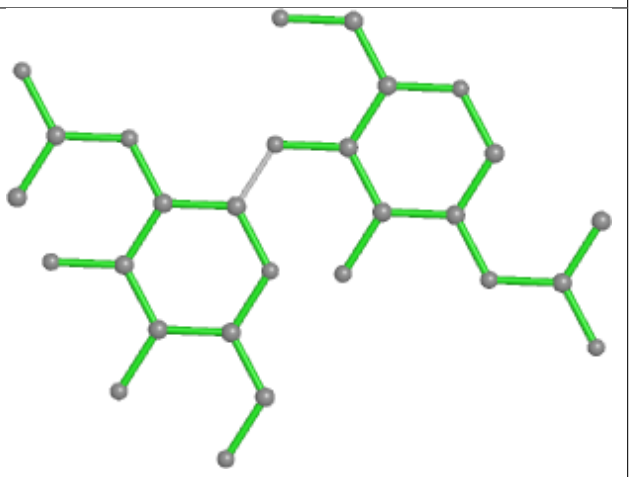


Rings

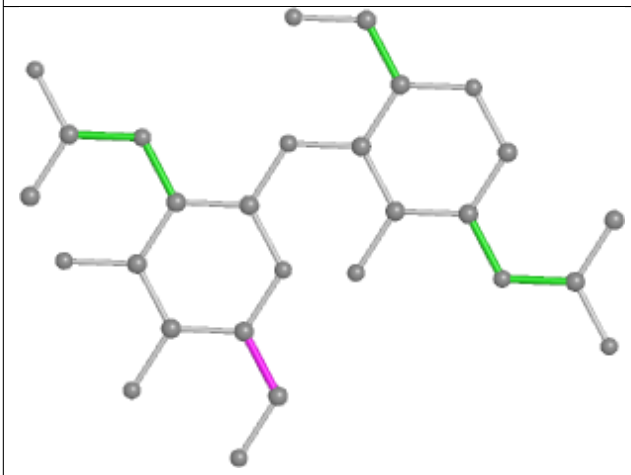
Oligosaccharide Chain T



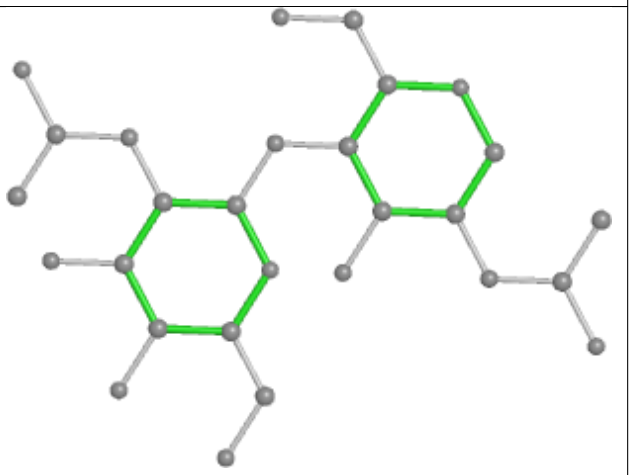
Bond lengths



Bond angles

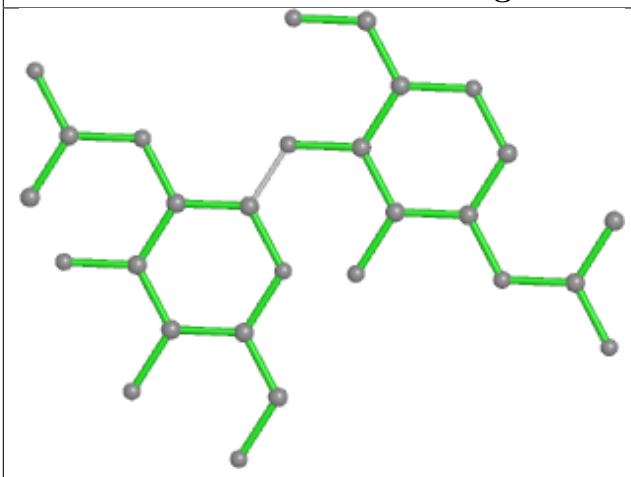


Torsions

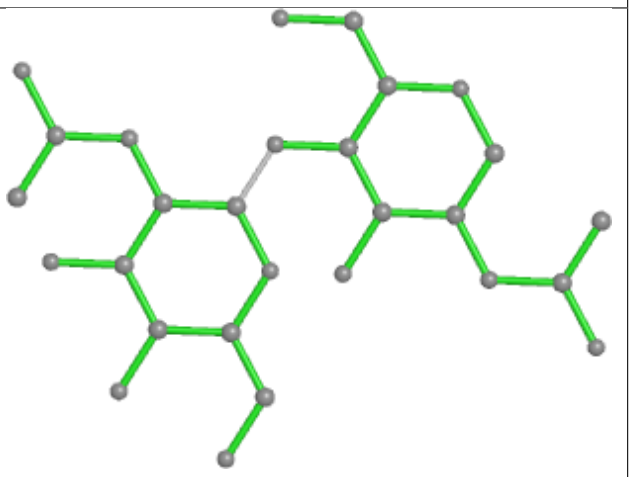


Rings

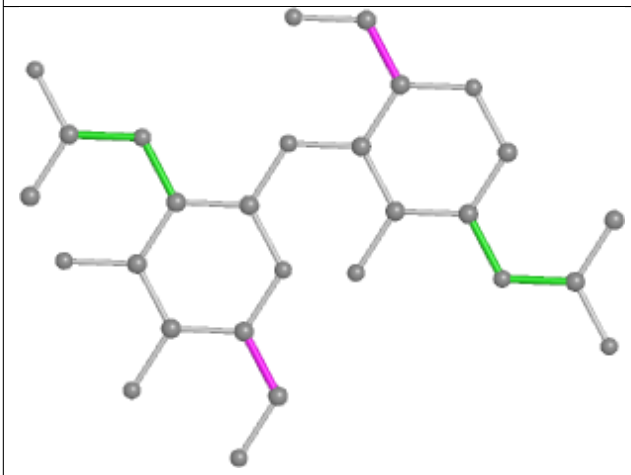
Oligosaccharide Chain U



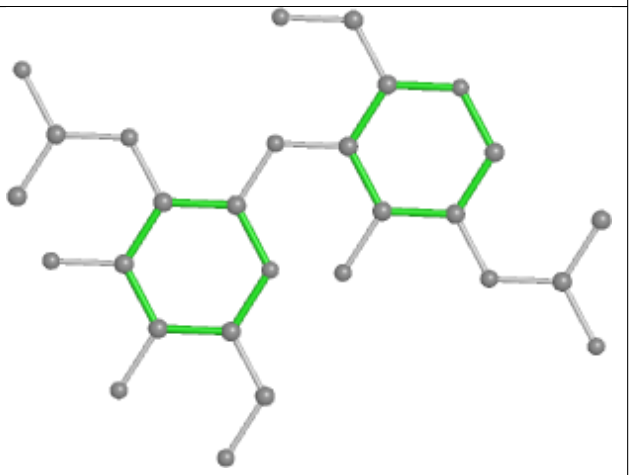
Bond lengths



Bond angles

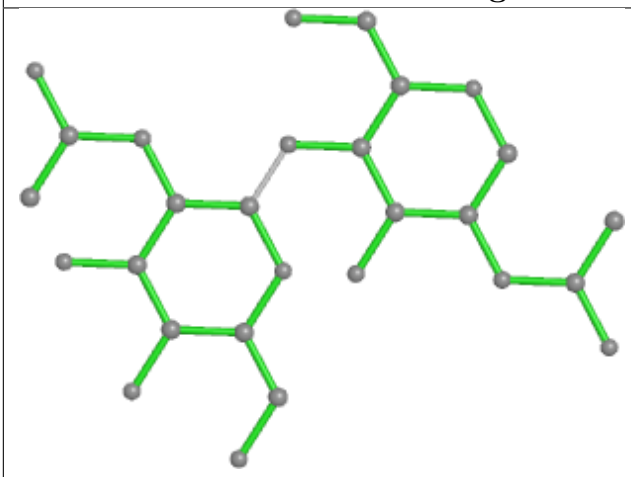


Torsions

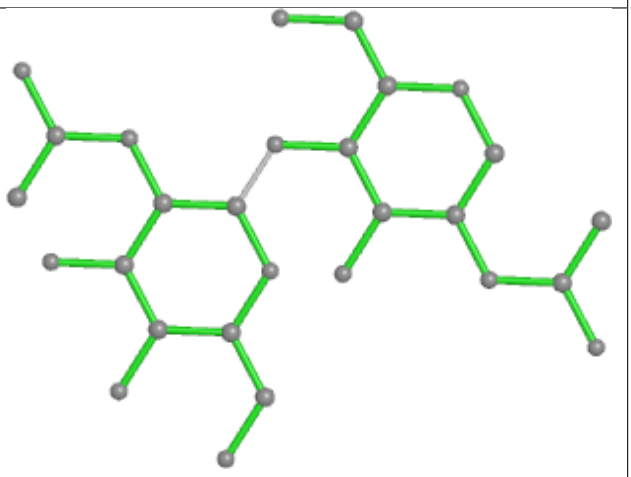


Rings

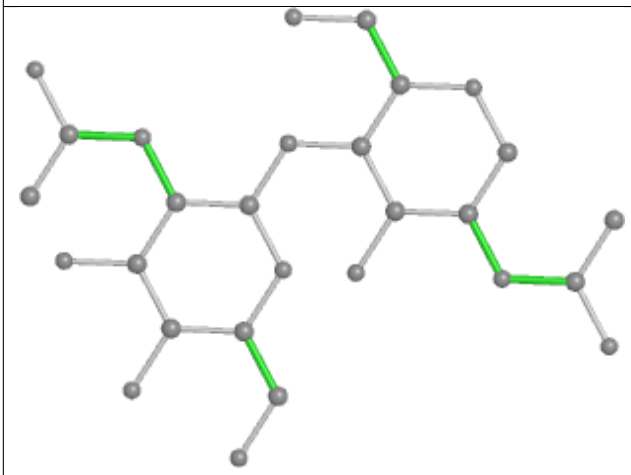
Oligosaccharide Chain W



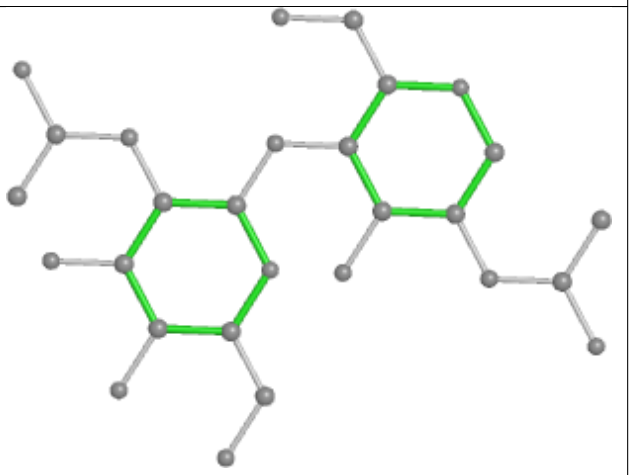
Bond lengths



Bond angles

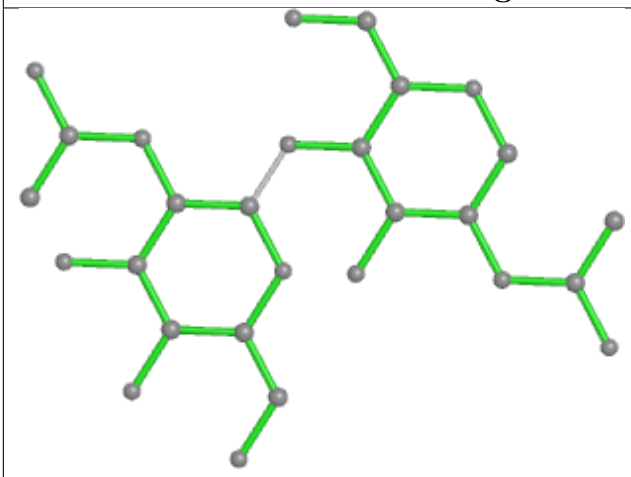


Torsions



Rings

Oligosaccharide Chain X



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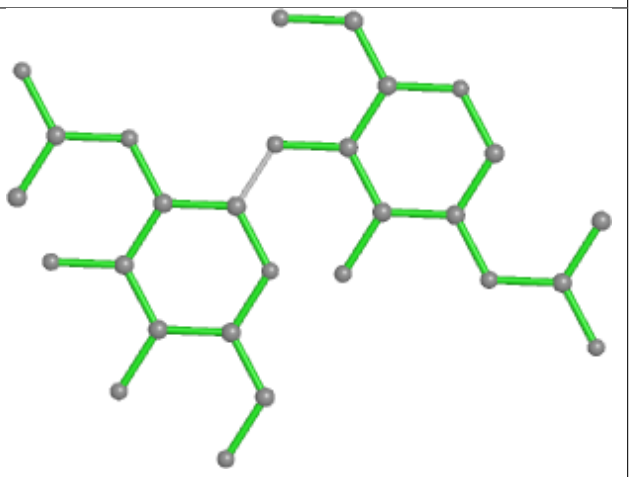
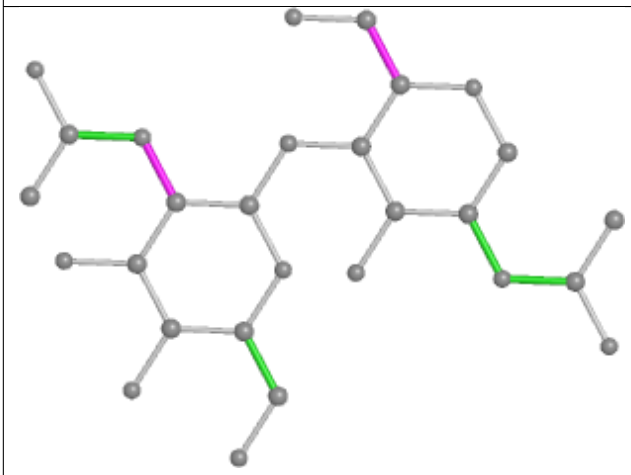


Bond angles



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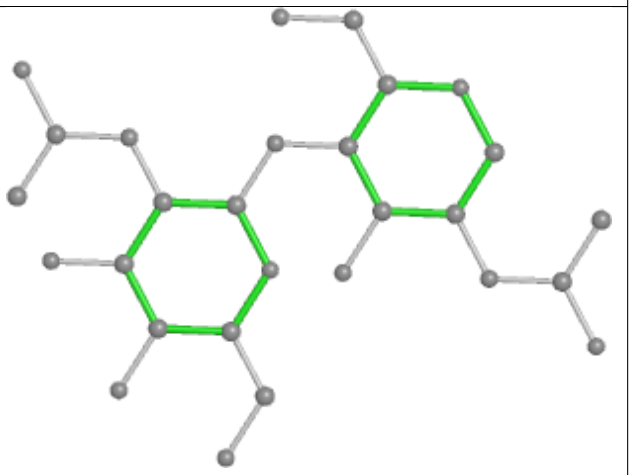
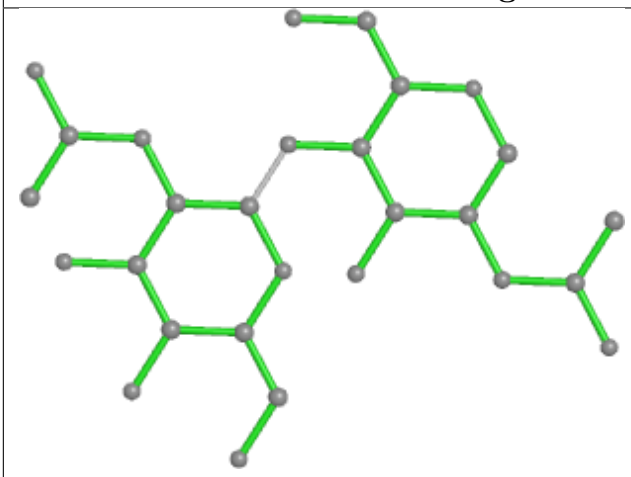


Rings

Oligosaccharide Chain g



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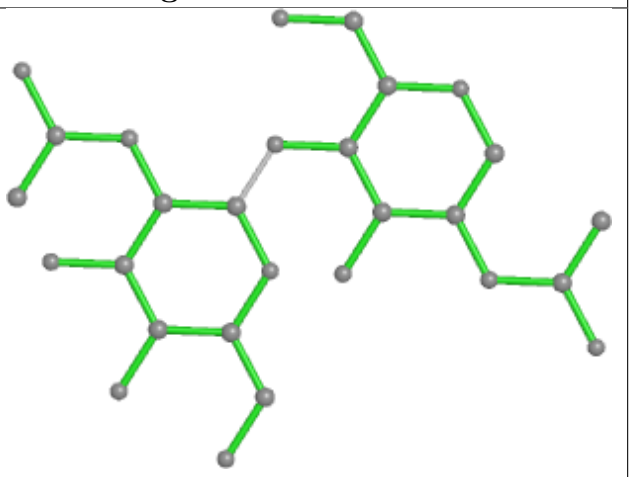

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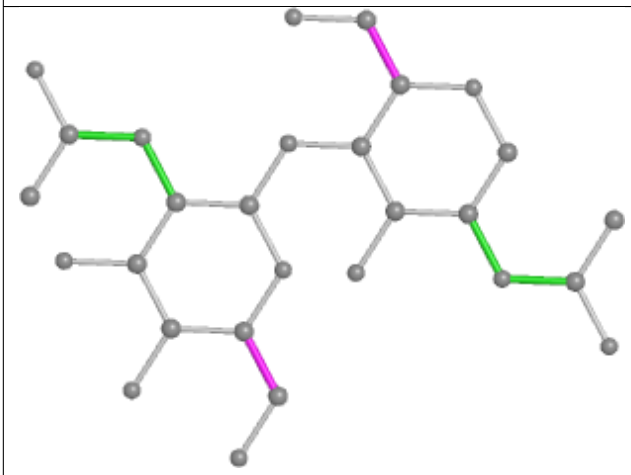

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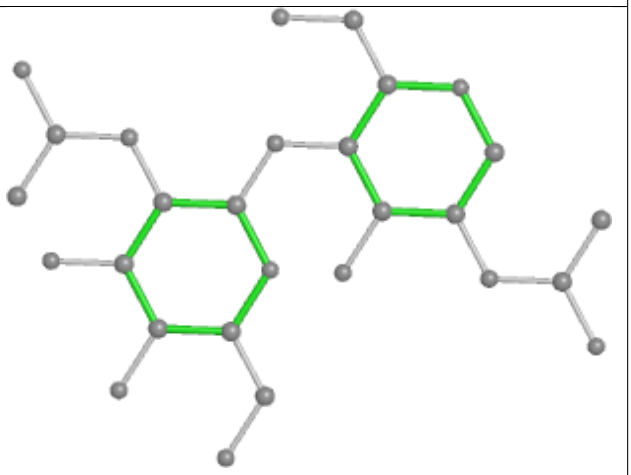
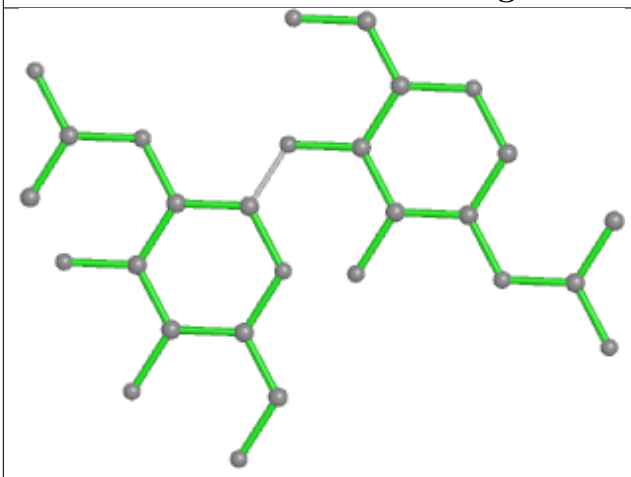


Rings

Oligosaccharide Chain h



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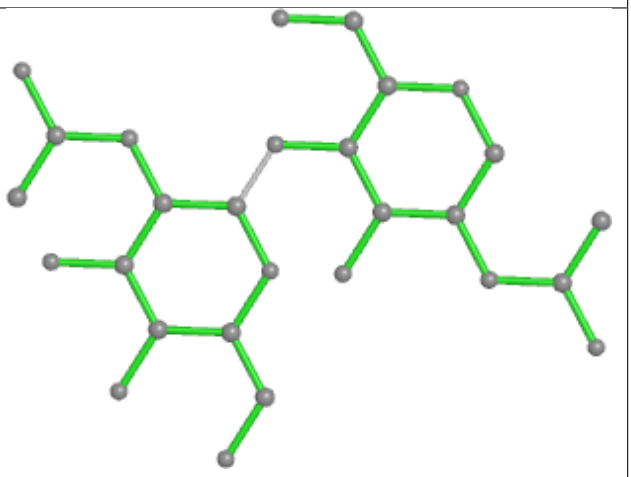
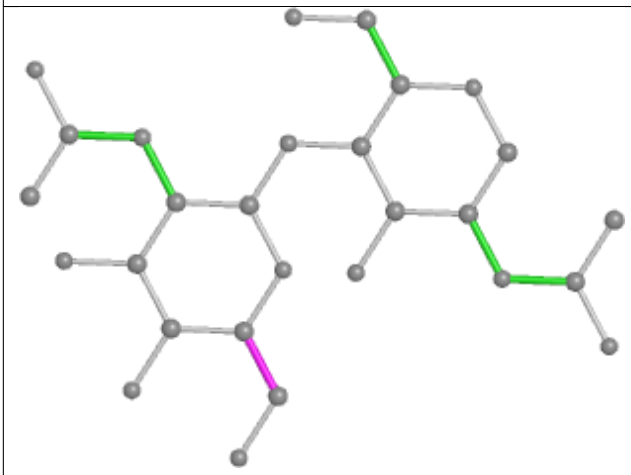


Bond angles



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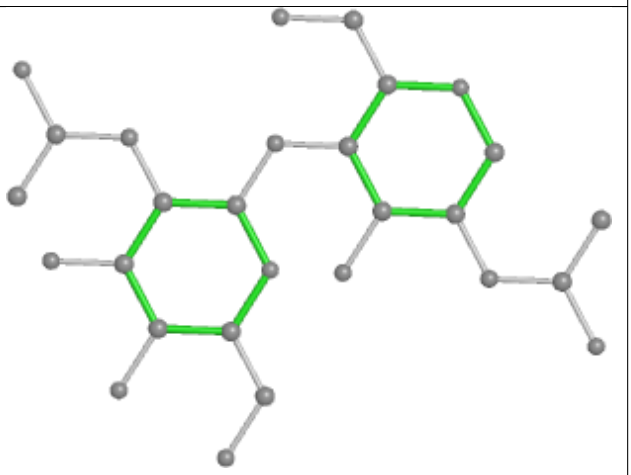
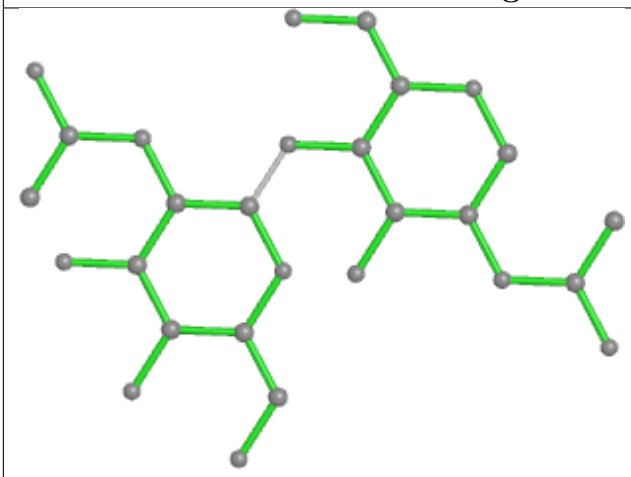


Rings

Oligosaccharide Chain j



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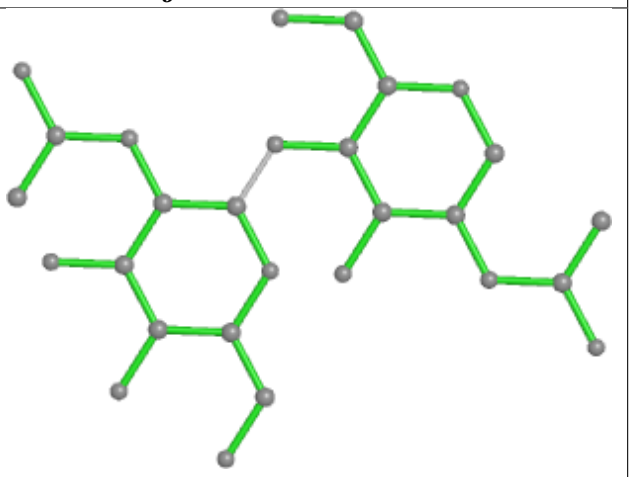

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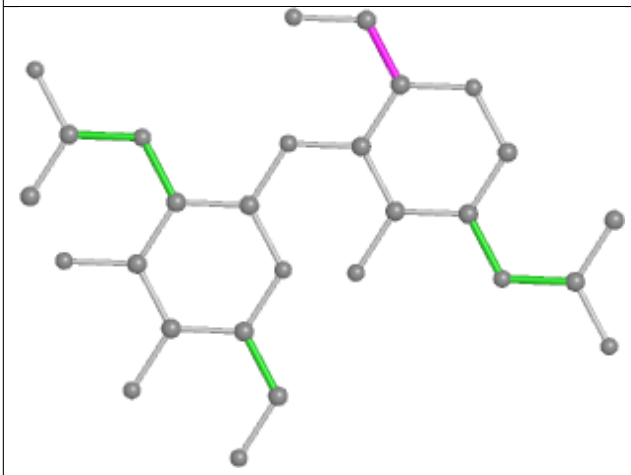

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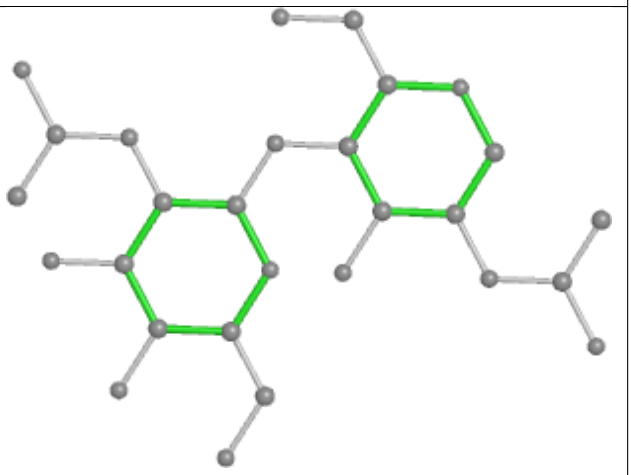
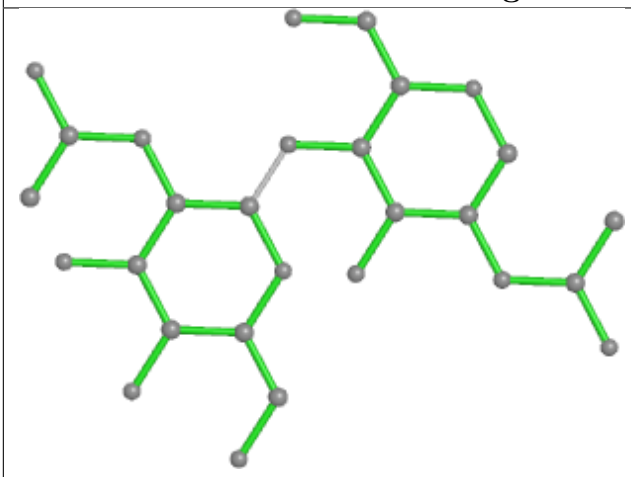


Rings

Oligosaccharide Chain l



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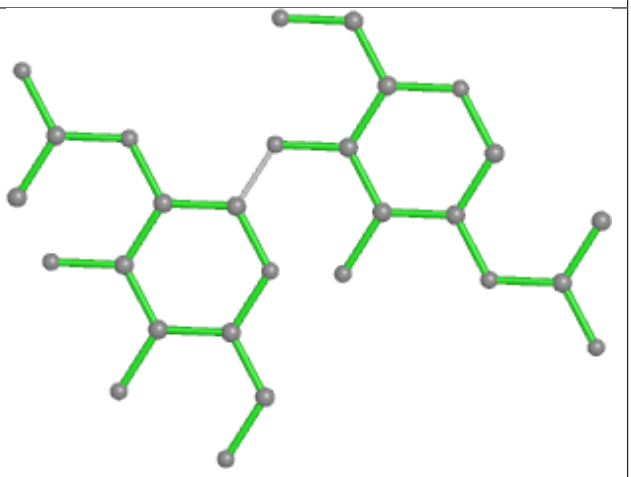
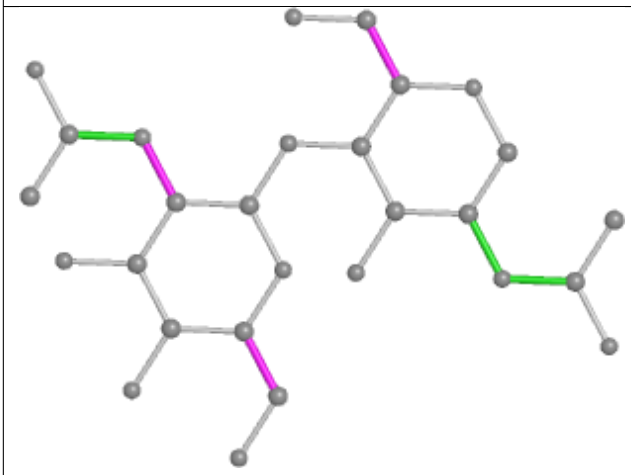


Bond angles



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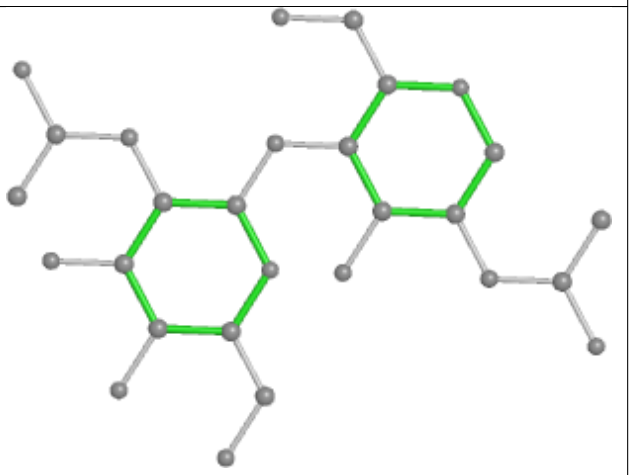
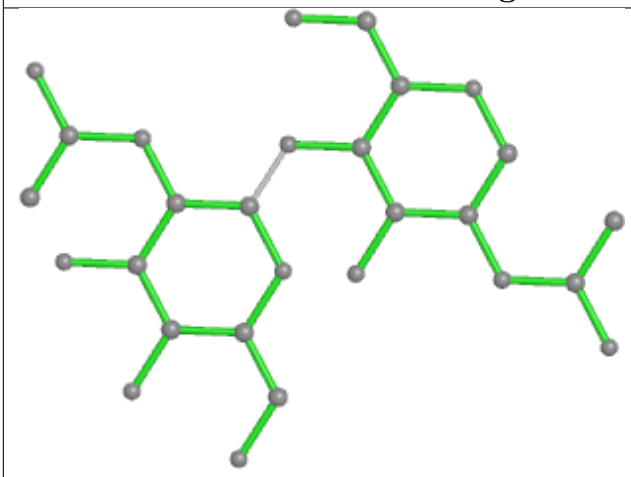


Rings

Oligosaccharide Chain o



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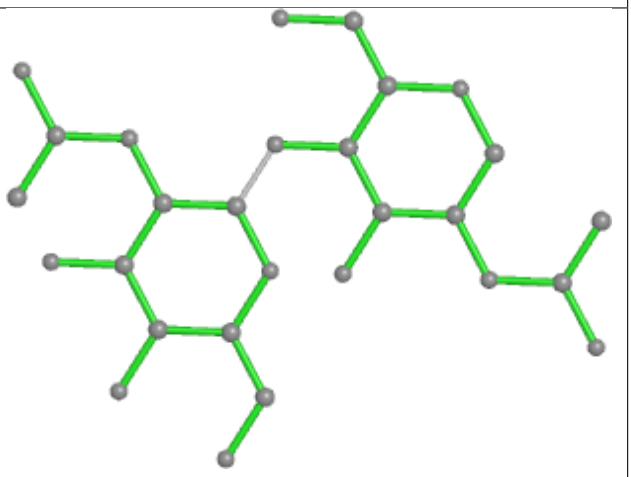
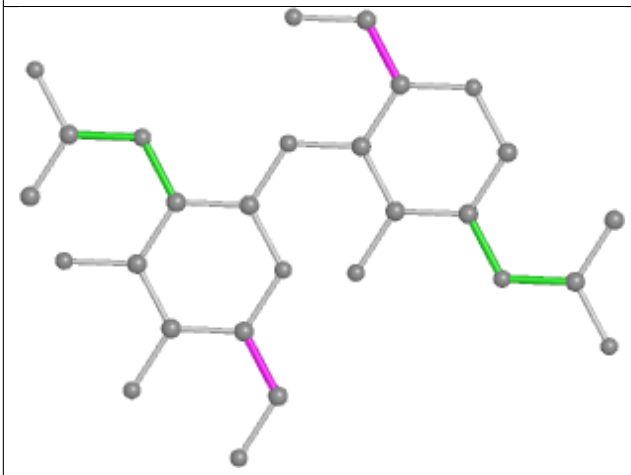


Bond angles



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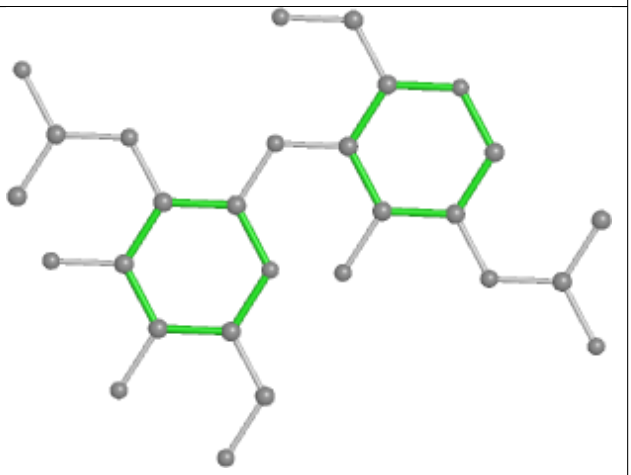
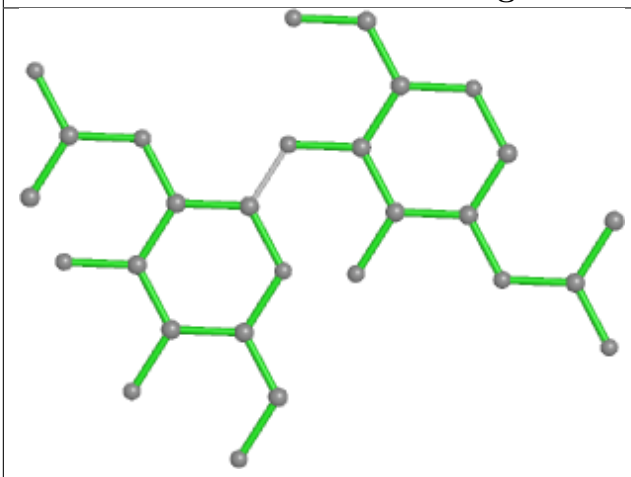


Rings

Oligosaccharide Chain p



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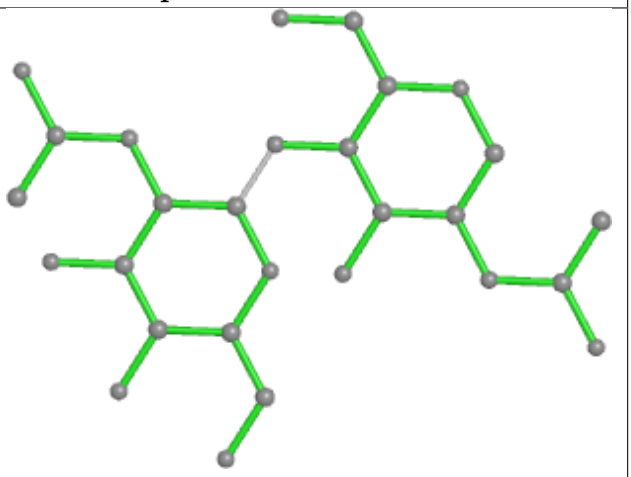

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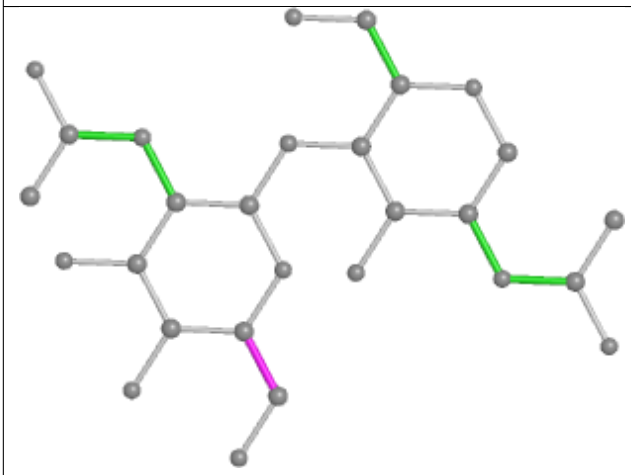

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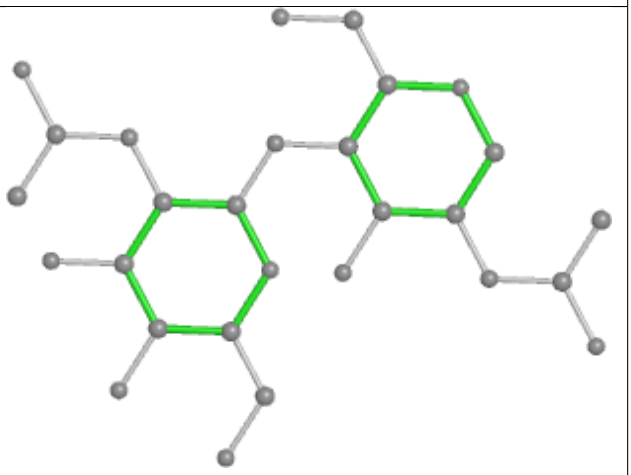
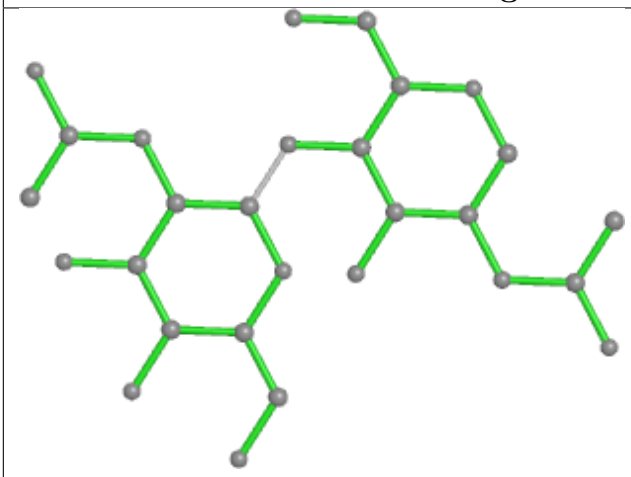


Rings

Oligosaccharide Chain r



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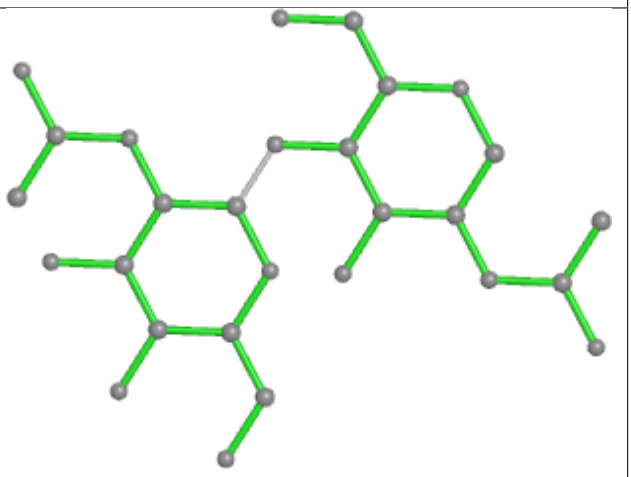
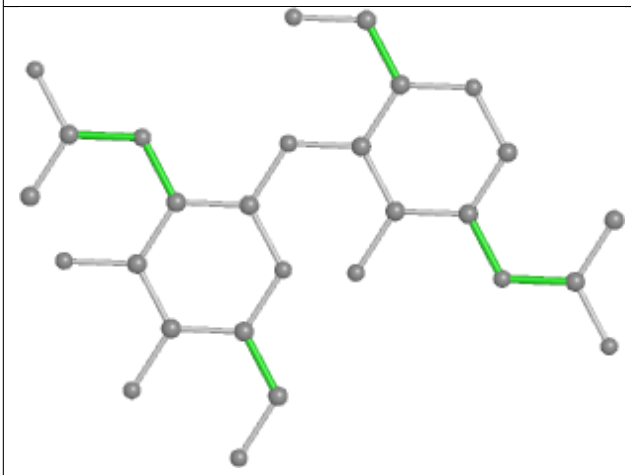


Bond angles



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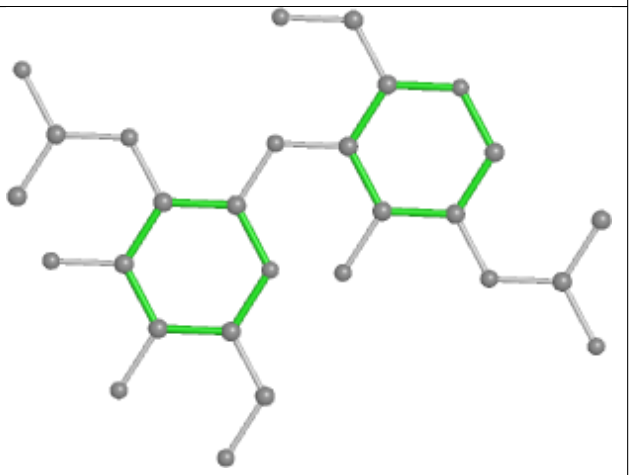
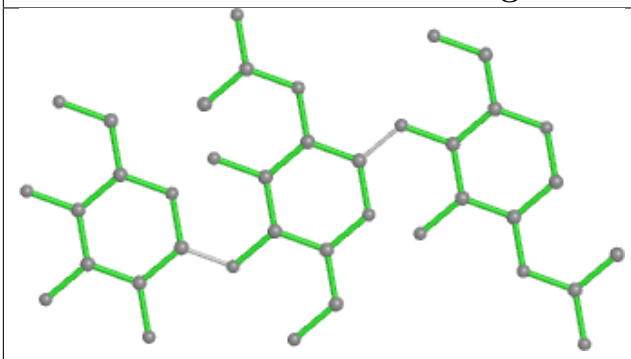


Rings

Oligosaccharide Chain I



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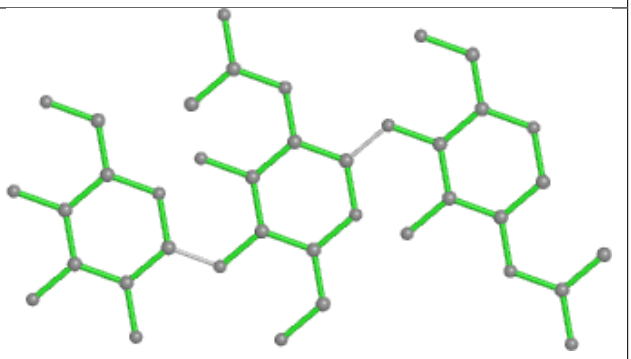

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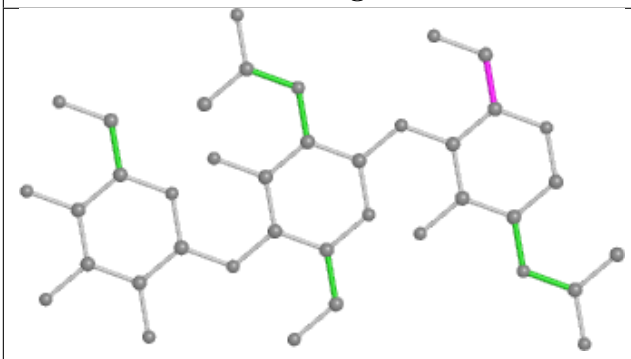

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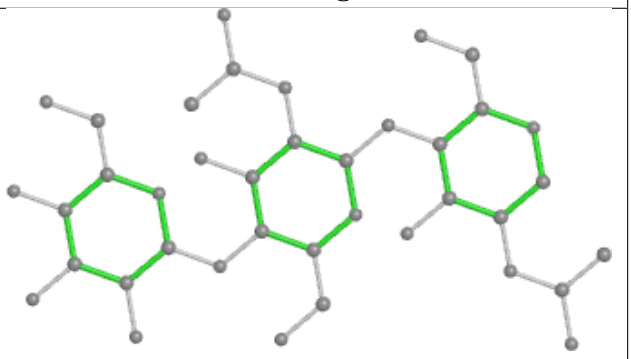
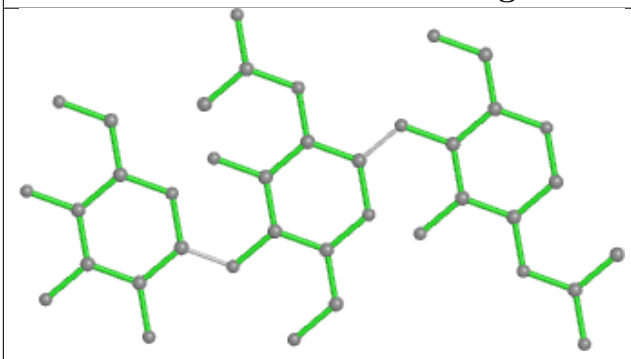


Rings

Oligosaccharide Chain J



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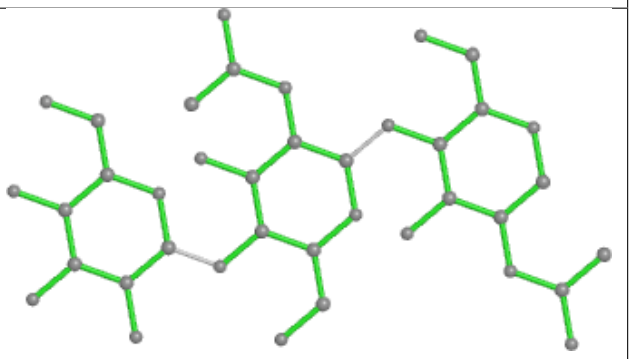
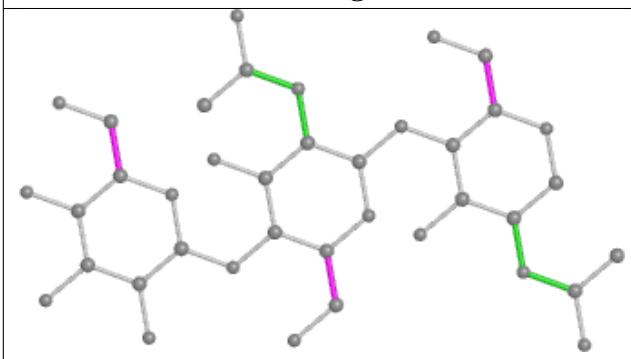
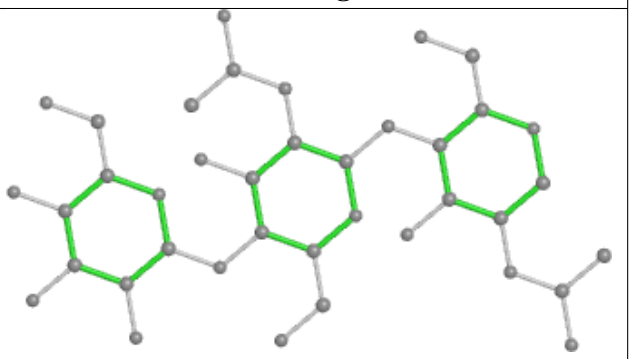


Bond angles

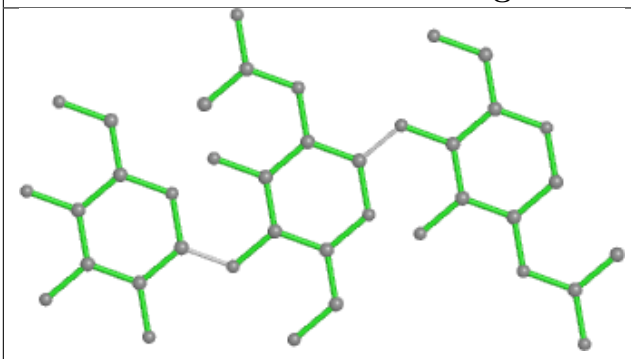


Torsions



Rings

Oligosaccharide Chain Y



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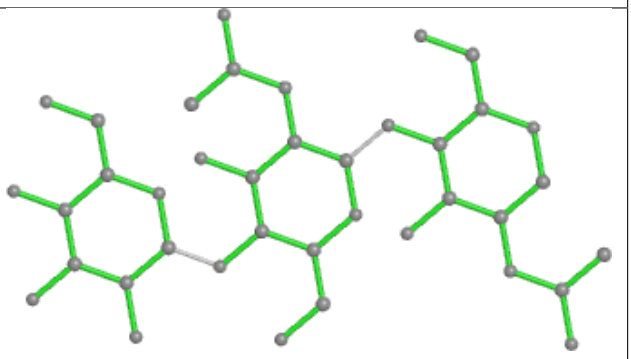
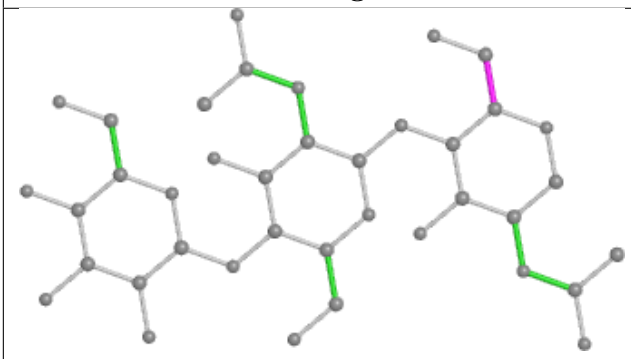
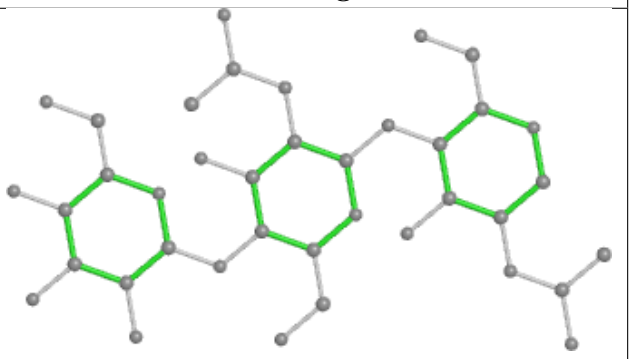


Bond angles

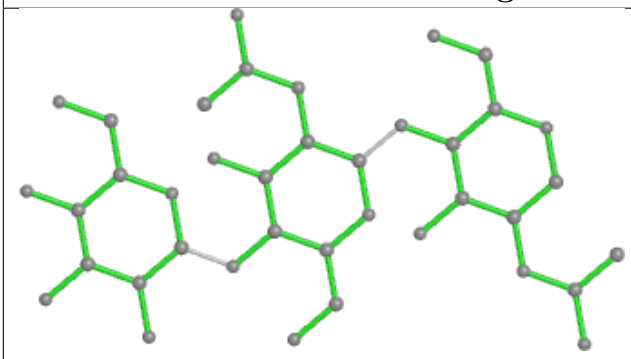


Torsions



Rings

Oligosaccharide Chain Z



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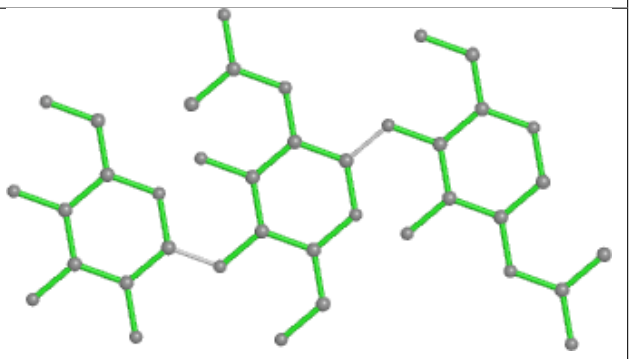
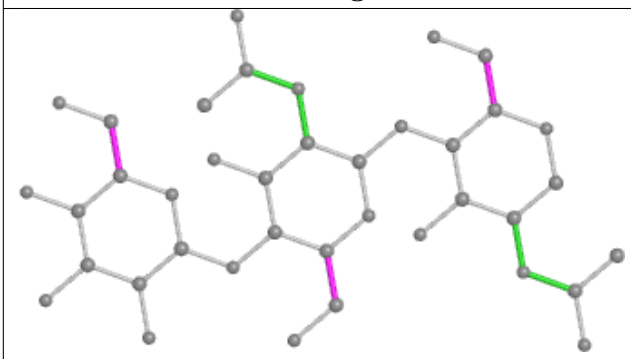
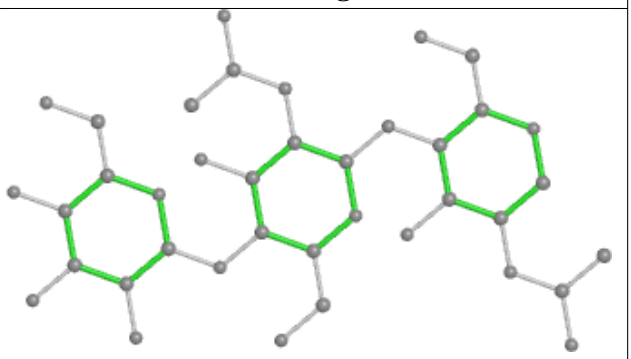


Bond angles

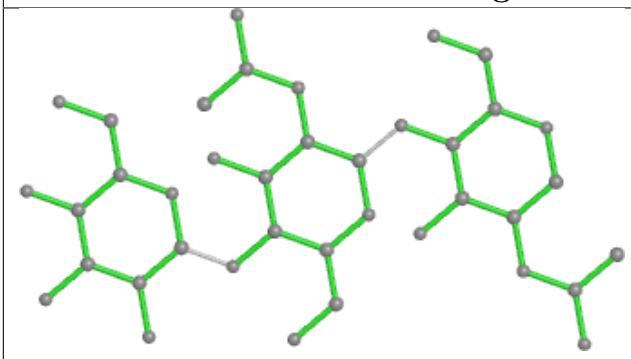


Torsions

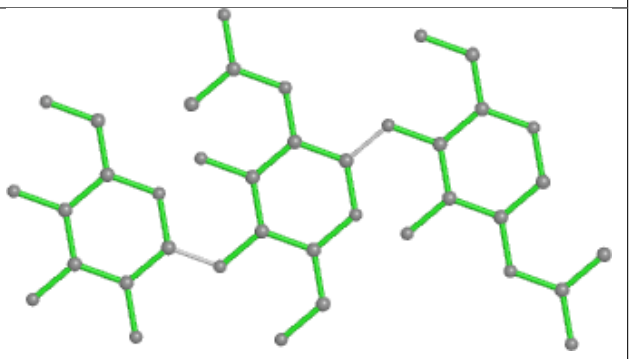


Rings

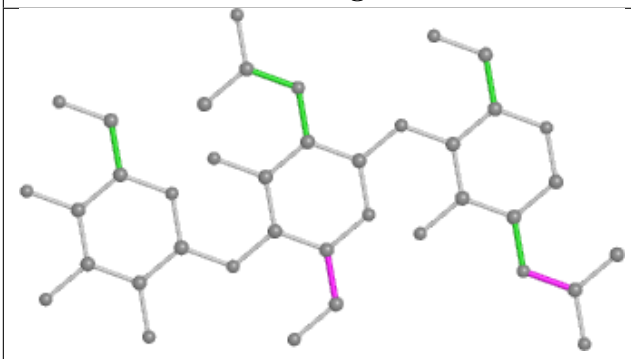
Oligosaccharide Chain m



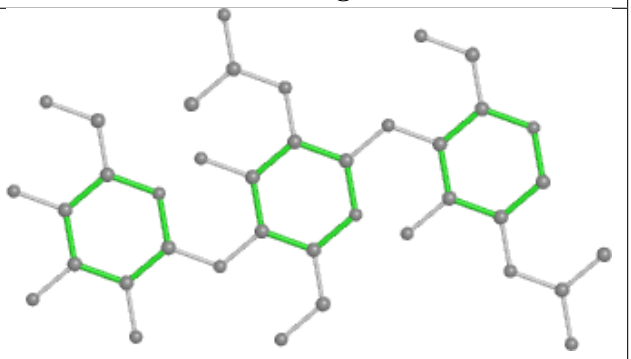
Bond lengths



Bond angles

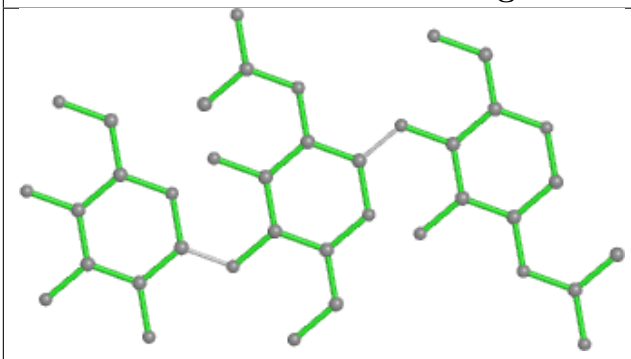


Torsions

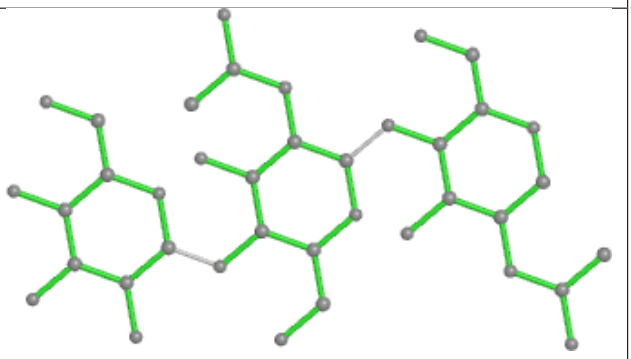


Rings

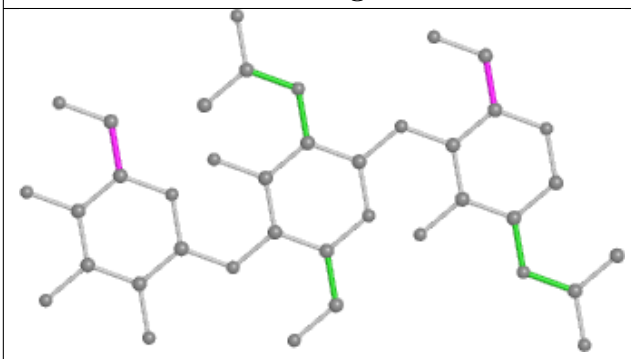
Oligosaccharide Chain n



Bond lengths



Bond angles



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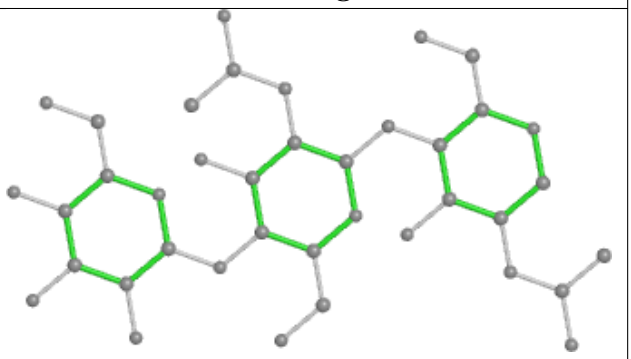
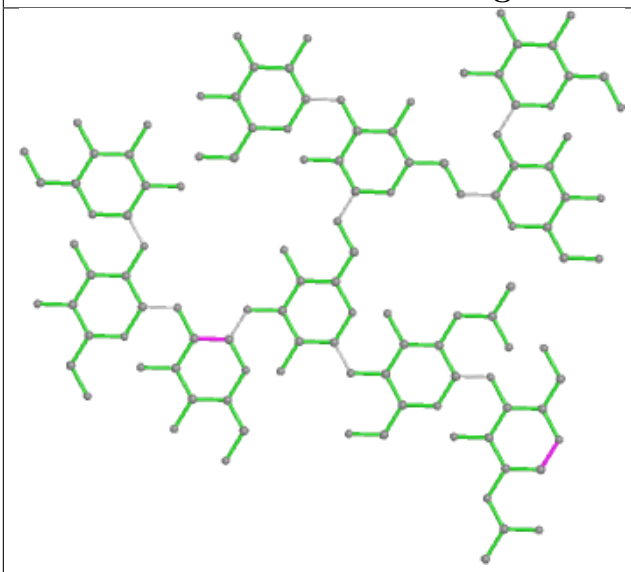
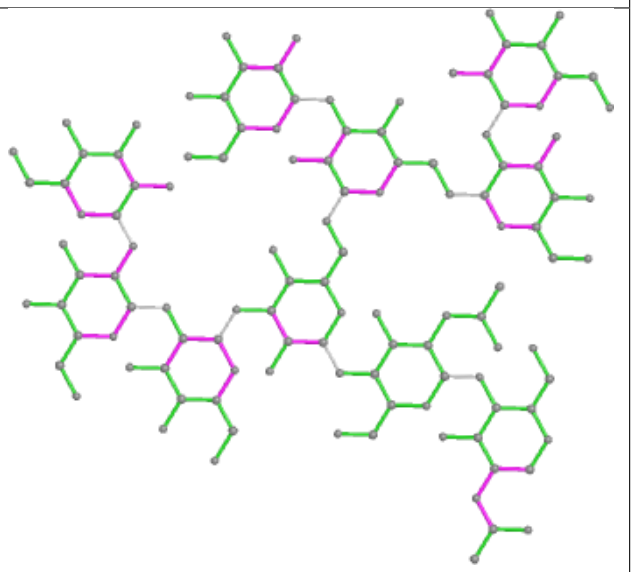


Rings

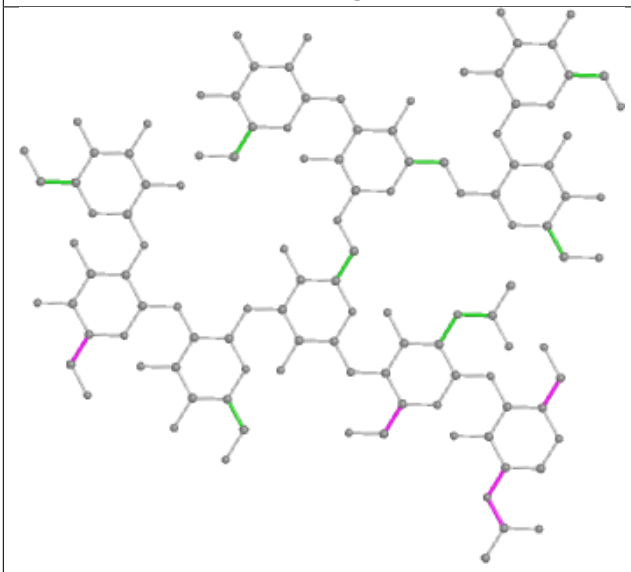
Oligosaccharide Chain N



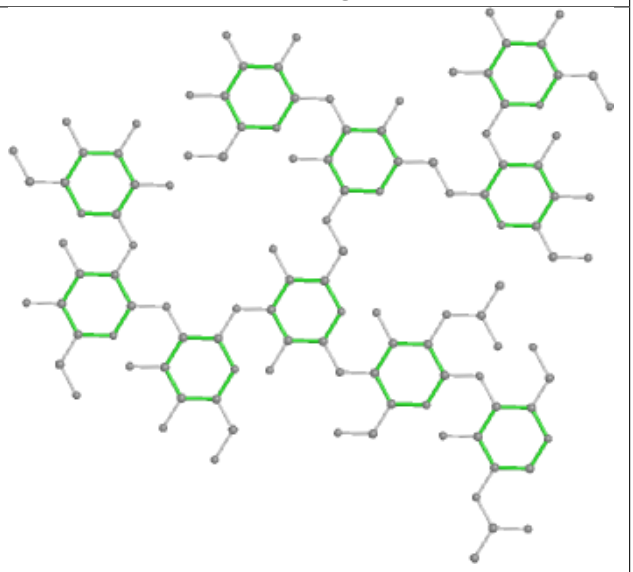
Bond lengths



Bond angles

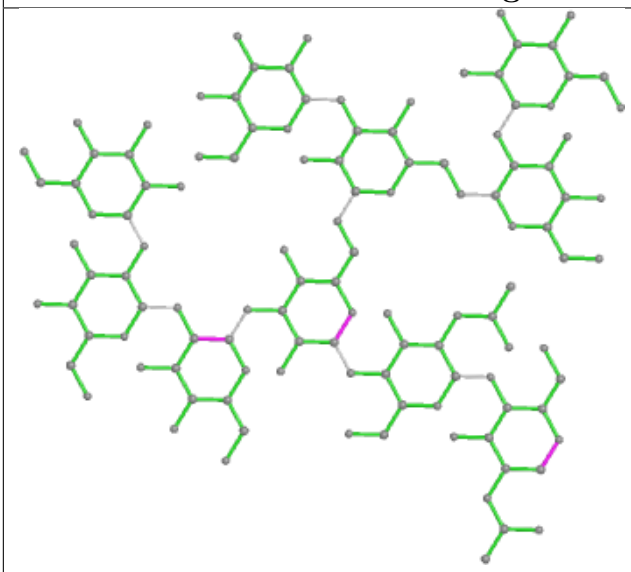


Torsions

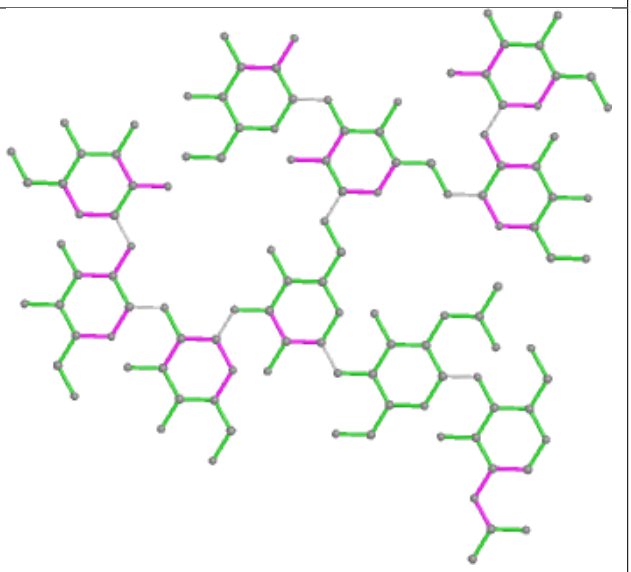


Rings

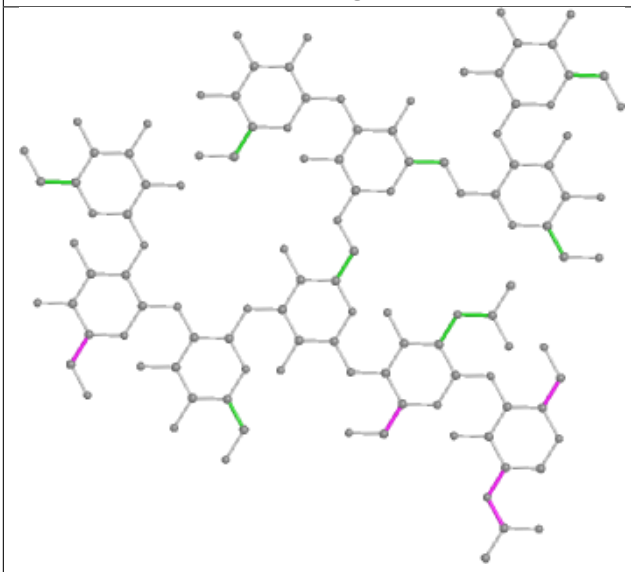
Oligosaccharide Chain i



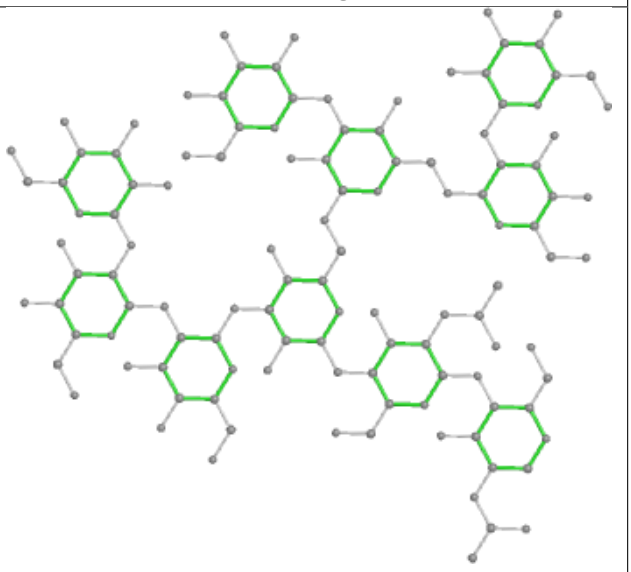
Bond lengths



Bond angles

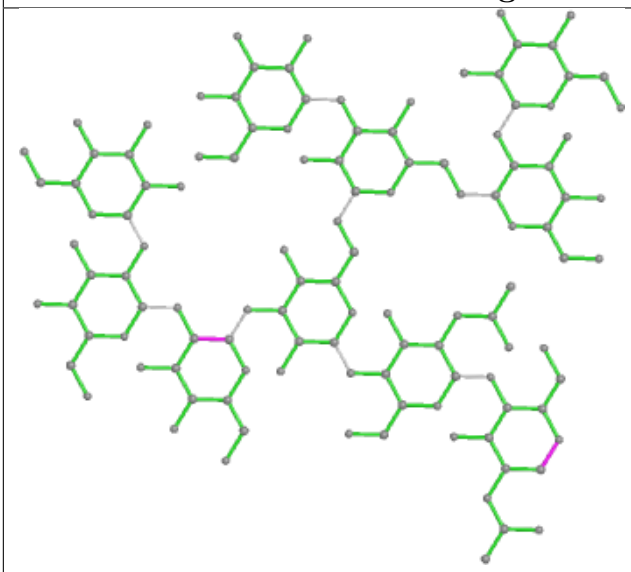


Torsions

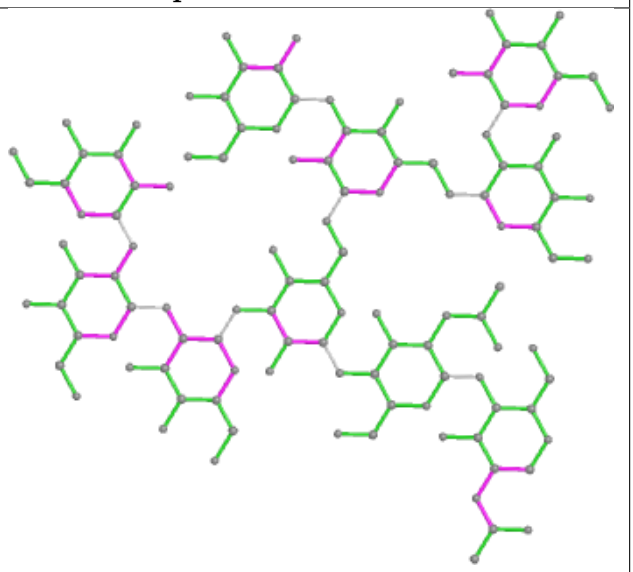


Rings

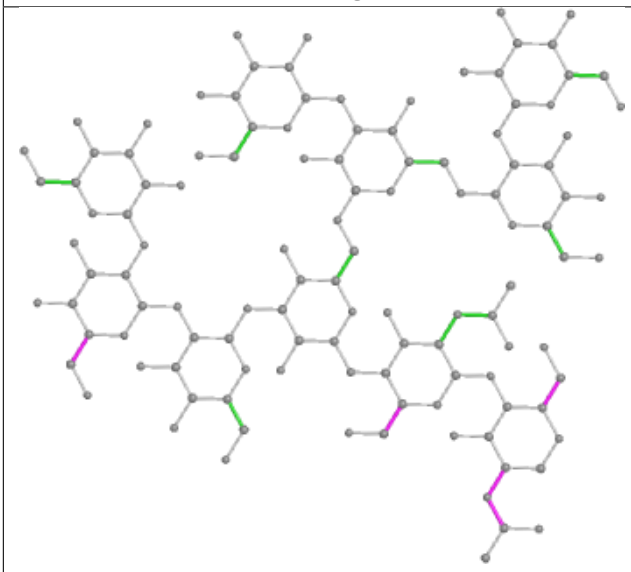
Oligosaccharide Chain q



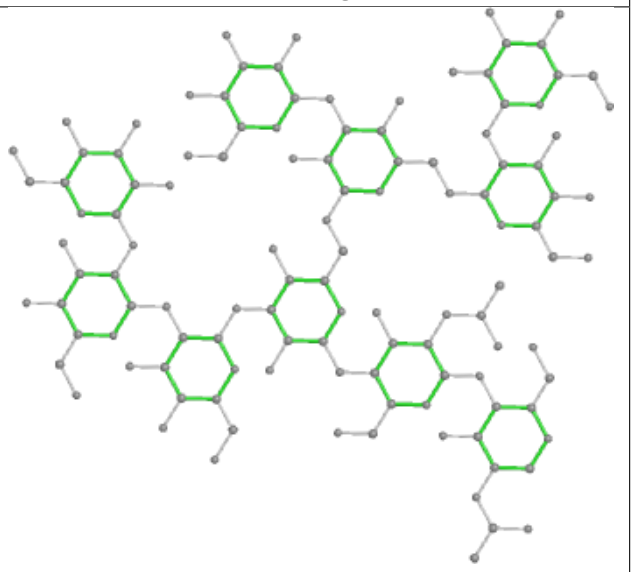
Bond lengths



Bond angles

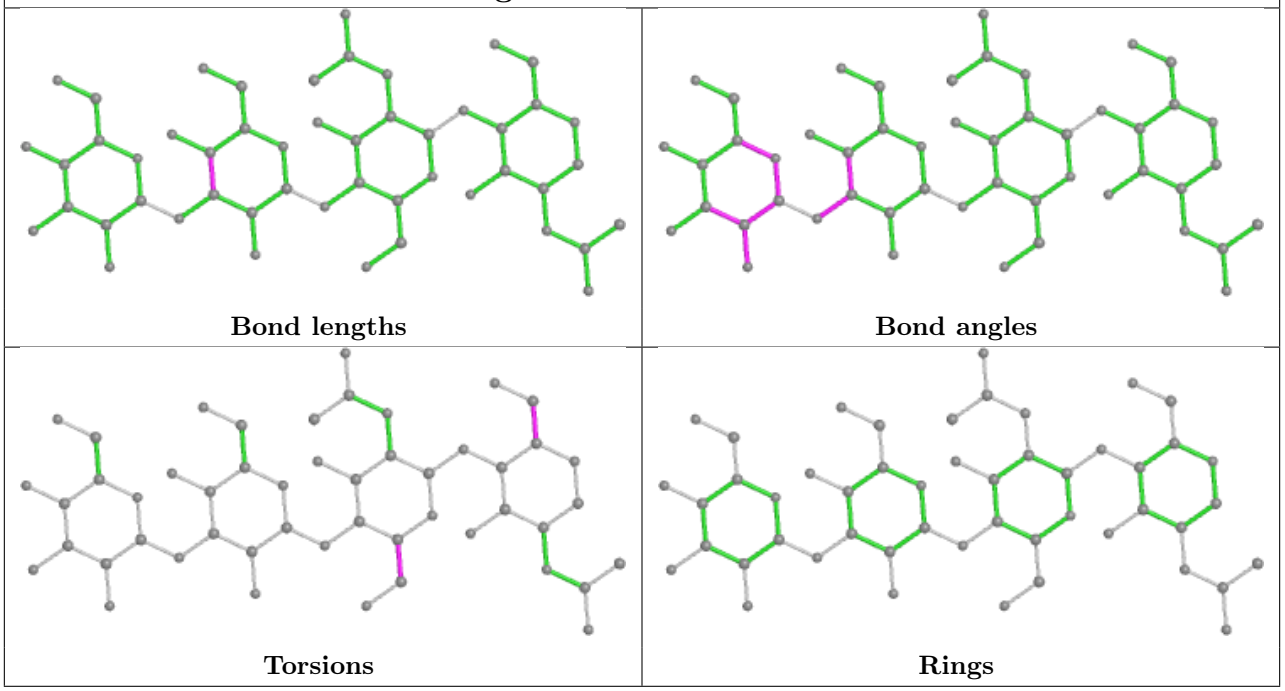


Torsions

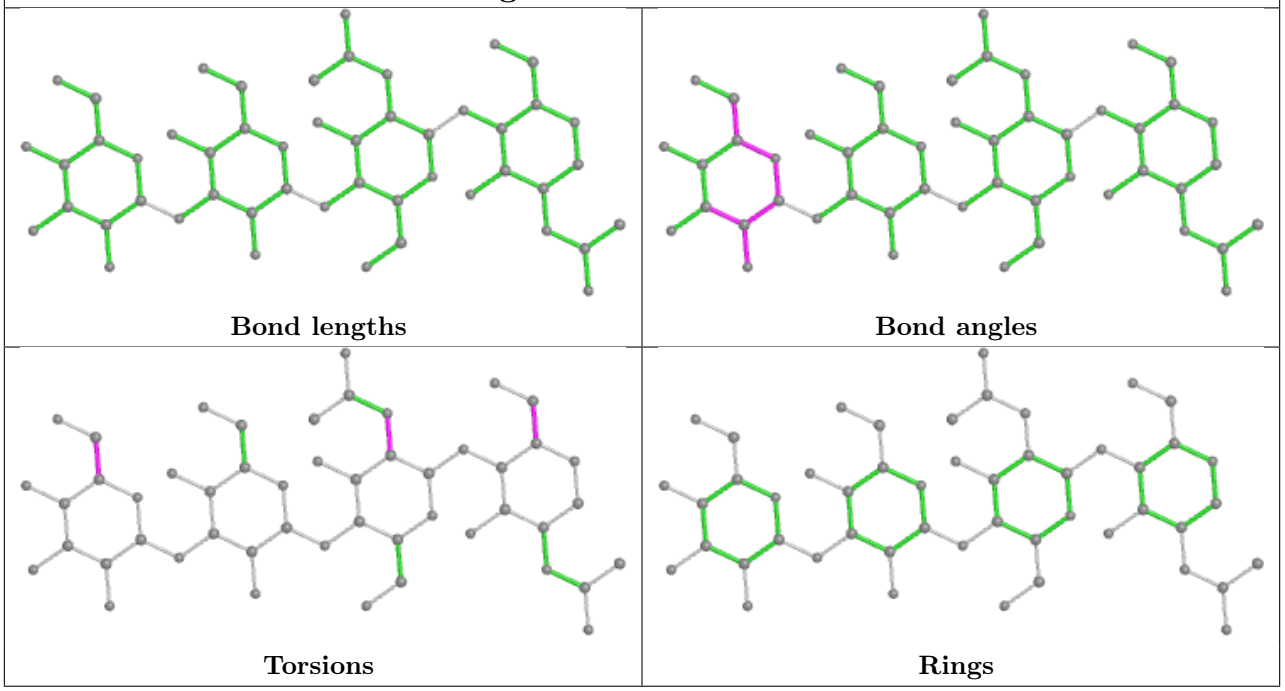


Rings

Oligosaccharide Chain V



Oligosaccharide Chain k



5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
11	NAG	G	605	4	14,14,15	0.27	0	17,19,21	0.44	0
11	NAG	e	607	4	14,14,15	0.19	0	17,19,21	0.43	0
11	NAG	R	604	4	14,14,15	0.28	0	17,19,21	0.44	0
11	NAG	G	603	4	14,14,15	0.28	0	17,19,21	0.41	0
11	NAG	B	701	1	14,14,15	0.27	0	17,19,21	0.46	0
11	NAG	e	604	4	14,14,15	0.21	0	17,19,21	0.49	0
11	NAG	H	703	1	14,14,15	0.18	0	17,19,21	0.42	0
11	NAG	R	601	4	14,14,15	0.39	0	17,19,21	0.49	0
11	NAG	G	608	4	14,14,15	0.43	0	17,19,21	0.56	0
11	NAG	a	701	1	14,14,15	0.27	0	17,19,21	0.47	0
11	NAG	e	603	4	14,14,15	0.27	0	17,19,21	0.41	0
11	NAG	e	606	4	14,14,15	0.31	0	17,19,21	0.49	0
11	NAG	G	607	4	14,14,15	0.21	0	17,19,21	0.44	0
11	NAG	R	602	4	14,14,15	0.26	0	17,19,21	0.41	0
11	NAG	R	605	4	14,14,15	0.28	0	17,19,21	0.49	0
11	NAG	B	703	1	14,14,15	0.20	0	17,19,21	0.43	0
11	NAG	e	608	4	14,14,15	0.31	0	17,19,21	0.49	0
11	NAG	e	605	4	14,14,15	0.25	0	17,19,21	0.47	0
11	NAG	R	603	4	14,14,15	0.23	0	17,19,21	0.50	0
11	NAG	a	702	1	14,14,15	0.26	0	17,19,21	0.40	0
11	NAG	G	606	4	14,14,15	0.30	0	17,19,21	0.48	0
11	NAG	R	606	4	14,14,15	0.20	0	17,19,21	0.43	0
11	NAG	G	602	4	14,14,15	0.30	0	17,19,21	0.47	0
11	NAG	G	604	4	14,14,15	0.24	0	17,19,21	0.47	0
11	NAG	H	701	1	14,14,15	0.26	0	17,19,21	0.47	0
11	NAG	G	601	4	14,14,15	0.40	0	17,19,21	0.48	0
11	NAG	a	703	1	14,14,15	0.22	0	17,19,21	0.42	0
11	NAG	e	602	4	14,14,15	0.27	0	17,19,21	0.47	0
11	NAG	H	702	1	14,14,15	0.28	0	17,19,21	1.51	2 (11%)
11	NAG	B	702	1	14,14,15	0.20	0	17,19,21	0.53	0
11	NAG	e	601	4	14,14,15	0.39	0	17,19,21	0.45	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
11	NAG	G	605	4	-	2/6/23/26	0/1/1/1
11	NAG	e	607	4	-	0/6/23/26	0/1/1/1
11	NAG	R	604	4	-	2/6/23/26	0/1/1/1
11	NAG	G	603	4	-	2/6/23/26	0/1/1/1
11	NAG	B	701	1	-	2/6/23/26	0/1/1/1
11	NAG	e	604	4	-	2/6/23/26	0/1/1/1
11	NAG	H	703	1	-	2/6/23/26	0/1/1/1
11	NAG	R	601	4	-	2/6/23/26	0/1/1/1
11	NAG	G	608	4	-	3/6/23/26	0/1/1/1
11	NAG	a	701	1	-	2/6/23/26	0/1/1/1
11	NAG	e	603	4	-	2/6/23/26	0/1/1/1
11	NAG	e	606	4	-	2/6/23/26	0/1/1/1
11	NAG	G	607	4	-	2/6/23/26	0/1/1/1
11	NAG	R	602	4	-	2/6/23/26	0/1/1/1
11	NAG	R	605	4	-	2/6/23/26	0/1/1/1
11	NAG	B	703	1	-	2/6/23/26	0/1/1/1
11	NAG	e	608	4	-	2/6/23/26	0/1/1/1
11	NAG	e	605	4	-	2/6/23/26	0/1/1/1
11	NAG	R	603	4	-	2/6/23/26	0/1/1/1
11	NAG	a	702	1	-	1/6/23/26	0/1/1/1
11	NAG	G	606	4	-	2/6/23/26	0/1/1/1
11	NAG	R	606	4	-	0/6/23/26	0/1/1/1
11	NAG	G	602	4	-	2/6/23/26	0/1/1/1
11	NAG	G	604	4	-	2/6/23/26	0/1/1/1
11	NAG	H	701	1	-	2/6/23/26	0/1/1/1
11	NAG	G	601	4	-	2/6/23/26	0/1/1/1
11	NAG	a	703	1	-	2/6/23/26	0/1/1/1
11	NAG	e	602	4	-	2/6/23/26	0/1/1/1
11	NAG	H	702	1	-	4/6/23/26	0/1/1/1
11	NAG	B	702	1	-	2/6/23/26	0/1/1/1
11	NAG	e	601	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	702	NAG	C2-N2-C7	5.02	130.05	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	702	NAG	C1-C2-N2	2.85	115.36	110.49

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	603	NAG	O5-C5-C6-O6
11	G	604	NAG	O5-C5-C6-O6
11	a	701	NAG	O5-C5-C6-O6
11	e	603	NAG	C4-C5-C6-O6
11	G	605	NAG	O5-C5-C6-O6
11	e	602	NAG	C4-C5-C6-O6
11	G	602	NAG	C4-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	R	605	NAG	O5-C5-C6-O6
11	G	603	NAG	C4-C5-C6-O6
11	R	602	NAG	O5-C5-C6-O6
11	e	604	NAG	O5-C5-C6-O6
11	e	605	NAG	O5-C5-C6-O6
11	e	606	NAG	O5-C5-C6-O6
11	G	604	NAG	C4-C5-C6-O6
11	R	603	NAG	C4-C5-C6-O6
11	e	605	NAG	C4-C5-C6-O6
11	R	601	NAG	O5-C5-C6-O6
11	R	605	NAG	C4-C5-C6-O6
11	R	604	NAG	O5-C5-C6-O6
11	e	602	NAG	O5-C5-C6-O6
11	e	608	NAG	O5-C5-C6-O6
11	e	604	NAG	C4-C5-C6-O6
11	G	602	NAG	O5-C5-C6-O6
11	e	603	NAG	O5-C5-C6-O6
11	G	605	NAG	C4-C5-C6-O6
11	G	603	NAG	O5-C5-C6-O6
11	e	606	NAG	C4-C5-C6-O6
11	G	606	NAG	O5-C5-C6-O6
11	a	701	NAG	C4-C5-C6-O6
11	H	701	NAG	O5-C5-C6-O6
11	R	602	NAG	C4-C5-C6-O6
11	a	703	NAG	O5-C5-C6-O6
11	G	608	NAG	C8-C7-N2-C2
11	G	608	NAG	O7-C7-N2-C2
11	H	702	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	H	702	NAG	O7-C7-N2-C2
11	B	701	NAG	C4-C5-C6-O6
11	H	701	NAG	C4-C5-C6-O6
11	R	604	NAG	C4-C5-C6-O6
11	G	606	NAG	C4-C5-C6-O6
11	G	601	NAG	O5-C5-C6-O6
11	G	608	NAG	O5-C5-C6-O6
11	a	703	NAG	C4-C5-C6-O6
11	R	601	NAG	C4-C5-C6-O6
11	e	608	NAG	C4-C5-C6-O6
11	H	702	NAG	C1-C2-N2-C7
11	B	702	NAG	O5-C5-C6-O6
11	e	601	NAG	O5-C5-C6-O6
11	H	702	NAG	O5-C5-C6-O6
11	G	607	NAG	C4-C5-C6-O6
11	a	702	NAG	O5-C5-C6-O6
11	G	607	NAG	O5-C5-C6-O6
11	B	703	NAG	C4-C5-C6-O6
11	B	703	NAG	O5-C5-C6-O6
11	H	703	NAG	C4-C5-C6-O6
11	G	601	NAG	C4-C5-C6-O6
11	H	703	NAG	O5-C5-C6-O6
11	B	702	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

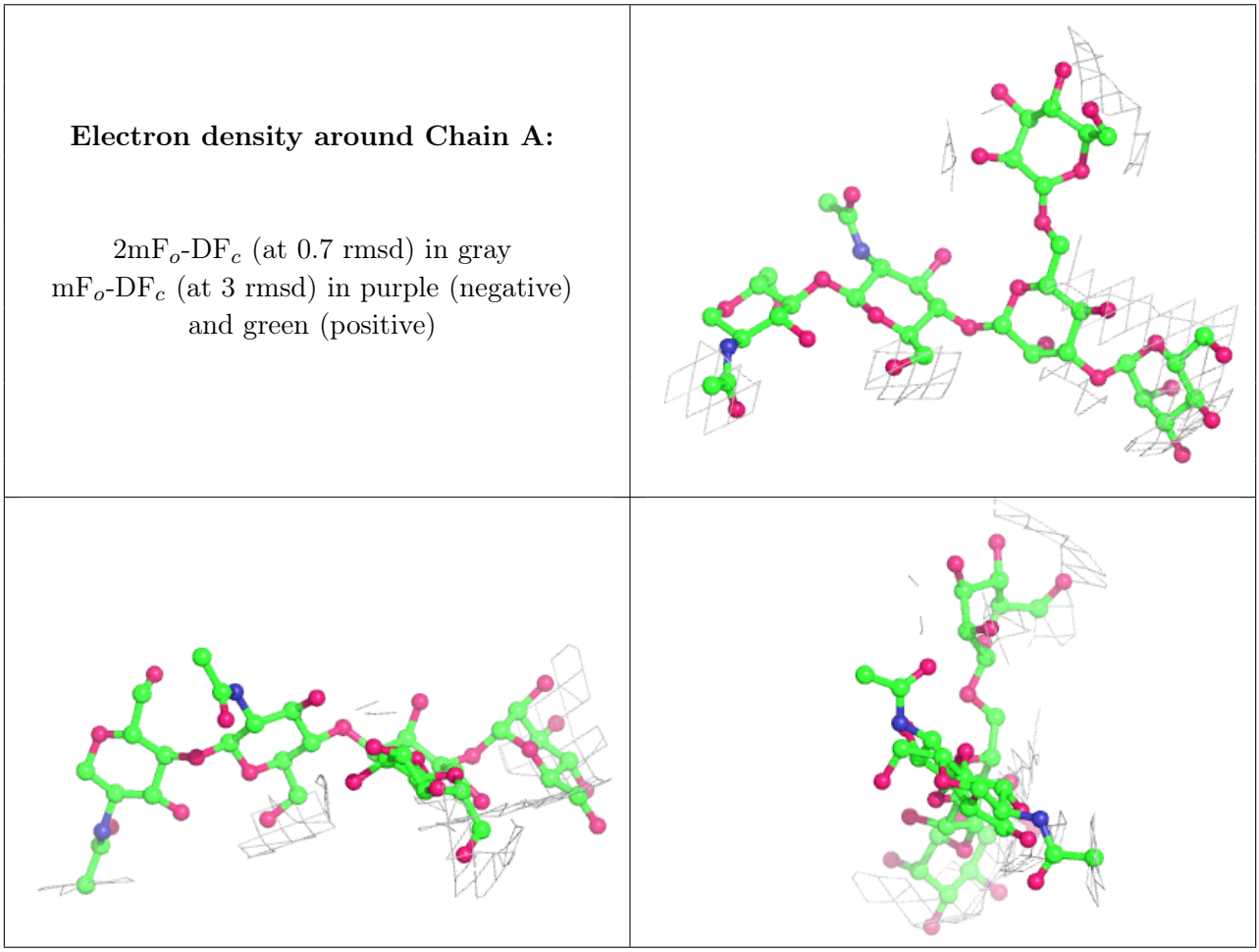
6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

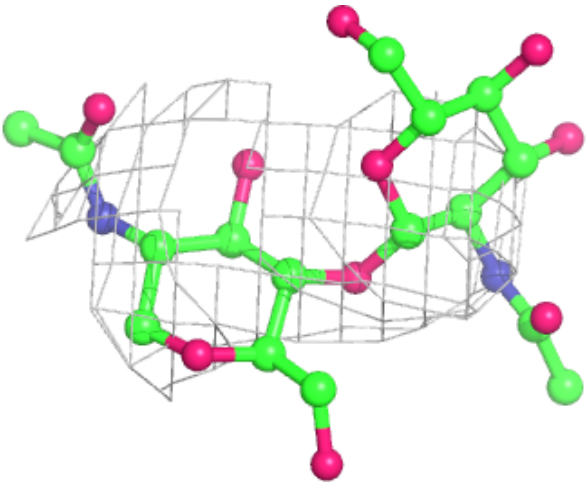
Unable to reproduce the depositors R factor - this section is therefore empty.

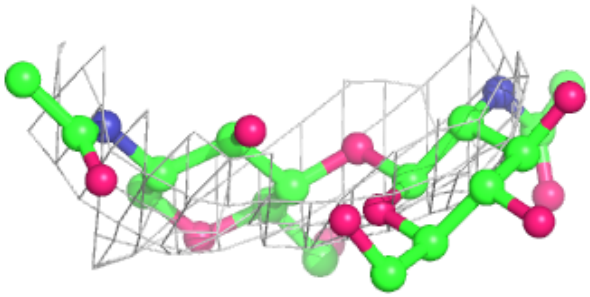
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

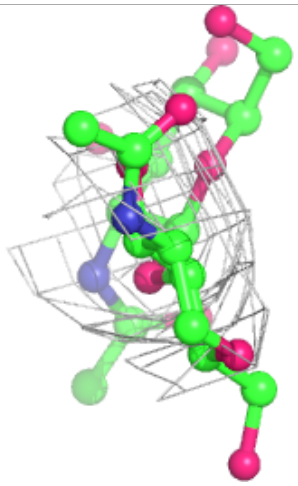


Electron density around Chain F:

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

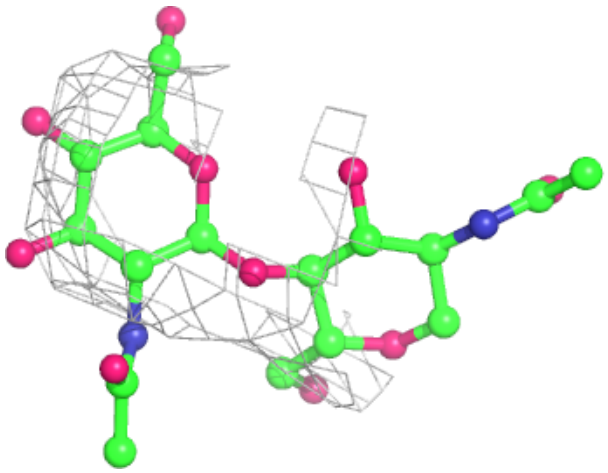


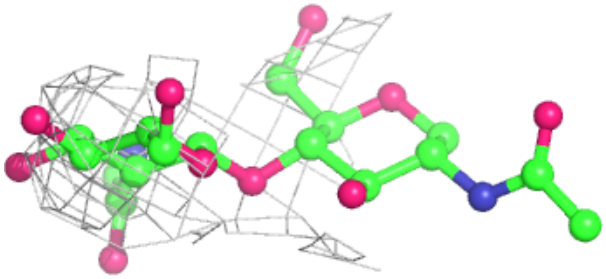


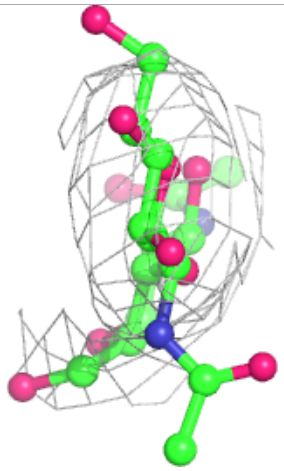


Electron density around Chain K:

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

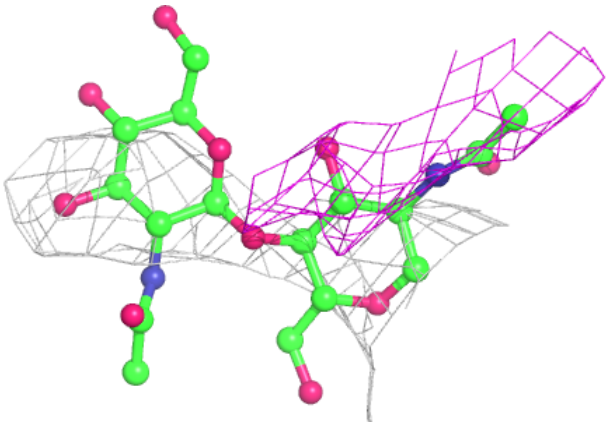


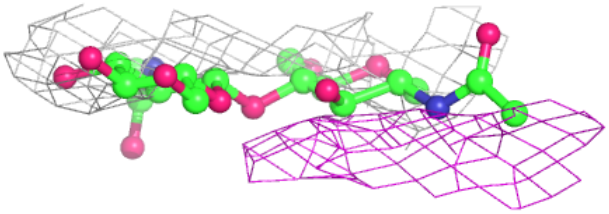


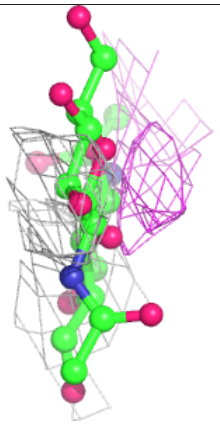


Electron density around Chain M:

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

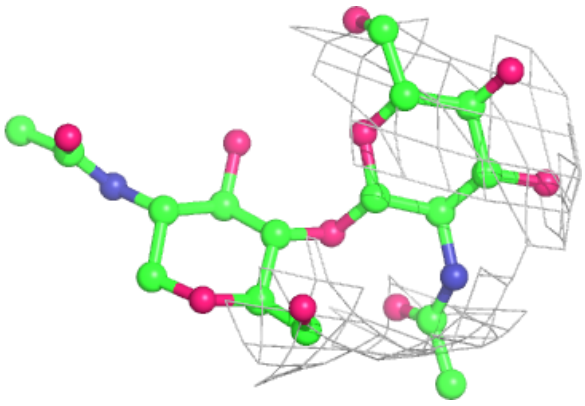


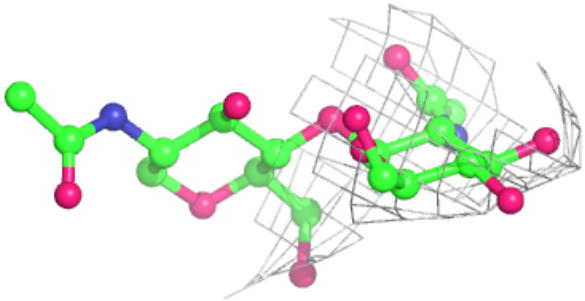


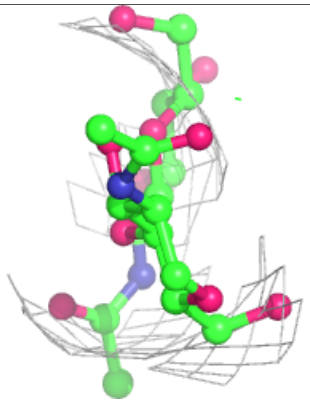


Electron density around Chain T:

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

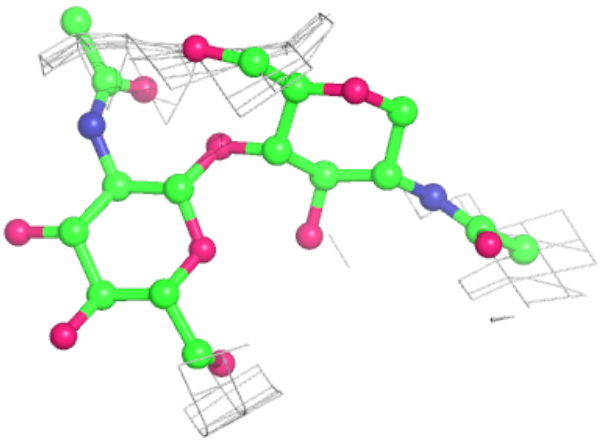


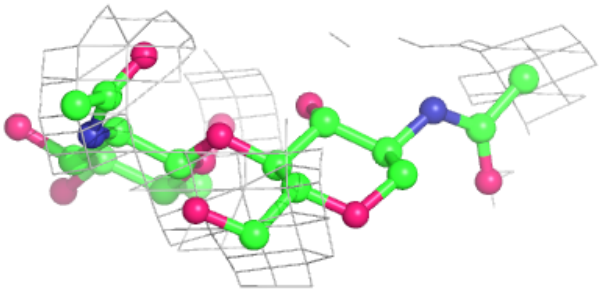


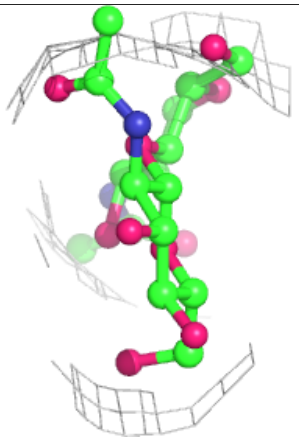


Electron density around Chain U:

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

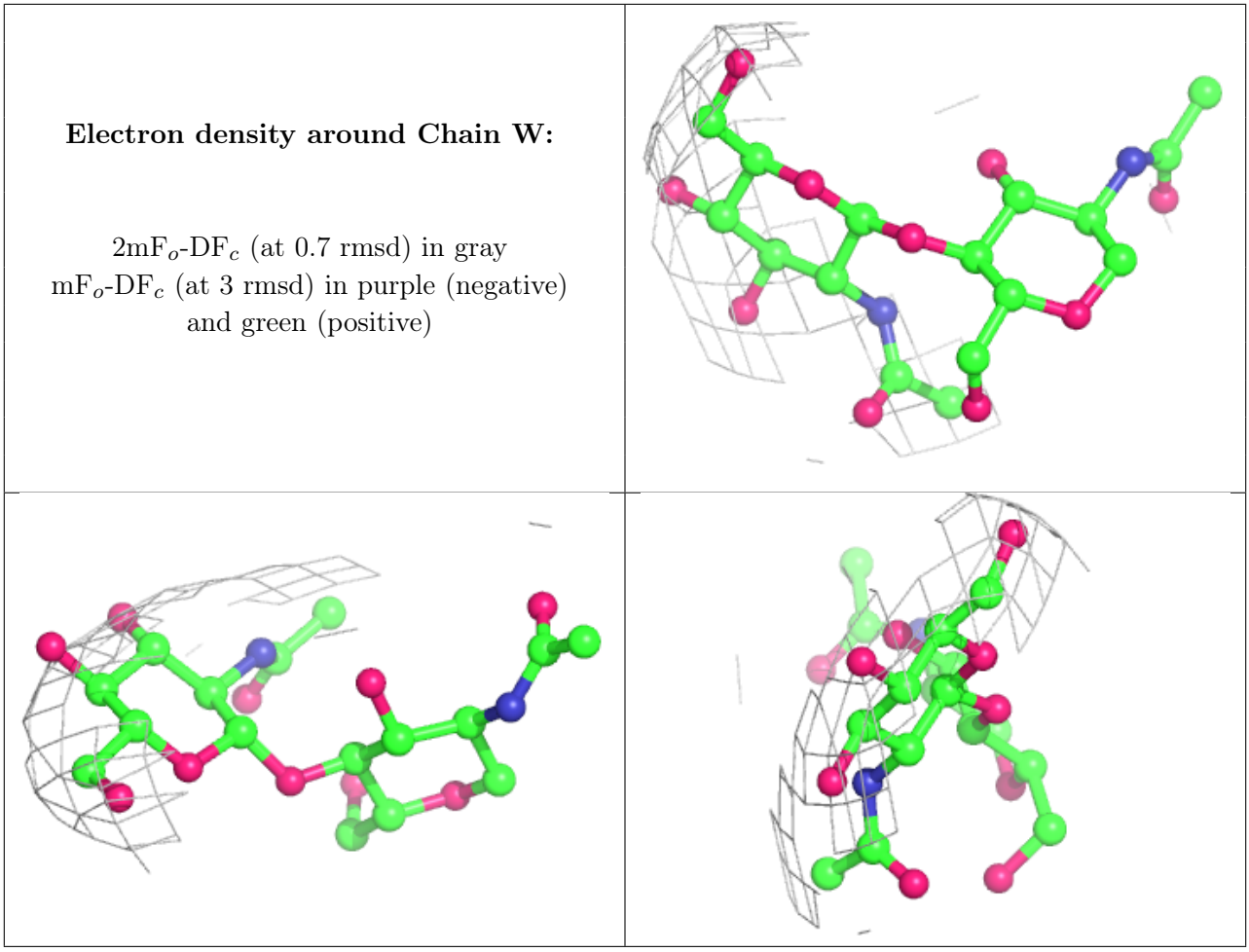






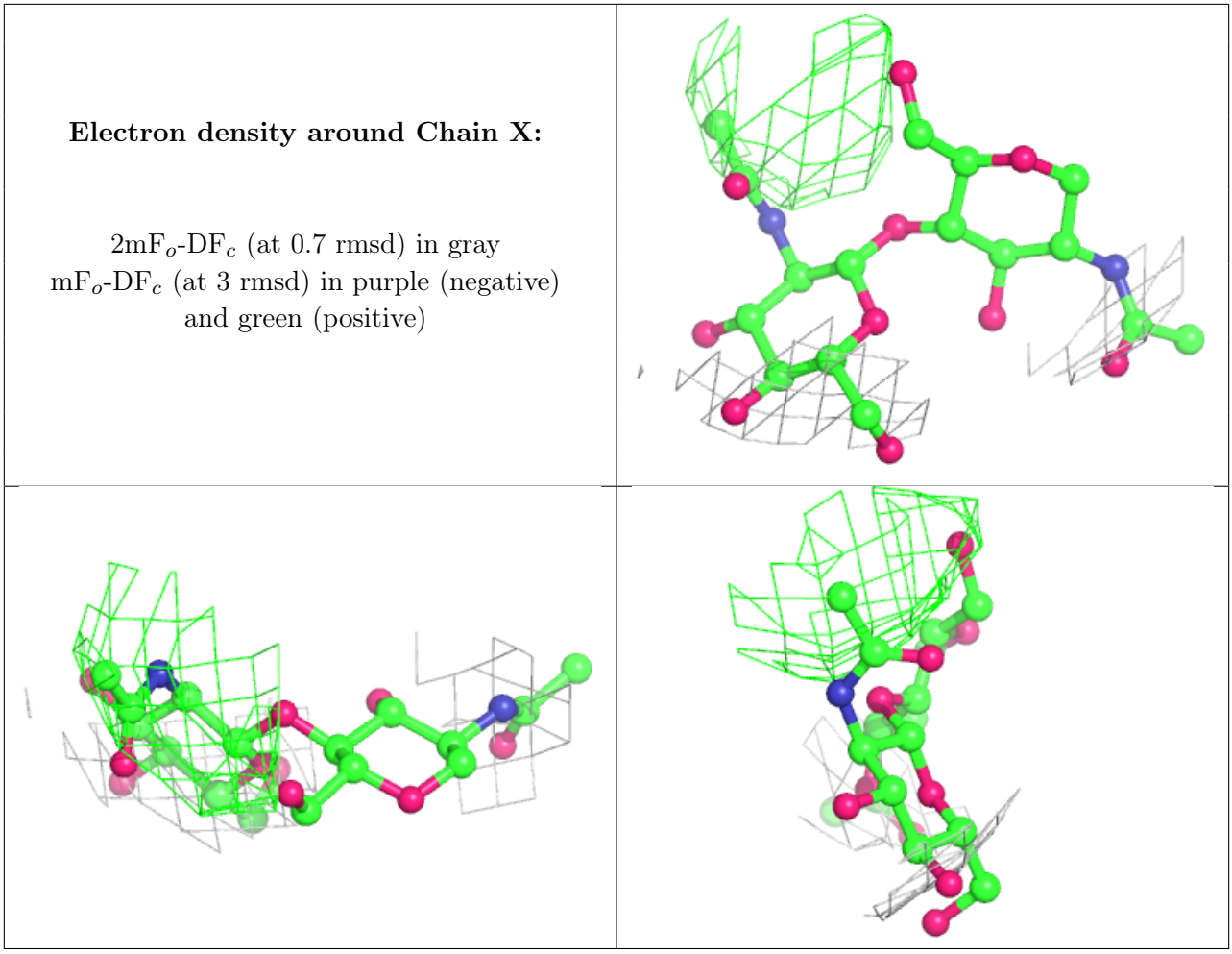
Electron density around Chain W:

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



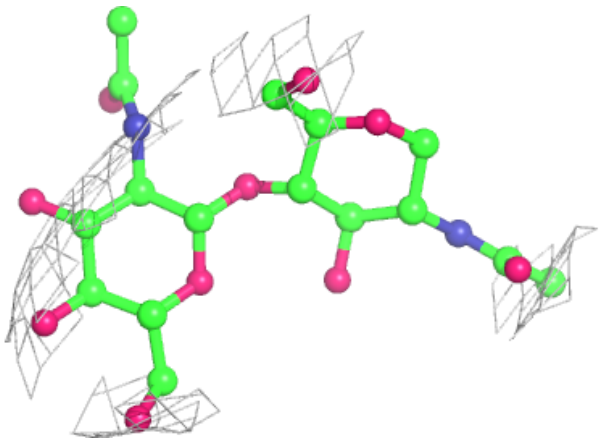
Electron density around Chain X:

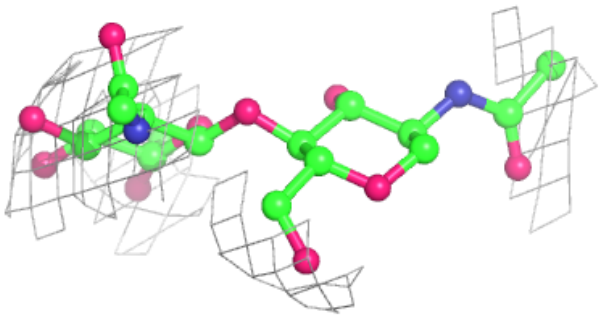
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

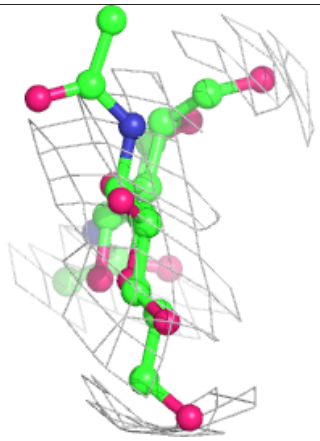


Electron density around Chain g:

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

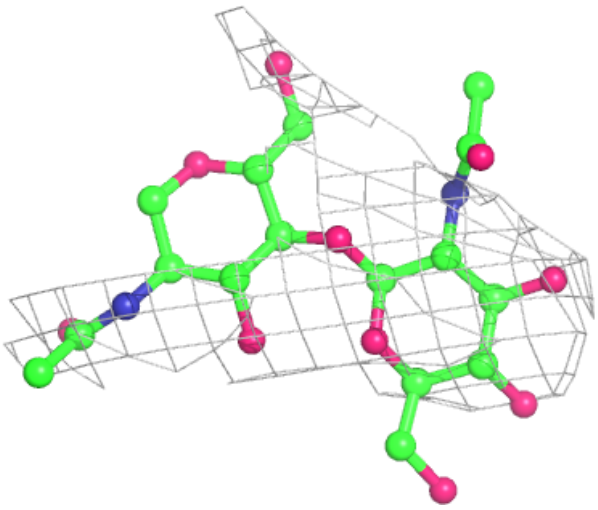


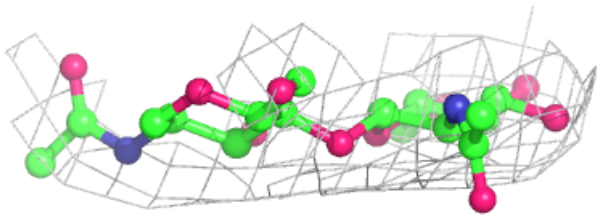


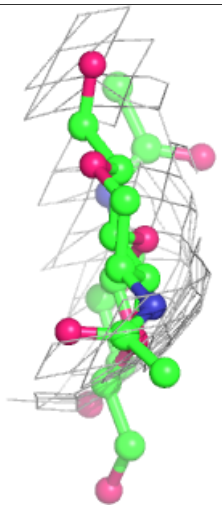


Electron density around Chain h:

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

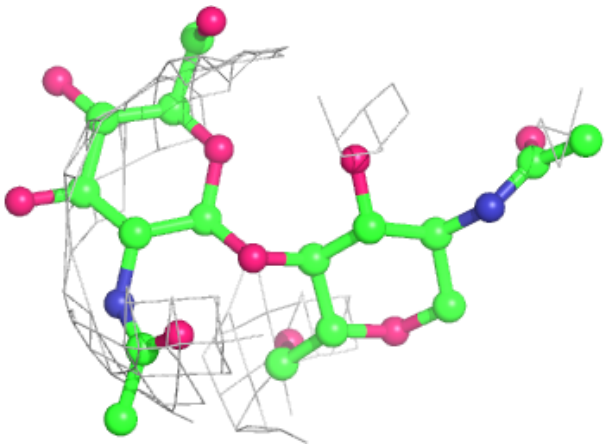


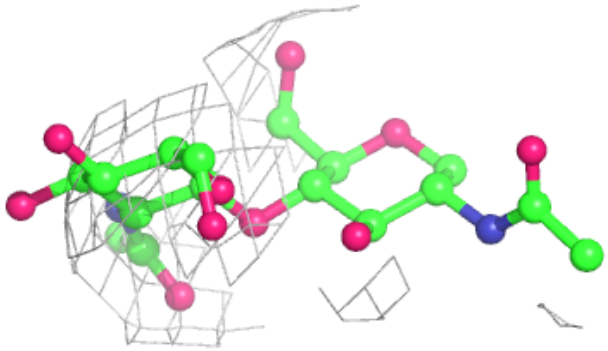


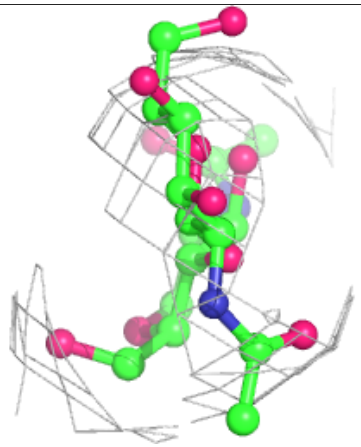


Electron density around Chain j:

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

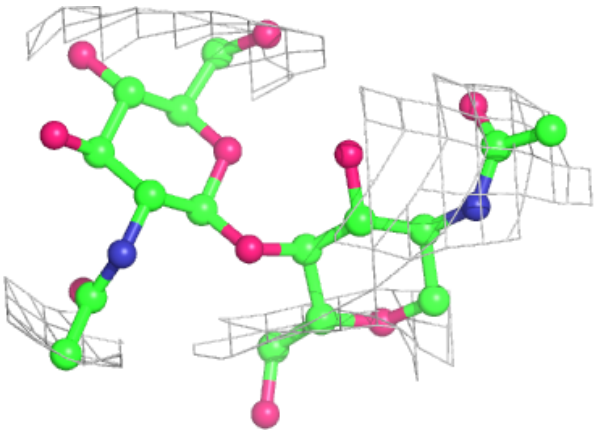


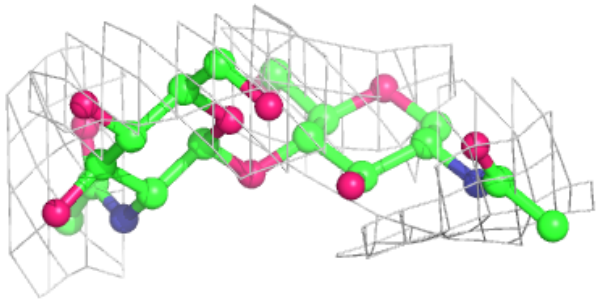


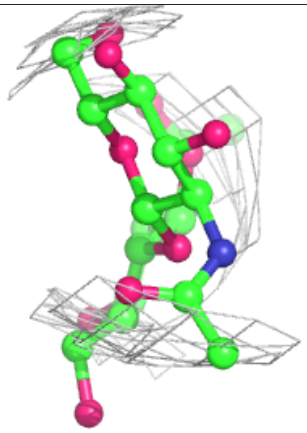


Electron density around Chain l:

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

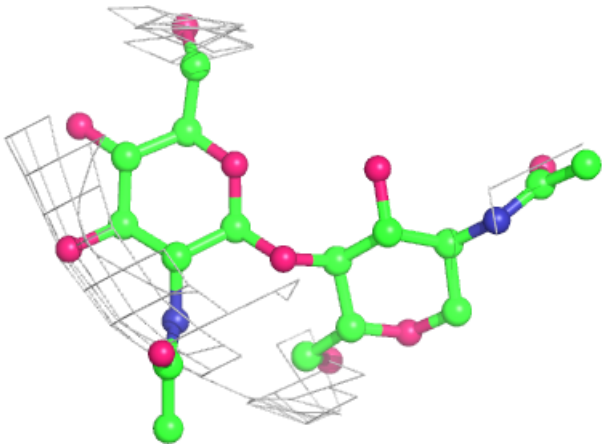


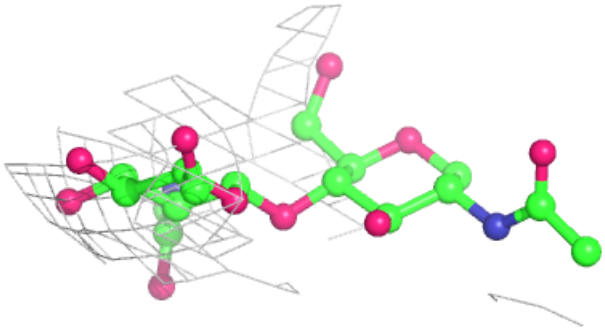


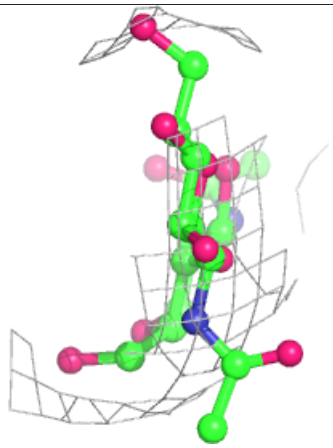


Electron density around Chain o:

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

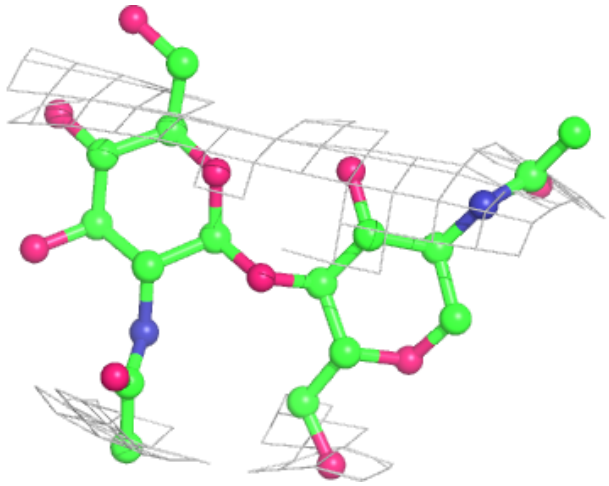


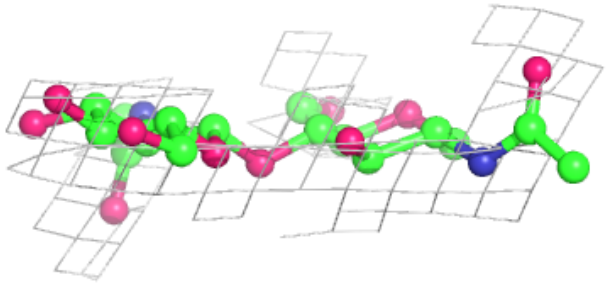


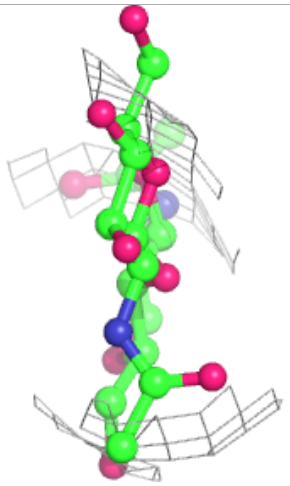


Electron density around Chain p:

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

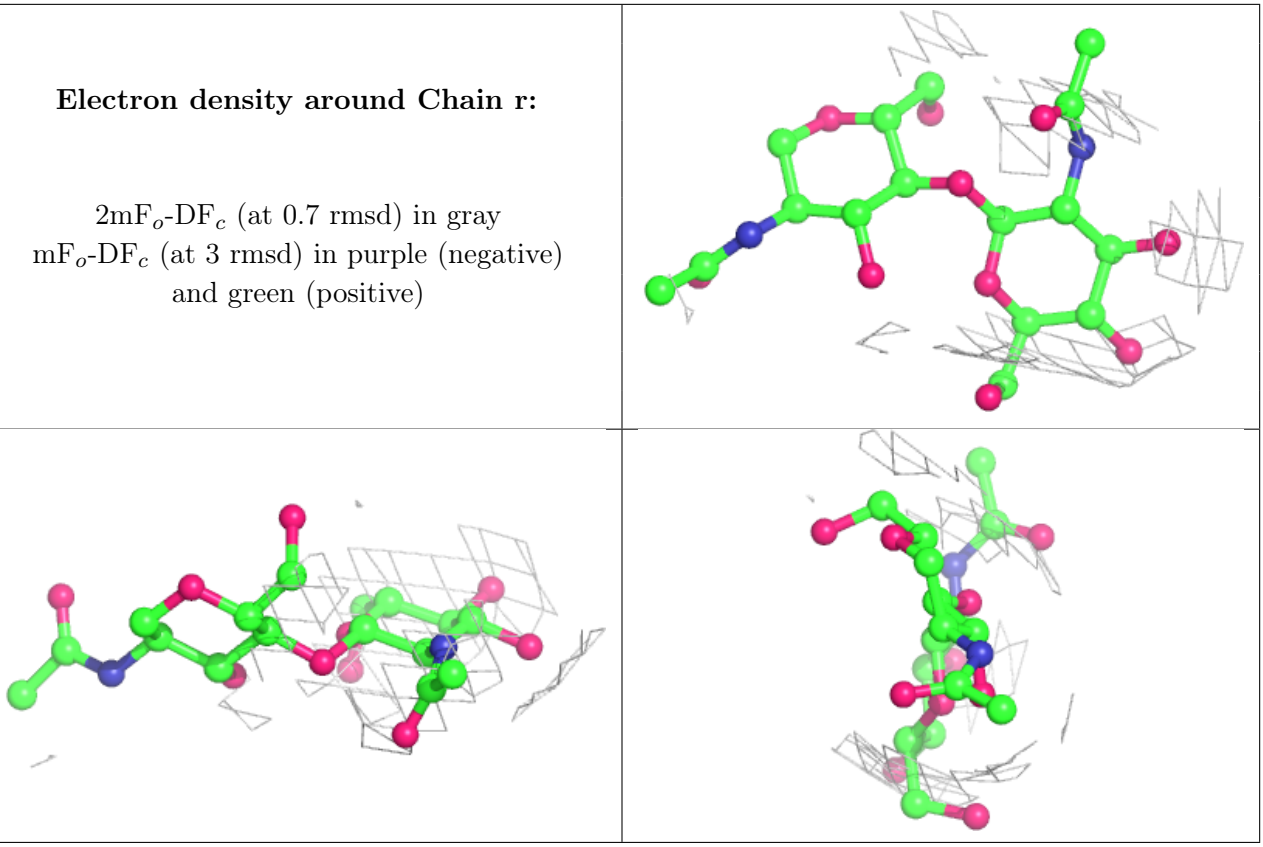






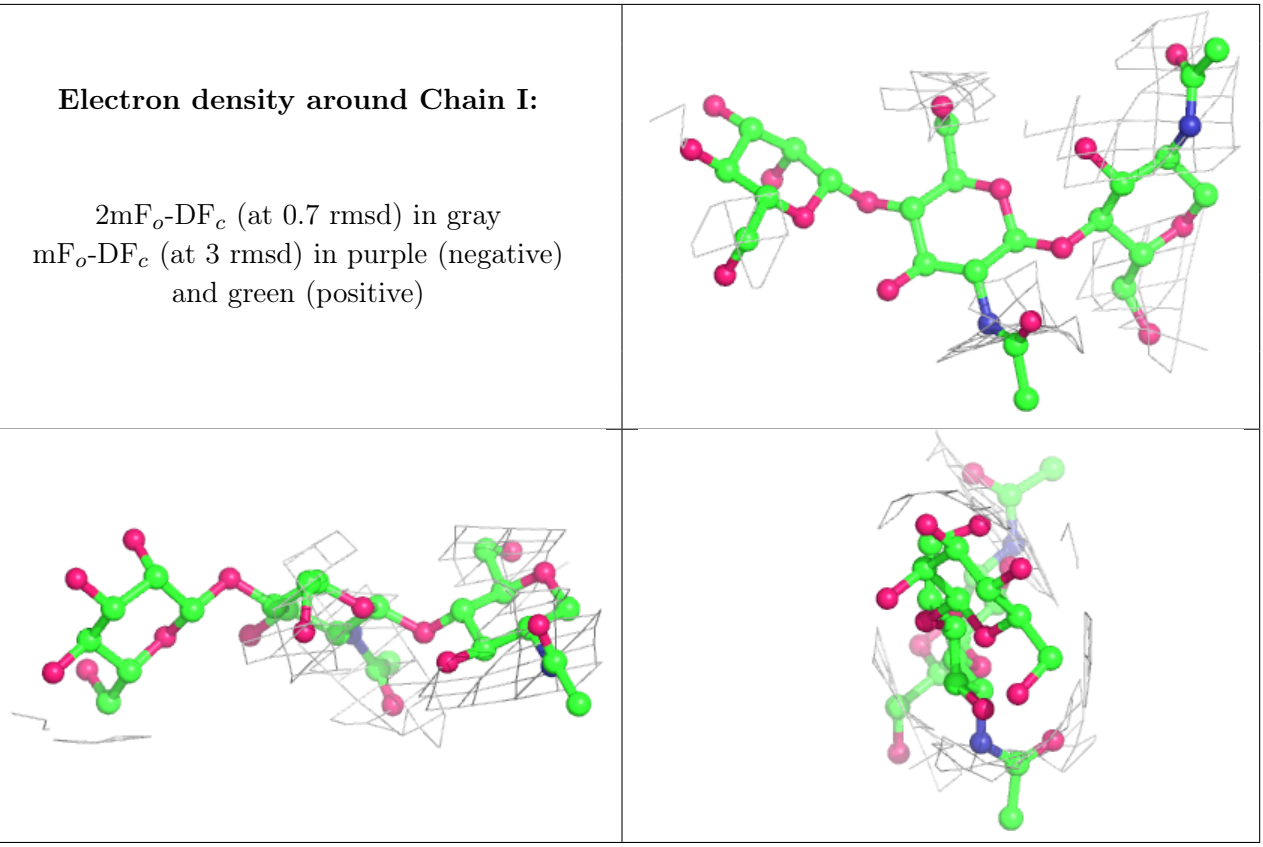
Electron density around Chain r:

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



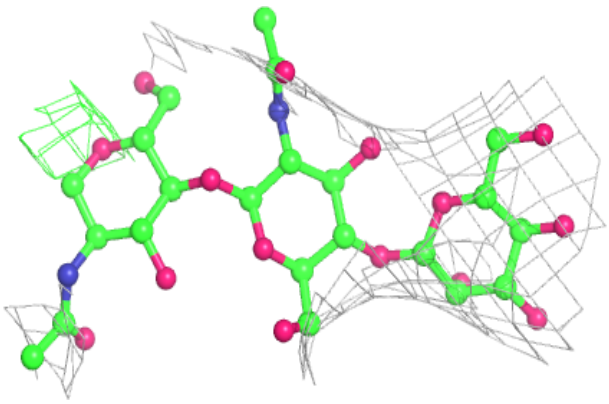
Electron density around Chain I:

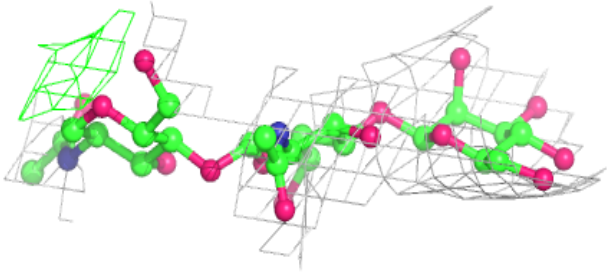
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

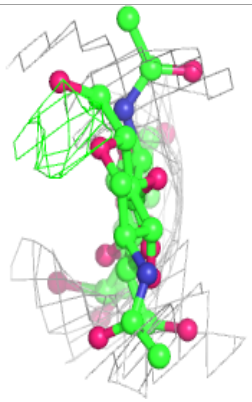


Electron density around Chain J:

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

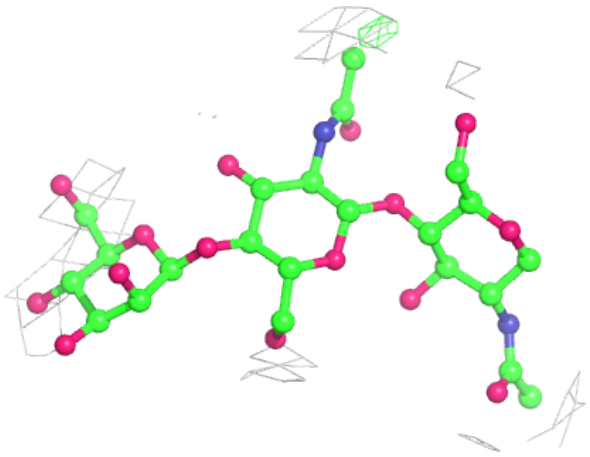


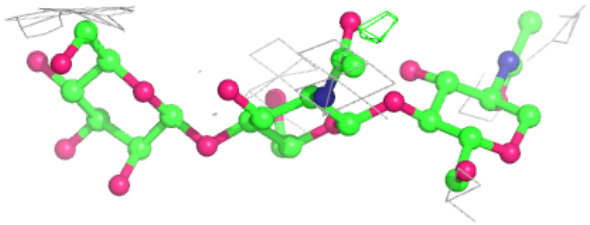


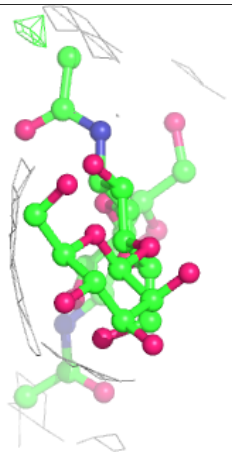


Electron density around Chain Y:

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

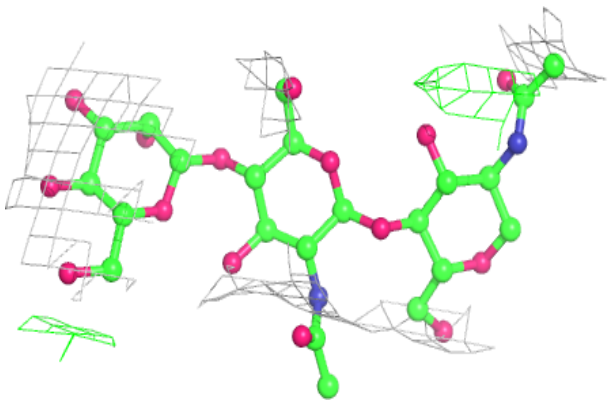


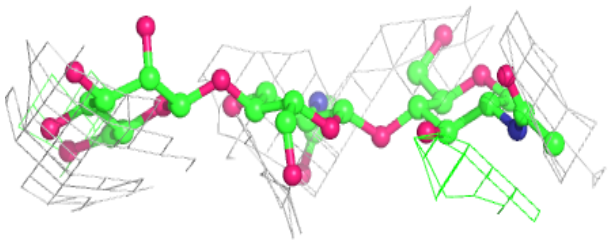


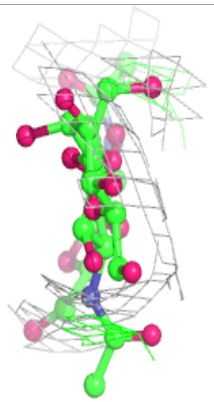


Electron density around Chain Z:

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

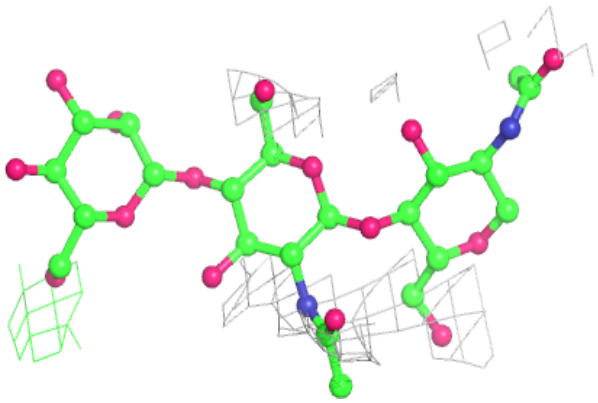


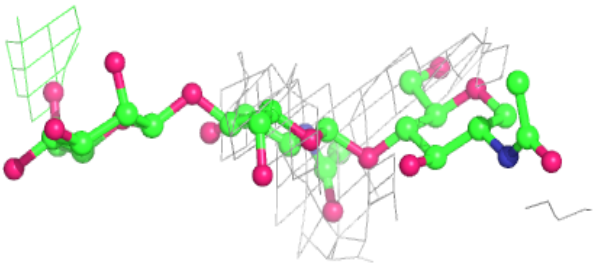


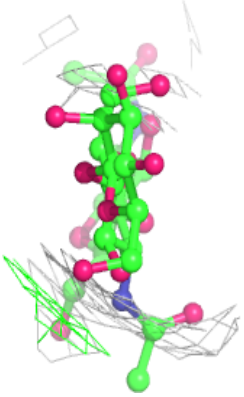


Electron density around Chain m:

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

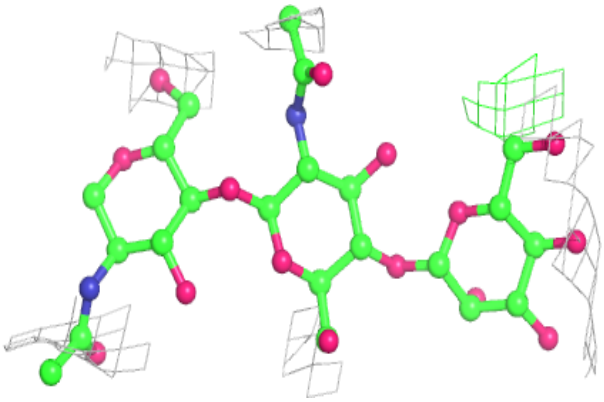


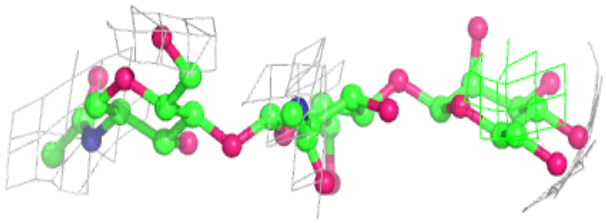


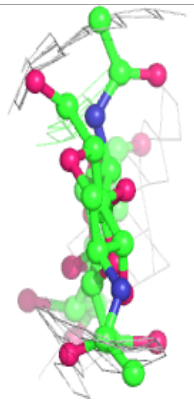


Electron density around Chain n:

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

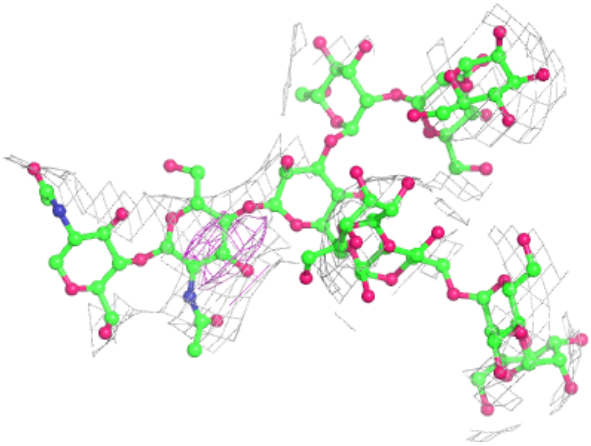


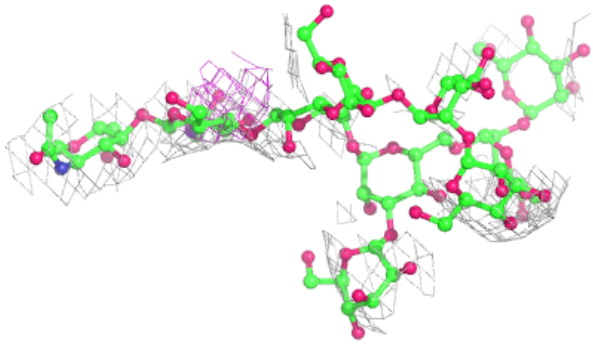


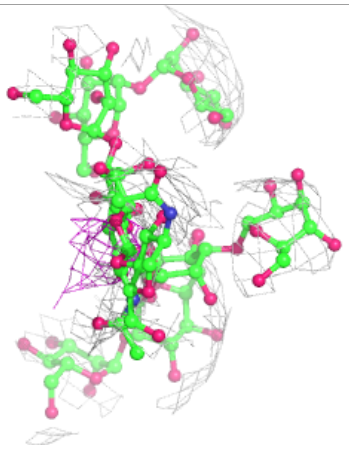


Electron density around Chain N:

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

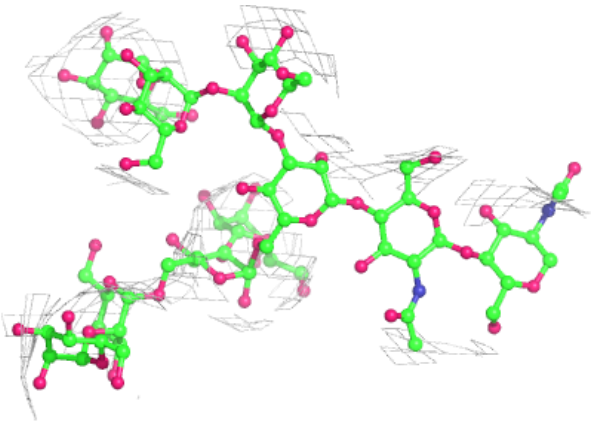


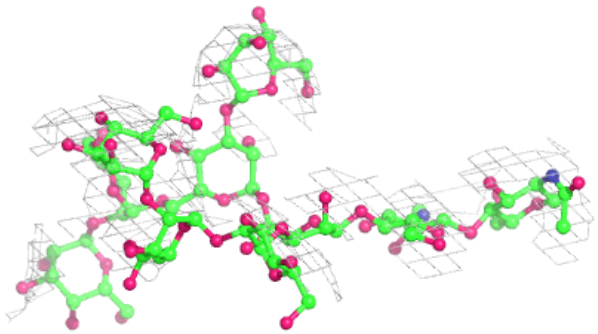


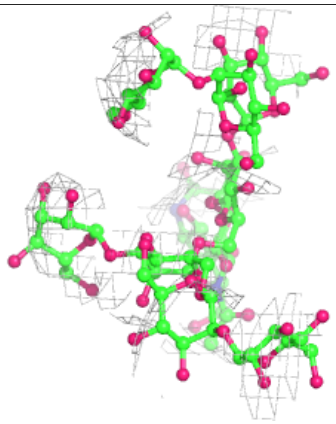


Electron density around Chain i:

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

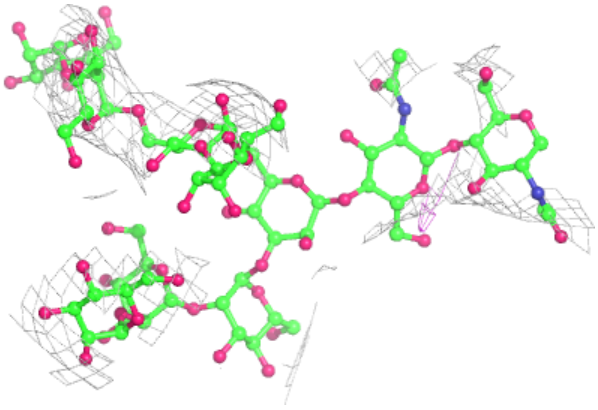


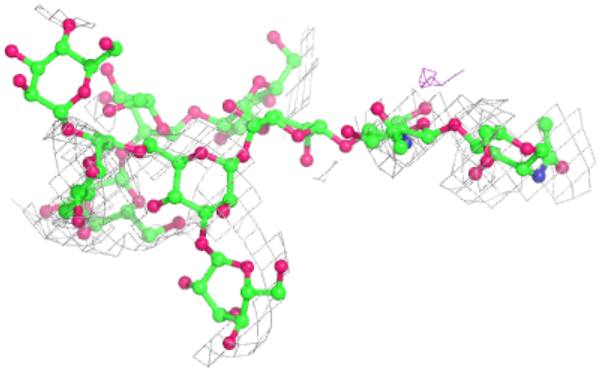


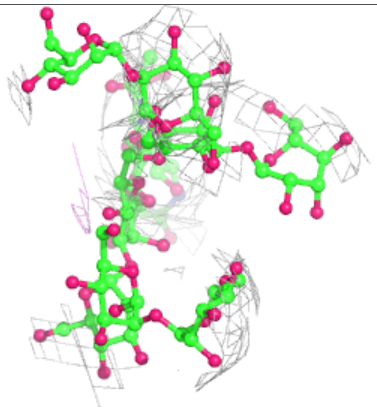


Electron density around Chain q:

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

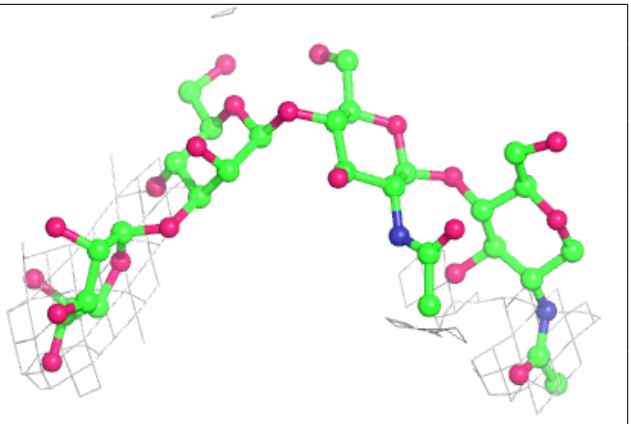


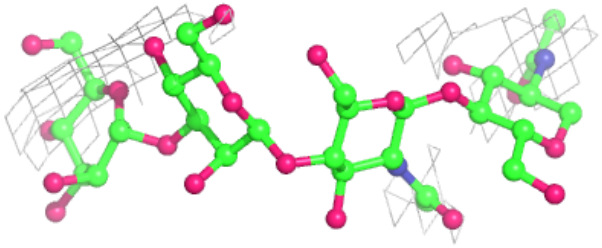


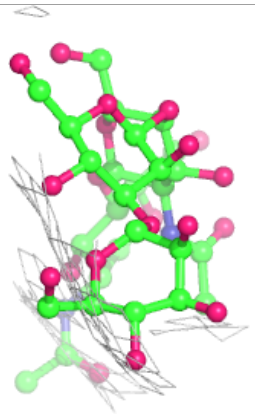


Electron density around Chain V:

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

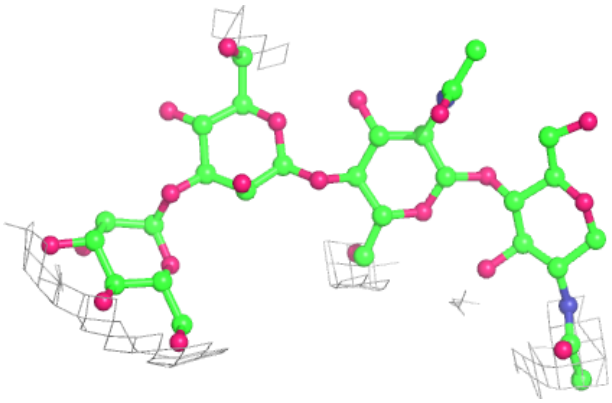


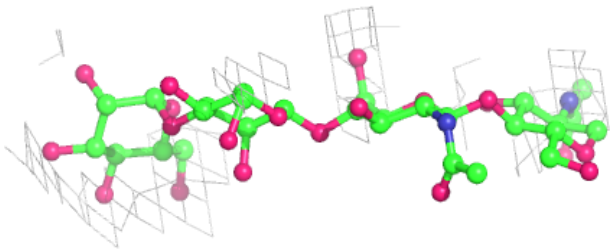


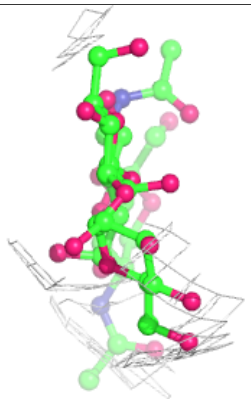


Electron density around Chain k:

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







6.4 Ligands (i)

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

6.5 Other polymers (i)

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