Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 05:56 AM EDT

PDB ID	:	4FQR
Title	:	Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin
Authors	:	Ekiert, D.C.; Wilson, I.A.
Deposited on	:	2012-06-25
Resolution	:	4.10 Å(reported)

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

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

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

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

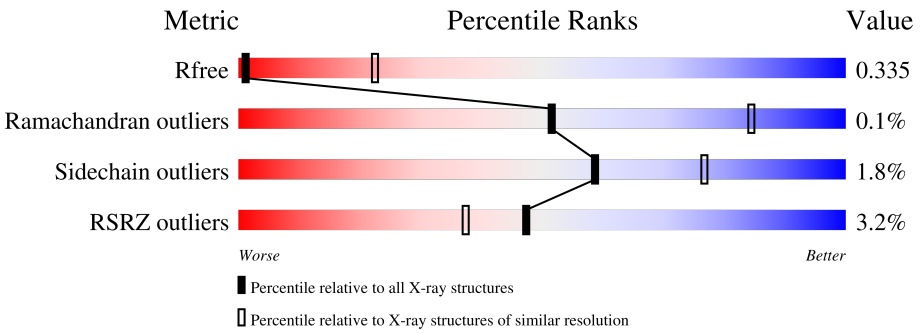
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	323	2% 97%
1	C	323	2% 97%
1	E	323	3% 97%
1	G	323	3% 98%
1	I	323	2% 97%
1	K	323	% 97%

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Mol	Chain	Length	Quality of chain
1	M	323	8% 97%
1	O	323	7% 97%
1	Q	323	5% 98%
1	S	323	7% 97%
1	U	323	2% 97%
1	W	323	5% 97%
2	B	174	2% 98%
2	D	174	4% 98%
2	F	174	5% 98%
2	H	174	2% 98%
2	J	174	3% 98%
2	L	174	5% 98%
2	N	174	9% 98%
2	P	174	5% 98%
2	R	174	% 98%
2	T	174	5% 98%
2	V	174	% 98%
2	X	174	3% 98%
3	a	241	% 96%
3	c	241	% 97%
3	e	241	7% 96%
3	g	241	3% 96%
3	i	241	% 96%
3	k	241	6% 96%
3	m	241	6% 97%

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Mol	Chain	Length	Quality of chain
3	o	241	6% 96%
3	q	241	3% 97%
3	s	241	5% 97%
3	u	241	% 96%
3	w	241	3% 96%
4	b	214	96%
4	d	214	95%
4	f	214	96%
4	h	214	% 94% 5%
4	j	214	96%
4	l	214	3% 96%
4	n	214	% 95%
4	p	214	3% 95% 5%
4	r	214	% 96%
4	t	214	% 96%
4	v	214	2% 95%
4	x	214	% 96%
5	0	4	100%
5	2	4	50% 50%
5	4	4	25% 75%
5	6	4	25% 75%
5	8	4	100%
5	AA	4	25% 75%
5	CA	4	25% 75%
5	EA	4	100%

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Mol	Chain	Length	Quality of chain
5	GA	4	25% 75%
5	IA	4	50% 50%
5	Y	4	25% 75%
5	y	4	75% 25%
6	1	2	50% 50%
6	3	2	100%
6	5	2	50% 50%
6	7	2	50% 50%
6	9	2	50% 50%
6	BA	2	50% 50%
6	DA	2	100%
6	FA	2	50% 50%
6	HA	2	50% 50%
6	JA	2	50% 50%
6	Z	2	100%
6	z	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	6	2	-	-	-	X
5	NAG	AA	2	-	-	-	X
5	MAN	AA	4	-	-	-	X
5	NAG	Y	1	-	-	-	X
6	NAG	3	2	-	-	-	X
6	NAG	7	2	-	-	-	X
7	NAG	A	601	-	-	-	X
7	NAG	C	501	-	-	-	X
7	NAG	E	601	-	-	-	X
7	NAG	F	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	G	502	-	-	-	X
7	NAG	M	502	-	-	-	X
7	NAG	O	501	-	-	-	X
7	NAG	Q	502	-	-	-	X
7	NAG	R	201	-	-	-	X
7	NAG	S	501	-	-	-	X
7	NAG	S	502	-	-	-	X
7	NAG	T	201	-	-	-	X
7	NAG	U	502	-	-	-	X
7	NAG	V	201	-	-	-	X
7	NAG	W	601	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 90792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2553	1598	450	491	14	0	12	0
1	C	318	2553	1598	450	491	14	0	12	0
1	E	318	2553	1598	450	491	14	0	12	0
1	G	318	2553	1598	450	491	14	0	12	0
1	I	318	2553	1598	450	491	14	0	12	0
1	K	318	2553	1598	450	491	14	0	12	0
1	M	318	2553	1598	450	491	14	0	12	0
1	O	318	2553	1598	450	491	14	0	12	0
1	Q	318	2553	1598	450	491	14	0	12	0
1	S	318	2553	1598	450	491	14	0	12	0
1	U	318	2553	1598	450	491	14	0	12	0
1	W	318	2553	1598	450	491	14	0	12	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
G	7	ALA	-	expression tag	UNP Q91MA7
G	8	ASP	-	expression tag	UNP Q91MA7
G	9	PRO	-	expression tag	UNP Q91MA7
G	10	GLY	-	expression tag	UNP Q91MA7
I	7	ALA	-	expression tag	UNP Q91MA7
I	8	ASP	-	expression tag	UNP Q91MA7
I	9	PRO	-	expression tag	UNP Q91MA7
I	10	GLY	-	expression tag	UNP Q91MA7
K	7	ALA	-	expression tag	UNP Q91MA7
K	8	ASP	-	expression tag	UNP Q91MA7
K	9	PRO	-	expression tag	UNP Q91MA7
K	10	GLY	-	expression tag	UNP Q91MA7
M	7	ALA	-	expression tag	UNP Q91MA7
M	8	ASP	-	expression tag	UNP Q91MA7
M	9	PRO	-	expression tag	UNP Q91MA7
M	10	GLY	-	expression tag	UNP Q91MA7
O	7	ALA	-	expression tag	UNP Q91MA7
O	8	ASP	-	expression tag	UNP Q91MA7
O	9	PRO	-	expression tag	UNP Q91MA7
O	10	GLY	-	expression tag	UNP Q91MA7
Q	7	ALA	-	expression tag	UNP Q91MA7
Q	8	ASP	-	expression tag	UNP Q91MA7
Q	9	PRO	-	expression tag	UNP Q91MA7
Q	10	GLY	-	expression tag	UNP Q91MA7
S	7	ALA	-	expression tag	UNP Q91MA7
S	8	ASP	-	expression tag	UNP Q91MA7
S	9	PRO	-	expression tag	UNP Q91MA7
S	10	GLY	-	expression tag	UNP Q91MA7
U	7	ALA	-	expression tag	UNP Q91MA7
U	8	ASP	-	expression tag	UNP Q91MA7
U	9	PRO	-	expression tag	UNP Q91MA7
U	10	GLY	-	expression tag	UNP Q91MA7
W	7	ALA	-	expression tag	UNP Q91MA7
W	8	ASP	-	expression tag	UNP Q91MA7
W	9	PRO	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
W	10	GLY	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1446	901	251	287	7	0	7	0
2	D	172	1446	901	251	287	7	0	7	0
2	F	172	1446	901	251	287	7	0	7	0
2	H	172	1446	901	251	287	7	0	7	0
2	J	172	1446	901	251	287	7	0	7	0
2	L	172	1446	901	251	287	7	0	7	0
2	N	172	1446	901	251	287	7	0	7	0
2	P	172	1446	901	251	287	7	0	7	0
2	R	172	1446	901	251	287	7	0	7	0
2	T	172	1446	901	251	287	7	0	7	0
2	V	172	1446	901	251	287	7	0	7	0
2	X	172	1446	901	251	287	7	0	7	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
H	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
J	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
L	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
N	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
P	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
R	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
V	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
X	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Broadly neutralizing antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	a	239	1806	1127	306	365	8	0	4	0
3	c	239	1806	1127	306	365	8	0	4	0
3	e	239	1806	1127	306	365	8	0	4	0
3	g	239	1806	1127	306	365	8	0	4	0
3	i	239	1806	1127	306	365	8	0	4	0
3	k	239	1806	1127	306	365	8	0	4	0
3	m	239	1806	1127	306	365	8	0	4	0
3	o	239	1806	1127	306	365	8	0	4	0
3	q	239	1806	1127	306	365	8	0	4	0
3	s	239	1806	1127	306	365	8	0	4	0
3	u	239	1806	1127	306	365	8	0	4	0
3	w	239	1806	1127	306	365	8	0	4	0

- Molecule 4 is a protein called Broadly neutralizing antibody C05, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	b	213	1648	1033	281	330	4	0	1	0
4	d	213	1648	1033	281	330	4	0	1	0
4	f	213	1648	1033	281	330	4	0	1	0
4	h	213	1648	1033	281	330	4	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	213	1648	1033	281	330	4	0	1	0
4	l	213	1648	1033	281	330	4	0	1	0
4	n	213	1648	1033	281	330	4	0	1	0
4	p	213	1648	1033	281	330	4	0	1	0
4	r	213	1648	1033	281	330	4	0	1	0
4	t	213	1648	1033	281	330	4	0	1	0
4	v	213	1648	1033	281	330	4	0	1	0
4	x	213	1648	1033	281	330	4	0	1	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	Y	4	50	28	2	20	0	0	0
5	y	4	50	28	2	20	0	0	0
5	0	4	50	28	2	20	0	0	0
5	2	4	50	28	2	20	0	0	0
5	4	4	50	28	2	20	0	0	0
5	6	4	50	28	2	20	0	0	0
5	8	4	50	28	2	20	0	0	0
5	AA	4	50	28	2	20	0	0	0

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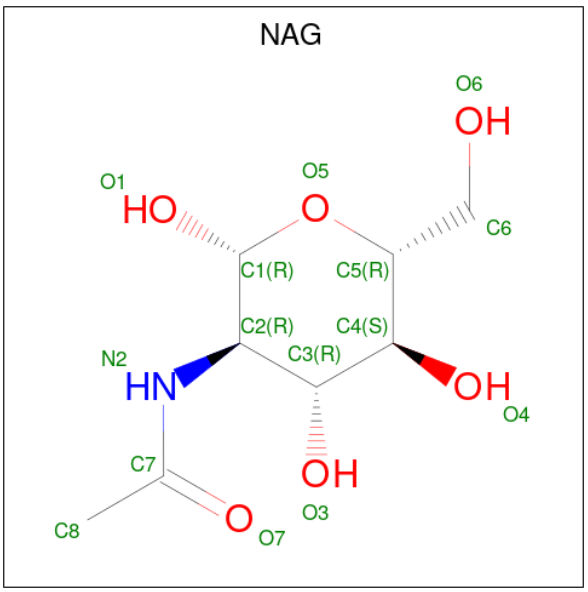
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	CA	4	50	28	2	20	0	0	0
			Total	C	N	O			
5	EA	4	50	28	2	20	0	0	0
			Total	C	N	O			
5	GA	4	50	28	2	20	0	0	0
			Total	C	N	O			
5	IA	4	50	28	2	20	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	Z	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	z	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	1	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	3	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	5	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	7	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	9	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	BA	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	DA	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	FA	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	HA	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	JA	2	28	16	2	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



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

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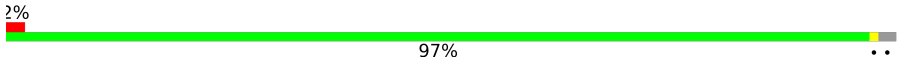
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	M	1	14	8	1	5	0	0
			Total	C	N	O		
7	M	1	14	8	1	5	0	0
			Total	C	N	O		
7	N	1	14	8	1	5	0	0
			Total	C	N	O		
7	O	1	14	8	1	5	0	0
			Total	C	N	O		
7	O	1	14	8	1	5	0	0
			Total	C	N	O		
7	P	1	14	8	1	5	0	0
			Total	C	N	O		
7	Q	1	14	8	1	5	0	0
			Total	C	N	O		
7	Q	1	14	8	1	5	0	0
			Total	C	N	O		
7	R	1	14	8	1	5	0	0
			Total	C	N	O		
7	S	1	14	8	1	5	0	0
			Total	C	N	O		
7	S	1	14	8	1	5	0	0
			Total	C	N	O		
7	T	1	14	8	1	5	0	0
			Total	C	N	O		
7	U	1	14	8	1	5	0	0
			Total	C	N	O		
7	U	1	14	8	1	5	0	0
			Total	C	N	O		
7	V	1	14	8	1	5	0	0
			Total	C	N	O		
7	W	1	14	8	1	5	0	0
			Total	C	N	O		
7	X	1	14	8	1	5	0	0

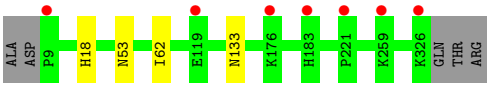
3 Residue-property plots (i)

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

• Molecule 1: Hemagglutinin HA1 chain

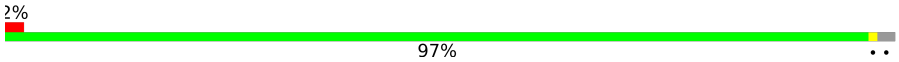
Chain A:

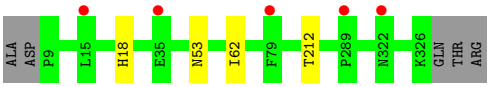




• Molecule 1: Hemagglutinin HA1 chain

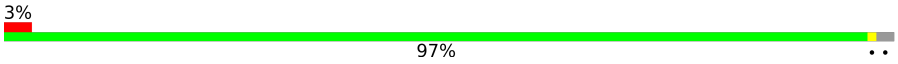
Chain C:





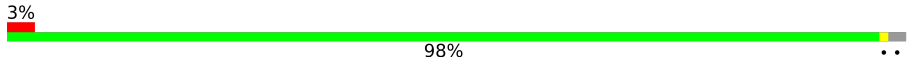
• Molecule 1: Hemagglutinin HA1 chain

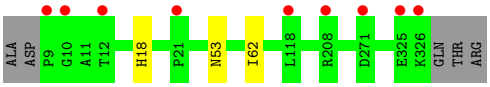
Chain E:



• Molecule 1: Hemagglutinin HA1 chain

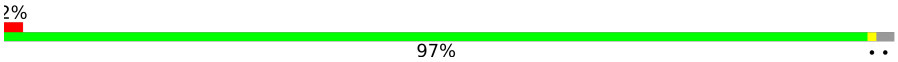
Chain G:

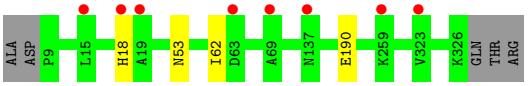




• Molecule 1: Hemagglutinin HA1 chain

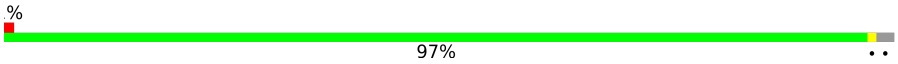
Chain I:

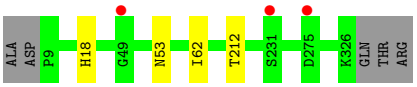




• Molecule 1: Hemagglutinin HA1 chain

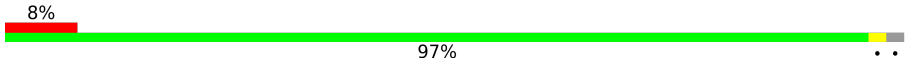
Chain K:

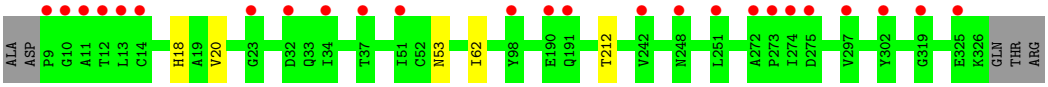




• Molecule 1: Hemagglutinin HA1 chain

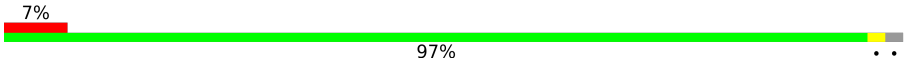
Chain M:

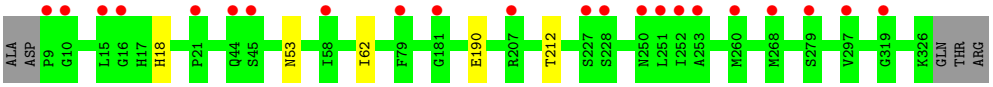




• Molecule 1: Hemagglutinin HA1 chain

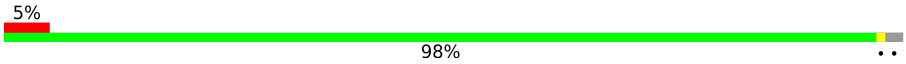
Chain O:

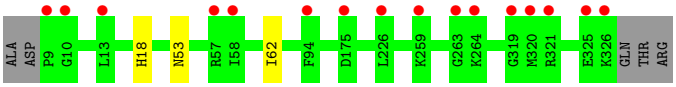




• Molecule 1: Hemagglutinin HA1 chain

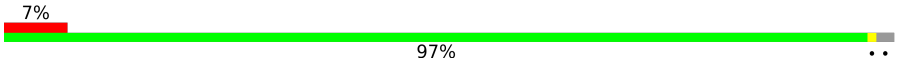
Chain Q:

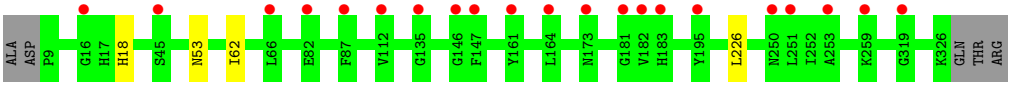




• Molecule 1: Hemagglutinin HA1 chain

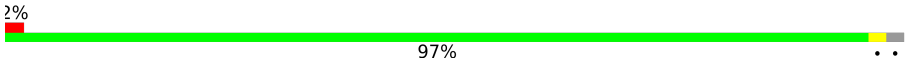
Chain S:

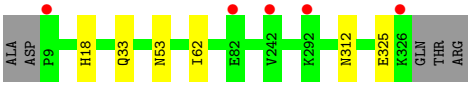




• Molecule 1: Hemagglutinin HA1 chain

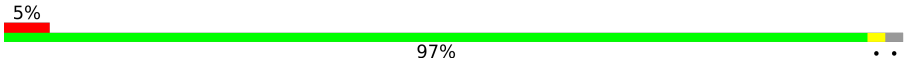
Chain U:

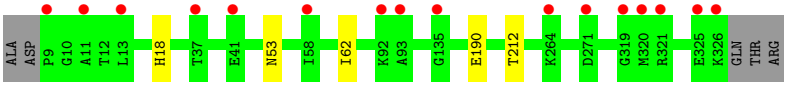




• Molecule 1: Hemagglutinin HA1 chain

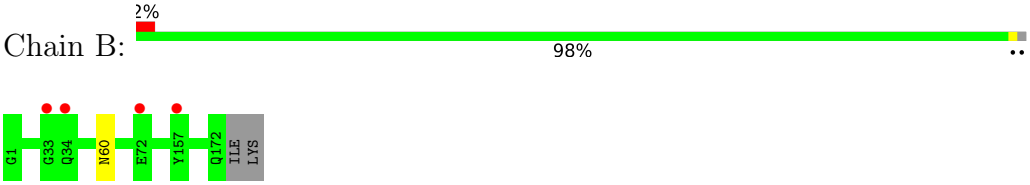
Chain W:





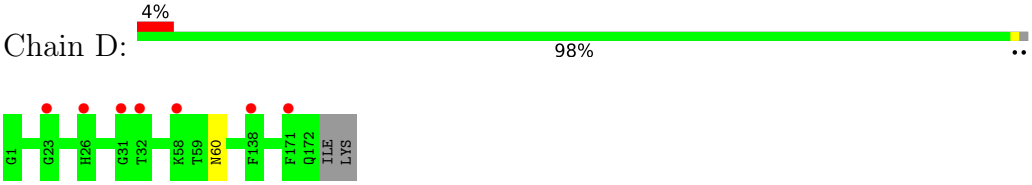
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



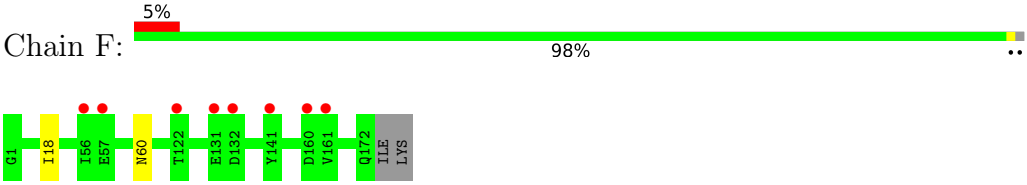
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



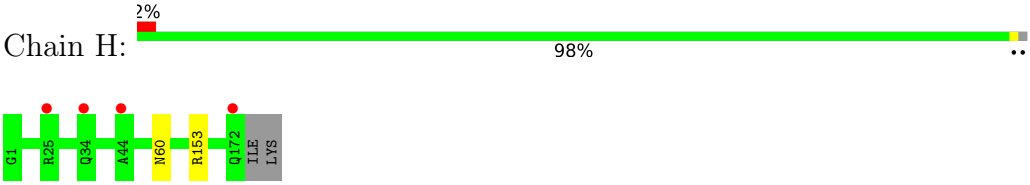
• Molecule 2: Hemagglutinin HA2 chain

Chain F:



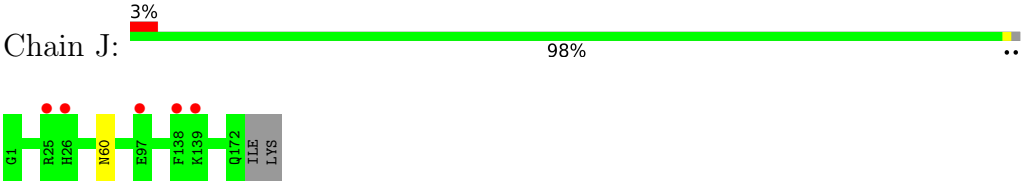
• Molecule 2: Hemagglutinin HA2 chain

Chain H:



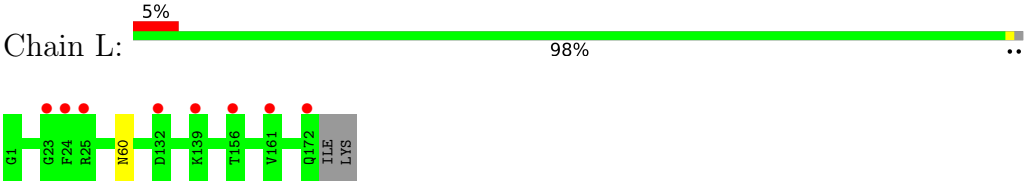
• Molecule 2: Hemagglutinin HA2 chain

Chain J:



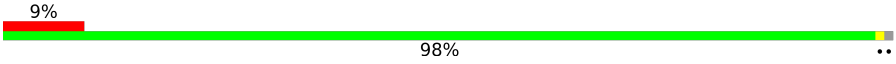
• Molecule 2: Hemagglutinin HA2 chain

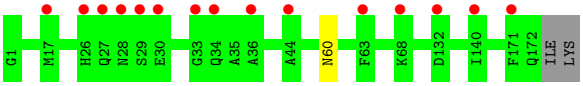
Chain L:



• Molecule 2: Hemagglutinin HA2 chain

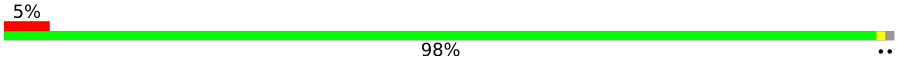
Chain N:

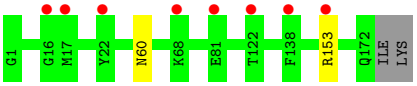




• Molecule 2: Hemagglutinin HA2 chain

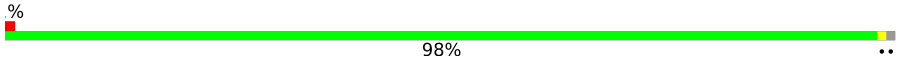
Chain P:

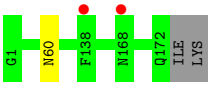




• Molecule 2: Hemagglutinin HA2 chain

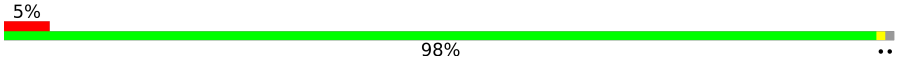
Chain R:

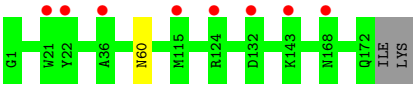




• Molecule 2: Hemagglutinin HA2 chain

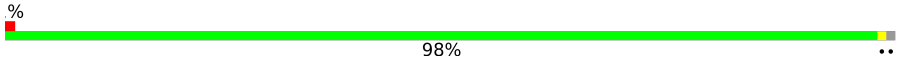
Chain T:

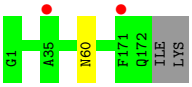




• Molecule 2: Hemagglutinin HA2 chain

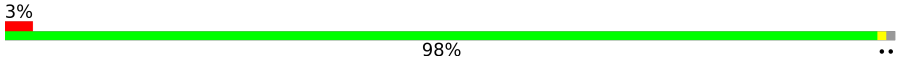
Chain V:

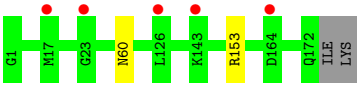




• Molecule 2: Hemagglutinin HA2 chain

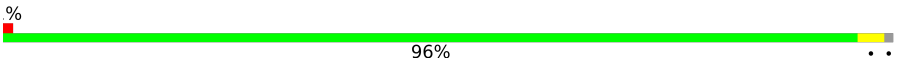
Chain X:

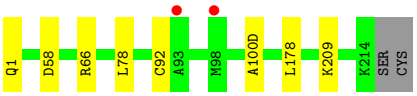




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

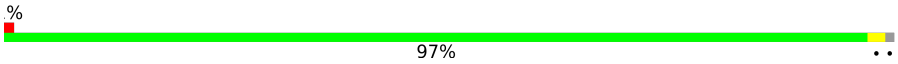
Chain a:





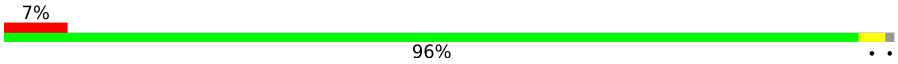
• Molecule 3: Broadly neutralizing antibody C05, heavy chain

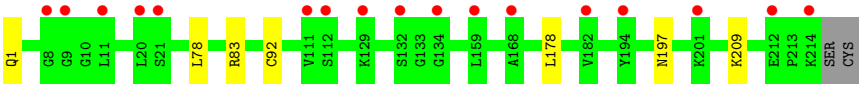
Chain c:



• Molecule 3: Broadly neutralizing antibody C05, heavy chain

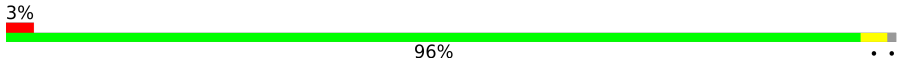
Chain e:

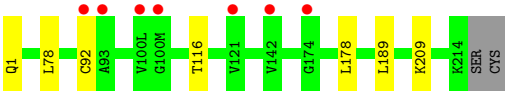




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

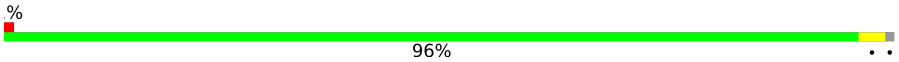
Chain g:

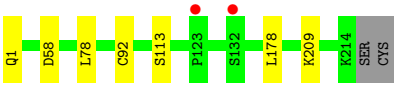




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

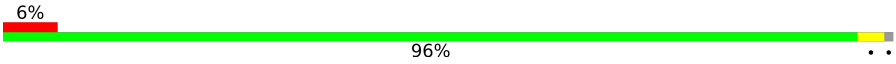
Chain i:

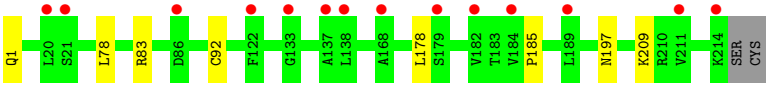




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

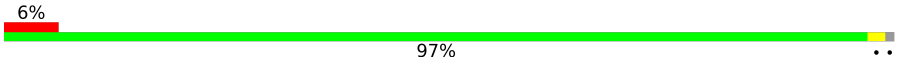
Chain k:

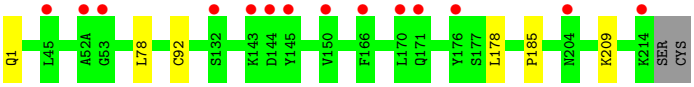




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

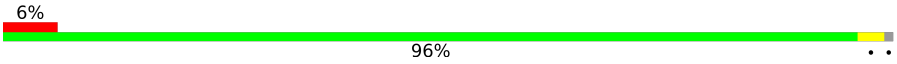
Chain m:

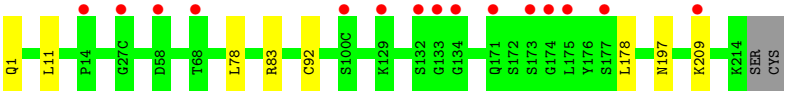




• Molecule 3: Broadly neutralizing antibody C05, heavy chain

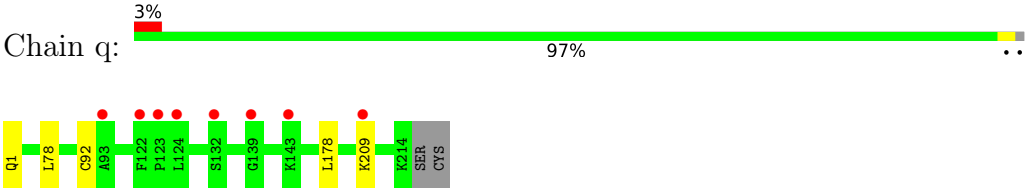
Chain o:





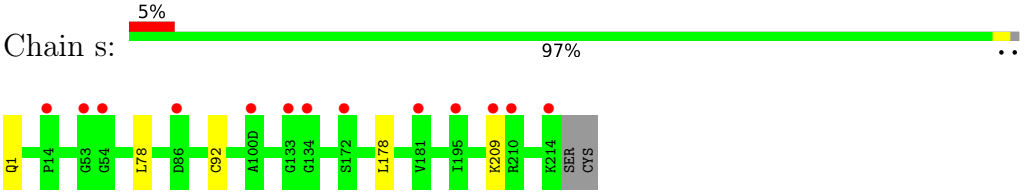
• Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain q:



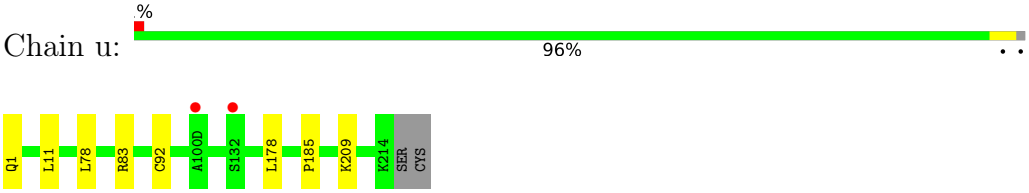
• Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain s:



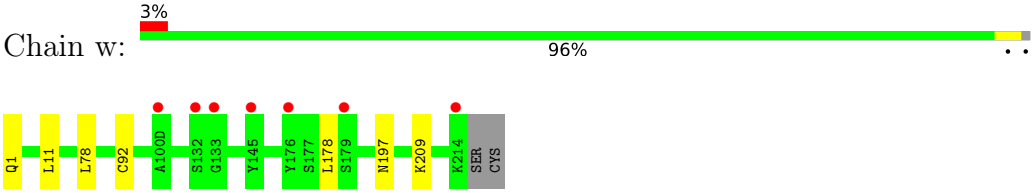
• Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain u:



• Molecule 3: Broadly neutralizing antibody C05, heavy chain

Chain w:

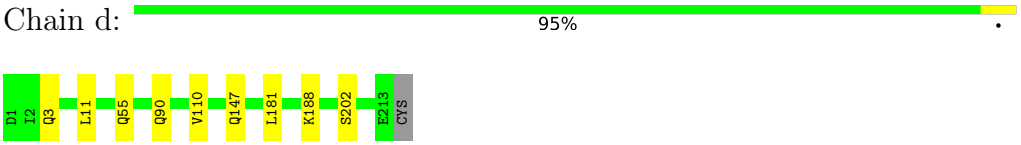


• Molecule 4: Broadly neutralizing antibody C05, light chain

Chain b:

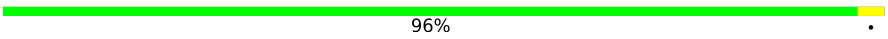
• Molecule 4: Broadly neutralizing antibody C05, light chain

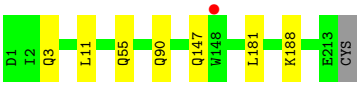
Chain d:



• Molecule 4: Broadly neutralizing antibody C05, light chain

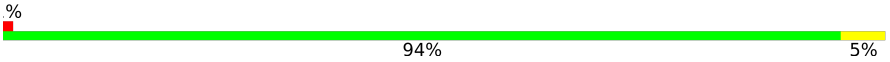
Chain f:





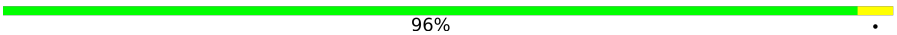
• Molecule 4: Broadly neutralizing antibody C05, light chain

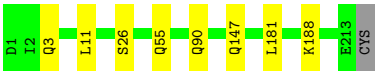
Chain h:



• Molecule 4: Broadly neutralizing antibody C05, light chain

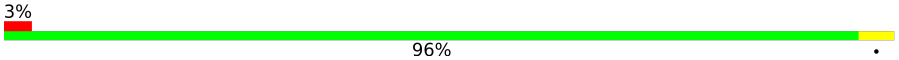
Chain j:

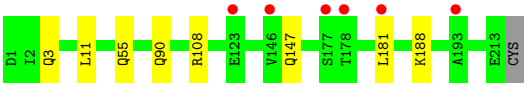




• Molecule 4: Broadly neutralizing antibody C05, light chain

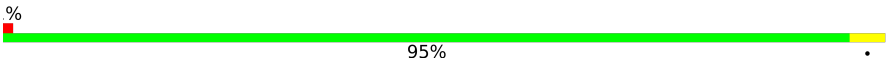
Chain l:

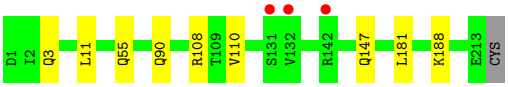




• Molecule 4: Broadly neutralizing antibody C05, light chain

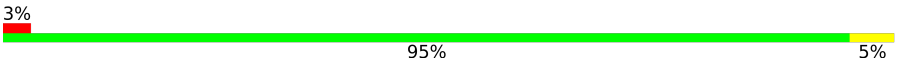
Chain n:

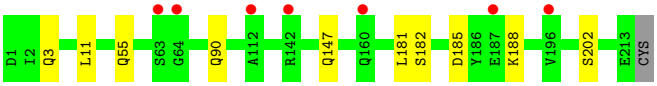




• Molecule 4: Broadly neutralizing antibody C05, light chain

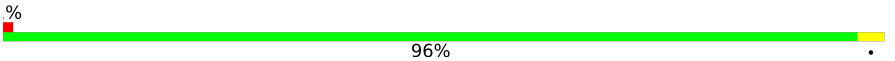
Chain p:

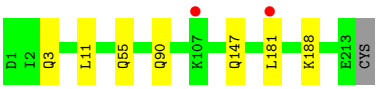




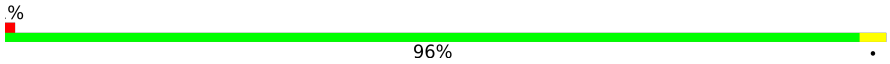
• Molecule 4: Broadly neutralizing antibody C05, light chain

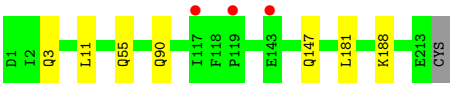
Chain r:



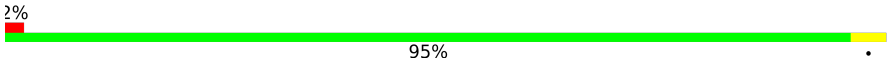


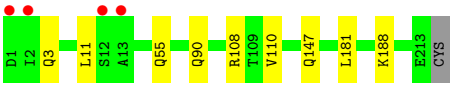
• Molecule 4: Broadly neutralizing antibody C05, light chain

Chain t: 

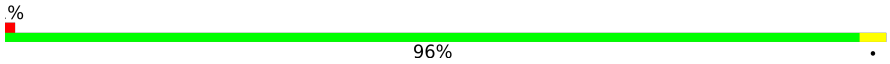


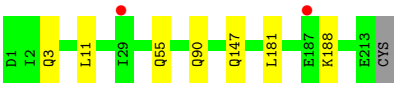
• Molecule 4: Broadly neutralizing antibody C05, light chain

Chain v: 



• Molecule 4: Broadly neutralizing antibody C05, light chain

Chain x: 



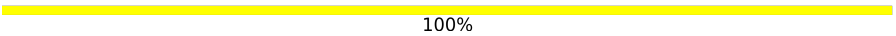
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

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

Chain y:

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

Chain 0: 

• Molecule 5: 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 2:

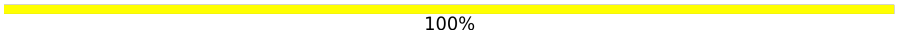
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

• Molecule 5: 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 6:

• Molecule 5: 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 8: 

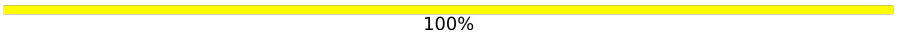
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:

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

Chain CA:

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

Chain EA: 

• Molecule 5: 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 GA: 25% 75%

NAG1 NAG2 BMA3 MAN4

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

Chain IA: 50% 50%

NAG1 NAG2 BMA3 MAN4

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

Chain Z: 100%

NAG1 NAG2

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

Chain z: 100%

NAG1 NAG2

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

Chain 1: 50% 50%

NAG1 NAG2

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

Chain 3: 100%

NAG1 NAG2

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

Chain 5: 50% 50%

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

Chain 7:

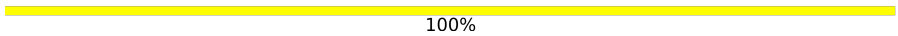
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:

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

Chain BA:

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

Chain DA: 

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

Chain FA:

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

Chain HA:

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

Chain JA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	142.02Å 158.62Å 178.50Å 89.95° 85.44° 84.37°	Depositor
Resolution (Å)	49.07 – 4.10 49.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	73.9 (49.07-4.10) 58.9 (49.07-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.309 , 0.334 0.312 , 0.335	Depositor DCC
R_{free} test set	4527 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 8.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	90792	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.42	0/2612	0.66	0/3558
1	C	0.39	0/2612	0.65	1/3558 (0.0%)
1	E	0.38	1/2612 (0.0%)	0.65	0/3558
1	G	0.39	0/2612	0.66	0/3558
1	I	0.48	2/2612 (0.1%)	0.69	2/3558 (0.1%)
1	K	0.39	0/2612	0.64	1/3558 (0.0%)
1	M	0.42	0/2612	0.68	2/3558 (0.1%)
1	O	0.41	1/2612 (0.0%)	0.65	1/3558 (0.0%)
1	Q	0.40	0/2612	0.66	0/3558
1	S	0.38	0/2612	0.66	1/3558 (0.0%)
1	U	0.44	1/2612 (0.0%)	0.68	1/3558 (0.0%)
1	W	0.42	1/2612 (0.0%)	0.65	1/3558 (0.0%)
2	B	0.37	0/1470	0.63	0/1975
2	D	0.36	0/1470	0.64	0/1975
2	F	0.41	0/1470	0.66	0/1975
2	H	0.37	0/1470	0.64	1/1975 (0.1%)
2	J	0.37	0/1470	0.63	0/1975
2	L	0.39	0/1470	0.64	0/1975
2	N	0.35	0/1470	0.63	0/1975
2	P	0.38	0/1470	0.63	1/1975 (0.1%)
2	R	0.36	0/1470	0.64	0/1975
2	T	0.36	0/1470	0.63	0/1975
2	V	0.37	0/1470	0.65	0/1975
2	X	0.36	0/1470	0.63	1/1975 (0.1%)
3	a	0.48	1/1837 (0.1%)	0.75	2/2500 (0.1%)
3	c	0.41	0/1837	0.68	0/2500
3	e	0.43	0/1837	0.71	0/2500
3	g	0.46	1/1837 (0.1%)	0.71	1/2500 (0.0%)
3	i	0.53	0/1837	0.79	1/2500 (0.0%)
3	k	0.42	0/1837	0.69	0/2500
3	m	0.41	0/1837	0.69	0/2500
3	o	0.43	0/1837	0.71	1/2500 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	q	0.43	0/1837	0.69	0/2500
3	s	0.42	0/1837	0.69	0/2500
3	u	0.41	0/1837	0.70	1/2500 (0.0%)
3	w	0.42	0/1837	0.69	1/2500 (0.0%)
4	b	0.45	0/1682	0.67	0/2280
4	d	0.50	1/1682 (0.1%)	0.72	0/2280
4	f	0.40	0/1682	0.66	0/2280
4	h	0.51	1/1682 (0.1%)	0.71	0/2280
4	j	0.44	0/1682	0.69	0/2280
4	l	0.44	0/1682	0.68	0/2280
4	n	0.48	1/1682 (0.1%)	0.69	0/2280
4	p	0.51	0/1682	0.78	4/2280 (0.2%)
4	r	0.39	0/1682	0.66	0/2280
4	t	0.37	0/1682	0.64	0/2280
4	v	0.48	1/1682 (0.1%)	0.70	0/2280
4	x	0.40	0/1682	0.66	0/2280
All	All	0.42	12/91212 (0.0%)	0.67	24/123756 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
3	k	0	1
3	m	0	1
3	u	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	GLU	CG-CD	-11.09	1.35	1.51
1	W	190	GLU	CB-CG	-7.77	1.37	1.52
3	a	100(D)	ALA	CA-CB	-7.11	1.37	1.52
3	g	116	THR	CB-CG2	-7.02	1.29	1.52
4	n	110	VAL	CB-CG2	-6.42	1.39	1.52
4	d	110	VAL	CB-CG2	-6.08	1.40	1.52
4	v	110	VAL	CB-CG2	-6.08	1.40	1.52
1	E	190	GLU	CB-CG	-6.05	1.40	1.52
1	U	325	GLU	CG-CD	-5.43	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	190	GLU	CB-CG	-5.37	1.42	1.52
1	I	190	GLU	CA-CB	-5.36	1.42	1.53
4	h	183	LYS	CE-NZ	-5.05	1.36	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	p	185	ASP	CB-CG-OD2	10.08	127.37	118.30
3	i	58	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	M	20	VAL	N-CA-C	-8.49	88.08	111.00
4	p	185	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	I	190	GLU	OE1-CD-OE2	7.20	131.93	123.30
3	a	58	ASP	CB-CG-OD1	-6.66	112.31	118.30
4	p	182	SER	CB-CA-C	-6.18	98.36	110.10
3	o	11	LEU	CB-CG-CD2	-6.07	100.68	111.00
3	u	11	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	I	190	GLU	CA-CB-CG	-5.64	100.99	113.40
1	S	226	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	K	212	THR	CA-CB-CG2	-5.45	104.77	112.40
3	g	189	LEU	CB-CG-CD2	-5.41	101.81	111.00
3	w	11	LEU	CB-CG-CD2	-5.29	102.01	111.00
3	a	66	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	O	212	THR	CA-CB-CG2	-5.19	105.13	112.40
4	p	185	ASP	N-CA-CB	5.13	119.84	110.60
1	W	212	THR	CA-CB-CG2	-5.12	105.23	112.40
2	P	153	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	M	212	THR	CA-CB-CG2	-5.05	105.33	112.40
1	U	325	GLU	N-CA-C	5.04	124.62	111.00
1	C	212	THR	CA-CB-CG2	-5.04	105.34	112.40
2	H	153	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	X	153	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	ILE	Mainchain
3	k	185	PRO	Mainchain
3	m	185	PRO	Mainchain
3	u	185	PRO	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	C	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	G	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	I	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	K	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	M	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	O	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	Q	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	S	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
1	U	328/323 (102%)	323 (98%)	4 (1%)	1 (0%)	41	75
1	W	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	41	75
2	B	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	D	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	F	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	H	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	J	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	L	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	N	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	P	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	R	177/174 (102%)	172 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	V	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	X	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
3	a	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	c	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	e	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	g	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	i	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	k	241/241 (100%)	235 (98%)	6 (2%)	0	100	100
3	m	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	o	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	q	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	s	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	u	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	w	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
4	b	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	d	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	f	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	h	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	j	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	l	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	n	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	p	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	r	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	t	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	v	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	x	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	11496/11424 (101%)	11268 (98%)	216 (2%)	12 (0%)	51	84

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE

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Mol	Chain	Res	Type
1	C	62	ILE
1	E	62	ILE
1	G	62	ILE
1	I	62	ILE
1	K	62	ILE
1	M	62	ILE
1	O	62	ILE
1	Q	62	ILE
1	S	62	ILE
1	U	62	ILE
1	W	62	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	C	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	E	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	G	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	I	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	K	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	M	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	O	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	Q	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	S	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	U	291/283 (103%)	289 (99%)	2 (1%)	84 90
1	W	291/283 (103%)	289 (99%)	2 (1%)	84 90
2	B	153/148 (103%)	152 (99%)	1 (1%)	84 90
2	D	153/148 (103%)	152 (99%)	1 (1%)	84 90
2	F	153/148 (103%)	152 (99%)	1 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	J	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	L	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	N	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	P	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	R	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	T	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	V	153/148 (103%)	152 (99%)	1 (1%)	84	90
2	X	153/148 (103%)	152 (99%)	1 (1%)	84	90
3	a	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	c	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	e	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	g	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	i	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	k	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	m	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	o	202/200 (101%)	196 (97%)	6 (3%)	41	64
3	q	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	s	202/200 (101%)	198 (98%)	4 (2%)	55	73
3	u	202/200 (101%)	197 (98%)	5 (2%)	47	68
3	w	202/200 (101%)	197 (98%)	5 (2%)	47	68
4	b	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	d	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	f	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	h	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	j	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	l	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	n	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	p	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	r	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	t	187/187 (100%)	180 (96%)	7 (4%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	v	187/187 (100%)	180 (96%)	7 (4%)	34	59
4	x	187/187 (100%)	180 (96%)	7 (4%)	34	59
All	All	9996/9816 (102%)	9818 (98%)	178 (2%)	59	77

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
2	B	60	ASN
1	C	18	HIS
1	C	53	ASN
2	D	60	ASN
1	E	18	HIS
1	E	53	ASN
2	F	60	ASN
1	G	18	HIS
1	G	53	ASN
2	H	60	ASN
1	I	18	HIS
1	I	53	ASN
2	J	60	ASN
1	K	18	HIS
1	K	53	ASN
2	L	60	ASN
1	M	18	HIS
1	M	53	ASN
2	N	60	ASN
1	O	18	HIS
1	O	53	ASN
2	P	60	ASN
1	Q	18	HIS
1	Q	53	ASN
2	R	60	ASN
1	S	18	HIS
1	S	53	ASN
2	T	60	ASN
1	U	18	HIS
1	U	53	ASN
2	V	60	ASN
1	W	18	HIS

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Mol	Chain	Res	Type
1	W	53	ASN
2	X	60	ASN
3	a	78	LEU
3	a	92	CYS
3	a	178	LEU
3	a	209	LYS
4	b	3	GLN
4	b	11	LEU
4	b	55	GLN
4	b	90	GLN
4	b	147	GLN
4	b	181	LEU
4	b	188	LYS
3	c	78	LEU
3	c	92	CYS
3	c	113	SER
3	c	178	LEU
3	c	209	LYS
4	d	3	GLN
4	d	11	LEU
4	d	55	GLN
4	d	90	GLN
4	d	147	GLN
4	d	181	LEU
4	d	188	LYS
3	e	78	LEU
3	e	83	ARG
3	e	92	CYS
3	e	178	LEU
3	e	197	ASN
3	e	209	LYS
4	f	3	GLN
4	f	11	LEU
4	f	55	GLN
4	f	90	GLN
4	f	147	GLN
4	f	181	LEU
4	f	188	LYS
3	g	78	LEU
3	g	92	CYS
3	g	178	LEU
3	g	209	LYS

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Mol	Chain	Res	Type
4	h	3	GLN
4	h	11	LEU
4	h	55	GLN
4	h	90	GLN
4	h	147	GLN
4	h	181	LEU
4	h	188	LYS
3	i	78	LEU
3	i	92	CYS
3	i	113	SER
3	i	178	LEU
3	i	209	LYS
4	j	3	GLN
4	j	11	LEU
4	j	55	GLN
4	j	90	GLN
4	j	147	GLN
4	j	181	LEU
4	j	188	LYS
3	k	78	LEU
3	k	83	ARG
3	k	92	CYS
3	k	178	LEU
3	k	197	ASN
3	k	209	LYS
4	l	3	GLN
4	l	11	LEU
4	l	55	GLN
4	l	90	GLN
4	l	147	GLN
4	l	181	LEU
4	l	188	LYS
3	m	78	LEU
3	m	92	CYS
3	m	178	LEU
3	m	209	LYS
4	n	3	GLN
4	n	11	LEU
4	n	55	GLN
4	n	90	GLN
4	n	147	GLN
4	n	181	LEU

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Mol	Chain	Res	Type
4	n	188	LYS
3	o	78	LEU
3	o	83	ARG
3	o	92	CYS
3	o	178	LEU
3	o	197	ASN
3	o	209	LYS
4	p	3	GLN
4	p	11	LEU
4	p	55	GLN
4	p	90	GLN
4	p	147	GLN
4	p	181	LEU
4	p	188	LYS
3	q	78	LEU
3	q	92	CYS
3	q	178	LEU
3	q	209	LYS
4	r	3	GLN
4	r	11	LEU
4	r	55	GLN
4	r	90	GLN
4	r	147	GLN
4	r	181	LEU
4	r	188	LYS
3	s	78	LEU
3	s	92	CYS
3	s	178	LEU
3	s	209	LYS
4	t	3	GLN
4	t	11	LEU
4	t	55	GLN
4	t	90	GLN
4	t	147	GLN
4	t	181	LEU
4	t	188	LYS
3	u	78	LEU
3	u	83	ARG
3	u	92	CYS
3	u	178	LEU
3	u	209	LYS
4	v	3	GLN

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Mol	Chain	Res	Type
4	v	11	LEU
4	v	55	GLN
4	v	90	GLN
4	v	147	GLN
4	v	181	LEU
4	v	188	LYS
3	w	78	LEU
3	w	92	CYS
3	w	178	LEU
3	w	197	ASN
3	w	209	LYS
4	x	3	GLN
4	x	11	LEU
4	x	55	GLN
4	x	90	GLN
4	x	147	GLN
4	x	181	LEU
4	x	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	137	ASN
1	A	189	GLN
2	B	53	ASN
2	B	60	ASN
2	B	125	GLN
1	C	53	ASN
2	D	53	ASN
2	D	60	ASN
2	D	125	GLN
1	E	53	ASN
1	E	189	GLN
1	E	211	GLN
2	F	53	ASN
2	F	60	ASN
2	F	125	GLN
1	G	53	ASN
2	H	53	ASN
2	H	60	ASN
2	H	125	GLN

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Mol	Chain	Res	Type
1	I	53	ASN
1	I	189	GLN
2	J	53	ASN
2	J	60	ASN
2	J	125	GLN
1	K	18	HIS
1	K	53	ASN
1	K	189	GLN
2	L	53	ASN
2	L	60	ASN
2	L	125	GLN
1	M	18	HIS
1	M	53	ASN
2	N	53	ASN
2	N	60	ASN
2	N	125	GLN
1	O	53	ASN
2	P	53	ASN
2	P	60	ASN
2	P	125	GLN
1	Q	53	ASN
1	Q	189	GLN
1	Q	211	GLN
2	R	53	ASN
2	R	60	ASN
2	R	125	GLN
1	S	53	ASN
1	S	189	GLN
2	T	53	ASN
2	T	60	ASN
2	T	125	GLN
1	U	18	HIS
1	U	53	ASN
2	V	53	ASN
2	V	60	ASN
2	V	125	GLN
1	W	53	ASN
2	X	53	ASN
2	X	60	ASN
2	X	125	GLN
3	a	192	GLN
4	b	55	GLN

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Mol	Chain	Res	Type
4	b	189	HIS
4	b	199	GLN
3	c	192	GLN
4	d	55	GLN
4	d	189	HIS
4	d	199	GLN
3	e	192	GLN
4	f	55	GLN
4	f	189	HIS
4	f	199	GLN
3	g	192	GLN
4	h	55	GLN
4	h	189	HIS
4	h	199	GLN
3	i	192	GLN
4	j	55	GLN
4	j	189	HIS
4	j	199	GLN
3	k	192	GLN
4	l	55	GLN
4	l	189	HIS
3	m	192	GLN
4	n	55	GLN
4	n	189	HIS
4	n	199	GLN
3	o	192	GLN
4	p	55	GLN
4	p	189	HIS
4	p	199	GLN
3	q	192	GLN
4	r	55	GLN
4	r	189	HIS
4	r	199	GLN
3	s	192	GLN
4	t	55	GLN
4	t	189	HIS
4	t	199	GLN
3	u	192	GLN
4	v	55	GLN
4	v	189	HIS
4	v	199	GLN
3	w	192	GLN

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Mol	Chain	Res	Type
4	x	55	GLN
4	x	189	HIS
4	x	199	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PCA	s	1	3	7,8,9	2.30	2 (28%)	9,10,12	2.32	5 (55%)
3	PCA	u	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.32	5 (55%)
3	PCA	c	1	3	7,8,9	2.20	2 (28%)	9,10,12	2.33	5 (55%)
3	PCA	k	1	3	7,8,9	2.15	2 (28%)	9,10,12	2.36	5 (55%)
3	PCA	i	1	3	7,8,9	2.24	2 (28%)	9,10,12	2.23	5 (55%)
3	PCA	g	1	3	7,8,9	2.09	2 (28%)	9,10,12	2.34	5 (55%)
3	PCA	m	1	3	7,8,9	2.14	2 (28%)	9,10,12	2.12	5 (55%)
3	PCA	a	1	3	7,8,9	2.29	2 (28%)	9,10,12	2.30	5 (55%)
3	PCA	q	1	3	7,8,9	2.11	2 (28%)	9,10,12	2.24	5 (55%)
3	PCA	w	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.27	5 (55%)
3	PCA	e	1	3	7,8,9	2.18	2 (28%)	9,10,12	2.31	5 (55%)
3	PCA	o	1	3	7,8,9	2.19	2 (28%)	9,10,12	2.25	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	s	1	3	-	0/0/11/13	0/1/1/1
3	PCA	u	1	3	-	0/0/11/13	0/1/1/1
3	PCA	c	1	3	-	0/0/11/13	0/1/1/1
3	PCA	k	1	3	-	0/0/11/13	0/1/1/1
3	PCA	i	1	3	-	0/0/11/13	0/1/1/1
3	PCA	g	1	3	-	0/0/11/13	0/1/1/1
3	PCA	m	1	3	-	0/0/11/13	0/1/1/1
3	PCA	a	1	3	-	0/0/11/13	0/1/1/1
3	PCA	q	1	3	-	0/0/11/13	0/1/1/1
3	PCA	w	1	3	-	0/0/11/13	0/1/1/1
3	PCA	e	1	3	-	0/0/11/13	0/1/1/1
3	PCA	o	1	3	-	0/0/11/13	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1	PCA	CD-N	4.80	1.47	1.34
3	s	1	PCA	CD-N	4.78	1.47	1.34
3	i	1	PCA	CD-N	4.77	1.47	1.34
3	c	1	PCA	CD-N	4.75	1.47	1.34
3	u	1	PCA	CD-N	4.73	1.47	1.34
3	k	1	PCA	CD-N	4.68	1.46	1.34
3	e	1	PCA	CD-N	4.66	1.46	1.34
3	o	1	PCA	CD-N	4.66	1.46	1.34
3	w	1	PCA	CD-N	4.63	1.46	1.34
3	g	1	PCA	CD-N	4.61	1.46	1.34
3	m	1	PCA	CD-N	4.60	1.46	1.34
3	q	1	PCA	CD-N	4.57	1.46	1.34
3	s	1	PCA	CA-N	3.61	1.50	1.46
3	a	1	PCA	CA-N	3.55	1.50	1.46
3	i	1	PCA	CA-N	3.32	1.50	1.46
3	w	1	PCA	CA-N	3.28	1.50	1.46
3	o	1	PCA	CA-N	3.26	1.50	1.46
3	e	1	PCA	CA-N	3.23	1.50	1.46
3	c	1	PCA	CA-N	3.18	1.50	1.46
3	u	1	PCA	CA-N	3.18	1.50	1.46
3	m	1	PCA	CA-N	3.14	1.50	1.46
3	k	1	PCA	CA-N	3.00	1.50	1.46
3	q	1	PCA	CA-N	2.99	1.50	1.46
3	g	1	PCA	CA-N	2.82	1.49	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	e	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	s	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	o	1	PCA	CB-CA-C	-3.59	107.76	112.70
3	a	1	PCA	CB-CA-C	-3.58	107.77	112.70
3	w	1	PCA	CB-CA-C	-3.55	107.81	112.70
3	g	1	PCA	CB-CA-C	-3.44	107.97	112.70
3	k	1	PCA	OE-CD-CG	-3.42	120.80	126.76
3	c	1	PCA	CB-CA-C	-3.41	108.01	112.70
3	u	1	PCA	OE-CD-CG	-3.37	120.89	126.76
3	q	1	PCA	CB-CA-C	-3.35	108.09	112.70
3	u	1	PCA	CB-CA-C	-3.34	108.11	112.70
3	c	1	PCA	OE-CD-CG	-3.31	120.98	126.76
3	a	1	PCA	OE-CD-CG	-3.28	121.04	126.76
3	k	1	PCA	CA-N-CD	-3.24	102.48	113.58
3	i	1	PCA	CA-N-CD	-3.19	102.66	113.58
3	s	1	PCA	OE-CD-CG	-3.17	121.23	126.76
3	g	1	PCA	OE-CD-CG	-3.17	121.24	126.76
3	g	1	PCA	CA-N-CD	-3.16	102.77	113.58
3	c	1	PCA	CA-N-CD	-3.12	102.90	113.58
3	i	1	PCA	OE-CD-CG	-3.09	121.36	126.76
3	m	1	PCA	CB-CA-C	-3.08	108.46	112.70
3	u	1	PCA	CA-N-CD	-3.07	103.06	113.58
3	w	1	PCA	CA-N-CD	-3.03	103.21	113.58
3	q	1	PCA	CA-N-CD	-3.01	103.26	113.58
3	w	1	PCA	OE-CD-CG	-3.00	121.54	126.76
3	o	1	PCA	OE-CD-CG	-2.98	121.57	126.76
3	k	1	PCA	CB-CA-C	-2.97	108.61	112.70
3	e	1	PCA	CA-N-CD	-2.96	103.45	113.58
3	o	1	PCA	CA-N-CD	-2.96	103.45	113.58
3	i	1	PCA	CB-CA-N	2.96	111.79	103.30
3	k	1	PCA	CB-CA-N	2.94	111.75	103.30
3	a	1	PCA	CA-N-CD	-2.93	103.53	113.58
3	e	1	PCA	OE-CD-CG	-2.93	121.64	126.76
3	m	1	PCA	CA-N-CD	-2.93	103.53	113.58
3	q	1	PCA	OE-CD-CG	-2.90	121.71	126.76
3	s	1	PCA	CA-N-CD	-2.90	103.67	113.58
3	g	1	PCA	CB-CA-N	2.85	111.47	103.30
3	i	1	PCA	CB-CA-C	-2.84	108.80	112.70
3	c	1	PCA	CB-CA-N	2.82	111.38	103.30
3	m	1	PCA	CB-CA-N	2.75	111.18	103.30
3	q	1	PCA	CB-CA-N	2.74	111.17	103.30
3	u	1	PCA	CB-CA-N	2.73	111.12	103.30
3	w	1	PCA	CB-CA-N	2.72	111.11	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	e	1	PCA	CB-CA-N	2.67	110.97	103.30
3	k	1	PCA	CG-CD-N	2.65	115.25	108.39
3	g	1	PCA	CG-CD-N	2.64	115.22	108.39
3	o	1	PCA	CB-CA-N	2.63	110.86	103.30
3	m	1	PCA	OE-CD-CG	-2.56	122.30	126.76
3	a	1	PCA	CB-CA-N	2.55	110.62	103.30
3	u	1	PCA	CG-CD-N	2.54	114.97	108.39
3	c	1	PCA	CG-CD-N	2.51	114.89	108.39
3	i	1	PCA	CG-CD-N	2.50	114.86	108.39
3	s	1	PCA	CB-CA-N	2.48	110.41	103.30
3	w	1	PCA	CG-CD-N	2.46	114.76	108.39
3	q	1	PCA	CG-CD-N	2.45	114.73	108.39
3	o	1	PCA	CG-CD-N	2.42	114.65	108.39
3	a	1	PCA	CG-CD-N	2.41	114.63	108.39
3	s	1	PCA	CG-CD-N	2.41	114.62	108.39
3	e	1	PCA	CG-CD-N	2.38	114.54	108.39
3	m	1	PCA	CG-CD-N	2.33	114.42	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

72 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	$\#\|Z\| > 2$
5	NAG	0	1	5,1	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
5	NAG	0	2	5	14,14,15	0.59	0	17,19,21	0.82	1 (5%)
5	BMA	0	3	5	11,11,12	0.75	0	15,15,17	1.00	1 (6%)
5	MAN	0	4	5	11,11,12	0.68	0	15,15,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	1	1	6,1	14,14,15	0.59	0	17,19,21	0.66	0
6	NAG	1	2	6	14,14,15	0.47	0	17,19,21	0.89	1 (5%)
5	NAG	2	1	5,1	14,14,15	0.63	0	17,19,21	0.99	0
5	NAG	2	2	5	14,14,15	0.56	0	17,19,21	0.80	0
5	BMA	2	3	5	11,11,12	0.76	0	15,15,17	1.18	1 (6%)
5	MAN	2	4	5	11,11,12	0.60	0	15,15,17	0.83	1 (6%)
6	NAG	3	1	6,1	14,14,15	0.51	0	17,19,21	0.86	1 (5%)
6	NAG	3	2	6	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
5	NAG	4	1	5,1	14,14,15	0.52	0	17,19,21	0.86	0
5	NAG	4	2	5	14,14,15	0.54	0	17,19,21	0.80	1 (5%)
5	BMA	4	3	5	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
5	MAN	4	4	5	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
6	NAG	5	1	6,1	14,14,15	0.59	0	17,19,21	0.68	0
6	NAG	5	2	6	14,14,15	0.51	0	17,19,21	0.78	1 (5%)
5	NAG	6	1	5,1	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
5	NAG	6	2	5	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
5	BMA	6	3	5	11,11,12	0.77	0	15,15,17	1.02	1 (6%)
5	MAN	6	4	5	11,11,12	0.62	0	15,15,17	0.69	0
6	NAG	7	1	6,1	14,14,15	0.57	0	17,19,21	0.60	0
6	NAG	7	2	6	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
5	NAG	8	1	5,1	14,14,15	0.46	0	17,19,21	1.19	1 (5%)
5	NAG	8	2	5	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
5	BMA	8	3	5	11,11,12	0.70	0	15,15,17	1.02	1 (6%)
5	MAN	8	4	5	11,11,12	0.64	0	15,15,17	0.99	1 (6%)
6	NAG	9	1	6,1	14,14,15	0.58	0	17,19,21	0.74	0
6	NAG	9	2	6	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
5	NAG	AA	1	5,1	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
5	NAG	AA	2	5	14,14,15	0.57	0	17,19,21	0.82	0
5	BMA	AA	3	5	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
5	MAN	AA	4	5	11,11,12	0.63	0	15,15,17	0.97	1 (6%)
6	NAG	BA	1	6,1	14,14,15	0.56	0	17,19,21	0.71	0
6	NAG	BA	2	6	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
5	NAG	CA	1	5,1	14,14,15	0.51	0	17,19,21	0.93	0
5	NAG	CA	2	5	14,14,15	0.55	0	17,19,21	0.99	1 (5%)
5	BMA	CA	3	5	11,11,12	0.79	0	15,15,17	1.04	1 (6%)
5	MAN	CA	4	5	11,11,12	0.63	0	15,15,17	0.82	1 (6%)
6	NAG	DA	1	6,1	14,14,15	0.60	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	DA	2	6	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
5	NAG	EA	1	5,1	14,14,15	0.46	0	17,19,21	0.98	1 (5%)
5	NAG	EA	2	5	14,14,15	0.54	0	17,19,21	1.06	2 (11%)
5	BMA	EA	3	5	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
5	MAN	EA	4	5	11,11,12	0.63	0	15,15,17	0.75	1 (6%)
6	NAG	FA	1	6,1	14,14,15	0.58	0	17,19,21	0.75	1 (5%)
6	NAG	FA	2	6	14,14,15	0.55	0	17,19,21	0.76	0
5	NAG	GA	1	5,1	14,14,15	0.55	0	17,19,21	1.10	0
5	NAG	GA	2	5	14,14,15	0.56	0	17,19,21	1.01	1 (5%)
5	BMA	GA	3	5	11,11,12	0.79	0	15,15,17	0.96	1 (6%)
5	MAN	GA	4	5	11,11,12	0.63	0	15,15,17	0.77	1 (6%)
6	NAG	HA	1	6,1	14,14,15	0.53	0	17,19,21	0.75	0
6	NAG	HA	2	6	14,14,15	0.52	0	17,19,21	0.84	1 (5%)
5	NAG	IA	1	5,1	14,14,15	0.48	0	17,19,21	0.98	0
5	NAG	IA	2	5	14,14,15	0.57	0	17,19,21	0.66	0
5	BMA	IA	3	5	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
5	MAN	IA	4	5	11,11,12	0.59	0	15,15,17	0.81	1 (6%)
6	NAG	JA	1	6,1	14,14,15	0.58	0	17,19,21	0.59	0
6	NAG	JA	2	6	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
5	NAG	Y	1	5,1	14,14,15	0.50	0	17,19,21	1.11	1 (5%)
5	NAG	Y	2	5	14,14,15	0.65	0	17,19,21	1.21	2 (11%)
5	BMA	Y	3	5	11,11,12	0.75	0	15,15,17	1.29	3 (20%)
5	MAN	Y	4	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	Z	1	6,1	14,14,15	0.55	0	17,19,21	0.55	0
6	NAG	Z	2	6	14,14,15	0.48	0	17,19,21	0.70	0
5	NAG	y	1	5,1	14,14,15	0.53	0	17,19,21	0.85	0
5	NAG	y	2	5	14,14,15	0.55	0	17,19,21	0.69	0
5	BMA	y	3	5	11,11,12	0.71	0	15,15,17	1.29	2 (13%)
5	MAN	y	4	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	z	1	6,1	14,14,15	0.61	0	17,19,21	0.79	1 (5%)
6	NAG	z	2	6	14,14,15	0.45	0	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	0	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	0/2/19/22	0/1/1/1
5	MAN	0	4	5	-	1/2/19/22	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	0/6/23/26	0/1/1/1
5	NAG	2	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	2	2	5	-	0/6/23/26	0/1/1/1
5	BMA	2	3	5	-	0/2/19/22	0/1/1/1
5	MAN	2	4	5	-	2/2/19/22	0/1/1/1
6	NAG	3	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
5	NAG	4	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	BMA	4	3	5	-	0/2/19/22	0/1/1/1
5	MAN	4	4	5	-	0/2/19/22	0/1/1/1
6	NAG	5	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	5	2	6	-	0/6/23/26	0/1/1/1
5	NAG	6	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	6	2	5	-	0/6/23/26	0/1/1/1
5	BMA	6	3	5	-	0/2/19/22	0/1/1/1
5	MAN	6	4	5	-	0/2/19/22	0/1/1/1
6	NAG	7	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
5	NAG	8	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	8	2	5	-	0/6/23/26	0/1/1/1
5	BMA	8	3	5	-	0/2/19/22	0/1/1/1
5	MAN	8	4	5	-	2/2/19/22	0/1/1/1
6	NAG	9	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	9	2	6	-	0/6/23/26	0/1/1/1
5	NAG	AA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	BA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	BA	2	6	-	0/6/23/26	0/1/1/1
5	NAG	CA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	CA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	CA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	CA	4	5	-	2/2/19/22	0/1/1/1
6	NAG	DA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	3	BMA	C1-C2-C3	3.68	114.19	109.67
5	2	3	BMA	C1-C2-C3	3.51	113.99	109.67
5	Y	2	NAG	O5-C5-C6	3.33	112.43	107.20
5	EA	3	BMA	C1-C2-C3	3.31	113.73	109.67
6	3	2	NAG	C1-O5-C5	3.30	116.67	112.19
5	8	1	NAG	C1-O5-C5	3.22	116.55	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	3	BMA	C1-C2-C3	3.09	113.46	109.67
5	y	3	BMA	C1-C2-C3	3.05	113.42	109.67
5	IA	3	BMA	C1-C2-C3	3.01	113.37	109.67
5	CA	3	BMA	C1-C2-C3	3.01	113.36	109.67
6	1	2	NAG	C1-O5-C5	2.92	116.16	112.19
5	GA	3	BMA	C1-C2-C3	2.87	113.19	109.67
5	AA	3	BMA	C1-C2-C3	2.86	113.18	109.67
5	6	3	BMA	C1-C2-C3	2.85	113.17	109.67
5	0	3	BMA	C1-C2-C3	2.83	113.15	109.67
5	8	3	BMA	C1-C2-C3	2.82	113.13	109.67
6	z	2	NAG	C1-O5-C5	2.82	116.01	112.19
6	7	2	NAG	C1-O5-C5	2.80	115.98	112.19
5	8	2	NAG	O5-C5-C6	2.72	111.47	107.20
5	Y	1	NAG	O5-C1-C2	-2.69	107.05	111.29
5	8	4	MAN	O5-C1-C2	-2.65	106.68	110.77
6	9	2	NAG	C1-O5-C5	2.63	115.76	112.19
5	EA	2	NAG	O5-C5-C6	2.63	111.33	107.20
6	JA	2	NAG	C1-O5-C5	2.61	115.73	112.19
5	4	4	MAN	O5-C1-C2	-2.60	106.75	110.77
5	6	2	NAG	O5-C5-C6	2.57	111.23	107.20
5	CA	2	NAG	O5-C5-C6	2.56	111.22	107.20
5	6	1	NAG	O5-C1-C2	-2.47	107.39	111.29
6	HA	2	NAG	C1-O5-C5	2.47	115.53	112.19
5	4	2	NAG	O5-C5-C6	2.44	111.03	107.20
6	5	2	NAG	C1-O5-C5	2.41	115.46	112.19
6	DA	2	NAG	C1-O5-C5	2.41	115.46	112.19
5	AA	4	MAN	O5-C1-C2	-2.41	107.06	110.77
6	DA	1	NAG	O5-C5-C6	2.29	110.79	107.20
5	y	3	BMA	O5-C5-C4	-2.26	105.34	110.83
5	IA	4	MAN	O5-C1-C2	-2.25	107.31	110.77
5	2	4	MAN	O5-C1-C2	-2.23	107.33	110.77
5	GA	2	NAG	O5-C5-C6	2.22	110.69	107.20
6	3	1	NAG	O5-C5-C6	2.20	110.66	107.20
5	0	4	MAN	O5-C1-C2	-2.20	107.38	110.77
5	0	2	NAG	O5-C5-C6	2.19	110.63	107.20
5	CA	4	MAN	O5-C1-C2	-2.18	107.40	110.77
5	EA	4	MAN	O5-C1-C2	-2.16	107.44	110.77
6	BA	2	NAG	C1-O5-C5	2.15	115.11	112.19
5	Y	2	NAG	C1-O5-C5	-2.14	109.29	112.19
5	Y	3	BMA	C1-O5-C5	2.13	115.08	112.19
5	AA	1	NAG	O5-C1-C2	-2.12	107.93	111.29
5	EA	1	NAG	C1-O5-C5	2.11	115.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	z	1	NAG	O5-C5-C6	2.11	110.50	107.20
6	FA	1	NAG	O5-C5-C6	2.08	110.46	107.20
5	Y	3	BMA	O5-C1-C2	2.07	113.96	110.77
5	GA	4	MAN	O5-C1-C2	-2.02	107.65	110.77
5	0	1	NAG	O5-C1-C2	-2.01	108.11	111.29
5	EA	2	NAG	O6-C6-C5	2.00	118.16	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

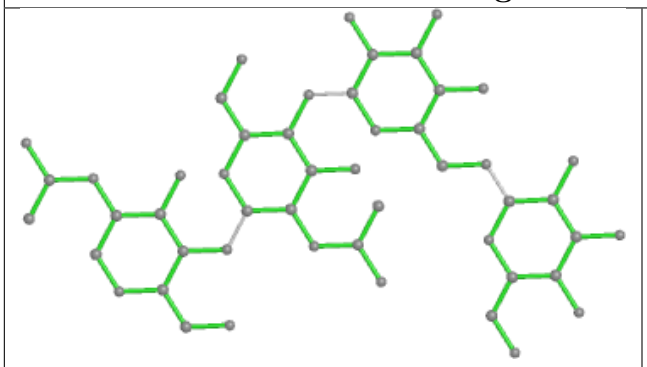
Mol	Chain	Res	Type	Atoms
5	8	4	MAN	C4-C5-C6-O6
5	EA	2	NAG	C4-C5-C6-O6
5	EA	2	NAG	O5-C5-C6-O6
5	AA	4	MAN	C4-C5-C6-O6
5	CA	4	MAN	C4-C5-C6-O6
5	8	4	MAN	O5-C5-C6-O6
5	Y	4	MAN	C4-C5-C6-O6
5	CA	4	MAN	O5-C5-C6-O6
5	2	4	MAN	C4-C5-C6-O6
5	GA	4	MAN	C4-C5-C6-O6
5	AA	4	MAN	O5-C5-C6-O6
5	EA	4	MAN	C4-C5-C6-O6
5	IA	4	MAN	C4-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	0	4	MAN	C4-C5-C6-O6
5	GA	4	MAN	O5-C5-C6-O6
5	GA	3	BMA	O5-C5-C6-O6
5	EA	4	MAN	O5-C5-C6-O6
5	2	4	MAN	O5-C5-C6-O6
5	IA	4	MAN	O5-C5-C6-O6

There are no ring outliers.

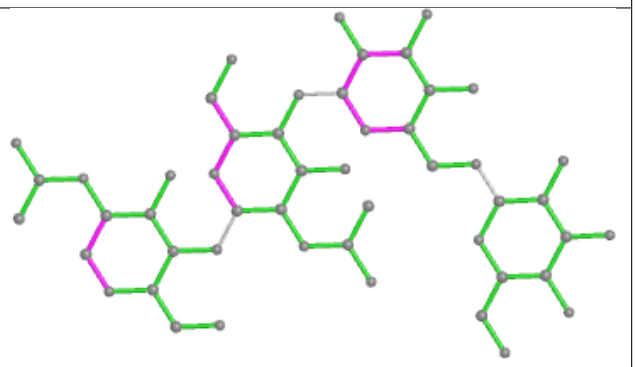
No monomer is involved in short contacts.

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

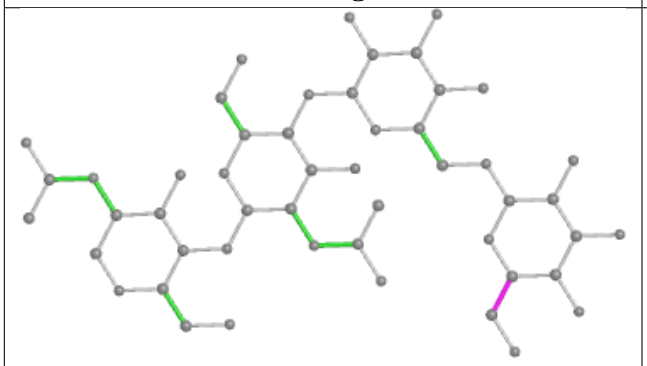
Oligosaccharide Chain Y



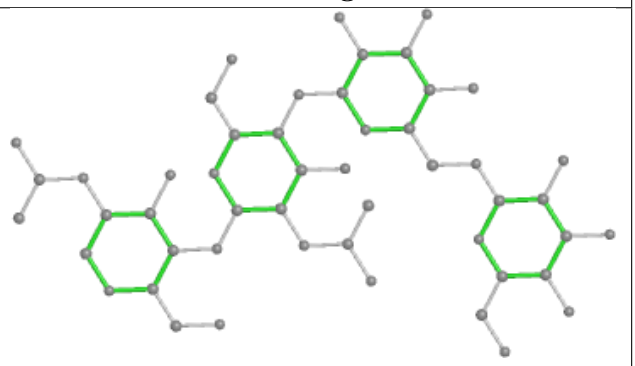
Bond lengths



Bond angles

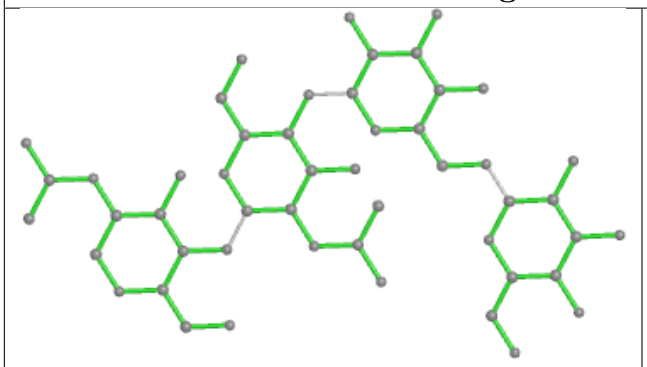


Torsions

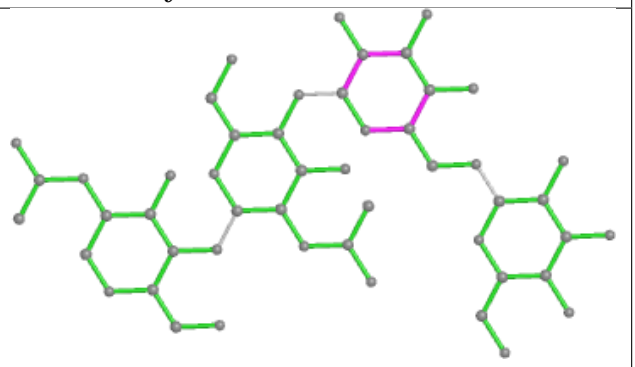


Rings

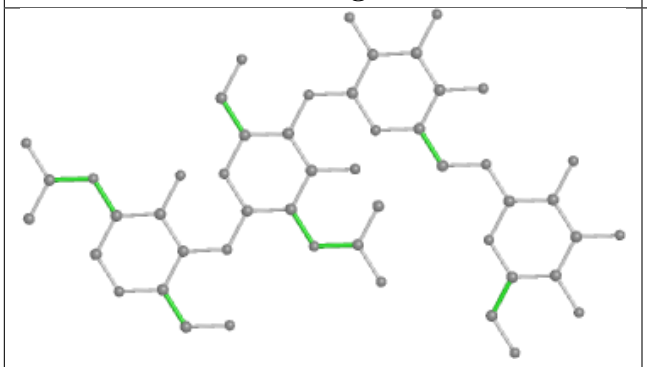
Oligosaccharide Chain y



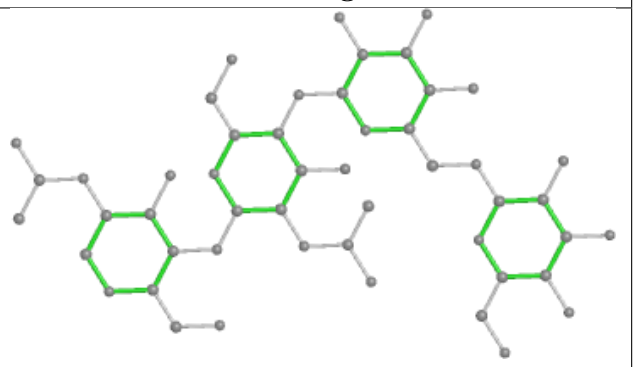
Bond lengths



Bond angles

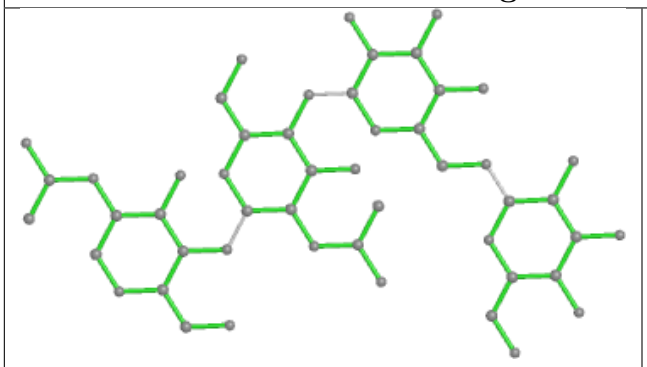


Torsions

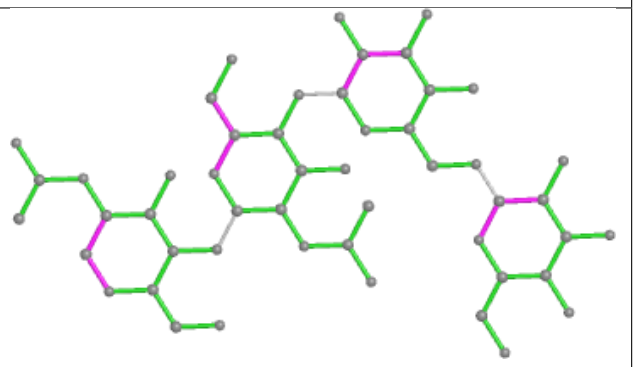


Rings

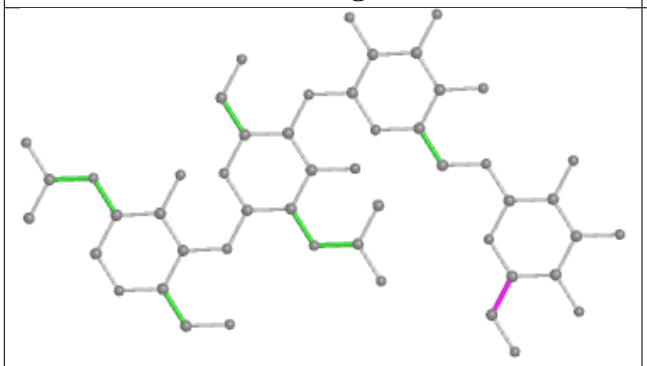
Oligosaccharide Chain 0



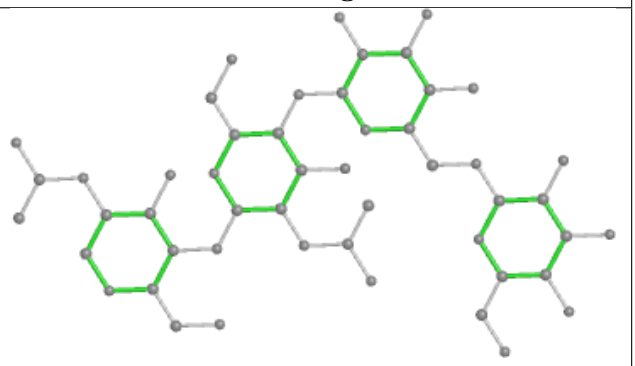
Bond lengths



Bond angles

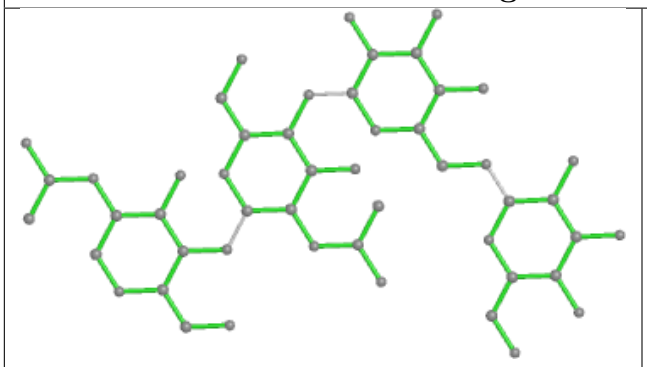


Torsions

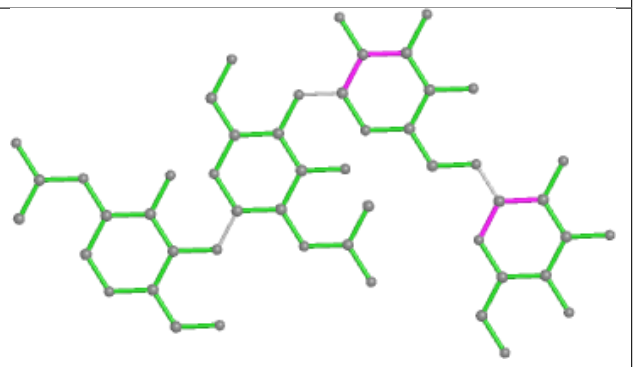


Rings

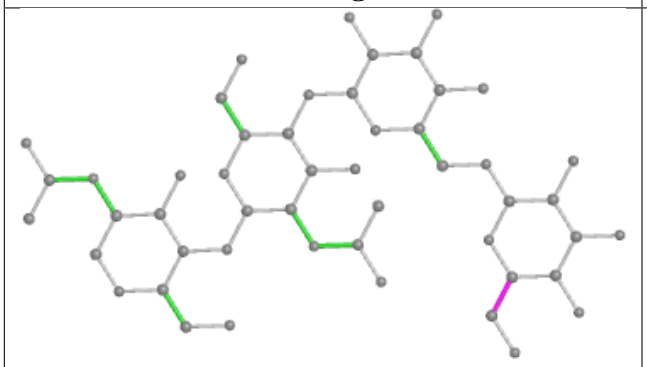
Oligosaccharide Chain 2



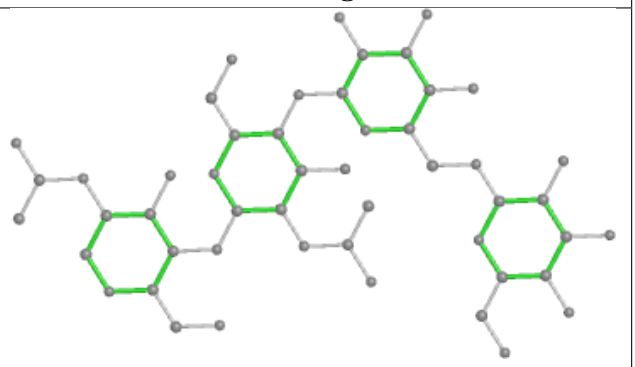
Bond lengths



Bond angles

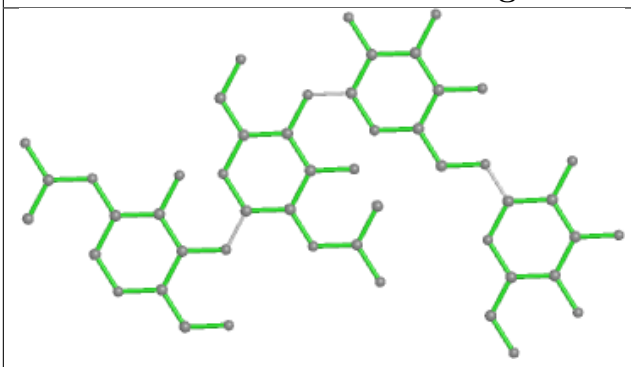


Torsions



Rings

Oligosaccharide Chain 4



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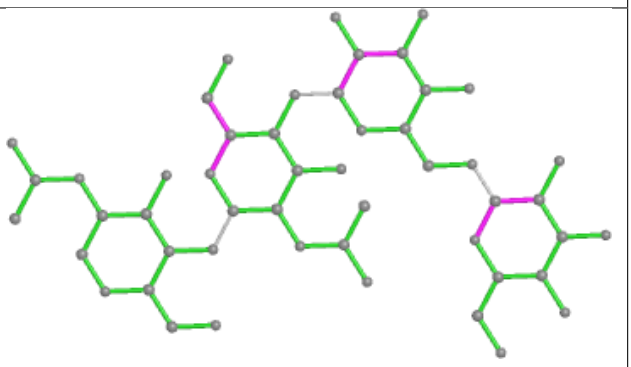
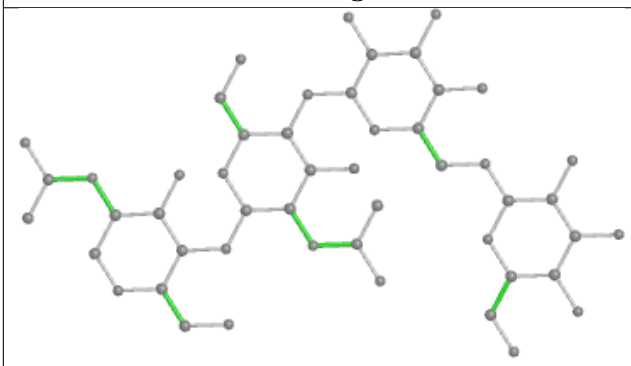


Bond angles



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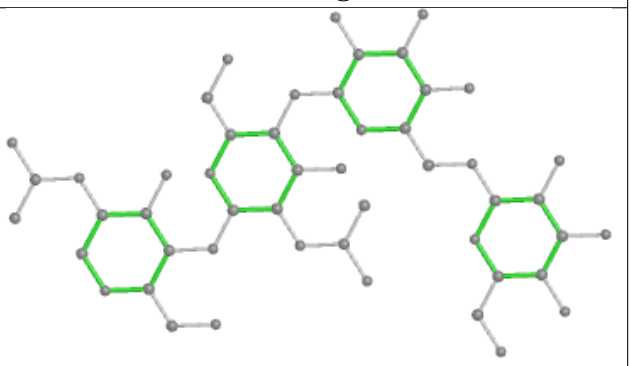
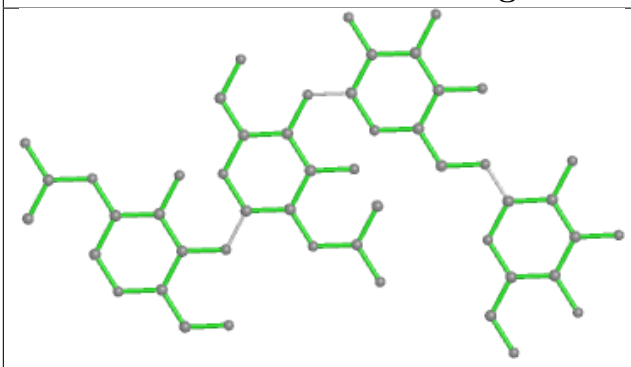


Rings

Oligosaccharide Chain 6



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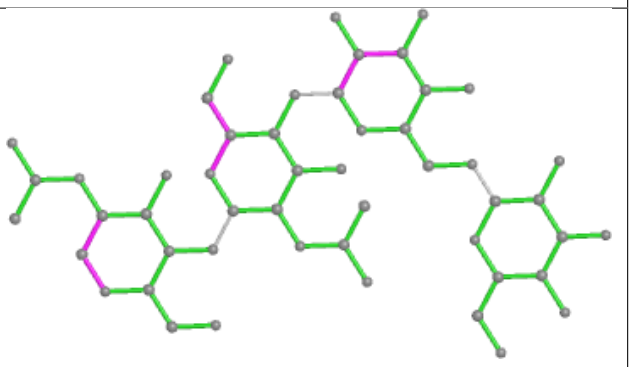
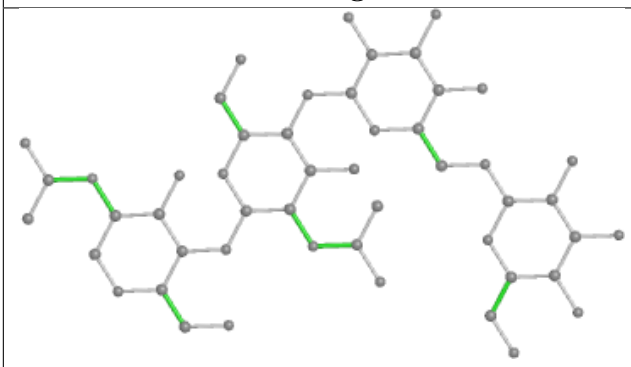


Bond angles



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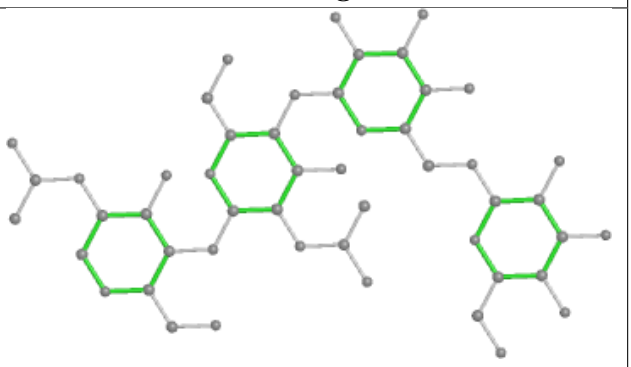
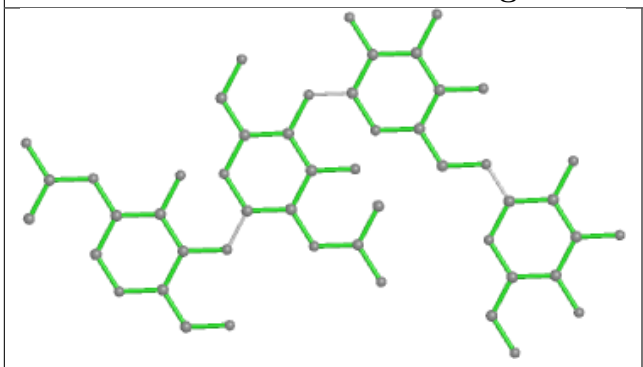
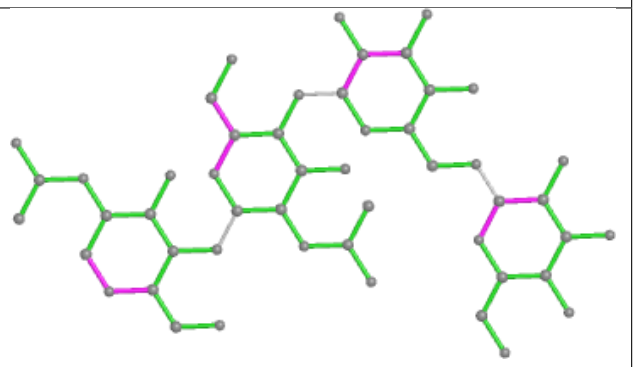


Rings

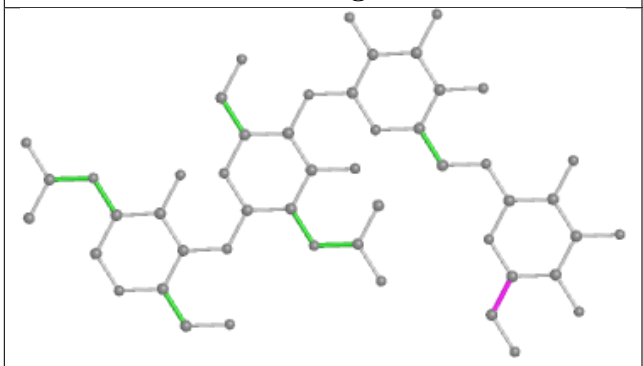
Oligosaccharide Chain 8



Bond lengths



Bond angles



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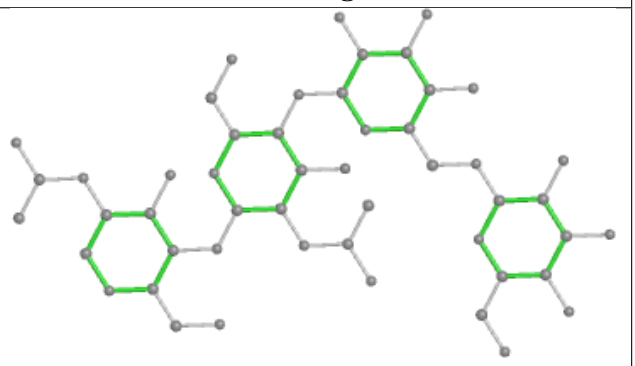
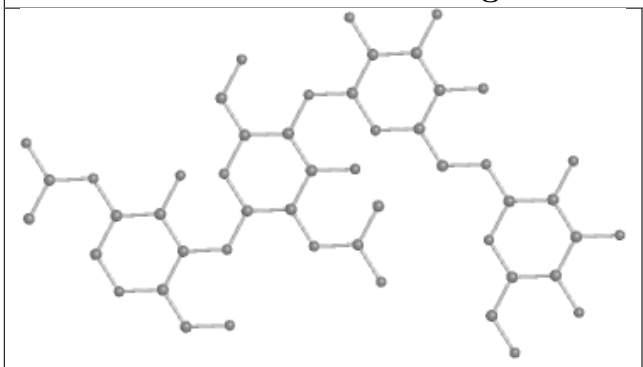
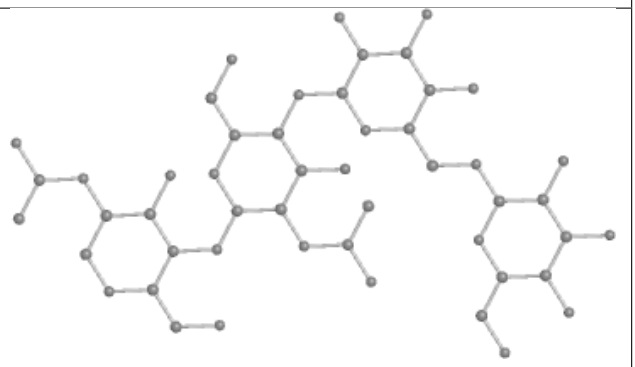


Rings

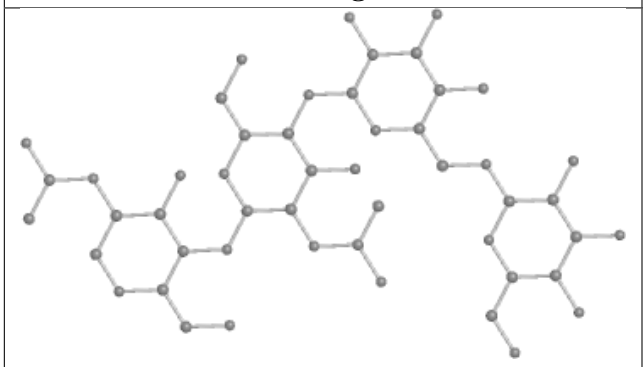
Oligosaccharide Chain AA



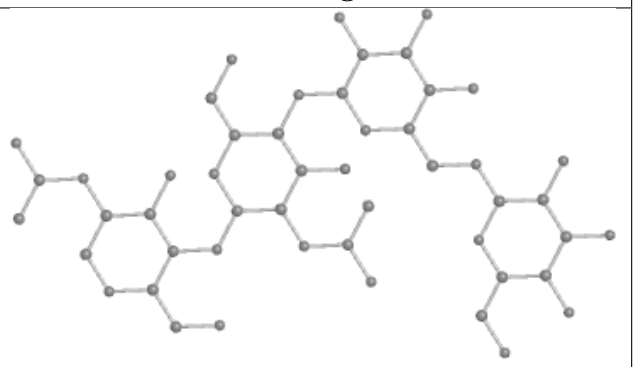
Bond lengths



Bond angles

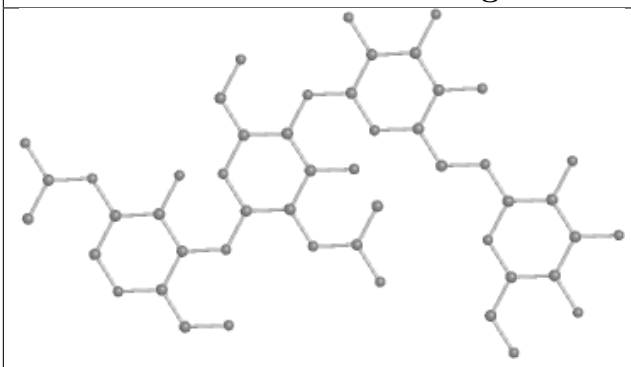


Torsions

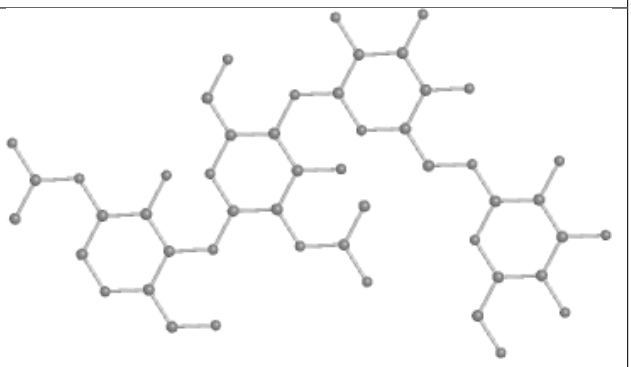


Rings

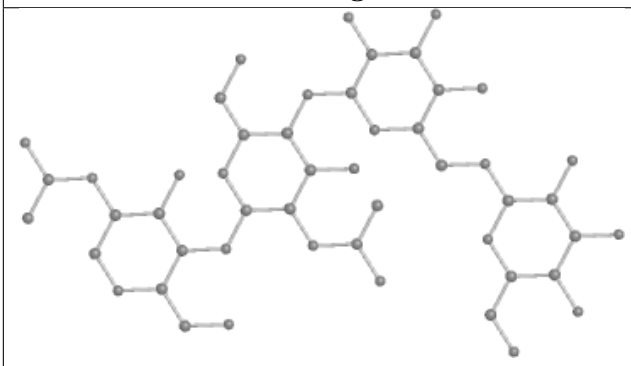
Oligosaccharide Chain CA



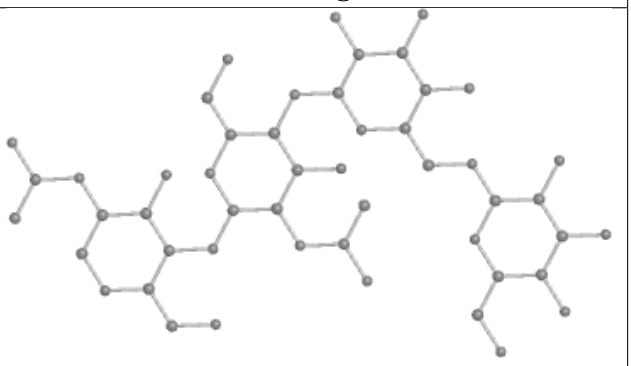
Bond lengths



Bond angles

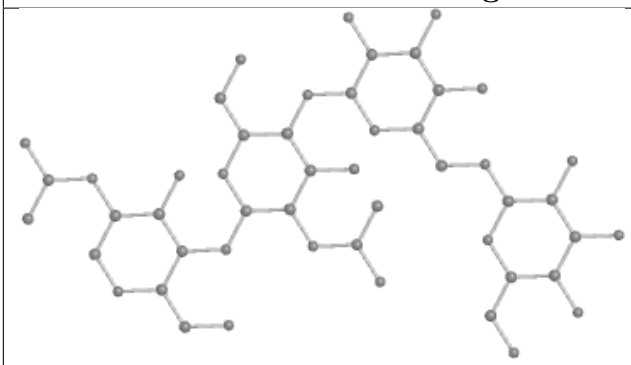


Torsions

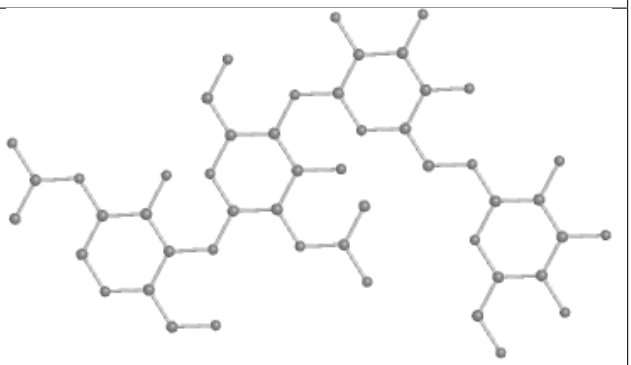


Rings

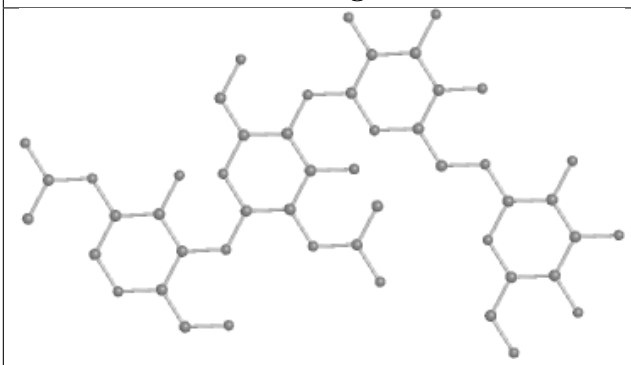
Oligosaccharide Chain EA



Bond lengths



Bond angles



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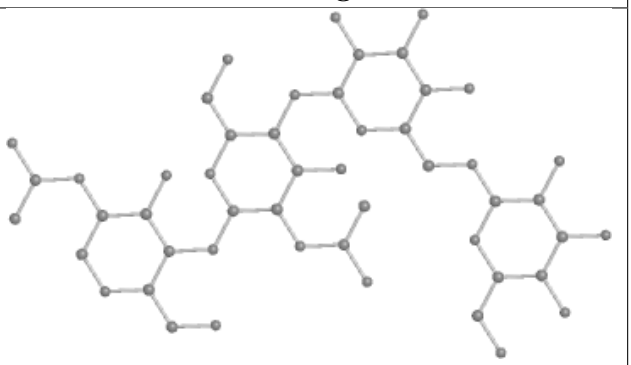
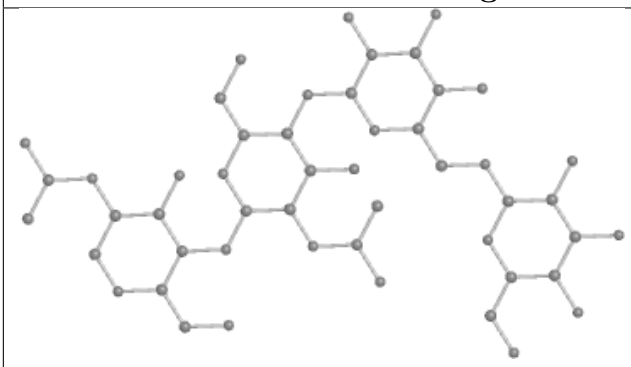


Rings

Oligosaccharide Chain GA



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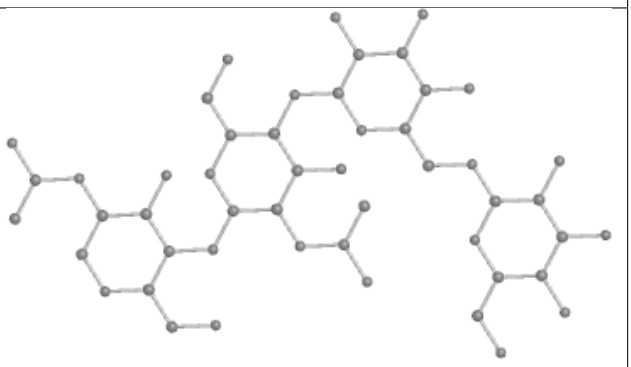

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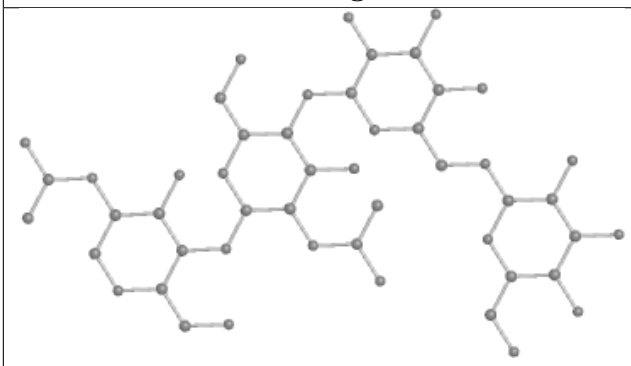

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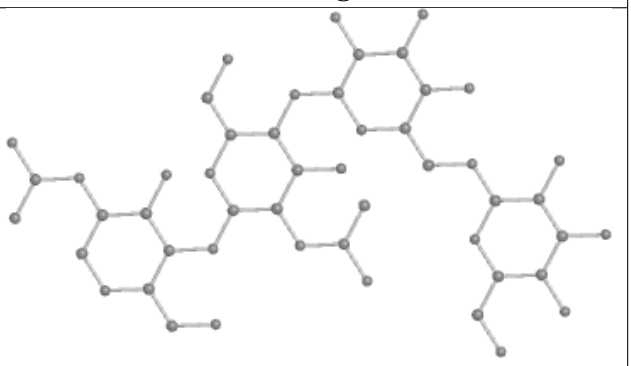
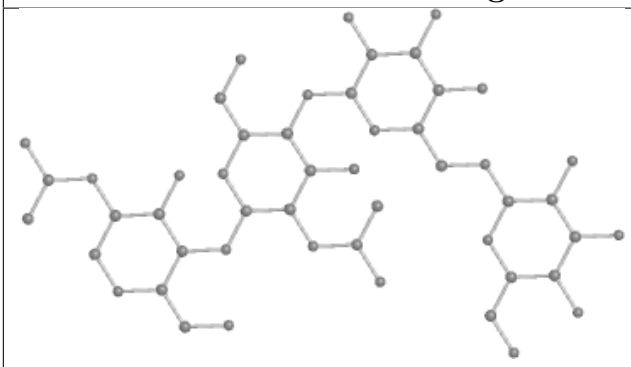


Rings

Oligosaccharide Chain IA



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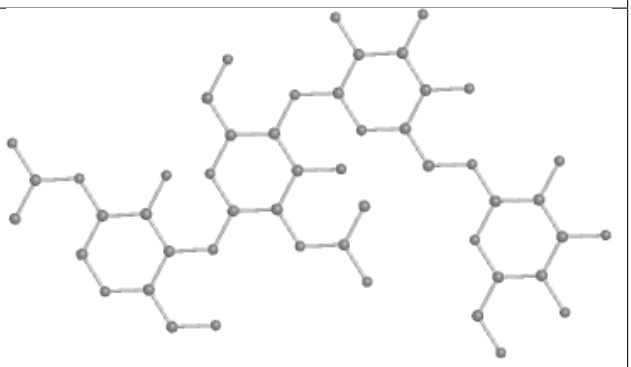

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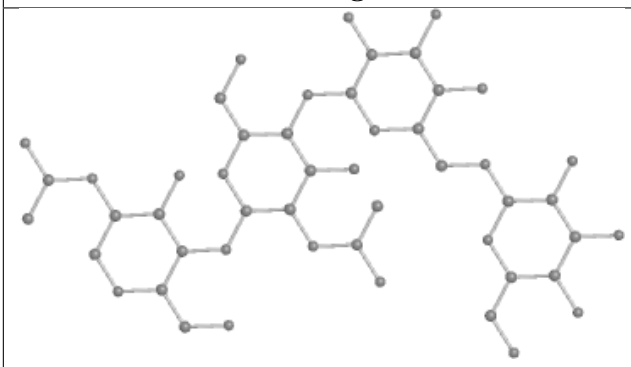

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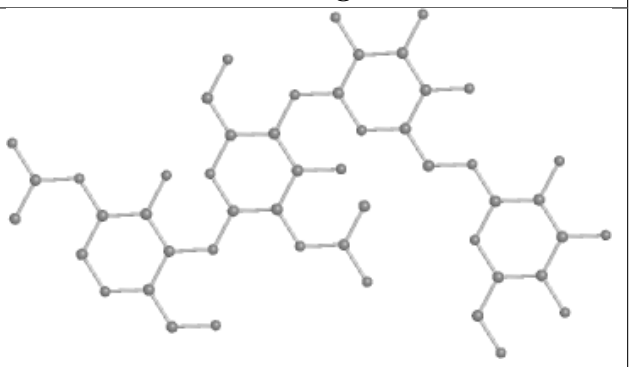
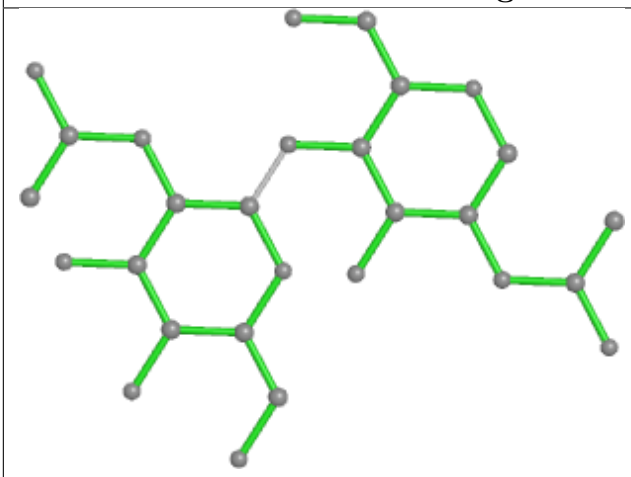
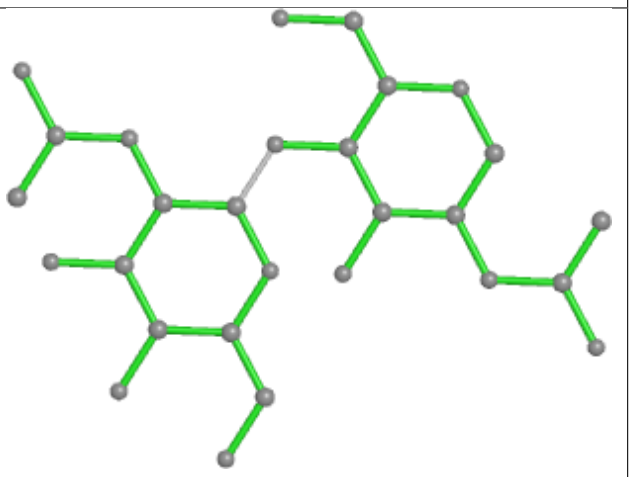
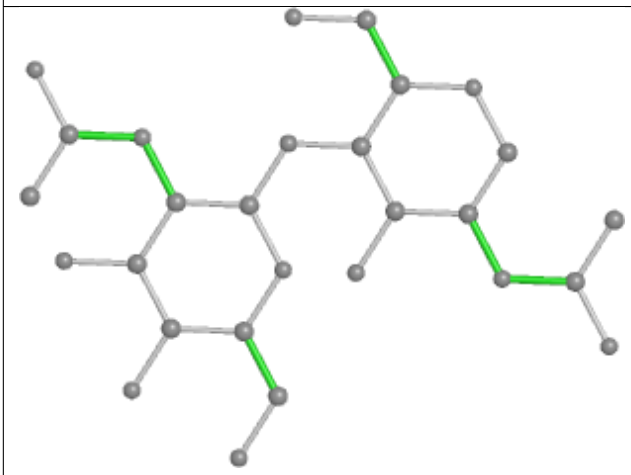
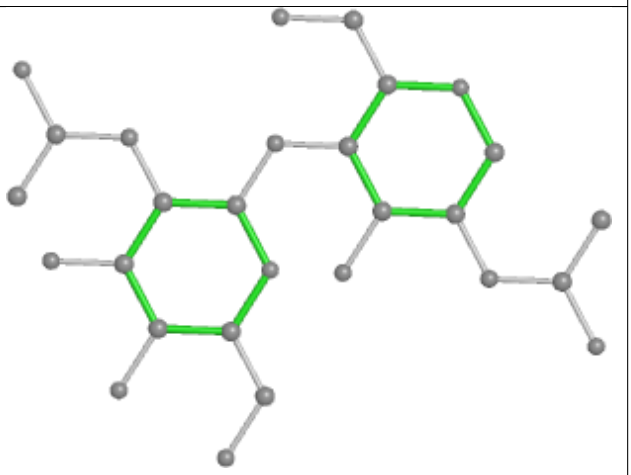
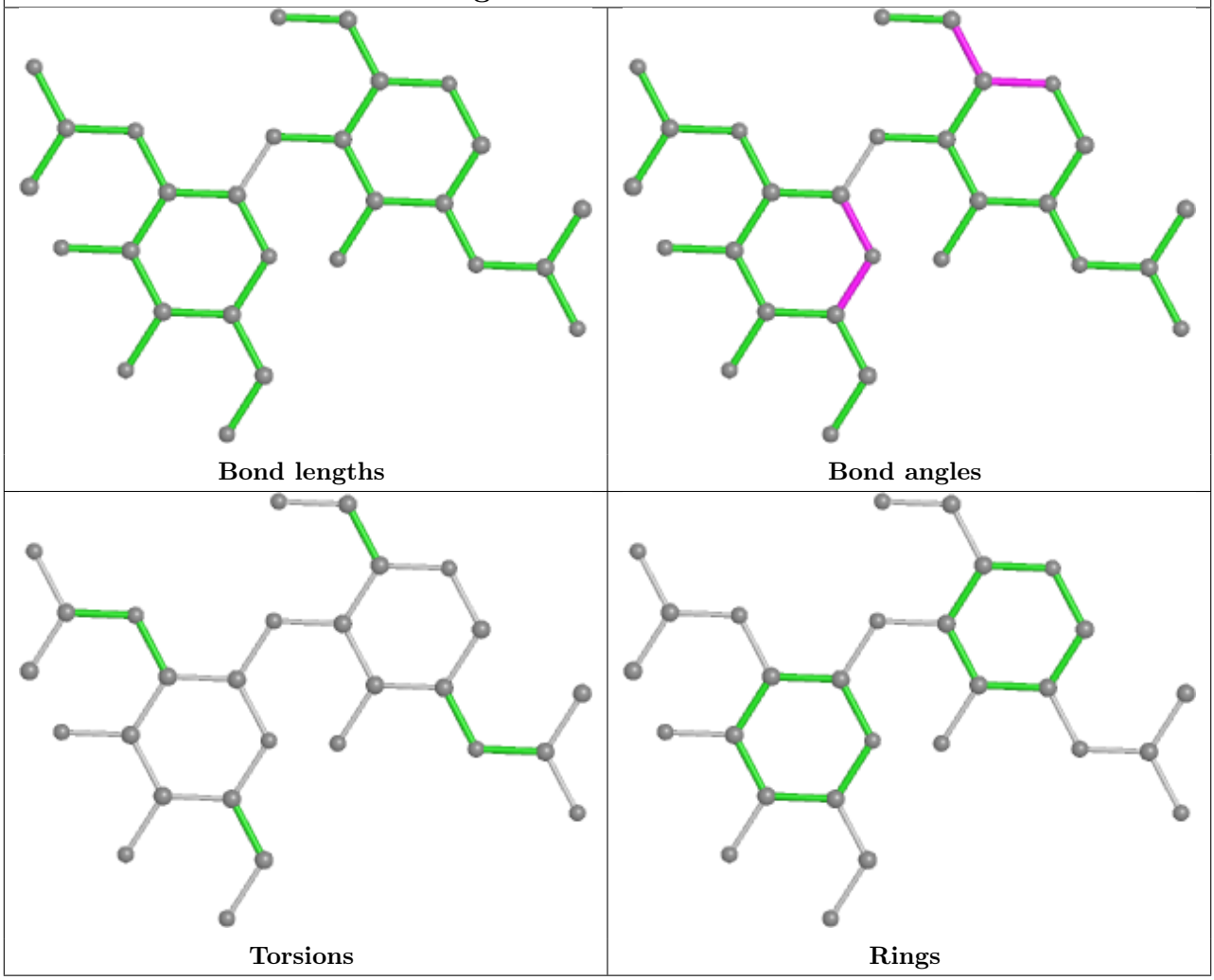


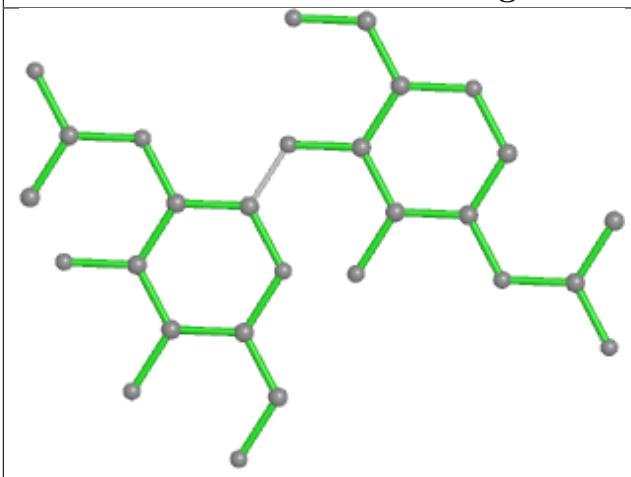
Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain z



Oligosaccharide Chain 1



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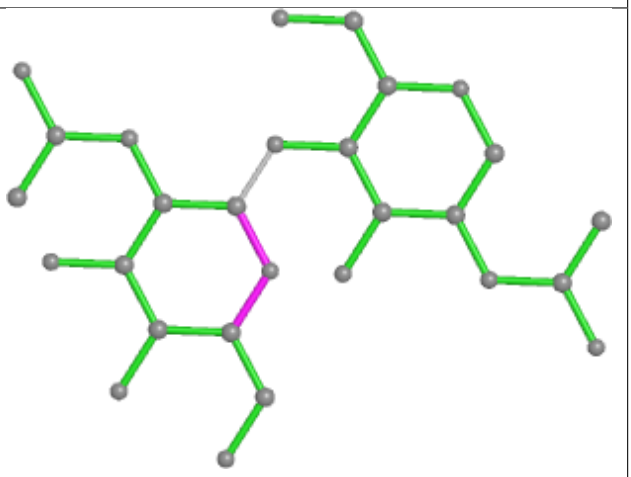
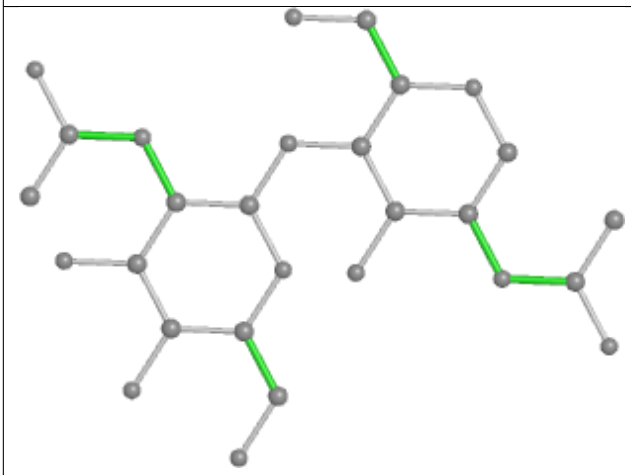


Bond angles



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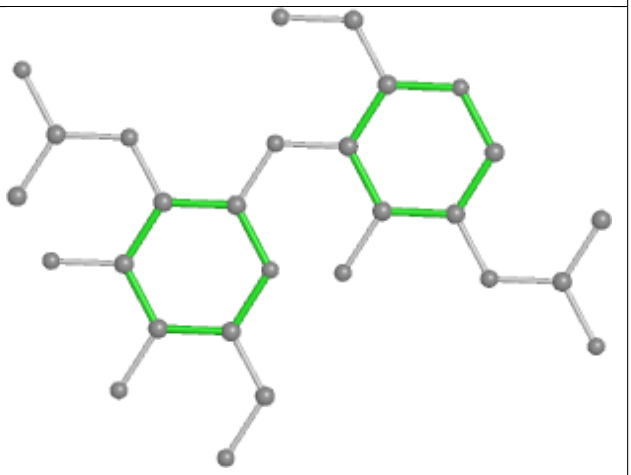
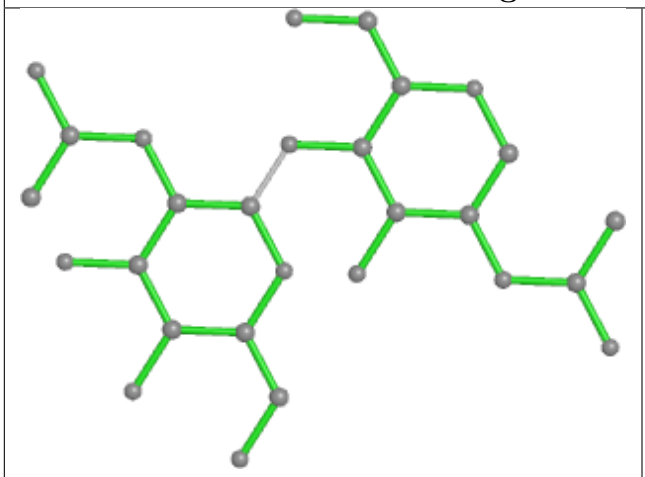


Rings

Oligosaccharide Chain 3



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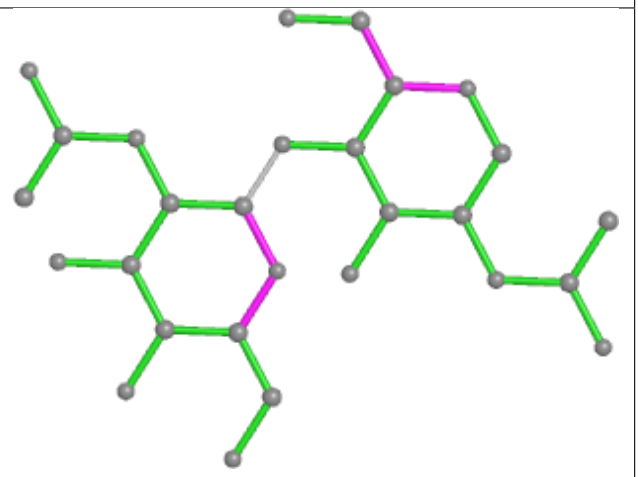

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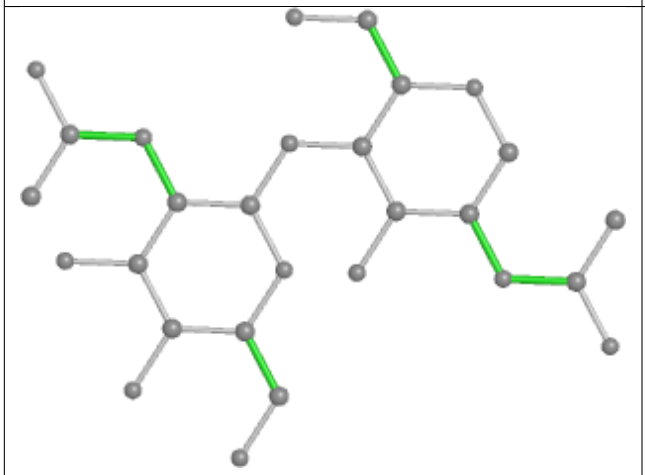

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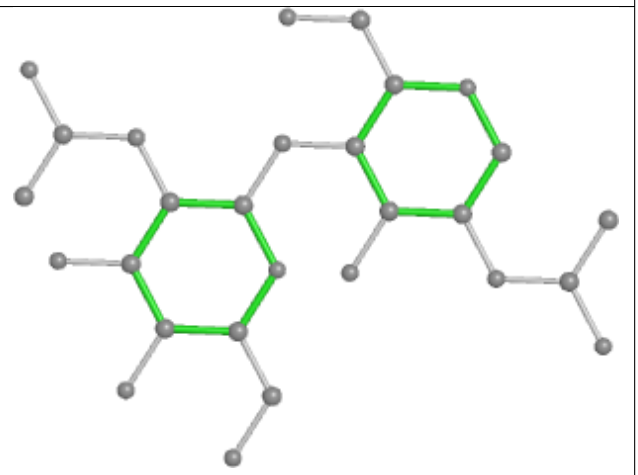
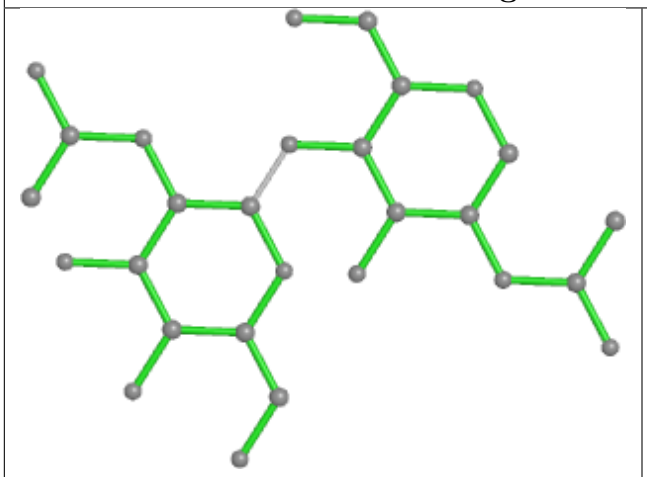


Rings

Oligosaccharide Chain 5



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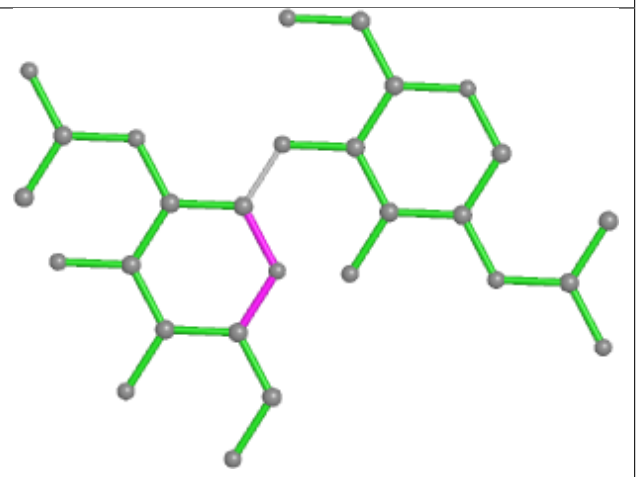

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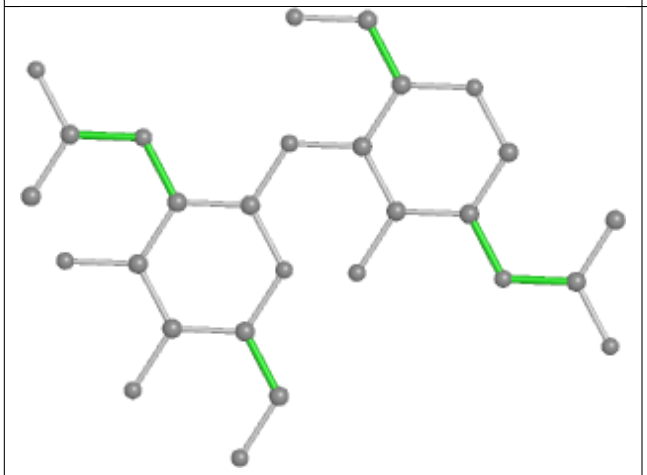

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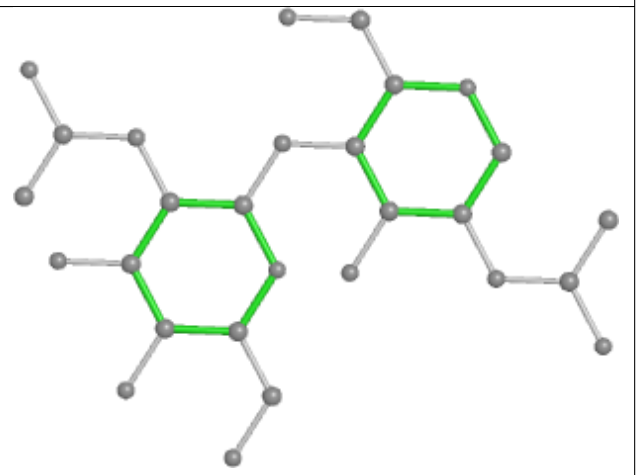
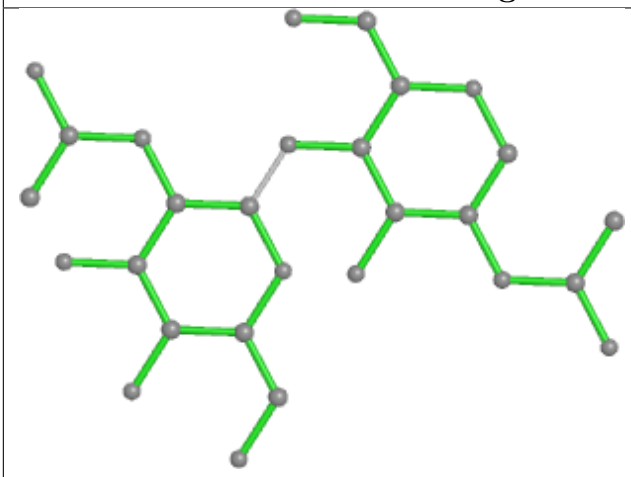


Rings

Oligosaccharide Chain 7



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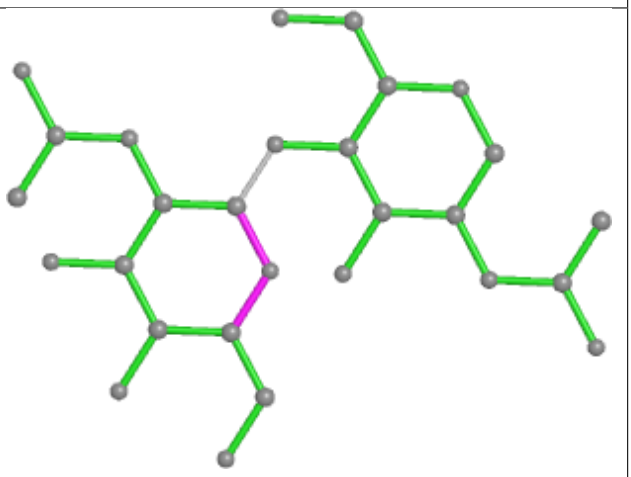

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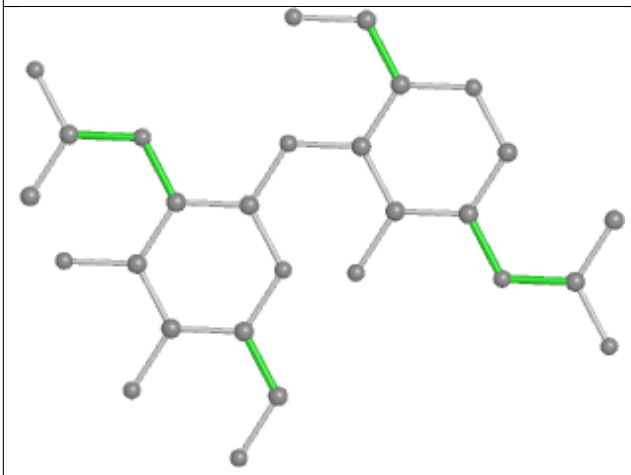

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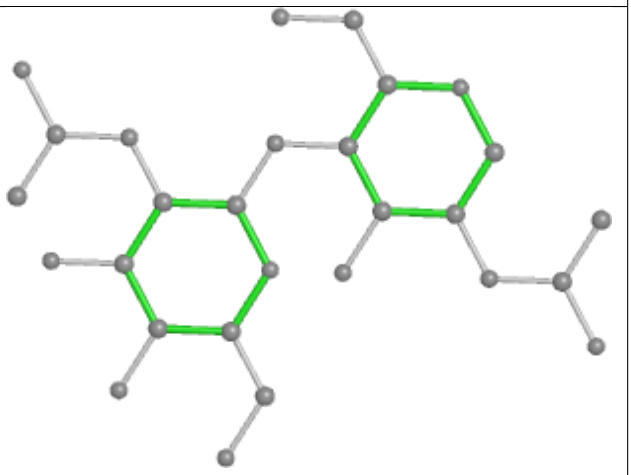
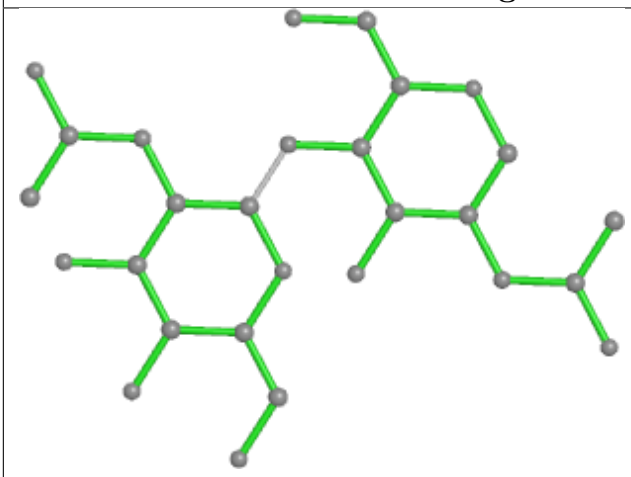


Rings

Oligosaccharide Chain 9



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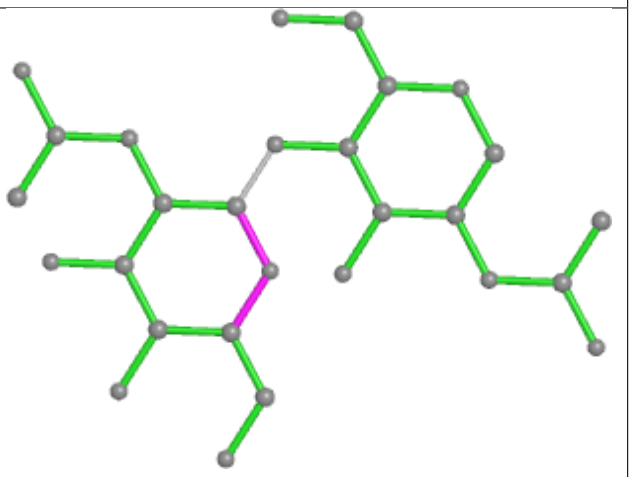

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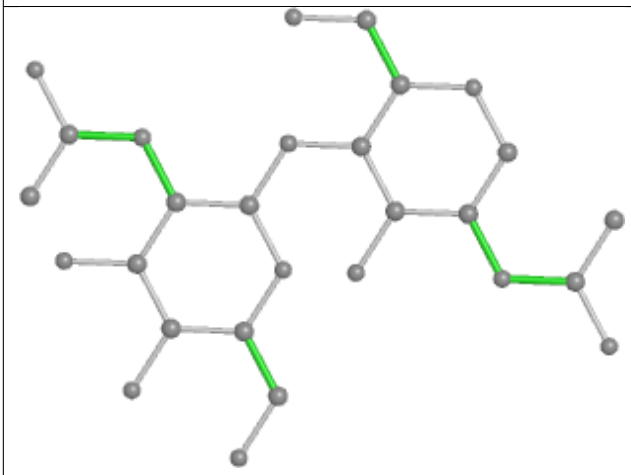

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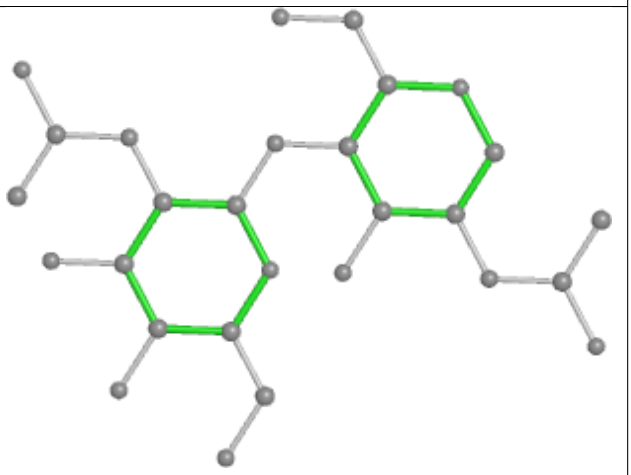
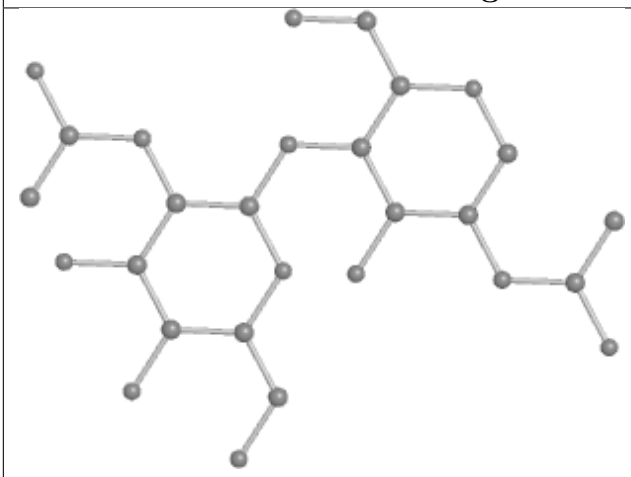
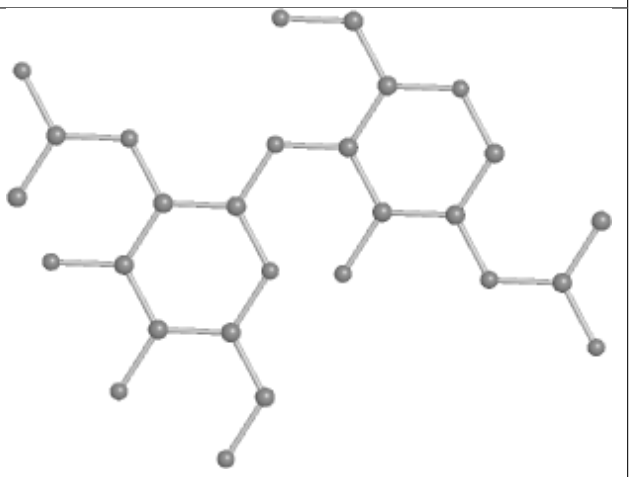
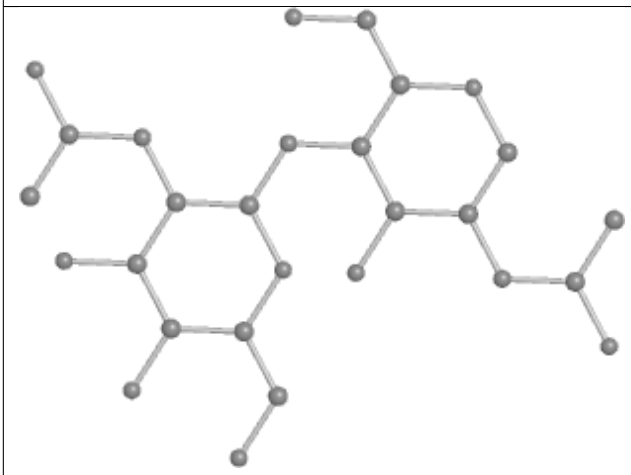
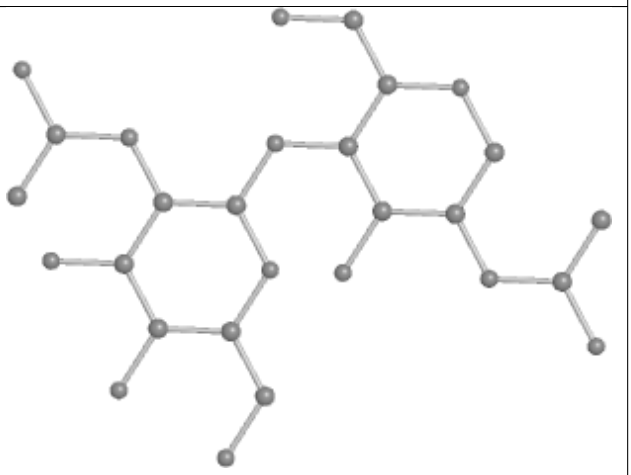


Rings

Oligosaccharide Chain BA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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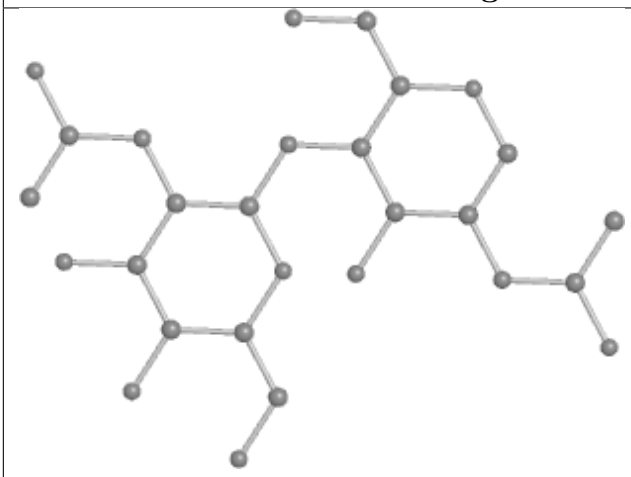
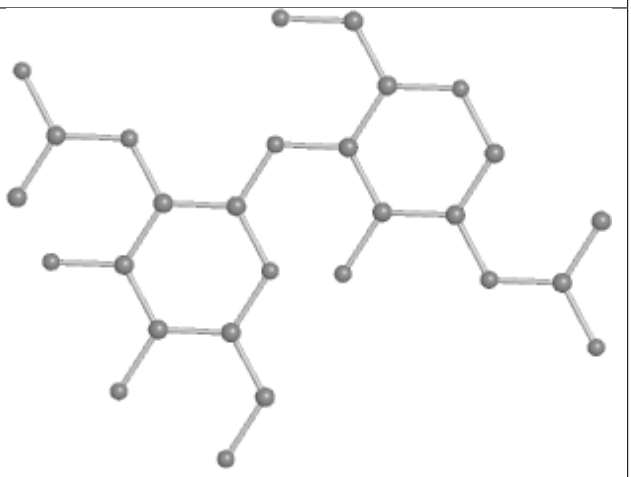
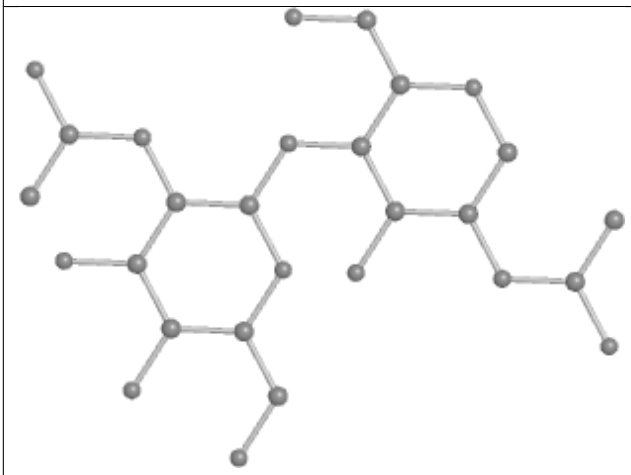
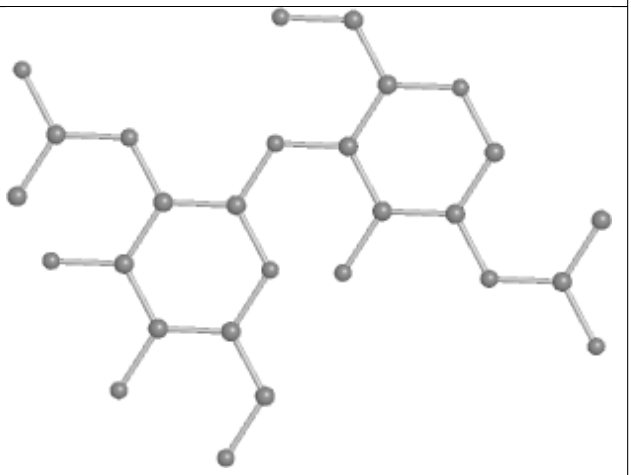
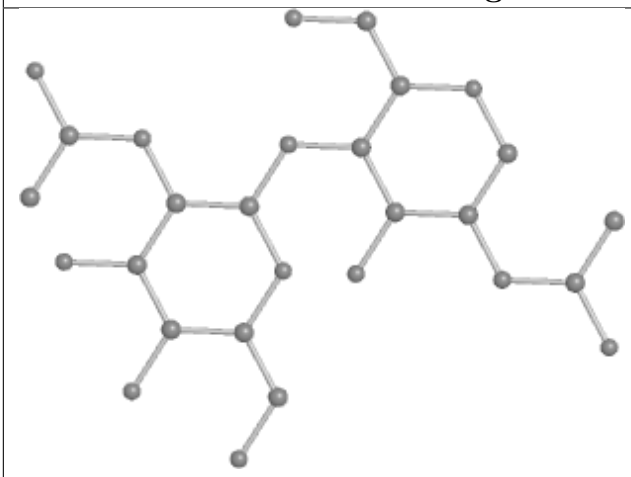
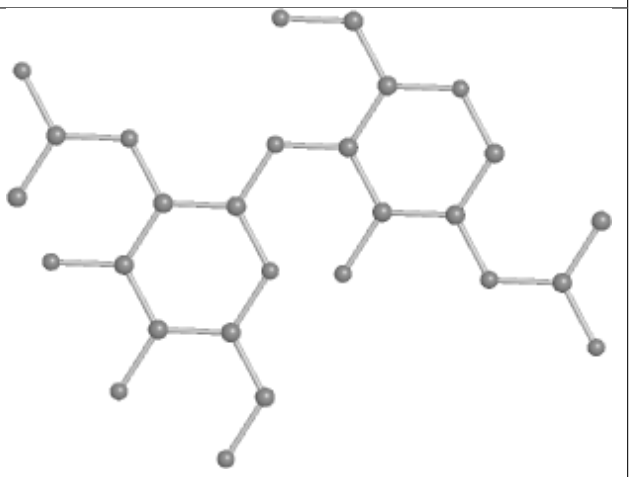
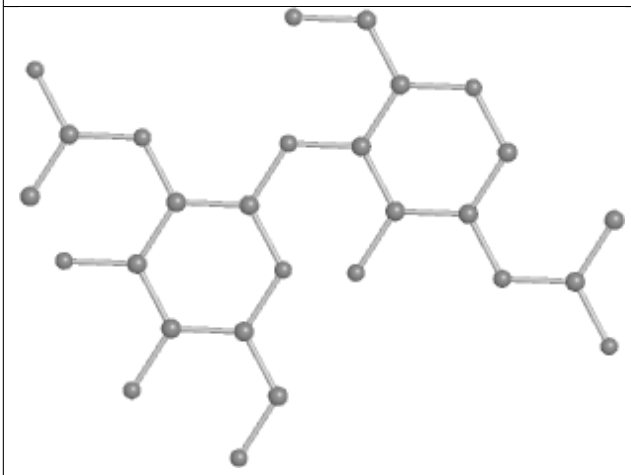
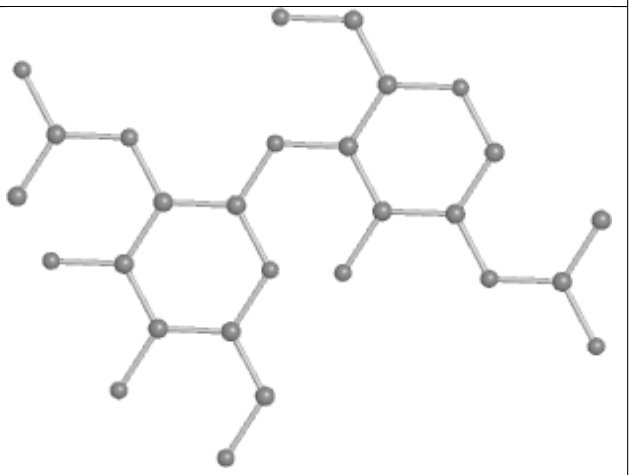
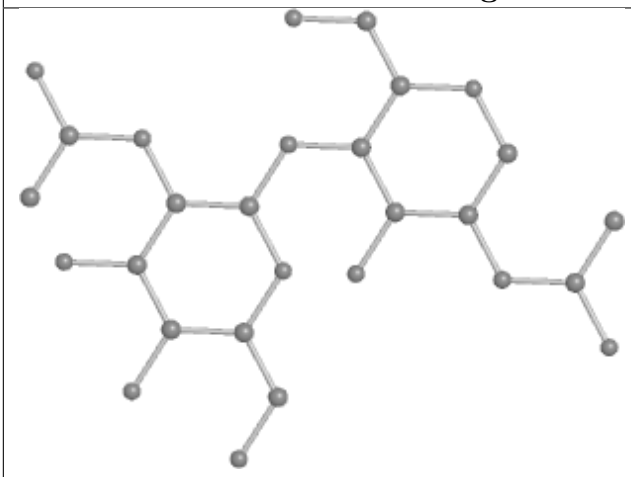
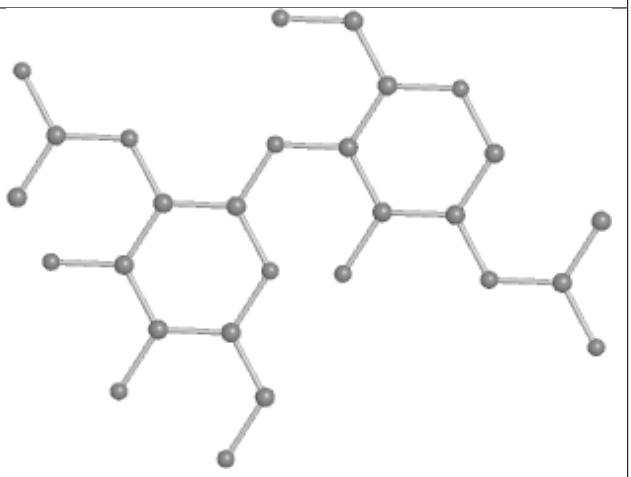
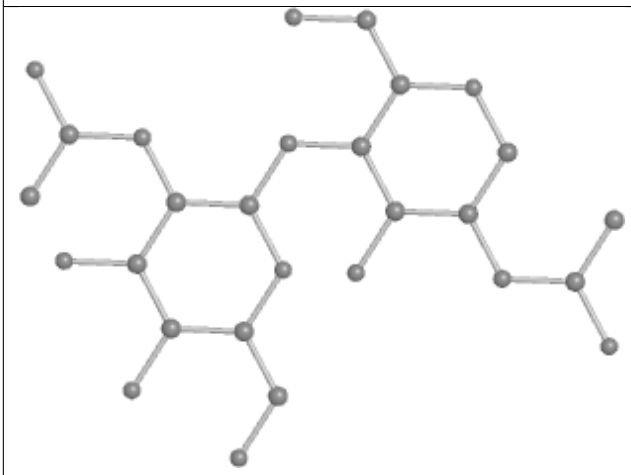
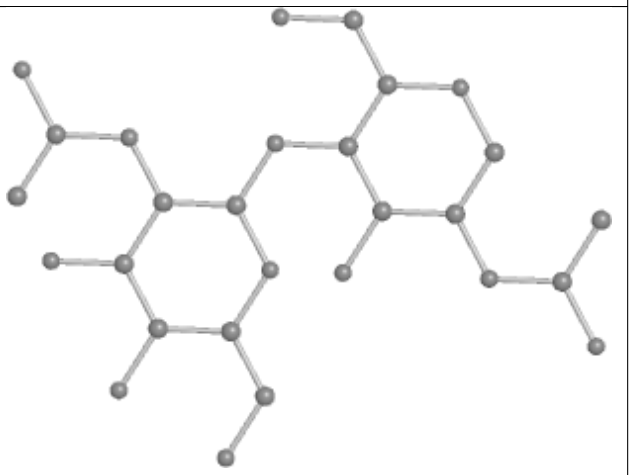
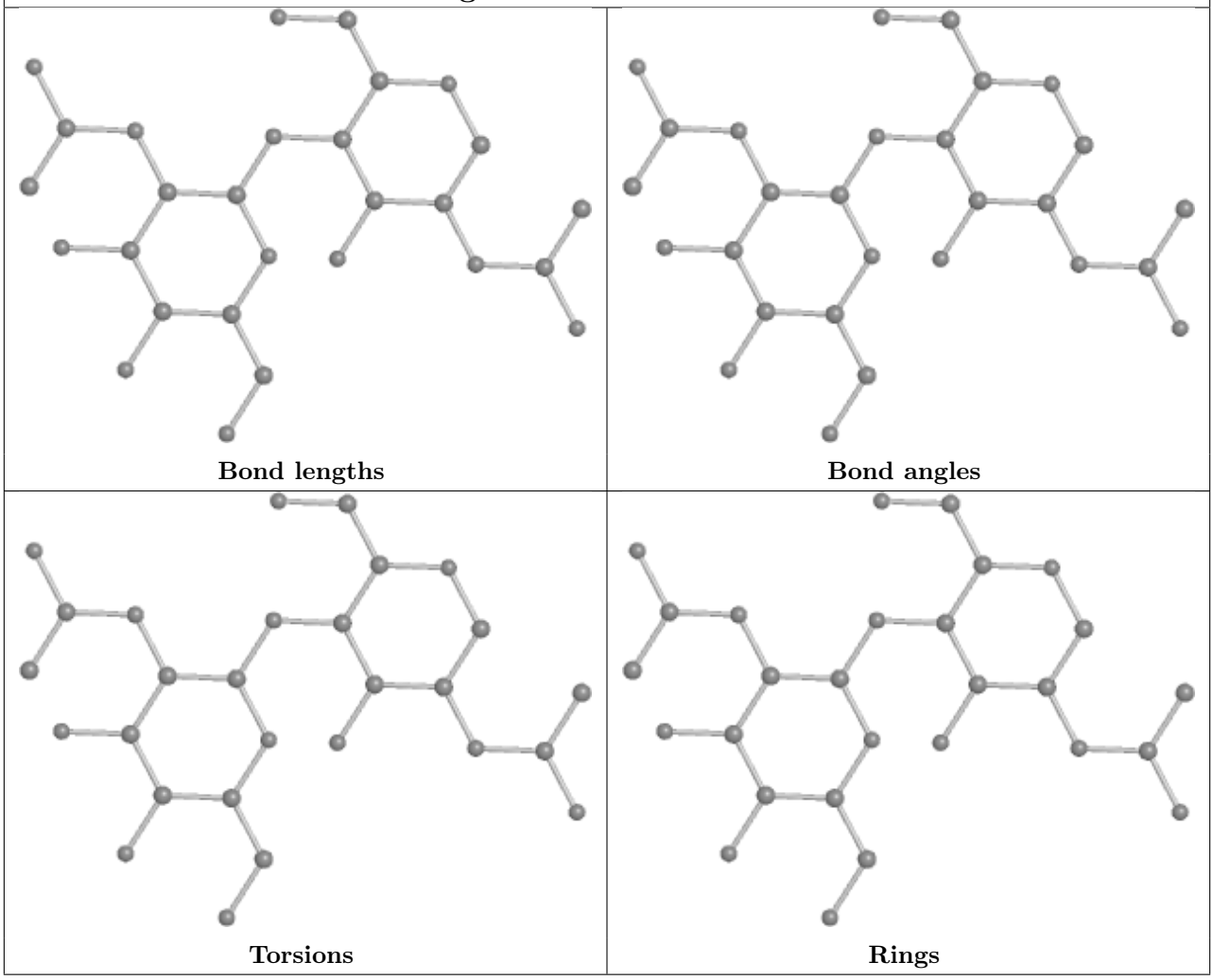
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain FA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain HA	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Oligosaccharide Chain JA



5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	601	1	14,14,15	1.56	2 (14%)	17,19,21	4.27	9 (52%)
7	NAG	E	601	1	14,14,15	0.47	0	17,19,21	1.40	2 (11%)
7	NAG	C	501	1	14,14,15	0.46	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	N	201	2	14,14,15	0.56	0	17,19,21	1.16	1 (5%)
7	NAG	S	501	1	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
7	NAG	B	201	2	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
7	NAG	L	201	2	14,14,15	0.56	0	17,19,21	0.91	0
7	NAG	Q	502	1	14,14,15	0.57	0	17,19,21	1.50	2 (11%)
7	NAG	M	502	1	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
7	NAG	D	201	2	14,14,15	0.53	0	17,19,21	1.20	1 (5%)
7	NAG	X	201	2	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
7	NAG	Q	501	1	14,14,15	0.44	0	17,19,21	1.05	1 (5%)
7	NAG	V	201	2	14,14,15	0.56	0	17,19,21	0.88	1 (5%)
7	NAG	G	501	1	14,14,15	0.40	0	17,19,21	1.07	1 (5%)
7	NAG	U	501	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)
7	NAG	J	201	2	14,14,15	0.52	0	17,19,21	1.22	1 (5%)
7	NAG	I	501	1	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
7	NAG	M	501	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
7	NAG	R	201	2	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
7	NAG	F	201	2	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
7	NAG	P	201	2	14,14,15	0.57	0	17,19,21	0.93	0
7	NAG	G	502	1	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
7	NAG	W	601	1	14,14,15	0.54	0	17,19,21	1.58	4 (23%)
7	NAG	H	201	2	14,14,15	0.58	0	17,19,21	0.92	1 (5%)
7	NAG	U	502	1	14,14,15	0.47	0	17,19,21	1.50	2 (11%)
7	NAG	S	502	1	14,14,15	0.52	0	17,19,21	1.57	3 (17%)
7	NAG	O	501	1	14,14,15	0.52	0	17,19,21	0.85	0
7	NAG	T	201	2	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
7	NAG	O	502	1	14,14,15	0.50	0	17,19,21	1.42	3 (17%)
7	NAG	K	601	1	14,14,15	0.48	0	17,19,21	1.59	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	E	601	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	N	201	2	-	0/6/23/26	0/1/1/1
7	NAG	S	501	1	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2	-	0/6/23/26	0/1/1/1
7	NAG	L	201	2	-	0/6/23/26	0/1/1/1
7	NAG	Q	502	1	-	0/6/23/26	0/1/1/1
7	NAG	M	502	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	0/6/23/26	0/1/1/1
7	NAG	X	201	2	-	0/6/23/26	0/1/1/1
7	NAG	Q	501	1	-	0/6/23/26	0/1/1/1
7	NAG	V	201	2	-	0/6/23/26	0/1/1/1
7	NAG	G	501	1	-	0/6/23/26	0/1/1/1
7	NAG	U	501	1	-	0/6/23/26	0/1/1/1
7	NAG	J	201	2	-	0/6/23/26	0/1/1/1
7	NAG	I	501	1	-	0/6/23/26	0/1/1/1
7	NAG	M	501	1	-	0/6/23/26	0/1/1/1
7	NAG	R	201	2	-	0/6/23/26	0/1/1/1
7	NAG	F	201	2	-	0/6/23/26	0/1/1/1
7	NAG	P	201	2	-	0/6/23/26	0/1/1/1
7	NAG	G	502	1	-	0/6/23/26	0/1/1/1
7	NAG	W	601	1	-	0/6/23/26	0/1/1/1
7	NAG	H	201	2	-	0/6/23/26	0/1/1/1
7	NAG	U	502	1	-	0/6/23/26	0/1/1/1
7	NAG	S	502	1	-	0/6/23/26	0/1/1/1
7	NAG	O	501	1	-	0/6/23/26	0/1/1/1
7	NAG	T	201	2	-	0/6/23/26	0/1/1/1
7	NAG	O	502	1	-	0/6/23/26	0/1/1/1
7	NAG	K	601	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	NAG	C2-N2	-4.00	1.39	1.46
7	A	601	NAG	C8-C7	-3.49	1.43	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	NAG	O5-C1-C2	-8.70	97.54	111.29
7	A	601	NAG	C2-N2-C7	-7.89	111.67	122.90
7	A	601	NAG	C4-C3-C2	-7.71	99.72	111.02
7	A	601	NAG	C8-C7-N2	-5.86	106.18	116.10
7	A	601	NAG	C3-C4-C5	-4.89	101.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	502	NAG	O5-C5-C6	4.45	114.17	107.20
7	K	601	NAG	O5-C5-C6	4.39	114.08	107.20
7	U	502	NAG	O5-C5-C6	4.36	114.04	107.20
7	A	601	NAG	O3-C3-C2	4.26	118.27	109.47
7	J	201	NAG	C1-O5-C5	4.21	117.90	112.19
7	A	601	NAG	O7-C7-N2	3.99	129.29	121.95
7	S	502	NAG	O5-C5-C6	3.82	113.19	107.20
7	M	502	NAG	O5-C5-C6	3.79	113.14	107.20
7	O	502	NAG	O5-C5-C6	3.69	113.00	107.20
7	D	201	NAG	C1-O5-C5	3.68	117.17	112.19
7	E	601	NAG	O5-C5-C6	3.48	112.65	107.20
7	G	502	NAG	O5-C5-C6	3.44	112.60	107.20
7	W	601	NAG	O5-C5-C6	3.37	112.48	107.20
7	F	201	NAG	C1-O5-C5	2.99	116.24	112.19
7	W	601	NAG	C1-O5-C5	2.90	116.12	112.19
7	R	201	NAG	C1-O5-C5	2.77	115.95	112.19
7	C	501	NAG	C1-O5-C5	2.72	115.88	112.19
7	S	502	NAG	C4-C3-C2	-2.71	107.05	111.02
7	N	201	NAG	C1-O5-C5	2.70	115.85	112.19
7	S	501	NAG	O5-C1-C2	-2.70	107.03	111.29
7	K	601	NAG	C4-C3-C2	-2.69	107.08	111.02
7	M	501	NAG	C1-O5-C5	2.63	115.75	112.19
7	S	501	NAG	C4-C3-C2	-2.60	107.20	111.02
7	W	601	NAG	C4-C3-C2	-2.51	107.34	111.02
7	M	501	NAG	C4-C3-C2	-2.49	107.37	111.02
7	G	501	NAG	C1-O5-C5	2.43	115.49	112.19
7	C	501	NAG	C4-C3-C2	-2.42	107.47	111.02
7	U	501	NAG	C4-C3-C2	-2.33	107.60	111.02
7	O	502	NAG	C4-C3-C2	-2.30	107.64	111.02
7	T	201	NAG	C1-O5-C5	2.29	115.29	112.19
7	X	201	NAG	C1-O5-C5	2.25	115.24	112.19
7	G	502	NAG	C4-C3-C2	-2.25	107.72	111.02
7	S	502	NAG	O7-C7-C8	-2.24	117.89	122.06
7	E	601	NAG	C4-C3-C2	-2.24	107.74	111.02
7	W	601	NAG	O7-C7-C8	-2.23	117.92	122.06
7	O	502	NAG	C1-O5-C5	2.23	115.21	112.19
7	Q	501	NAG	O5-C5-C6	2.22	110.69	107.20
7	A	601	NAG	C1-O5-C5	-2.20	109.21	112.19
7	A	601	NAG	C1-C2-N2	-2.20	106.74	110.49
7	U	502	NAG	C4-C3-C2	-2.14	107.88	111.02
7	M	502	NAG	C4-C3-C2	-2.14	107.88	111.02
7	V	201	NAG	C1-O5-C5	2.12	115.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	501	NAG	C4-C3-C2	-2.12	107.92	111.02
7	H	201	NAG	C1-O5-C5	2.09	115.02	112.19
7	Q	502	NAG	O7-C7-C8	-2.08	118.19	122.06
7	B	201	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	NAG	C8-C7-N2-C2
7	A	601	NAG	O7-C7-N2-C2
7	C	501	NAG	C8-C7-N2-C2
7	C	501	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/323 (98%)	0.22	7 (2%)	62	52	33, 40, 68, 127	0
1	C	318/323 (98%)	0.15	5 (1%)	72	62	24, 43, 70, 106	0
1	E	318/323 (98%)	0.19	9 (2%)	53	42	30, 41, 77, 116	0
1	G	318/323 (98%)	0.08	9 (2%)	53	42	21, 33, 78, 132	0
1	I	318/323 (98%)	0.24	8 (2%)	57	47	25, 42, 64, 102	0
1	K	318/323 (98%)	0.05	3 (0%)	84	77	29, 42, 61, 112	0
1	M	318/323 (98%)	0.52	25 (7%)	12	11	58, 70, 100, 141	0
1	O	318/323 (98%)	0.42	22 (6%)	16	13	38, 61, 90, 116	0
1	Q	318/323 (98%)	0.22	16 (5%)	28	24	40, 49, 72, 115	0
1	S	318/323 (98%)	0.40	21 (6%)	18	15	43, 60, 76, 109	0
1	U	318/323 (98%)	0.13	5 (1%)	72	62	33, 42, 74, 121	0
1	W	318/323 (98%)	0.23	16 (5%)	28	24	31, 38, 91, 159	0
2	B	172/174 (98%)	0.03	4 (2%)	60	51	34, 61, 97, 111	0
2	D	172/174 (98%)	0.27	7 (4%)	37	30	40, 58, 81, 85	0
2	F	172/174 (98%)	0.18	8 (4%)	31	26	46, 61, 92, 97	0
2	H	172/174 (98%)	0.15	4 (2%)	60	51	15, 74, 123, 133	0
2	J	172/174 (98%)	0.22	5 (2%)	51	41	39, 61, 89, 96	0
2	L	172/174 (98%)	0.19	8 (4%)	31	26	23, 54, 94, 102	0
2	N	172/174 (98%)	0.34	15 (8%)	10	9	40, 87, 125, 133	0
2	P	172/174 (98%)	0.30	8 (4%)	31	26	40, 81, 115, 128	0
2	R	172/174 (98%)	0.04	2 (1%)	79	70	33, 61, 100, 111	0
2	T	172/174 (98%)	0.22	8 (4%)	31	26	43, 70, 121, 136	0
2	V	172/174 (98%)	0.01	2 (1%)	79	70	35, 57, 102, 115	0
2	X	172/174 (98%)	0.14	5 (2%)	51	41	36, 76, 130, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
3	a	238/241 (98%)	-0.02	2 (0%)	86	79	23, 37, 62, 74	0
3	c	238/241 (98%)	0.06	3 (1%)	77	68	26, 36, 54, 59	0
3	e	238/241 (98%)	0.30	17 (7%)	16	13	45, 66, 75, 83	0
3	g	238/241 (98%)	0.17	7 (2%)	51	41	18, 39, 95, 107	0
3	i	238/241 (98%)	0.08	2 (0%)	86	79	23, 30, 59, 70	0
3	k	238/241 (98%)	0.25	14 (5%)	22	18	50, 65, 91, 107	0
3	m	238/241 (98%)	0.14	14 (5%)	22	18	39, 47, 73, 86	0
3	o	238/241 (98%)	0.39	15 (6%)	20	16	70, 85, 107, 124	0
3	q	238/241 (98%)	0.18	8 (3%)	45	36	38, 54, 81, 91	0
3	s	238/241 (98%)	0.34	13 (5%)	25	21	63, 81, 100, 126	0
3	u	238/241 (98%)	0.02	2 (0%)	86	79	42, 57, 74, 86	0
3	w	238/241 (98%)	0.14	7 (2%)	51	41	28, 47, 83, 97	0
4	b	213/214 (99%)	-0.08	0	100	100	17, 28, 62, 66	0
4	d	213/214 (99%)	-0.08	0	100	100	23, 39, 67, 73	0
4	f	213/214 (99%)	-0.13	1 (0%)	91	85	44, 54, 86, 97	0
4	h	213/214 (99%)	0.05	3 (1%)	75	65	20, 33, 85, 91	0
4	j	213/214 (99%)	-0.05	0	100	100	23, 31, 66, 80	0
4	l	213/214 (99%)	-0.02	6 (2%)	53	42	54, 79, 103, 107	0
4	n	213/214 (99%)	0.04	3 (1%)	75	65	33, 44, 55, 62	0
4	p	213/214 (99%)	0.10	7 (3%)	46	37	70, 79, 105, 111	0
4	r	213/214 (99%)	-0.07	2 (0%)	84	77	33, 53, 68, 73	0
4	t	213/214 (99%)	-0.09	3 (1%)	75	65	47, 68, 105, 115	0
4	v	213/214 (99%)	-0.01	4 (1%)	66	58	34, 48, 84, 93	0
4	x	213/214 (99%)	0.03	2 (0%)	84	77	25, 41, 54, 59	0
All	All	11292/11424 (98%)	0.15	357 (3%)	47	37	15, 51, 98, 159	0

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	133	GLY	7.9
1	Q	10	GLY	7.6
1	W	326	LYS	7.0
3	w	132	SER	7.0
2	N	27	GLN	6.4

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Mol	Chain	Res	Type	RSRZ
2	D	23	GLY	6.2
3	s	133	GLY	6.0
1	M	37	THR	5.8
1	W	9	PRO	5.5
1	Q	9	PRO	5.3
3	e	20	LEU	5.2
1	O	9	PRO	4.9
1	E	9	PRO	4.9
1	A	9	PRO	4.8
1	O	251	LEU	4.8
3	k	21[A]	SER	4.7
2	D	32	THR	4.6
1	G	9	PRO	4.4
2	N	26	HIS	4.4
2	N	63	PHE	4.4
2	N	29	SER	4.3
1	M	12	THR	4.3
4	v	1	ASP	4.3
4	l	177	SER	4.3
1	M	9	PRO	4.2
3	w	214	LYS	4.2
1	S	16	GLY	4.1
1	O	319	GLY	4.1
1	Q	264	LYS	4.1
1	W	319	GLY	4.0
1	O	15	LEU	4.0
1	S	82	GLU	4.0
2	T	132	ASP	3.9
1	S	251	LEU	3.9
2	X	23	GLY	3.8
1	W	325	GLU	3.7
3	o	174	GLY	3.7
3	e	214	LYS	3.7
1	M	242	VAL	3.7
1	W	37	THR	3.7
1	O	252	ILE	3.6
2	L	161	VAL	3.6
2	N	171	PHE	3.6
1	O	181	GLY	3.6
1	M	274[A]	ILE	3.6
2	L	25	ARG	3.6
2	J	26	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
4	p	64	GLY	3.5
1	M	319	GLY	3.5
2	F	57	GLU	3.5
3	u	132	SER	3.5
1	M	302	TYR	3.4
3	e	9	GLY	3.4
3	k	211	VAL	3.4
3	e	8	GLY	3.4
3	m	176	TYR	3.4
3	w	176	TYR	3.4
2	P	22	TYR	3.4
2	F	161	VAL	3.4
2	D	31	GLY	3.4
3	q	123	PRO	3.4
2	F	132	ASP	3.4
3	o	175	LEU	3.4
2	H	25	ARG	3.3
1	M	13	LEU	3.3
2	L	139	LYS	3.3
2	B	33	GLY	3.3
3	o	134	GLY	3.3
1	M	51	ILE	3.3
2	N	132	ASP	3.3
1	O	250	ASN	3.3
1	E	10	GLY	3.2
4	t	119	PRO	3.2
4	l	181	LEU	3.2
1	M	273	PRO	3.2
4	h	200	GLY	3.2
1	A	326	LYS	3.2
1	O	10	GLY	3.2
3	s	209	LYS	3.2
1	Q	325	GLU	3.2
3	k	137	ALA	3.2
3	k	214	LYS	3.2
1	M	325	GLU	3.2
2	J	25	ARG	3.2
1	M	11	ALA	3.1
3	o	209	LYS	3.1
1	Q	320	MET	3.1
2	X	17[A]	MET	3.1
3	e	21[A]	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	297	VAL	3.1
2	H	44	ALA	3.1
1	E	12	THR	3.0
1	E	58	ILE	3.0
2	N	36	ALA	3.0
3	w	179	SER	3.0
2	N	33	GLY	3.0
1	Q	259	LYS	3.0
3	m	144	ASP	2.9
1	M	10	GLY	2.9
1	M	190	GLU	2.9
1	S	183	HIS	2.9
1	O	268	MET	2.9
3	o	129	LYS	2.9
3	e	132	SER	2.9
1	I	323	VAL	2.9
1	O	45	SER	2.9
3	e	134	GLY	2.9
4	p	196	VAL	2.9
1	O	79	PHE	2.9
3	k	138	LEU	2.9
2	H	172	GLN	2.9
2	X	143	LYS	2.9
4	v	2	ILE	2.9
1	Q	321[A]	ARG	2.9
4	h	125	LEU	2.9
2	T	168	ASN	2.9
2	N	28	ASN	2.9
3	s	86	ASP	2.9
1	G	208	ARG	2.8
3	m	145	TYR	2.8
3	s	214	LYS	2.8
2	F	122	THR	2.8
1	Q	57	ARG	2.8
3	g	174	GLY	2.8
3	k	189	LEU	2.8
3	g	92	CYS	2.8
1	G	271	ASP	2.8
3	w	145	TYR	2.8
1	E	18	HIS	2.8
1	S	135	GLY	2.8
1	G	21	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	17[A]	MET	2.7
3	m	132	SER	2.7
3	o	68	THR	2.7
1	G	10	GLY	2.7
1	S	181	GLY	2.7
3	m	204	ASN	2.7
1	G	325	GLU	2.7
1	U	326	LYS	2.7
3	e	11	LEU	2.7
2	D	26	HIS	2.7
1	M	32[A]	ASP	2.7
2	D	58	LYS	2.7
1	M	297	VAL	2.7
1	O	260[A]	MET	2.7
4	p	142	ARG	2.7
3	e	111	VAL	2.7
1	G	12	THR	2.7
3	k	182	VAL	2.7
1	A	221	PRO	2.7
1	Q	263	GLY	2.6
2	F	131	GLU	2.6
2	N	30	GLU	2.6
2	L	24	PHE	2.6
1	M	272	ALA	2.6
1	W	41	GLU	2.6
3	m	53	GLY	2.6
4	l	193	ALA	2.6
1	E	175	ASP	2.6
3	g	93	ALA	2.6
1	W	92	LYS	2.6
1	M	248	ASN	2.6
2	J	97	GLU	2.6
1	S	45	SER	2.6
3	g	100(M)	GLY	2.6
3	e	194	TYR	2.6
1	Q	175	ASP	2.6
1	I	19	ALA	2.6
1	W	264	LYS	2.6
1	W	321[A]	ARG	2.6
1	O	58	ILE	2.6
3	s	195	ILE	2.6
2	P	138	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	c	214	LYS	2.5
1	W	13	LEU	2.5
2	B	72	GLU	2.5
3	k	133	GLY	2.5
3	c	54	GLY	2.5
2	R	138	PHE	2.5
3	s	100(D)	ALA	2.5
1	Q	326	LYS	2.5
1	W	271	ASP	2.5
1	C	15	LEU	2.5
3	o	14	PRO	2.5
1	E	304	ALA	2.5
3	o	58	ASP	2.5
1	G	118	LEU	2.5
2	N	34	GLN	2.5
2	T	115	MET	2.5
1	O	16	GLY	2.5
1	E	229	ARG	2.5
2	D	171	PHE	2.5
3	q	132	SER	2.5
1	W	320	MET	2.5
1	O	207[A]	ARG	2.5
4	t	117	ILE	2.5
1	C	35	GLU	2.5
2	T	21	TRP	2.5
1	S	146	GLY	2.5
2	P	68	LYS	2.5
2	N	140	ILE	2.5
1	S	161	TYR	2.5
1	O	279	SER	2.5
3	o	173	SER	2.5
3	c	100(J)	ASP	2.4
2	P	16	GLY	2.4
4	v	12	SER	2.4
1	W	93	ALA	2.4
1	S	147	PHE	2.4
4	l	123	GLU	2.4
3	s	172	SER	2.4
3	s	181	VAL	2.4
3	g	121	VAL	2.4
1	M	98	TYR	2.4
1	K	49	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	34	GLN	2.4
1	S	173	ASN	2.4
4	t	143	GLU	2.4
1	I	259	LYS	2.4
1	E	306	PRO	2.4
3	k	86	ASP	2.4
1	W	135	GLY	2.4
1	M	23	GLY	2.3
1	G	326	LYS	2.3
1	O	253	ALA	2.3
2	D	138	PHE	2.3
2	N	44	ALA	2.3
1	A	259	LYS	2.3
3	m	45	LEU	2.3
2	T	22	TYR	2.3
1	M	251	LEU	2.3
1	U	292	LYS	2.3
3	q	122	PHE	2.3
3	s	14	PRO	2.3
3	s	210	ARG	2.3
1	A	119	GLU	2.3
1	S	164	LEU	2.3
3	q	124	LEU	2.3
3	s	53	GLY	2.3
3	s	54	GLY	2.3
2	X	164	ASP	2.3
2	J	139	LYS	2.3
3	m	214	LYS	2.3
3	o	171	GLN	2.3
4	p	187	GLU	2.3
3	a	98	MET	2.3
3	k	122	PHE	2.3
3	e	212	GLU	2.3
3	m	52(A)	ALA	2.3
2	R	168	ASN	2.3
1	O	228[A]	SER	2.3
4	n	132	VAL	2.3
4	r	107	LYS	2.3
3	w	133	GLY	2.2
4	x	29	ILE	2.2
2	V	35	ALA	2.2
1	C	322	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	126	LEU	2.2
1	Q	226	LEU	2.2
3	k	20	LEU	2.2
1	U	242	VAL	2.2
2	N	17[A]	MET	2.2
3	i	123	PRO	2.2
1	Q	58	ILE	2.2
1	S	195	TYR	2.2
1	S	250	ASN	2.2
2	T	36	ALA	2.2
3	e	168	ALA	2.2
3	k	184	VAL	2.2
4	r	181	LEU	2.2
2	H	34	GLN	2.2
1	S	319	GLY	2.2
3	q	209	LYS	2.2
2	F	56	ILE	2.2
1	A	183	HIS	2.2
3	q	139	GLY	2.2
1	I	18	HIS	2.2
1	Q	319	GLY	2.2
3	i	132	SER	2.2
3	u	100(D)	ALA	2.2
4	p	160	GLN	2.2
1	M	14	CYS	2.2
1	S	259	LYS	2.2
1	W	11	ALA	2.2
2	J	138	PHE	2.2
3	a	93	ALA	2.2
4	v	13	ALA	2.2
1	S	112	VAL	2.2
2	L	23	GLY	2.2
3	w	100(D)	ALA	2.2
1	S	182	VAL	2.2
2	L	156	THR	2.2
3	m	143	LYS	2.2
4	p	63	SER	2.2
1	I	15	LEU	2.1
1	Q	94	PHE	2.1
1	O	227[A]	SER	2.1
3	m	170	LEU	2.1
4	n	131	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	n	142	ARG	2.1
1	A	176	LYS	2.1
3	g	142	VAL	2.1
3	m	166	PHE	2.1
2	B	157	TYR	2.1
2	N	68	LYS	2.1
1	C	79	PHE	2.1
3	k	179	SER	2.1
2	P	122	THR	2.1
3	e	129	LYS	2.1
4	f	148	TRP	2.1
1	O	44	GLN	2.1
2	L	132	ASP	2.1
2	P	153	ARG	2.1
2	P	81	GLU	2.1
3	o	132	SER	2.1
3	q	93	ALA	2.1
1	Q	13	LEU	2.1
3	e	159	LEU	2.1
4	h	110	VAL	2.1
4	p	112	ALA	2.1
1	U	9	PRO	2.1
1	S	87	PHE	2.1
3	o	100(C)	SER	2.1
1	K	275[A]	ASP	2.1
2	L	172	GLN	2.1
2	T	124	ARG	2.1
3	q	143	LYS	2.1
2	T	143	LYS	2.1
1	C	289	PRO	2.1
1	I	69	ALA	2.1
1	M	34	ILE	2.1
1	M	191	GLN	2.1
3	e	182	VAL	2.0
1	K	231	SER	2.0
1	I	63	ASP	2.0
3	k	168	ALA	2.0
1	S	253	ALA	2.0
2	F	160	ASP	2.0
3	e	112	SER	2.0
4	l	146	VAL	2.0
1	I	137	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	m	171	GLN	2.0
3	g	100(L)	VAL	2.0
4	x	187	GLU	2.0
3	o	27(C)	GLY	2.0
3	s	134	GLY	2.0
3	o	177	SER	2.0
1	W	58	ILE	2.0
1	S	66	LEU	2.0
4	l	178	THR	2.0
2	V	171	PHE	2.0
1	O	21	PRO	2.0
1	M	275[A]	ASP	2.0
3	m	150	VAL	2.0
2	F	141	TYR	2.0
1	U	82	GLU	2.0
3	e	201	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PCA	o	1	8/9	0.77	0.26	77,78,79,79	0
3	PCA	i	1	8/9	0.82	0.34	32,32,33,33	0
3	PCA	e	1	8/9	0.86	0.29	54,56,59,62	0
3	PCA	u	1	8/9	0.86	0.30	54,55,56,56	0
3	PCA	q	1	8/9	0.87	0.24	57,57,58,58	0
3	PCA	c	1	8/9	0.88	0.25	36,37,38,39	0
3	PCA	a	1	8/9	0.90	0.21	36,36,37,38	0
3	PCA	k	1	8/9	0.90	0.20	50,52,54,57	0
3	PCA	s	1	8/9	0.90	0.18	63,64,64,64	0
3	PCA	m	1	8/9	0.90	0.17	40,41,41,41	0
3	PCA	w	1	8/9	0.91	0.17	27,27,27,29	0
3	PCA	g	1	8/9	0.94	0.17	35,36,38,38	0

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	AA	4	11/12	0.45	0.53	78,81,81,82	0
5	BMA	AA	3	11/12	0.46	0.38	66,70,72,75	0
5	BMA	8	3	11/12	0.47	0.31	78,82,85,86	0
5	BMA	GA	3	11/12	0.54	0.31	62,67,72,72	0
5	BMA	0	3	11/12	0.60	0.26	64,68,72,73	0
6	NAG	7	2	14/15	0.61	0.41	54,62,69,69	0
5	MAN	8	4	11/12	0.68	0.35	88,92,93,93	0
6	NAG	1	2	14/15	0.70	0.33	75,83,89,90	0
5	BMA	CA	3	11/12	0.70	0.27	82,87,91,92	0
5	BMA	EA	3	11/12	0.71	0.27	72,75,77,79	0
5	BMA	IA	3	11/12	0.71	0.27	68,73,76,76	0
5	NAG	6	2	14/15	0.72	0.50	51,60,69,71	0
5	MAN	6	4	11/12	0.72	0.34	84,87,89,90	0
5	NAG	Y	1	14/15	0.72	0.40	45,48,60,61	0
5	BMA	4	3	11/12	0.72	0.26	65,69,73,73	0
6	NAG	BA	1	14/15	0.72	0.36	71,77,82,84	0
5	MAN	CA	4	11/12	0.73	0.30	92,96,98,98	0
5	NAG	IA	1	14/15	0.73	0.32	39,46,56,57	0
5	MAN	Y	4	11/12	0.73	0.40	78,80,84,84	0
5	MAN	2	4	11/12	0.74	0.30	62,65,66,67	0
5	BMA	y	3	11/12	0.74	0.23	44,48,51,53	0
5	MAN	4	4	11/12	0.74	0.33	75,78,80,80	0
6	NAG	FA	2	14/15	0.74	0.26	70,80,86,87	0
6	NAG	3	2	14/15	0.76	0.54	49,58,66,66	0
5	BMA	2	3	11/12	0.76	0.24	51,55,58,60	0
6	NAG	9	1	14/15	0.76	0.36	70,73,76,76	0
5	MAN	IA	4	11/12	0.76	0.26	78,81,84,84	0
5	NAG	IA	2	14/15	0.76	0.32	43,52,61,63	0
5	BMA	Y	3	11/12	0.77	0.22	70,74,78,78	0
6	NAG	9	2	14/15	0.77	0.30	70,79,89,89	0
6	NAG	5	2	14/15	0.77	0.24	62,74,81,82	0
5	BMA	6	3	11/12	0.77	0.23	75,79,82,83	0
5	NAG	8	2	14/15	0.78	0.22	66,69,71,74	0
6	NAG	1	1	14/15	0.78	0.24	60,66,70,74	0
5	NAG	Y	2	14/15	0.79	0.28	45,54,65,65	0
5	NAG	EA	2	14/15	0.79	0.38	52,58,68,69	0
6	NAG	FA	1	14/15	0.79	0.29	59,63,67,70	0

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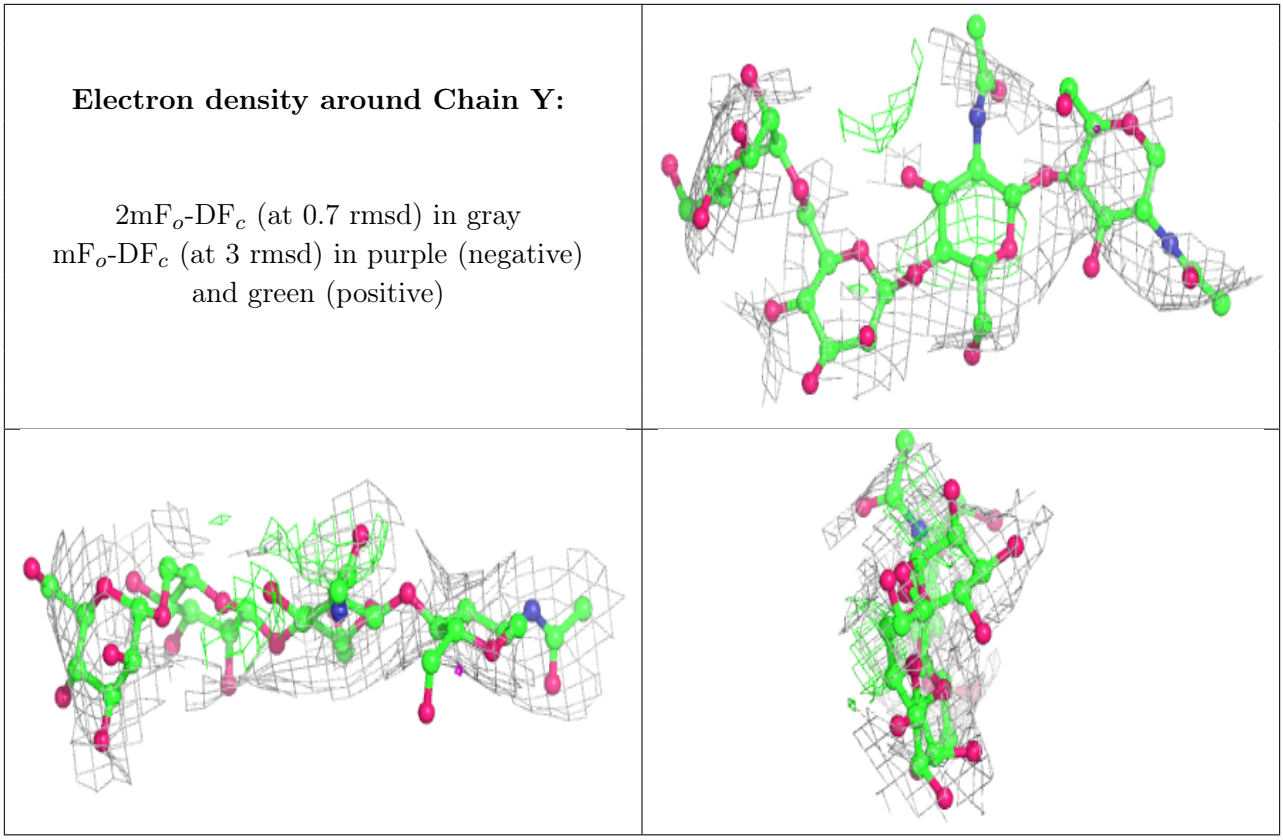
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	Z	2	14/15	0.79	0.36	51,59,65,65	0
6	NAG	BA	2	14/15	0.80	0.31	82,93,102,102	0
5	NAG	6	1	14/15	0.80	0.27	49,56,67,67	0
5	NAG	AA	2	14/15	0.80	0.41	47,52,59,62	0
6	NAG	5	1	14/15	0.81	0.39	50,57,61,63	0
6	NAG	Z	1	14/15	0.82	0.25	37,40,44,49	0
6	NAG	DA	2	14/15	0.82	0.36	59,67,73,73	0
5	NAG	CA	2	14/15	0.82	0.42	57,66,77,78	0
6	NAG	z	2	14/15	0.82	0.26	45,52,59,60	0
6	NAG	HA	1	14/15	0.82	0.53	42,44,47,47	0
6	NAG	z	1	14/15	0.83	0.33	43,45,49,50	0
5	NAG	y	2	14/15	0.83	0.21	32,34,37,40	0
5	MAN	0	4	11/12	0.83	0.27	76,78,80,81	0
5	MAN	GA	4	11/12	0.83	0.24	74,78,81,82	0
5	NAG	GA	2	14/15	0.84	0.27	44,46,55,58	0
5	MAN	EA	4	11/12	0.84	0.29	81,83,84,84	0
6	NAG	7	1	14/15	0.84	0.30	40,47,50,53	0
6	NAG	JA	2	14/15	0.84	0.28	67,78,86,87	0
6	NAG	DA	1	14/15	0.85	0.33	46,50,54,57	0
6	NAG	JA	1	14/15	0.85	0.26	53,60,66,68	0
5	NAG	EA	1	14/15	0.85	0.19	53,58,69,69	0
5	NAG	CA	1	14/15	0.86	0.23	54,60,70,71	0
6	NAG	3	1	14/15	0.86	0.21	37,42,47,49	0
5	NAG	0	1	14/15	0.87	0.28	40,46,56,56	0
5	NAG	0	2	14/15	0.88	0.25	46,50,58,60	0
6	NAG	HA	2	14/15	0.88	0.32	48,56,62,63	0
5	NAG	4	2	14/15	0.89	0.23	42,50,60,62	0
5	MAN	y	4	11/12	0.90	0.20	56,59,60,61	0
5	NAG	8	1	14/15	0.91	0.26	66,67,68,68	0
5	NAG	2	2	14/15	0.91	0.21	30,37,45,47	0
5	NAG	AA	1	14/15	0.91	0.19	43,49,57,58	0
5	NAG	GA	1	14/15	0.93	0.17	41,43,48,48	0
5	NAG	2	1	14/15	0.93	0.25	26,32,41,42	0
5	NAG	y	1	14/15	0.94	0.24	30,32,34,34	0
5	NAG	4	1	14/15	0.95	0.25	40,47,57,58	0

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

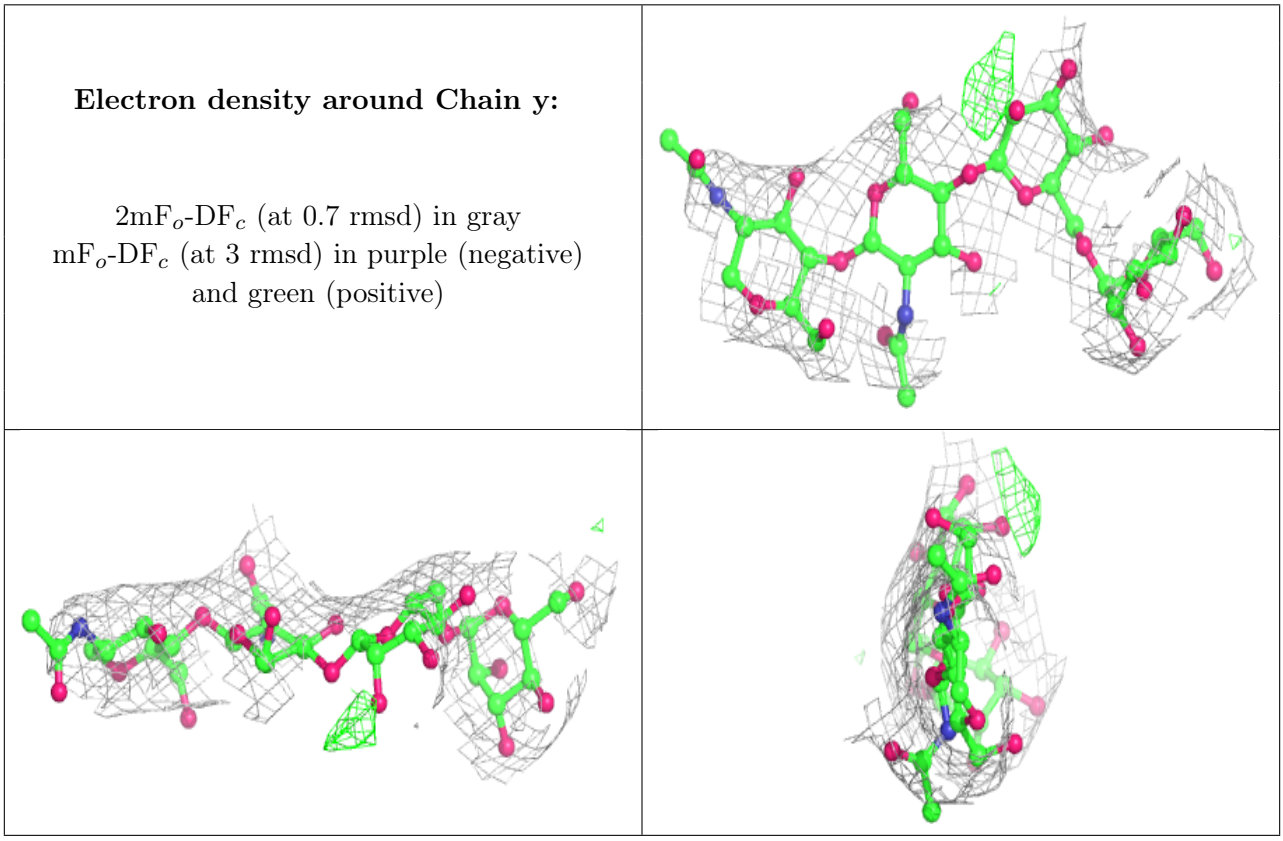
Electron density around Chain Y:

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



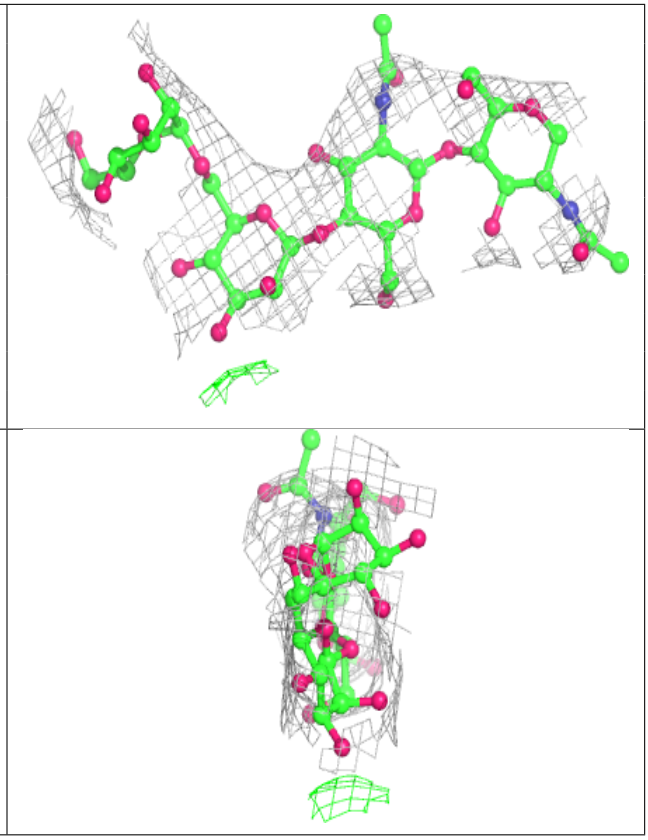
Electron density around Chain y:

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



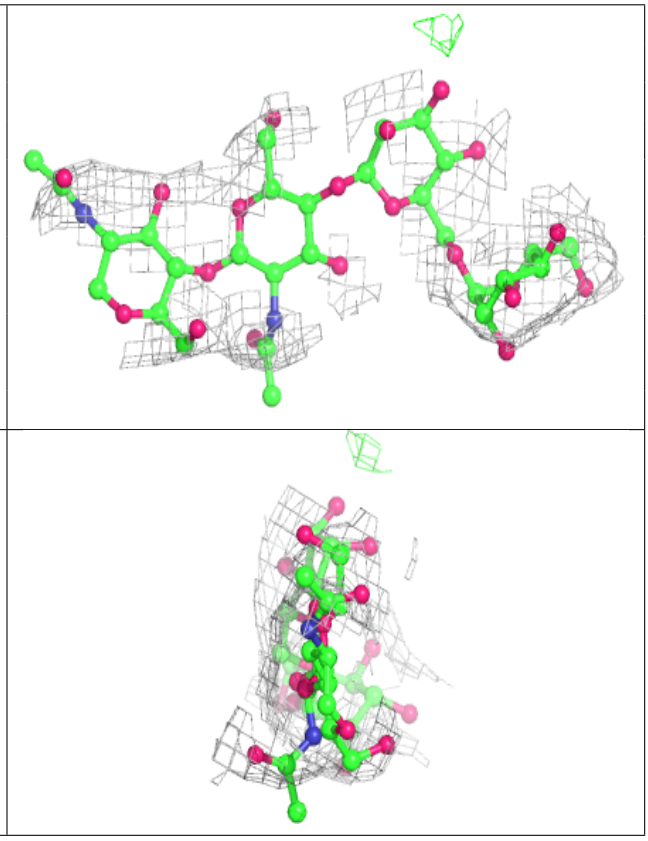
Electron density around Chain 0:

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



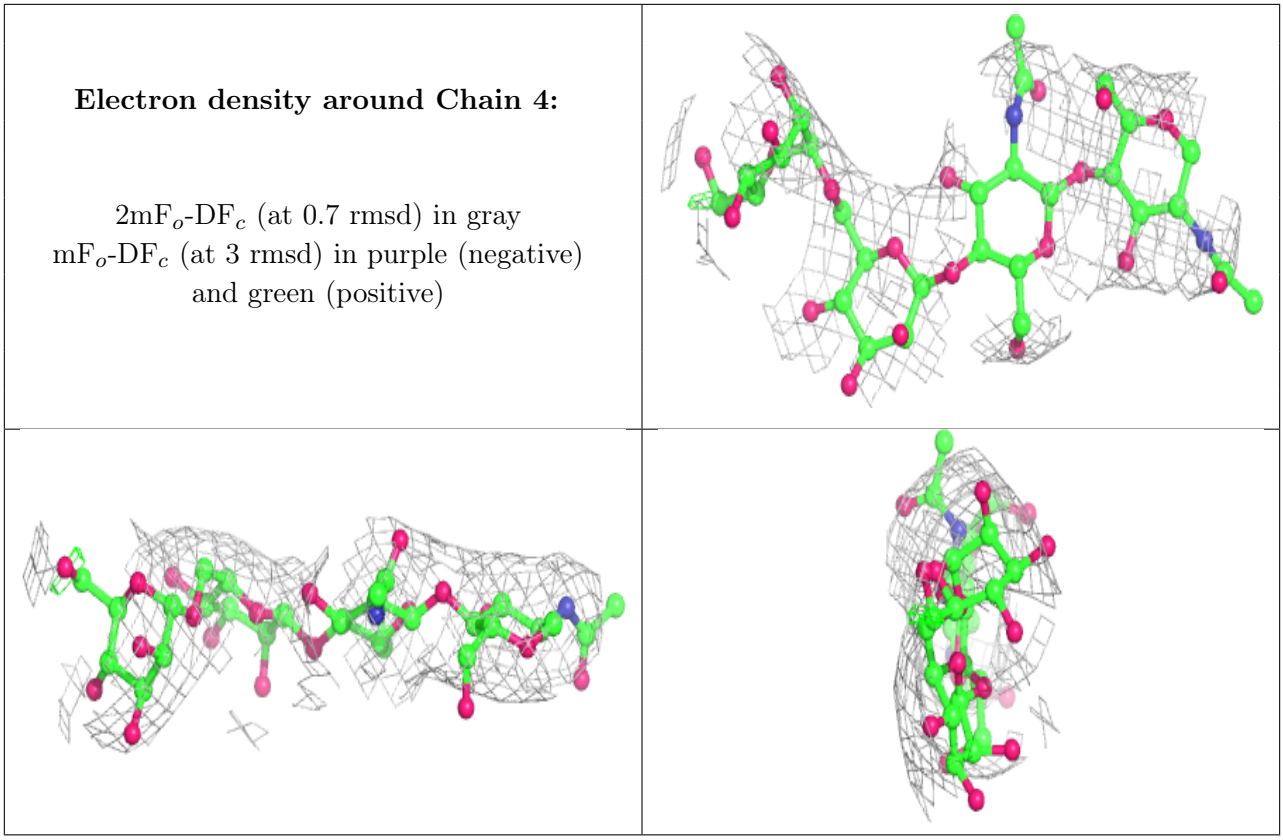
Electron density around Chain 2:

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



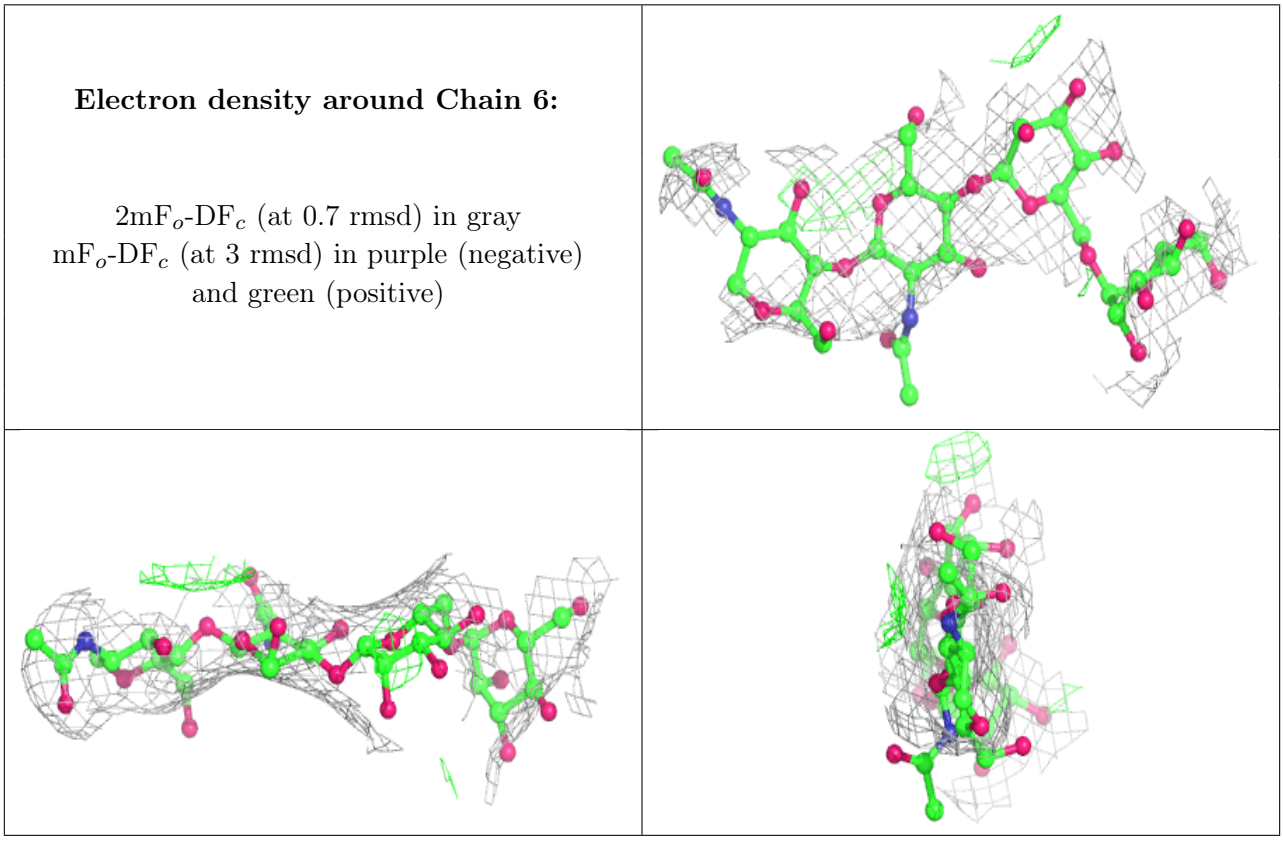
Electron density around Chain 4:

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



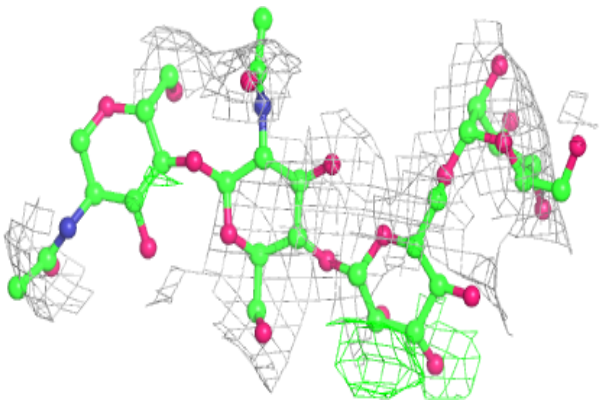
Electron density around Chain 6:

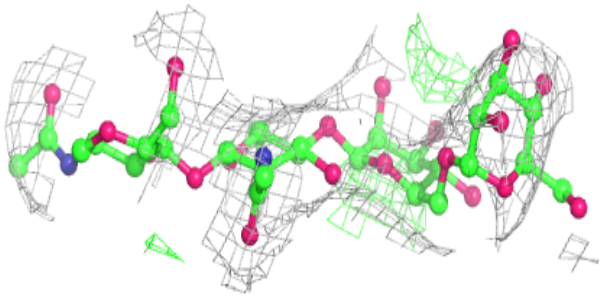
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

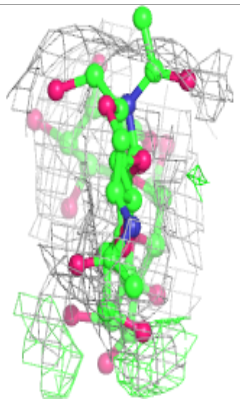


Electron density around Chain 8:

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

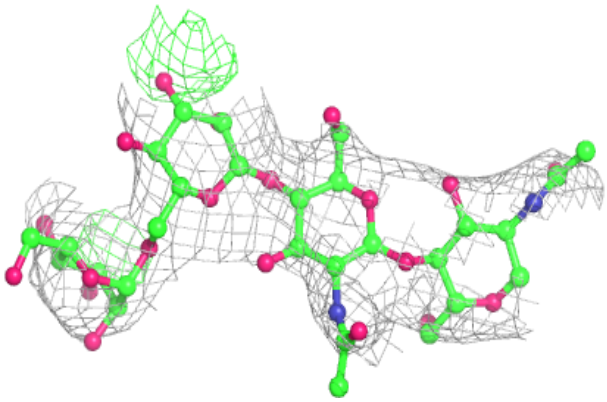


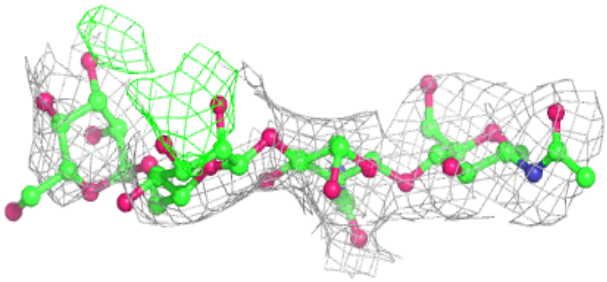


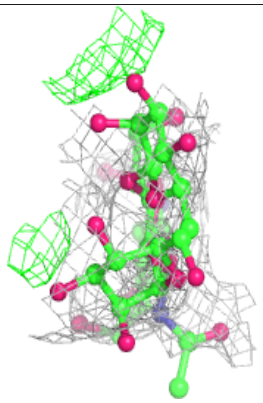


Electron density around Chain AA:

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

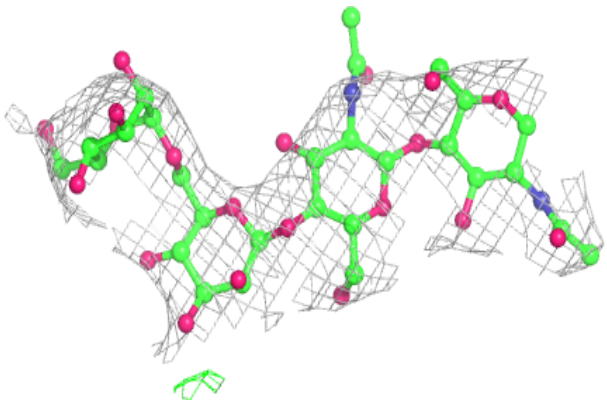


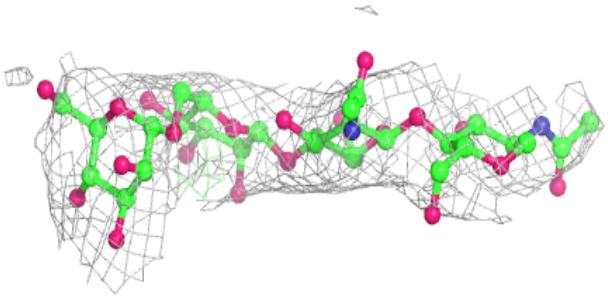


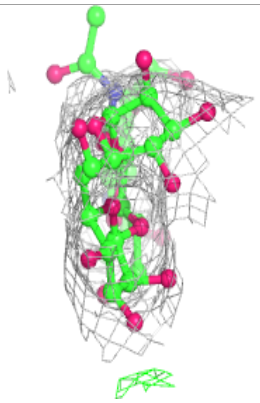


Electron density around Chain CA:

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

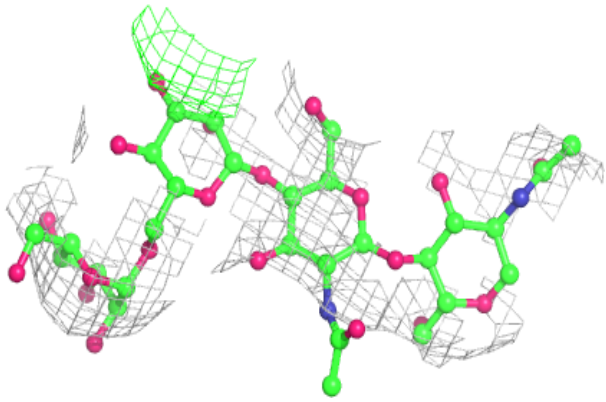


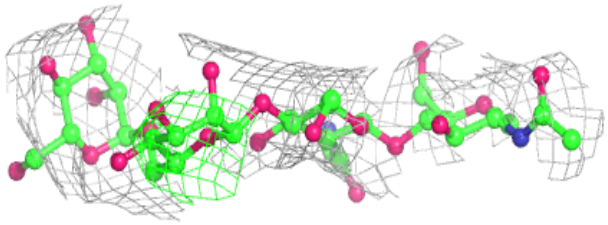


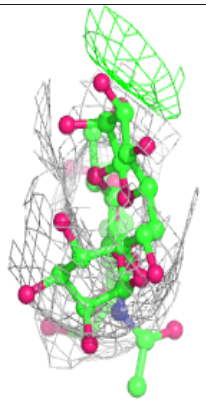


Electron density around Chain EA:

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

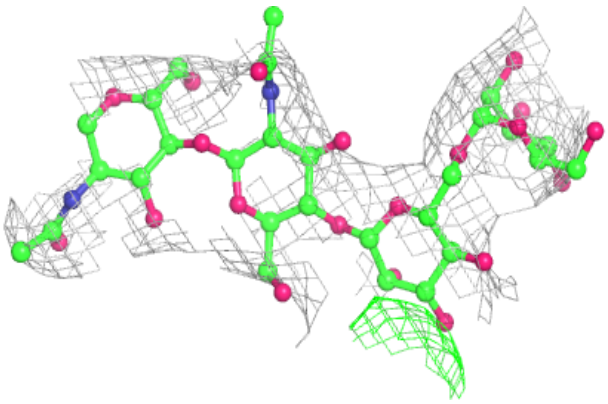


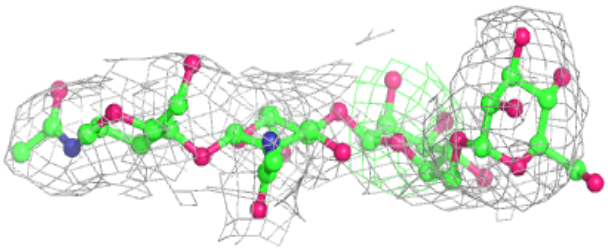


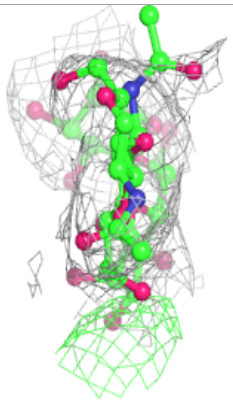


Electron density around Chain GA:

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

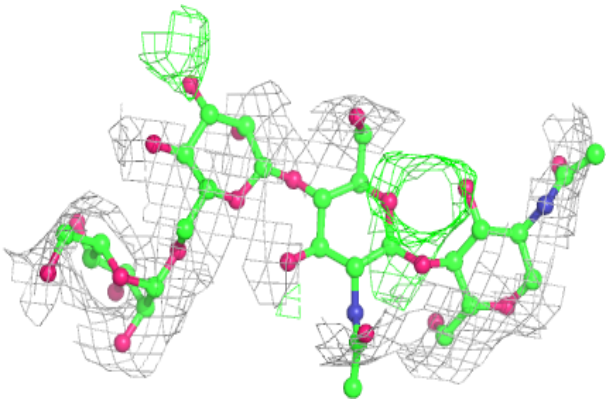


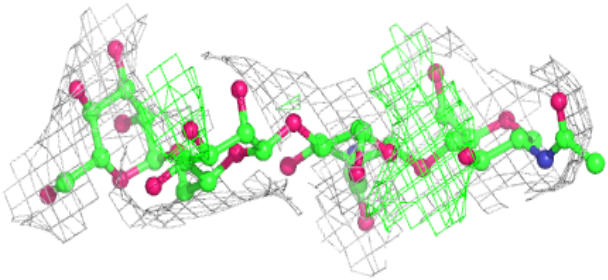


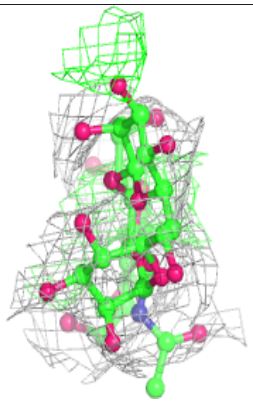


Electron density around Chain IA:

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

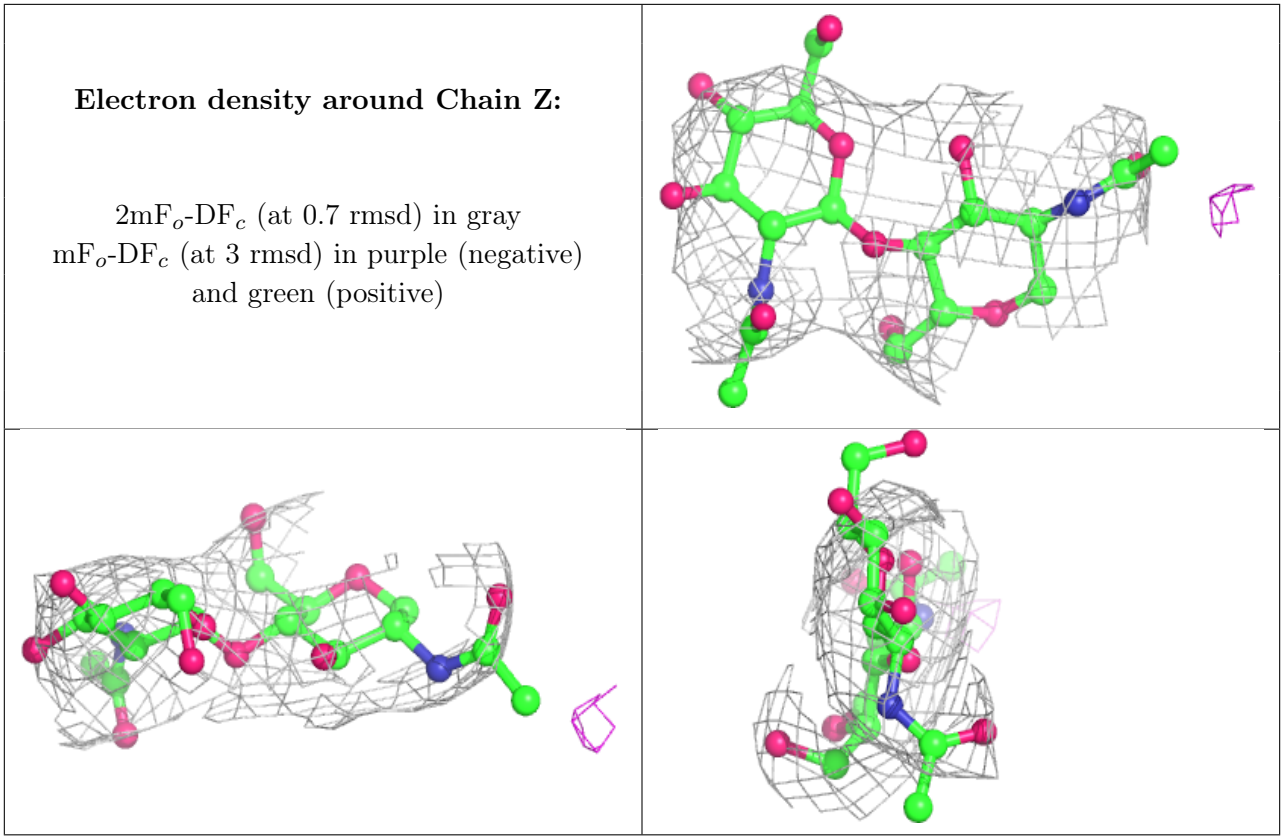






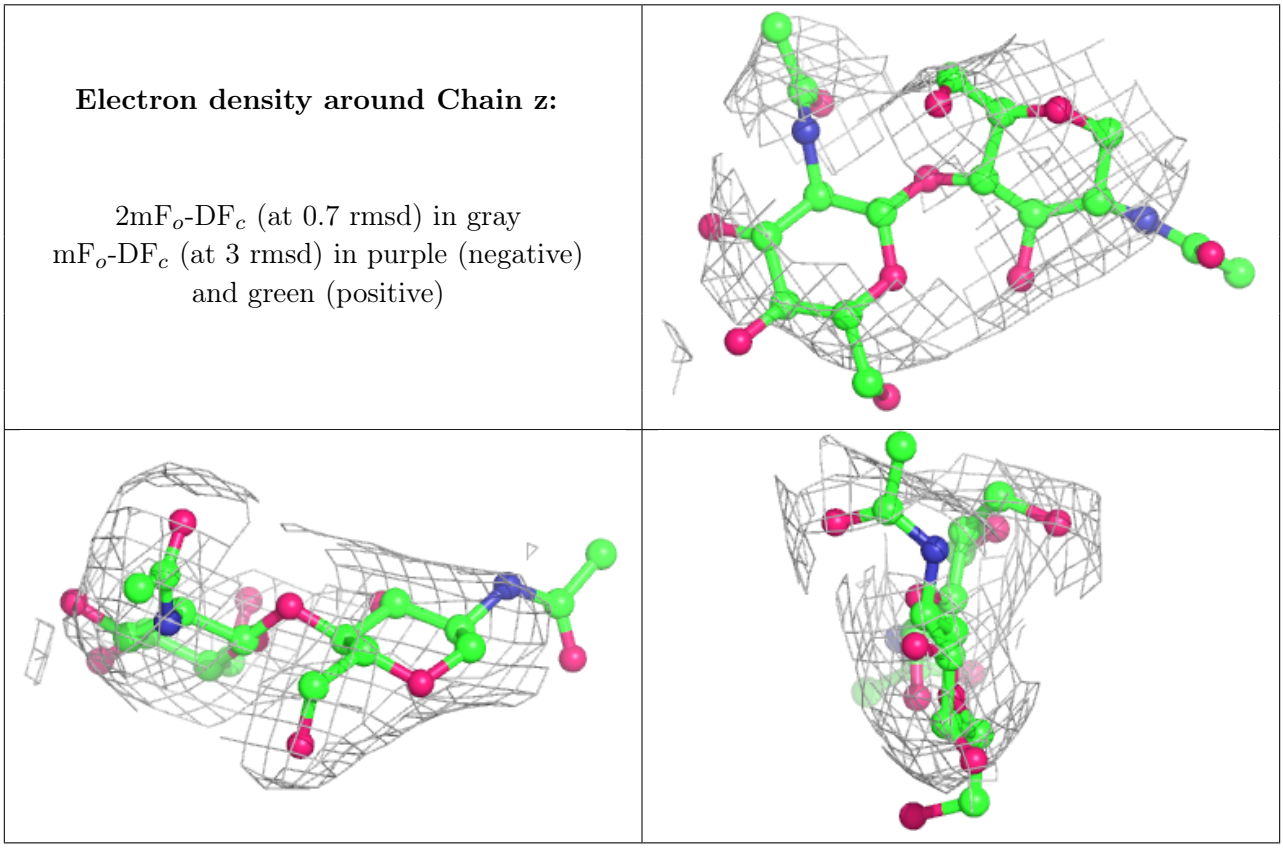
Electron density around Chain Z:

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



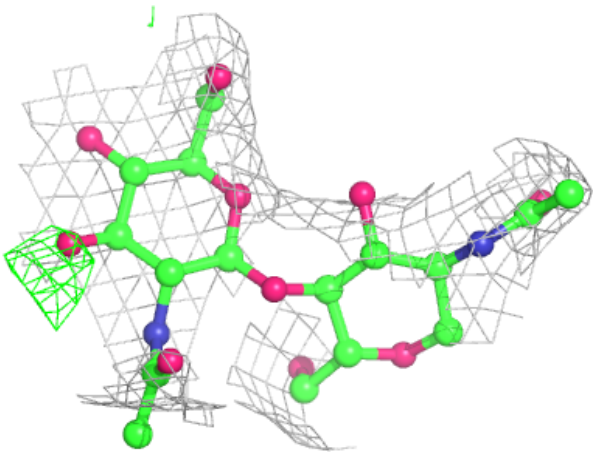
Electron density around Chain z:

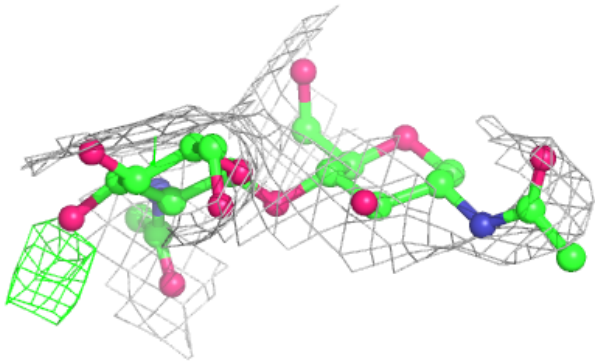
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

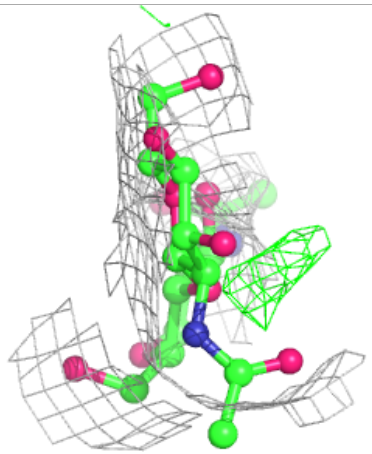


Electron density around Chain 1:

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

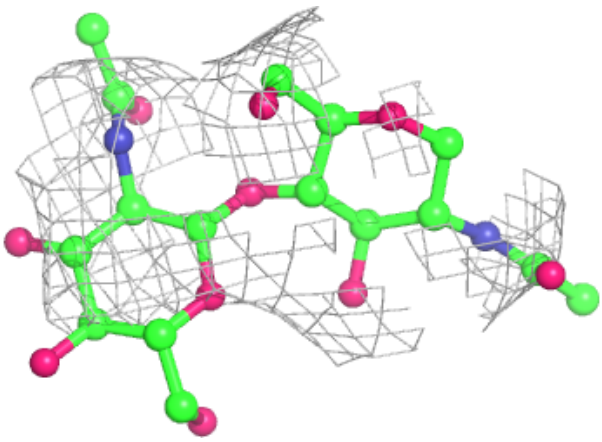


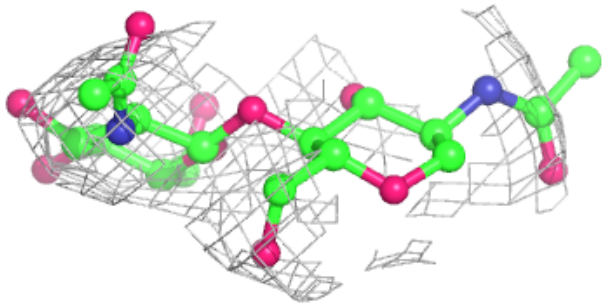


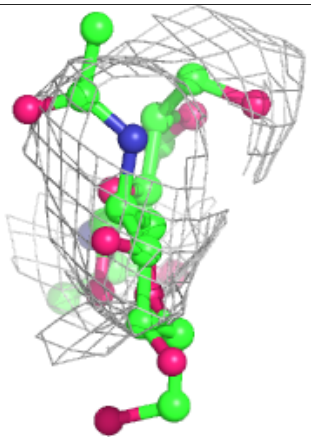


Electron density around Chain 3:

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

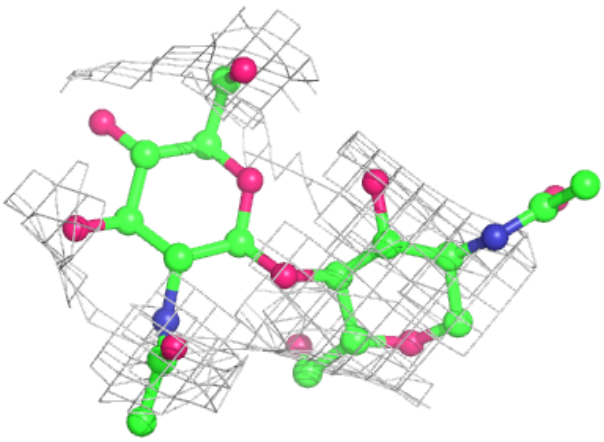


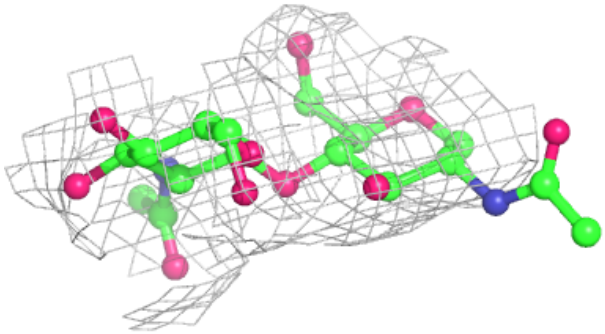


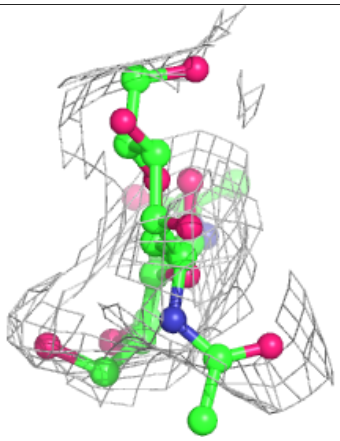


Electron density around Chain 5:

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

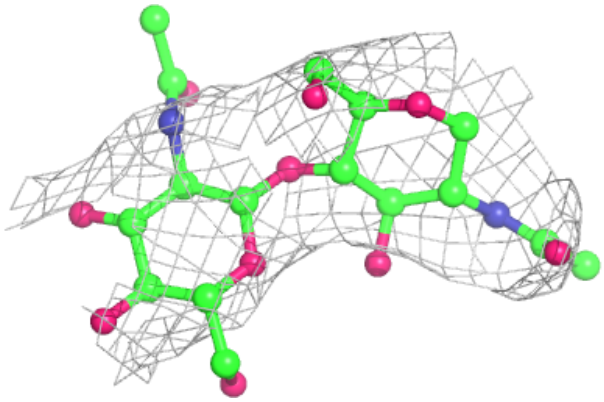


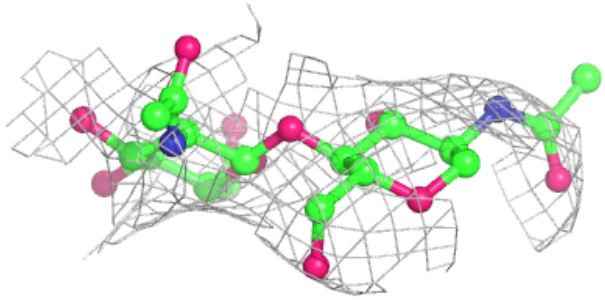


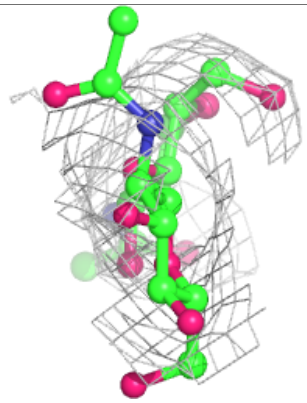


Electron density around Chain 7:

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

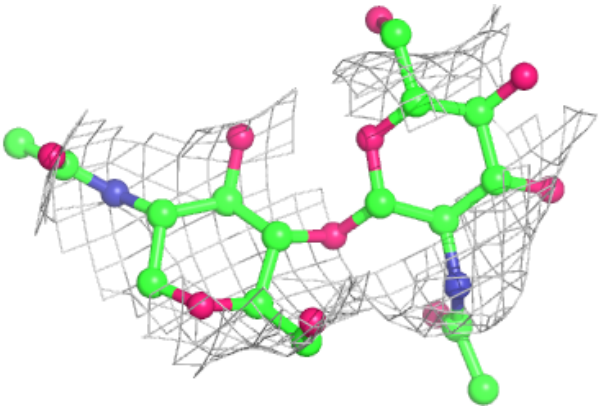


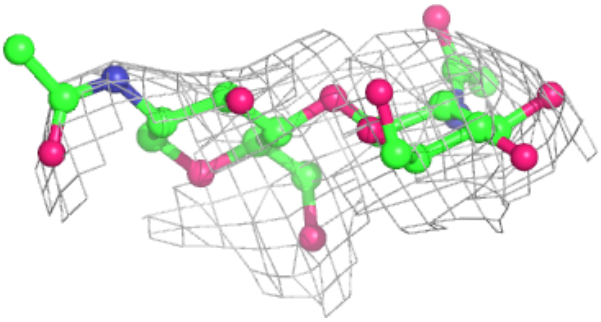


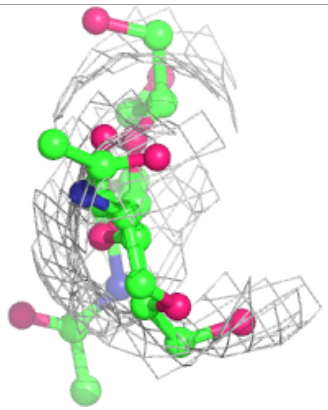


Electron density around Chain 9:

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

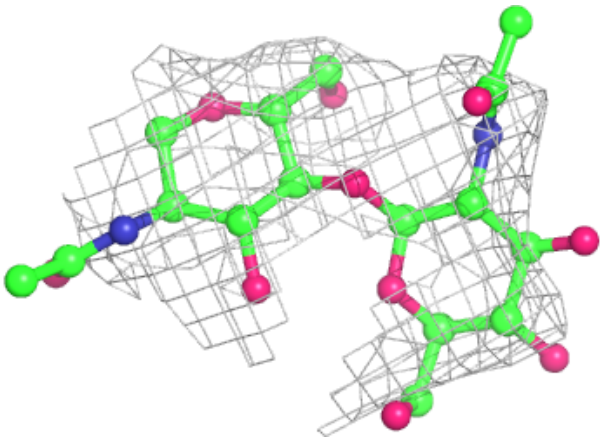


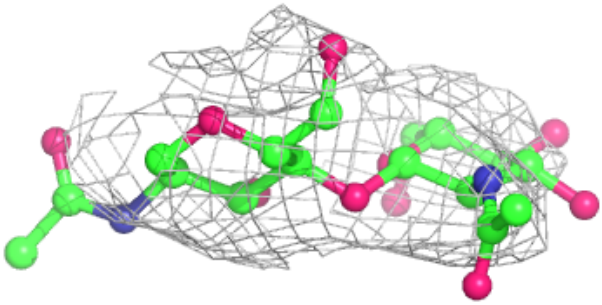


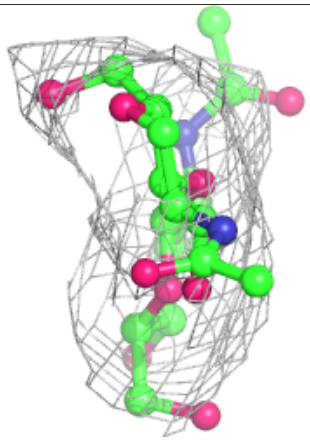


Electron density around Chain BA:

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

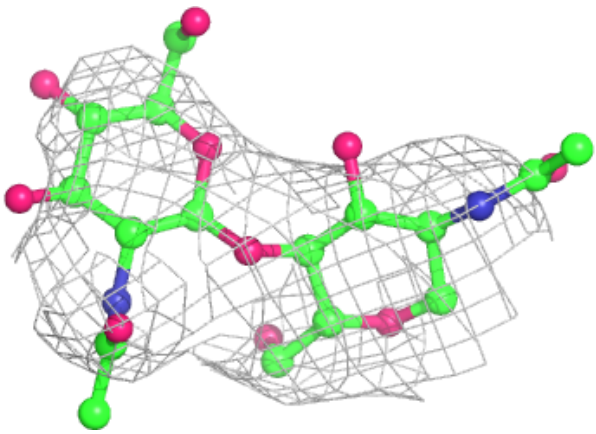


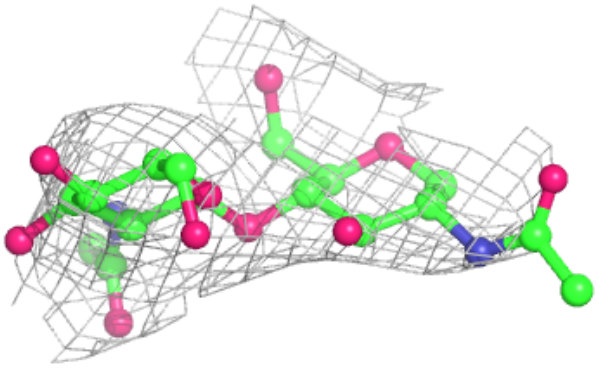


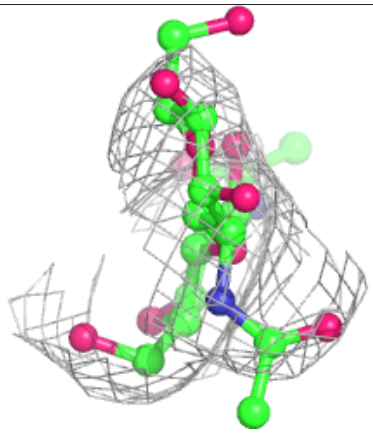


Electron density around Chain DA:

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

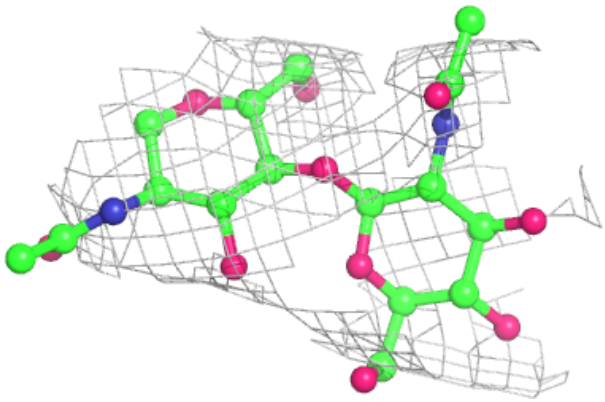


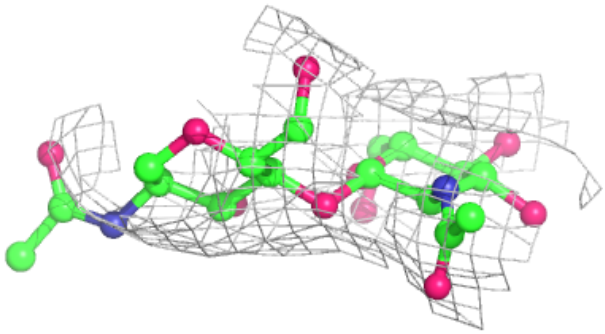


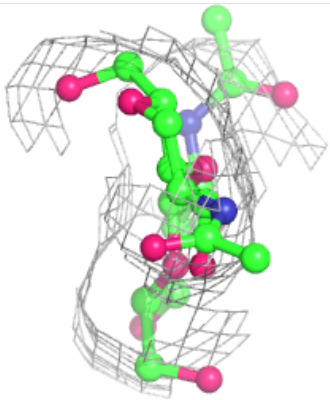


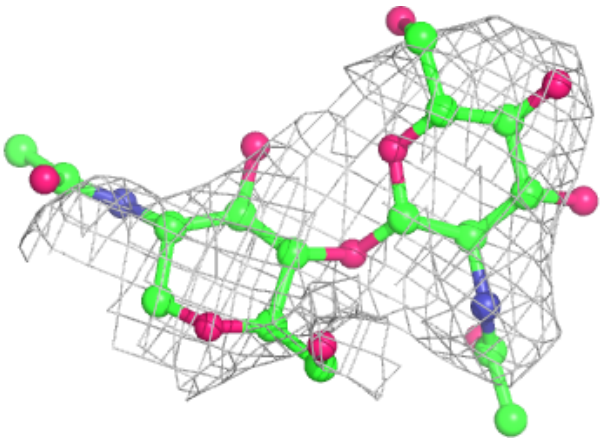
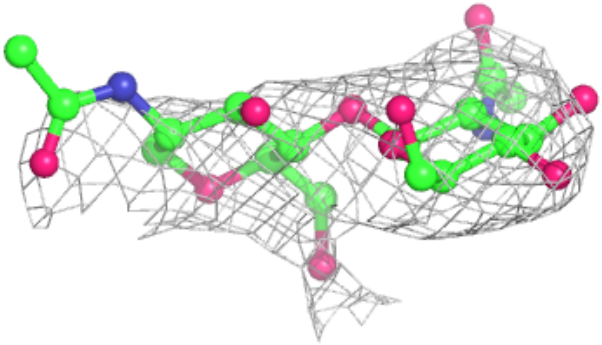
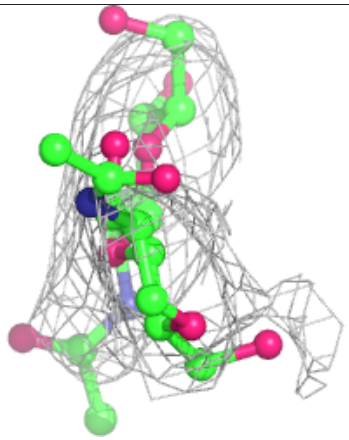
Electron density around Chain FA:

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



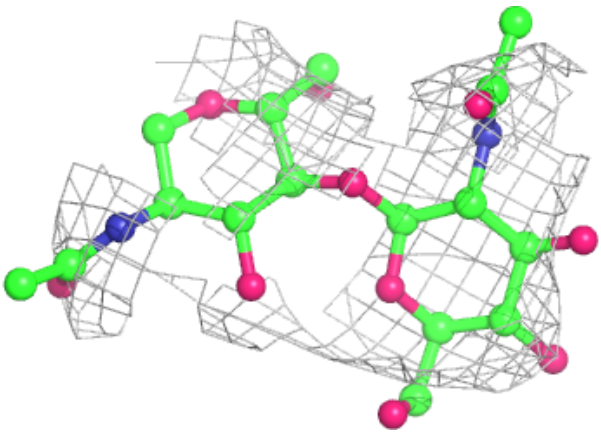


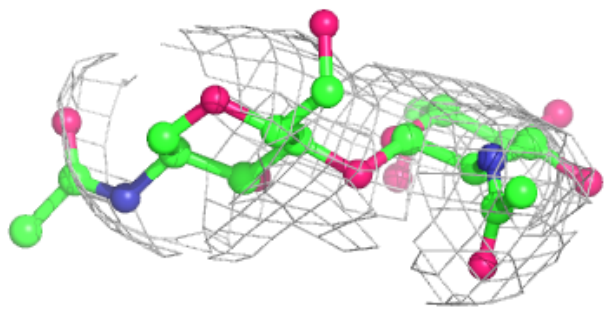


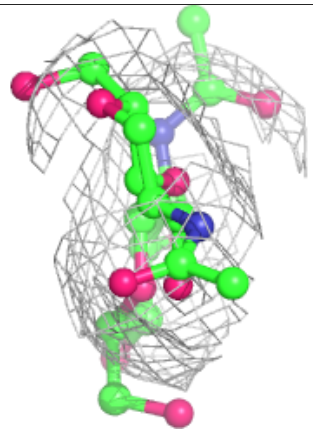
Electron density around Chain HA: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around Chain JA:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	R	201	14/15	0.35	0.60	100,111,117,117	0
7	NAG	M	502	14/15	0.40	0.58	75,76,77,78	0
7	NAG	E	601	14/15	0.43	0.43	59,64,66,67	0
7	NAG	U	502	14/15	0.45	0.61	46,48,50,51	0
7	NAG	G	502	14/15	0.49	0.70	42,47,49,51	0
7	NAG	Q	502	14/15	0.49	0.65	61,67,70,71	0
7	NAG	N	201	14/15	0.52	0.34	109,114,121,122	0
7	NAG	P	201	14/15	0.55	0.37	96,101,106,107	0
7	NAG	A	601	14/15	0.55	0.46	38,44,45,46	0
7	NAG	W	601	14/15	0.55	0.40	45,51,52,54	0
7	NAG	S	502	14/15	0.57	0.42	65,69,74,75	0
7	NAG	T	201	14/15	0.59	0.47	93,100,105,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	O	502	14/15	0.61	0.37	74,78,81,83	0
7	NAG	K	601	14/15	0.63	0.34	58,64,66,68	0
7	NAG	L	201	14/15	0.63	0.38	81,89,95,96	0
7	NAG	V	201	14/15	0.64	0.58	83,85,91,93	0
7	NAG	O	501	14/15	0.64	0.63	90,98,105,108	0
7	NAG	X	201	14/15	0.66	0.34	119,129,138,140	0
7	NAG	J	201	14/15	0.67	0.39	73,75,79,80	0
7	NAG	I	501	14/15	0.68	0.36	66,74,81,84	0
7	NAG	H	201	14/15	0.69	0.33	115,125,133,134	0
7	NAG	D	201	14/15	0.71	0.38	73,75,77,78	0
7	NAG	S	501	14/15	0.72	0.48	71,78,84,87	0
7	NAG	C	501	14/15	0.74	0.42	66,69,74,76	0
7	NAG	B	201	14/15	0.75	0.27	80,89,94,96	0
7	NAG	F	201	14/15	0.76	0.45	88,93,99,100	0
7	NAG	G	501	14/15	0.78	0.30	68,75,84,87	0
7	NAG	M	501	14/15	0.84	0.23	89,92,96,98	0
7	NAG	U	501	14/15	0.84	0.26	66,70,75,78	0
7	NAG	Q	501	14/15	0.85	0.24	66,74,80,83	0

6.5 Other polymers (i)

There are no such residues in this entry.