wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 03:25 PM EDT

PDB ID	:	6TYB
Title	:	Isolation and Structure of an Antibody that Fully Neutralizes Isolate SIV-mac239 Reveals Functional Similarity of SIV and HIV Glycan Shields
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2019-08-08
Resolution	:	2.30 Å(reported)

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

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

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

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

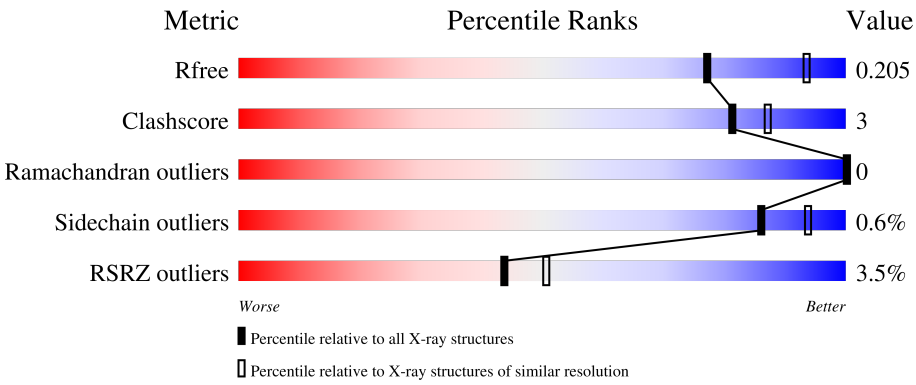
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	G	358	4%, 91%, 5%, •
2	C	187	7%, 86%, • •, 10%
3	H	238	2%, 91%, 5%, 5%
4	L	214	92%, 7%
5	A	7	86%, 14%

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Mol	Chain	Length	Quality of chain
5	F	7	57% 43%
5	I	7	43% 43% 14%
6	B	2	100%
7	D	3	33% 67%
8	E	7	43% 57%
9	J	6	50% 50%
9	K	6	50% 50%
10	M	5	40% 40% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	M	4	-	-	-	X
10	MAN	M	5	-	-	-	X
5	MAN	A	6	-	-	-	X
5	MAN	F	6	-	-	-	X
5	MAN	F	7	-	-	-	X
5	BMA	I	3	-	-	-	X
5	MAN	I	5	-	-	-	X
6	NAG	B	2	-	-	-	X
9	MAN	J	6	-	-	-	X
9	MAN	K	5	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 8525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	345	2806	1773	493	519	21	0	1	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	196	GLY	-	linker	UNP E7CWP5
G	197	SER	-	linker	UNP E7CWP5
G	198	GLY	-	linker	UNP E7CWP5
G	300	GLY	-	linker	UNP E7CWP5
G	301	GLY	-	linker	UNP E7CWP5
G	302	SER	-	linker	UNP E7CWP5
G	320	GLY	-	linker	UNP E7CWP5
G	321	GLY	-	linker	UNP E7CWP5
G	322	SER	-	linker	UNP E7CWP5
G	323	GLY	-	linker	UNP E7CWP5
G	494	GLY	-	expression tag	UNP E7CWP5
G	495	LEU	-	expression tag	UNP E7CWP5
G	496	GLU	-	expression tag	UNP E7CWP5
G	497	VAL	-	expression tag	UNP E7CWP5
G	498	LEU	-	expression tag	UNP E7CWP5
G	499	PHE	-	expression tag	UNP E7CWP5
G	500	GLN	-	expression tag	UNP E7CWP5

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	169	1307	817	226	259	5	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	GLN	CYS	conflict	UNP F6XGD3
C	179	GLY	-	expression tag	UNP F6XGD3
C	180	SER	-	expression tag	UNP F6XGD3
C	181	GLY	-	expression tag	UNP F6XGD3
C	182	LEU	-	expression tag	UNP F6XGD3
C	183	GLU	-	expression tag	UNP F6XGD3
C	184	VAL	-	expression tag	UNP F6XGD3
C	185	LEU	-	expression tag	UNP F6XGD3
C	186	PHE	-	expression tag	UNP F6XGD3
C	187	GLN	-	expression tag	UNP F6XGD3

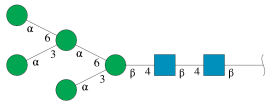
- Molecule 3 is a protein called NEUTRALIZING ANTIBODY ITS90.03 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	227	1738	1105	283	344	6	0	0	0

- Molecule 4 is a protein called NEUTRALIZING ANTIBODY ITS90.03 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	213	1645	1031	278	331	5	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

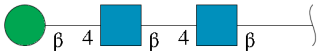


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	A	7	83	46	2	35	0	0	0
5	F	7	83	46	2	35	0	0	0
5	I	7	83	46	2	35	0	0	0

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

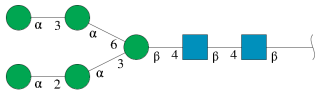
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	B	2	28	16	2	10	0	0	0

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



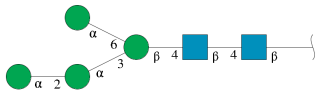
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	D	3	39	22	2	15	0	0	0

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



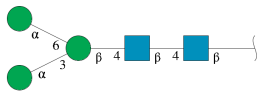
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	E	7	83	46	2	35	0	0	0

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



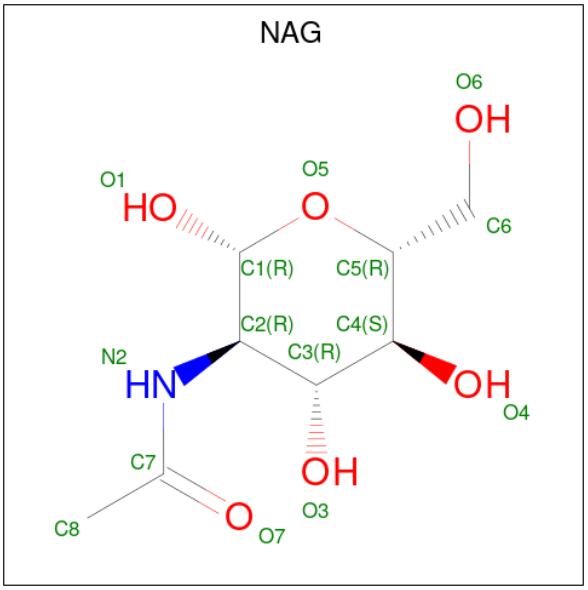
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	J	6	72	40	2	30	0	0	0
9	K	6	72	40	2	30	0	0	0

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



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

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



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

- Molecule 12 is water.

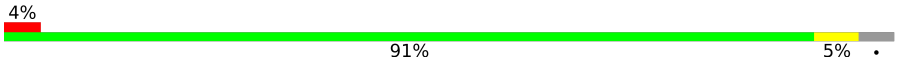
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	G	220	220	220	0	0
			Total	O		
12	C	27	27	27	0	0
			Total	O		
12	H	94	94	94	0	0
			Total	O		
12	L	56	56	56	0	0

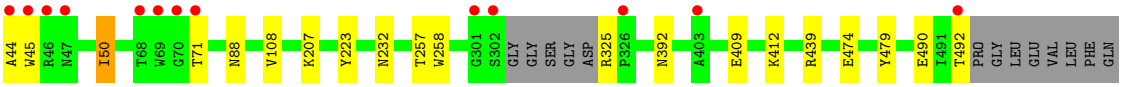
3 Residue-property plots (i)

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

• Molecule 1: Envelope glycoprotein gp160

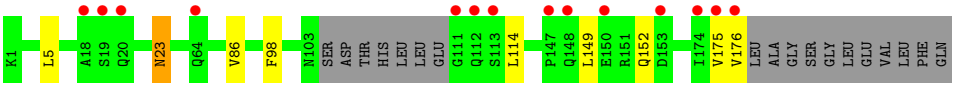
Chain G:





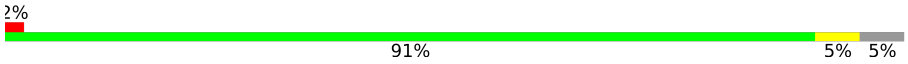
• Molecule 2: T-cell surface glycoprotein CD4

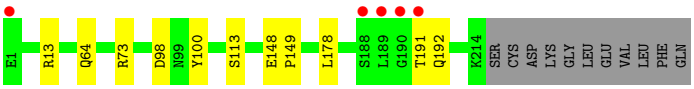
Chain C:



• Molecule 3: NEUTRALIZING ANTIBODY ITS90.03 FAB HEAVY CHAIN

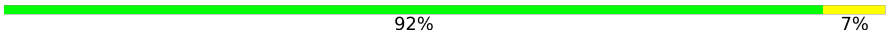
Chain H:

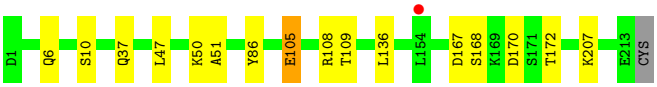




• Molecule 4: NEUTRALIZING ANTIBODY ITS90.03 FAB LIGHT CHAIN

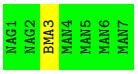
Chain L:





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

Chain A:



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

Chain F: 57% 43%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

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

Chain I: 43% 43% 14%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

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

Chain B: 100%

NAG1 NAG2

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

Chain D: 33% 67%

NAG1 NAG2 BMA3

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

Chain E: 43% 57%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

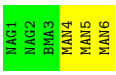
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

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

Chain K:



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

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	197.14Å 197.14Å 178.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.87 – 2.30 35.87 – 2.31	Depositor EDS
% Data completeness (in resolution range)	75.9 (35.87-2.30) 66.5 (35.87-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.31Å)	Xtriage
Refinement program	PHENIX dev_3584	Depositor
R, R_{free}	0.178 , 0.210 0.178 , 0.205	Depositor DCC
R_{free} test set	3115 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8525	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	G	0.28	0/2885	0.50	0/3921
2	C	0.26	0/1327	0.49	0/1784
3	H	0.27	0/1789	0.48	0/2441
4	L	0.26	0/1681	0.47	0/2282
All	All	0.27	0/7682	0.49	0/10428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2806	0	2680	14	0
2	C	1307	0	1334	11	0
3	H	1738	0	1662	7	0
4	L	1645	0	1600	9	0
5	A	83	0	70	0	0
5	F	83	0	70	3	0
5	I	83	0	70	1	0
6	B	28	0	25	0	0
7	D	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	83	0	70	0	0
9	J	72	0	61	0	0
9	K	72	0	61	0	0
10	M	61	0	52	1	0
11	G	28	0	26	0	0
12	C	27	0	0	0	0
12	G	220	0	0	1	0
12	H	94	0	0	1	0
12	L	56	0	0	0	0
All	All	8525	0	7815	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 42 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:3:BMA:H2	5:F:7:MAN:H5	1.52	0.91
2:C:175:VAL:HG12	2:C:176:VAL:HG22	1.62	0.79
4:L:10:SER:OG	4:L:105:GLU:OE2	2.09	0.70
4:L:170:ASP:OD1	4:L:172:THR:OG1	2.11	0.67
1:G:392:ASN:HB3	1:G:412:LYS:HG2	1.77	0.65

There are no symmetry-related clashes.

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	G	342/358 (96%)	333 (97%)	9 (3%)	0	100	100
2	C	166/187 (89%)	155 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	225/238 (94%)	219 (97%)	6 (3%)	0	100	100
4	L	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	944/997 (95%)	912 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	G	307/315 (98%)	305 (99%)	2 (1%)	84	92
2	C	152/167 (91%)	151 (99%)	1 (1%)	84	92
3	H	196/206 (95%)	195 (100%)	1 (0%)	88	95
4	L	186/187 (100%)	185 (100%)	1 (0%)	88	95
All	All	841/875 (96%)	836 (99%)	5 (1%)	86	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	50	ILE
1	G	409	GLU
2	C	23	ASN
3	H	64	GLN
4	L	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	232	ASN
1	G	422	GLN
2	C	88	ASN
3	H	204	ASN

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Mol	Chain	Res	Type
4	L	160	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

50 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	A	1	1,5	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	A	2	5	14,14,15	0.27	0	17,19,21	0.82	0
5	BMA	A	3	5	11,11,12	0.30	0	15,15,17	0.96	1 (6%)
5	MAN	A	4	5	11,11,12	0.24	0	15,15,17	0.86	0
5	MAN	A	5	5	11,11,12	0.26	0	15,15,17	0.84	0
5	MAN	A	6	5	11,11,12	0.25	0	15,15,17	0.84	0
5	MAN	A	7	5	11,11,12	0.24	0	15,15,17	0.89	0
6	NAG	B	1	1,6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	B	2	6	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	D	1	1,7	14,14,15	0.59	0	17,19,21	0.79	1 (5%)
7	NAG	D	2	7	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
7	BMA	D	3	7	11,11,12	0.23	0	15,15,17	0.86	0
8	NAG	E	1	1,8	14,14,15	0.24	0	17,19,21	0.48	0
8	NAG	E	2	8	14,14,15	0.33	0	17,19,21	0.42	0
8	BMA	E	3	8	11,11,12	0.64	0	15,15,17	0.68	0
8	MAN	E	4	8	11,11,12	0.71	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	MAN	E	5	8	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
8	MAN	E	6	8	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
8	MAN	E	7	8	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
5	NAG	F	1	1,5	14,14,15	0.42	0	17,19,21	0.59	0
5	NAG	F	2	5	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
5	BMA	F	3	5	11,11,12	0.29	0	15,15,17	0.72	0
5	MAN	F	4	5	11,11,12	0.39	0	15,15,17	0.70	0
5	MAN	F	5	5	11,11,12	0.24	0	15,15,17	0.73	0
5	MAN	F	6	5	11,11,12	0.28	0	15,15,17	0.96	0
5	MAN	F	7	5	11,11,12	0.20	0	15,15,17	0.97	0
5	NAG	I	1	1,5	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	I	2	5	14,14,15	0.18	0	17,19,21	0.41	0
5	BMA	I	3	5	11,11,12	0.34	0	15,15,17	0.94	0
5	MAN	I	4	5	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
5	MAN	I	5	5	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
5	MAN	I	6	5	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
5	MAN	I	7	5	11,11,12	0.29	0	15,15,17	0.88	0
9	NAG	J	1	9,1	14,14,15	0.34	0	17,19,21	0.50	0
9	NAG	J	2	9	14,14,15	0.30	0	17,19,21	0.38	0
9	BMA	J	3	9	11,11,12	0.51	0	15,15,17	0.79	0
9	MAN	J	4	9	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
9	MAN	J	5	9	11,11,12	0.69	0	15,15,17	0.96	2 (13%)
9	MAN	J	6	9	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
9	NAG	K	1	9,1	14,14,15	0.33	0	17,19,21	0.55	0
9	NAG	K	2	9	14,14,15	0.26	0	17,19,21	0.37	0
9	BMA	K	3	9	11,11,12	0.67	0	15,15,17	0.78	0
9	MAN	K	4	9	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
9	MAN	K	5	9	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
9	MAN	K	6	9	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
10	NAG	M	1	1,10	14,14,15	0.17	0	17,19,21	0.41	0
10	NAG	M	2	10	14,14,15	0.24	0	17,19,21	0.39	0
10	BMA	M	3	10	11,11,12	0.54	0	15,15,17	0.76	0
10	MAN	M	4	10	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
10	MAN	M	5	10	11,11,12	0.70	0	15,15,17	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
5	BMA	A	3	5	-	0/2/19/22	0/1/1/1
5	MAN	A	4	5	-	0/2/19/22	0/1/1/1
5	MAN	A	5	5	-	0/2/19/22	0/1/1/1
5	MAN	A	6	5	-	0/2/19/22	0/1/1/1
5	MAN	A	7	5	-	0/2/19/22	0/1/1/1
6	NAG	B	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	2/6/23/26	0/1/1/1
7	NAG	D	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3	7	-	0/2/19/22	0/1/1/1
8	NAG	E	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	2	8	-	2/6/23/26	0/1/1/1
8	BMA	E	3	8	-	0/2/19/22	0/1/1/1
8	MAN	E	4	8	-	2/2/19/22	0/1/1/1
8	MAN	E	5	8	-	2/2/19/22	0/1/1/1
8	MAN	E	6	8	-	0/2/19/22	0/1/1/1
8	MAN	E	7	8	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
5	MAN	I	6	5	-	0/2/19/22	0/1/1/1
5	MAN	I	7	5	-	0/2/19/22	0/1/1/1
9	NAG	J	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	2/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	0/1/1/1
9	MAN	J	5	9	-	0/2/19/22	0/1/1/1
9	MAN	J	6	9	-	0/2/19/22	0/1/1/1
9	NAG	K	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	2/2/19/22	0/1/1/1
9	MAN	K	5	9	-	1/2/19/22	0/1/1/1
9	MAN	K	6	9	-	0/2/19/22	0/1/1/1
10	NAG	M	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	MAN	M	4	10	-	0/2/19/22	0/1/1/1
10	MAN	M	5	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	2	NAG	O4-C4-C3	-3.05	103.30	110.35
9	J	4	MAN	C1-O5-C5	2.71	115.86	112.19
5	F	2	NAG	O5-C1-C2	-2.63	107.14	111.29
9	K	4	MAN	C1-O5-C5	2.61	115.72	112.19
8	E	7	MAN	C1-O5-C5	2.48	115.56	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	3	BMA	C4-C5-C6-O6
9	K	4	MAN	O5-C5-C6-O6
9	J	3	BMA	O5-C5-C6-O6
5	F	4	MAN	C4-C5-C6-O6
9	K	4	MAN	C4-C5-C6-O6

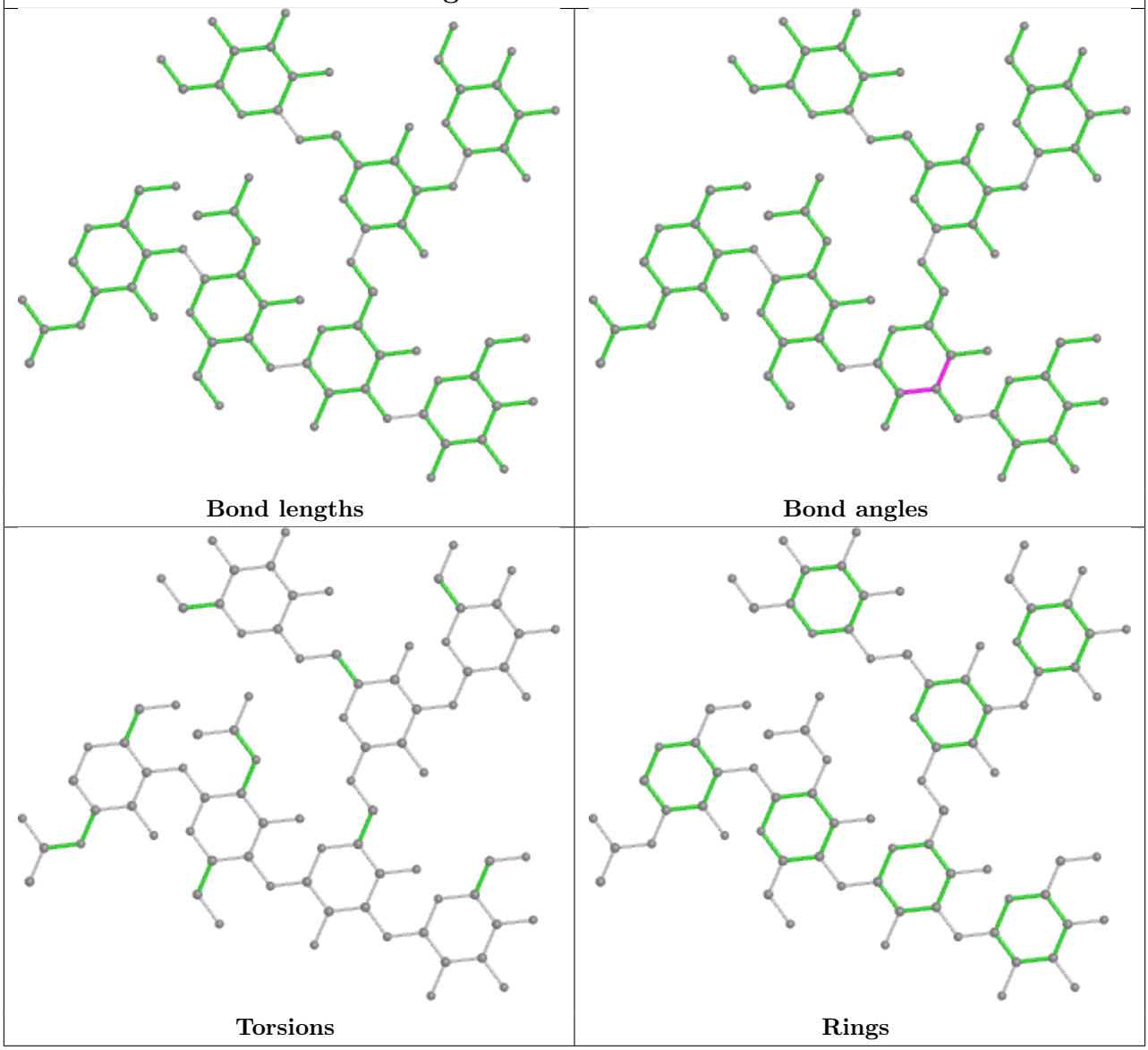
There are no ring outliers.

6 monomers are involved in 5 short contacts:

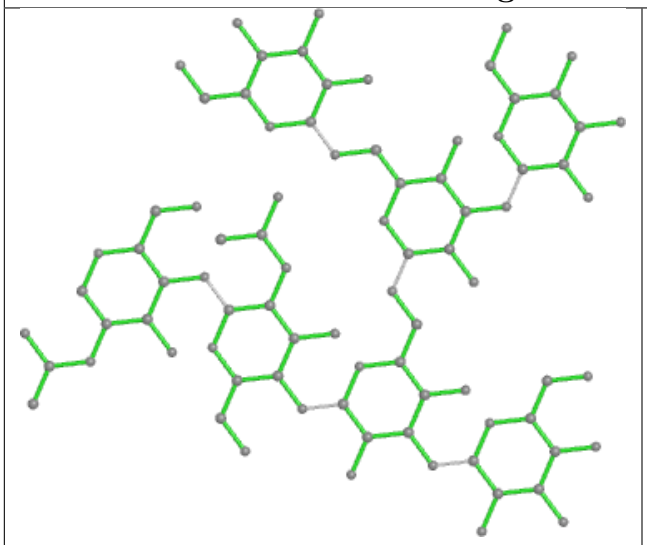
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	3	BMA	1	0
10	M	3	BMA	1	0
5	F	3	BMA	3	0
10	M	4	MAN	1	0
5	I	4	MAN	1	0
5	F	7	MAN	3	0

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

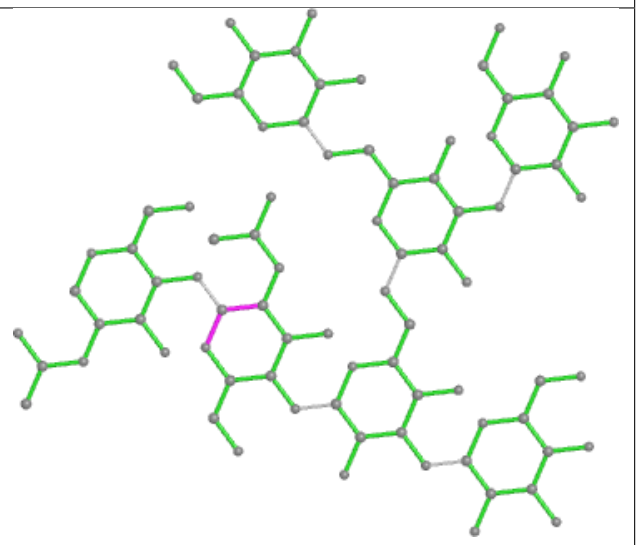
Oligosaccharide Chain A



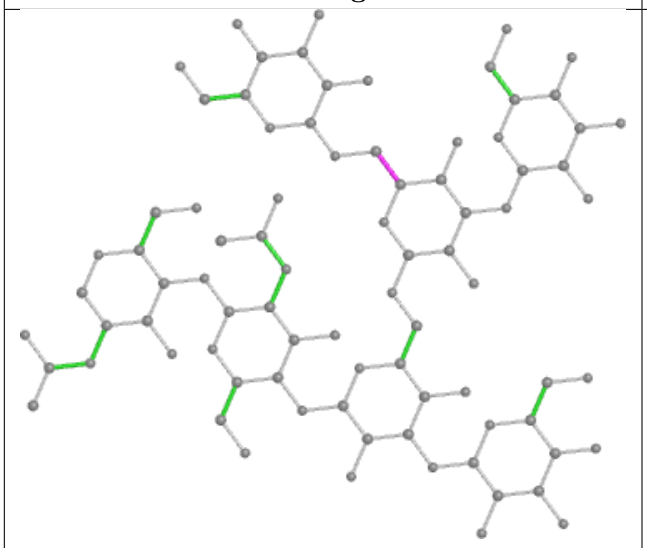
Oligosaccharide Chain F



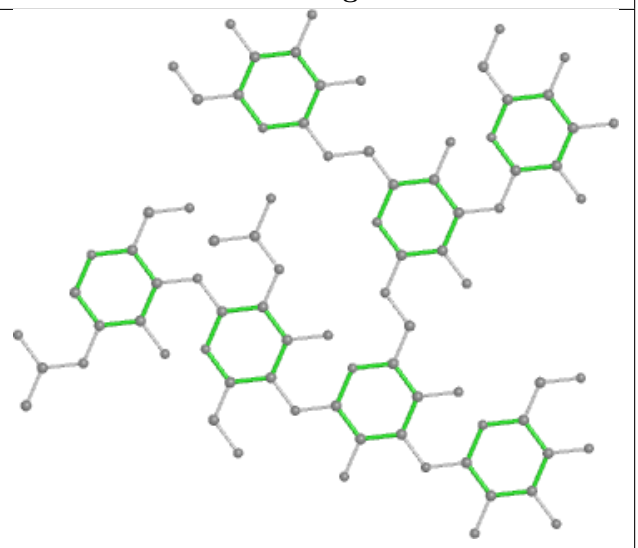
Bond lengths



Bond angles

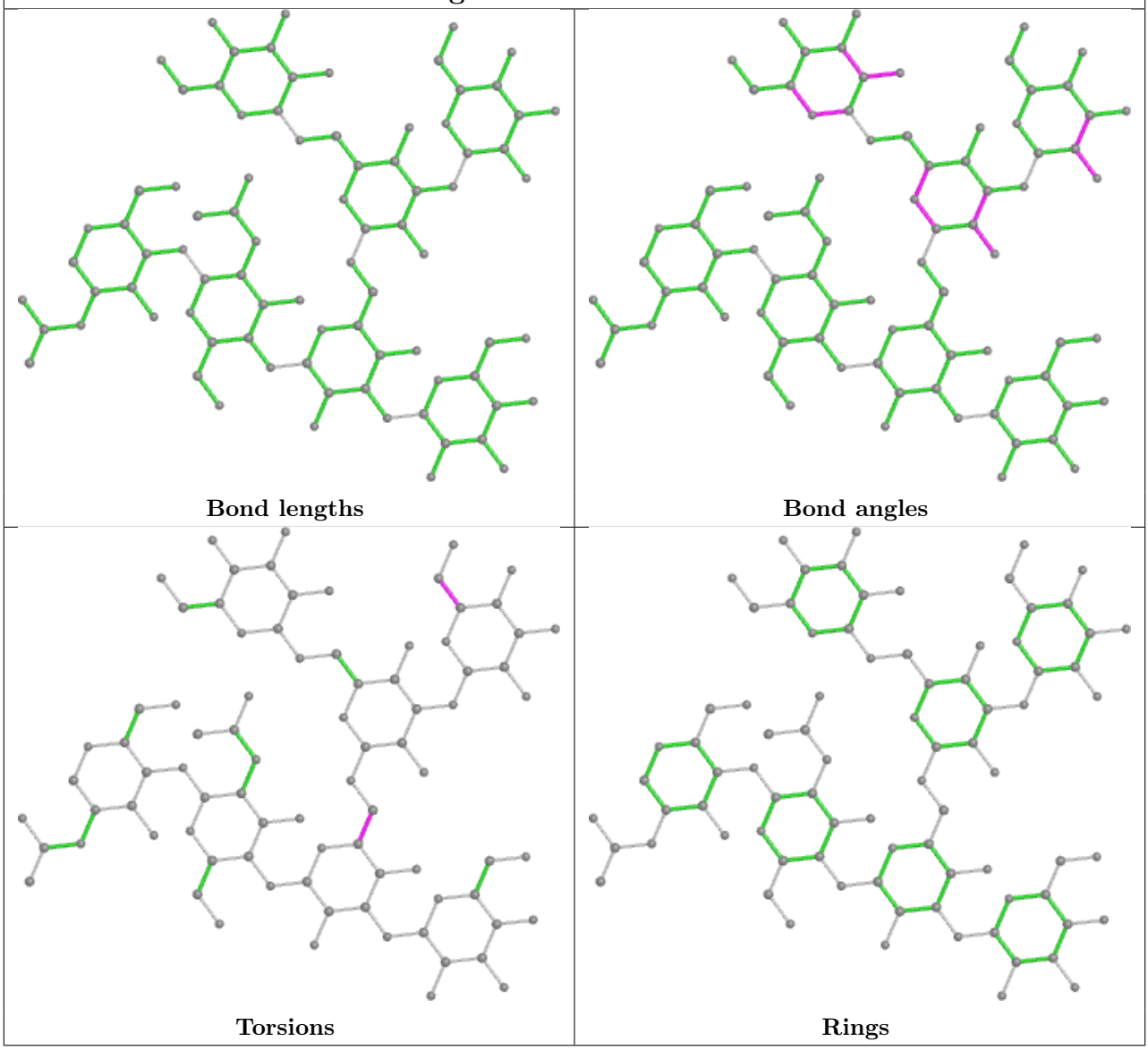


Torsions

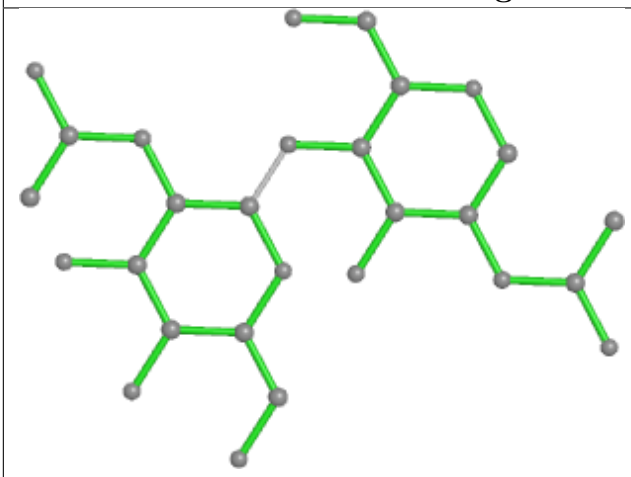


Rings

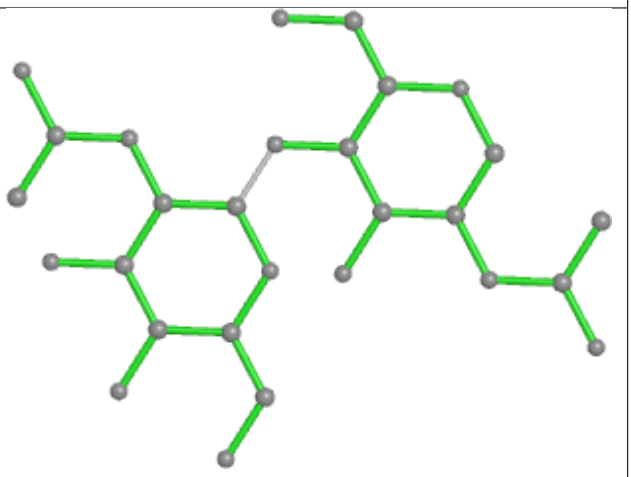
Oligosaccharide Chain I



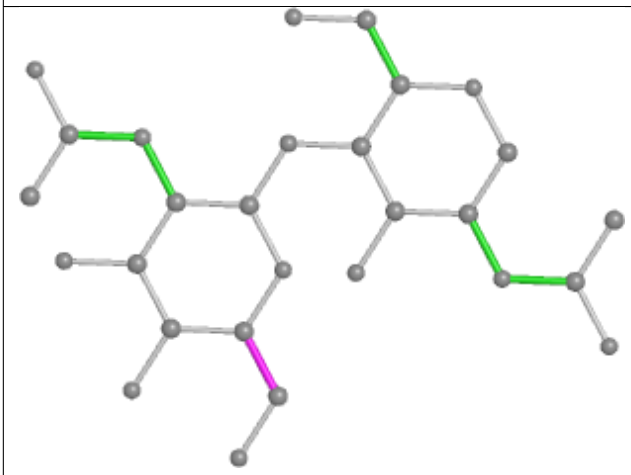
Oligosaccharide Chain B



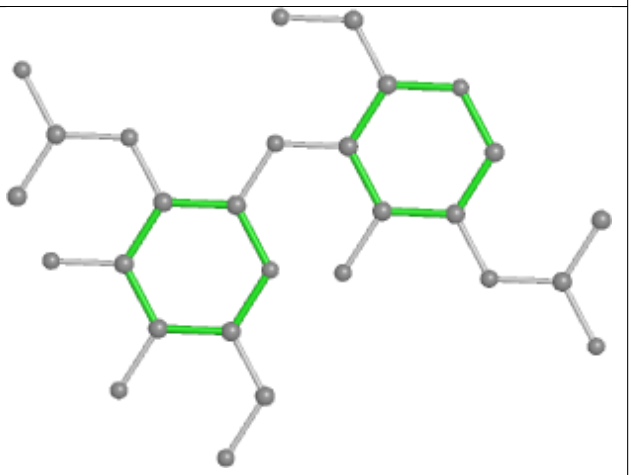
Bond lengths



Bond angles

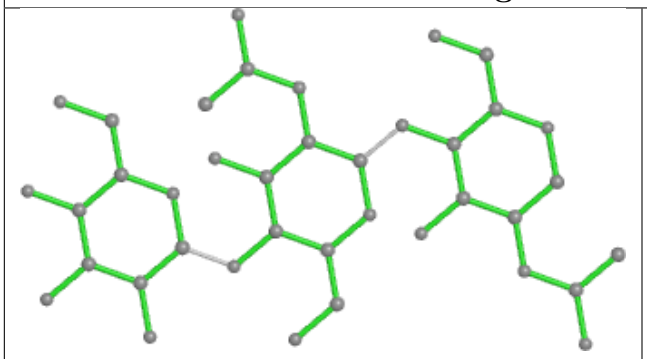


Torsions

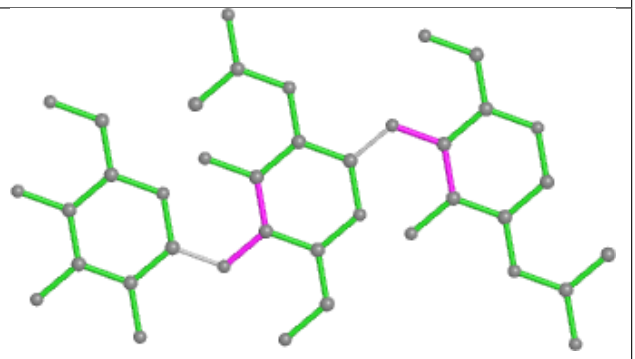


Rings

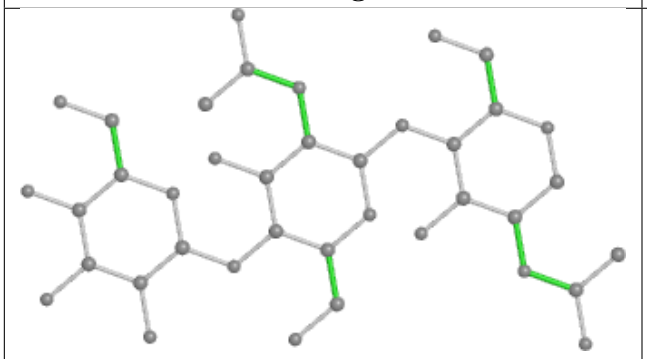
Oligosaccharide Chain D



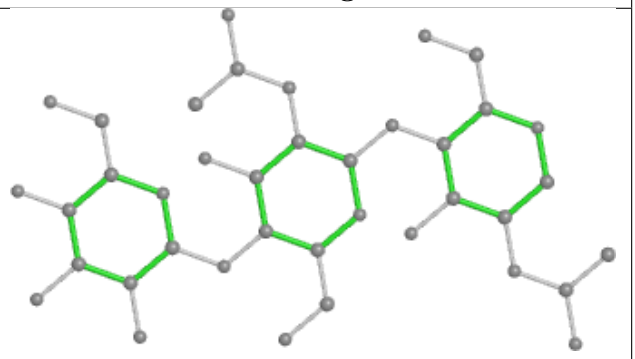
Bond lengths



Bond angles

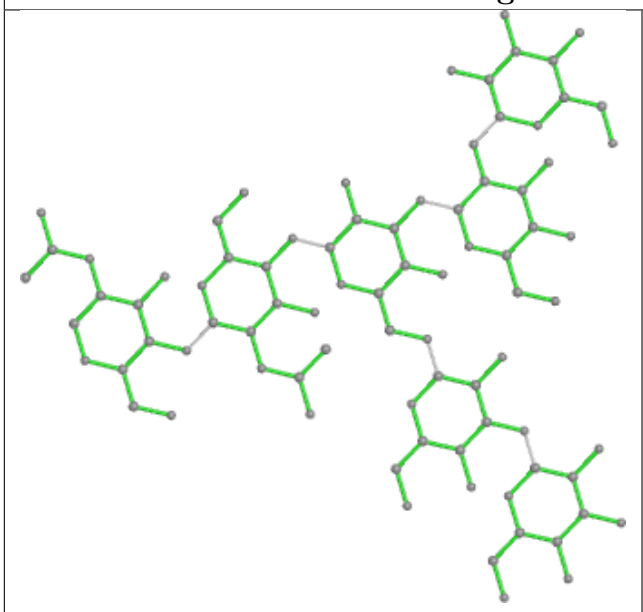


Torsions

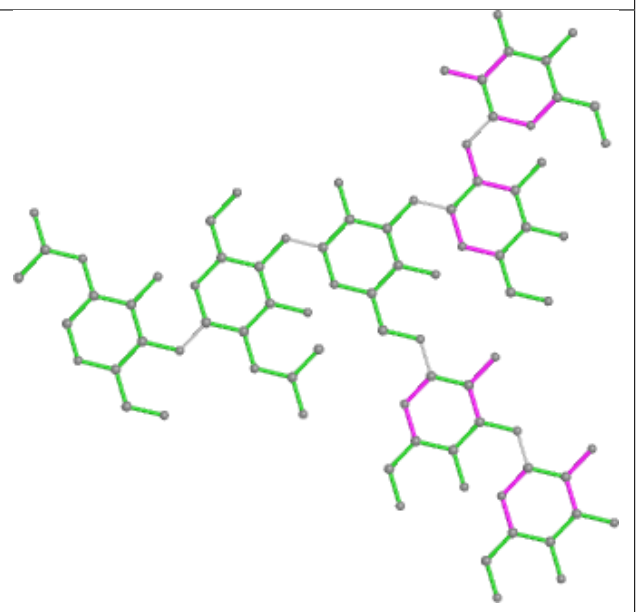


Rings

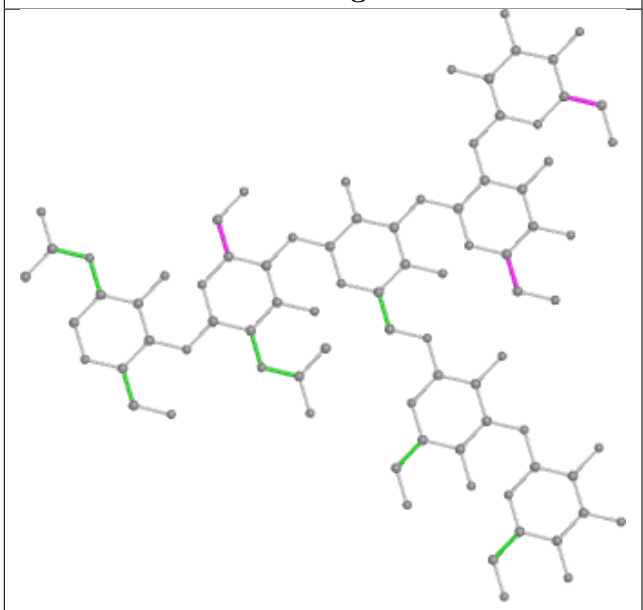
Oligosaccharide Chain E



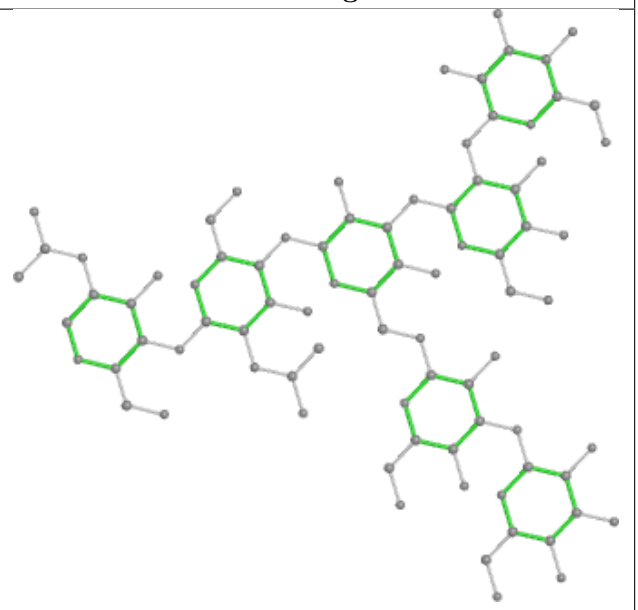
Bond lengths



Bond angles

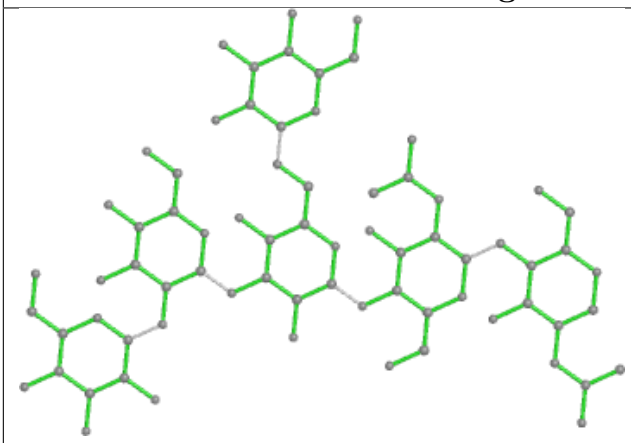


Torsions

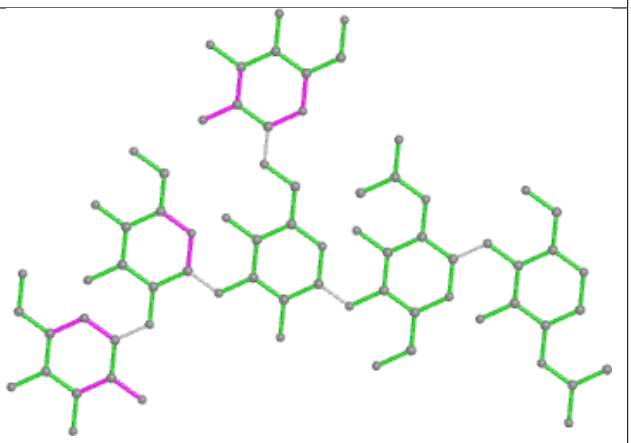


Rings

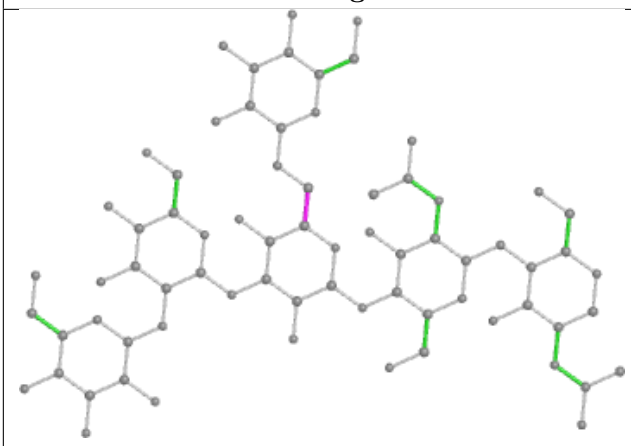
Oligosaccharide Chain J



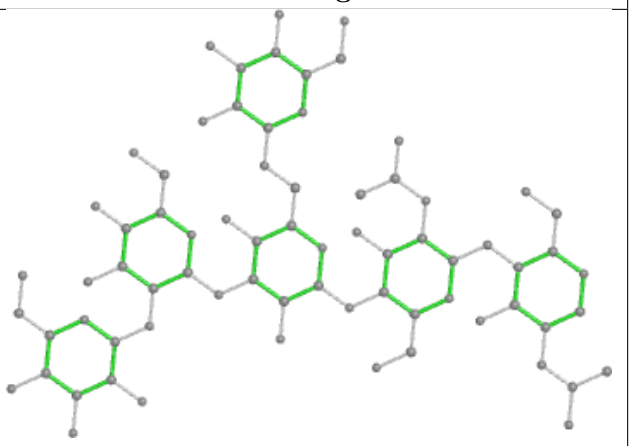
Bond lengths



Bond angles

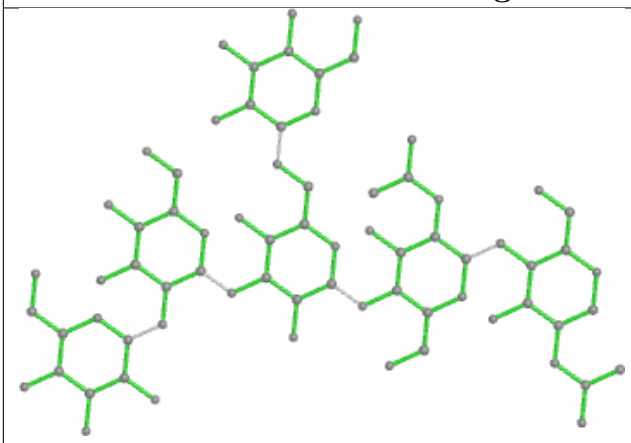


Torsions

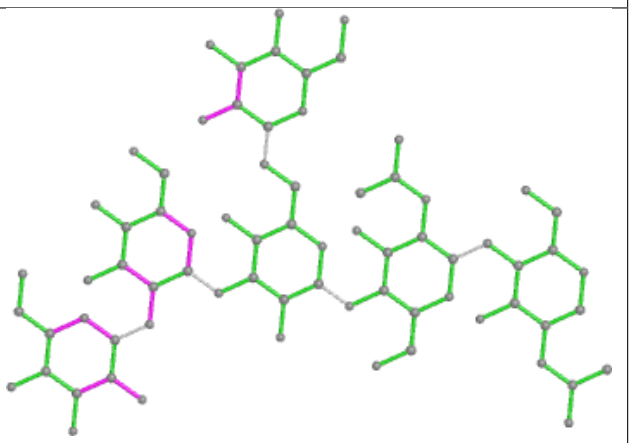


Rings

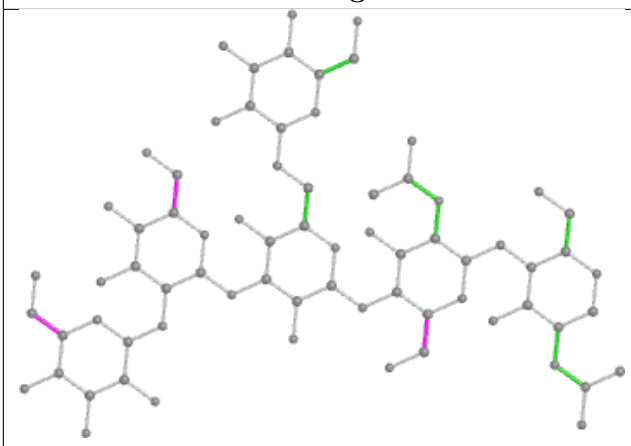
Oligosaccharide Chain K



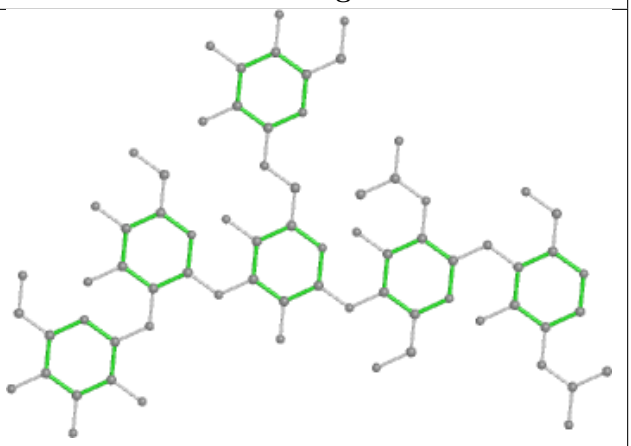
Bond lengths



Bond angles

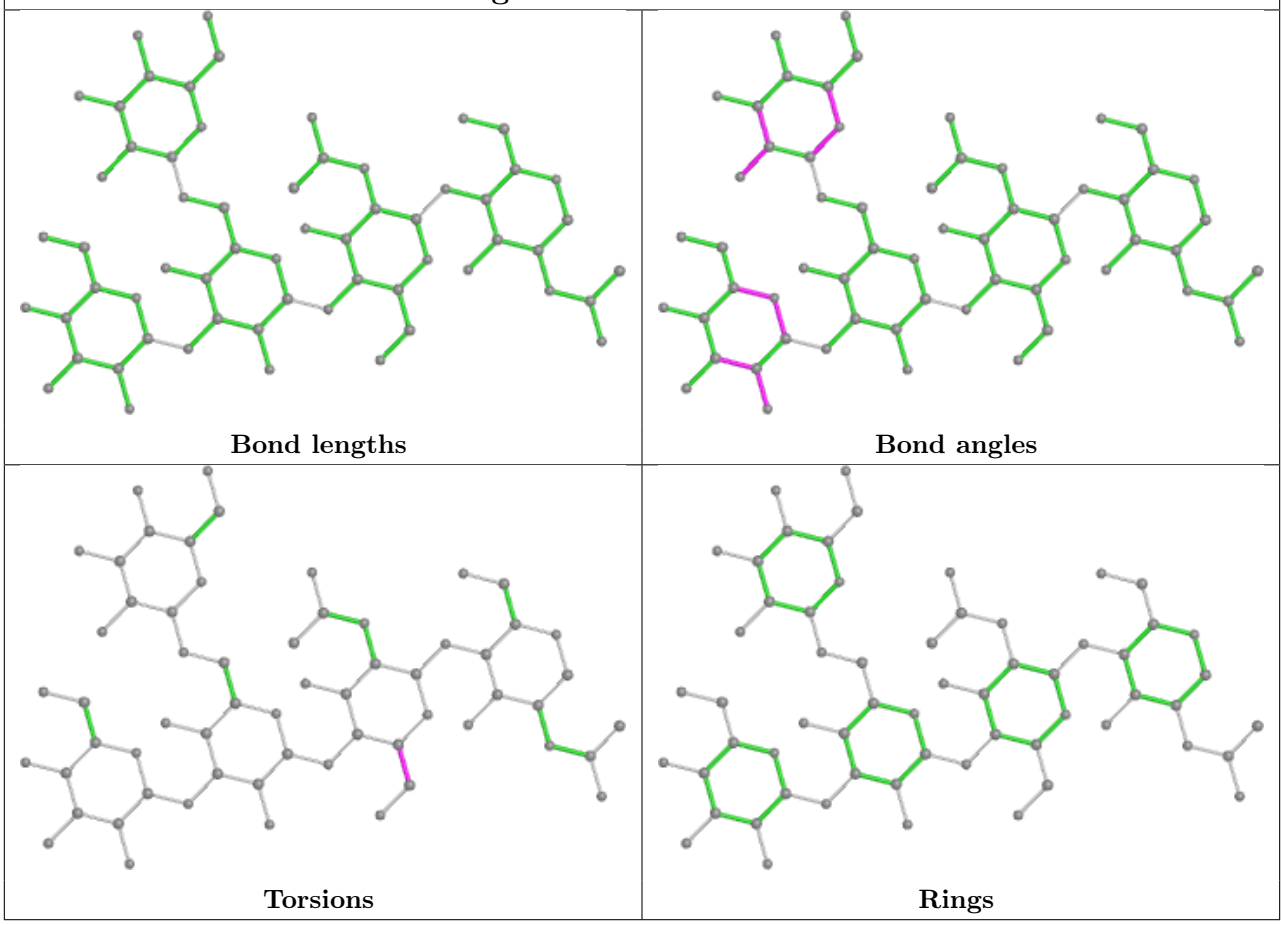


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	G	1446	1	14,14,15	0.24	0	17,19,21	0.47	0
11	NAG	G	1291	1	14,14,15	0.22	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	G	1446	1	-	2/6/23/26	0/1/1/1
11	NAG	G	1291	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	1446	NAG	C1-C2-N2-C7
11	G	1446	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	G	345/358 (96%)	-0.07	13 (3%)	40	47	15, 30, 83, 116	0
2	C	169/187 (90%)	0.16	14 (8%)	11	15	23, 64, 112, 134	0
3	H	227/238 (95%)	-0.37	5 (2%)	62	69	21, 44, 85, 111	0
4	L	213/214 (99%)	-0.18	1 (0%)	91	94	25, 57, 83, 100	0
All	All	954/997 (95%)	-0.13	33 (3%)	44	51	15, 45, 96, 134	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	302	SER	6.9
1	G	45	TRP	5.9
2	C	19	SER	4.5
1	G	492	THR	4.3
3	H	189	LEU	4.2

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

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

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
8	MAN	E	5	11/12	0.59	0.36	74,118,128,134	0
6	NAG	B	2	14/15	0.60	0.50	83,121,135,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BMA	D	3	11/12	0.62	0.38	122,133,140,144	0
10	MAN	M	5	11/12	0.62	0.52	114,137,148,149	0
9	MAN	K	5	11/12	0.64	0.49	116,126,134,136	0
9	MAN	K	6	11/12	0.69	0.31	80,100,108,111	0
5	BMA	I	3	11/12	0.72	0.49	116,134,145,148	0
5	MAN	I	6	11/12	0.72	0.39	102,128,131,133	0
10	MAN	M	4	11/12	0.74	0.45	96,117,129,135	0
5	MAN	F	6	11/12	0.74	0.41	93,121,129,129	0
5	MAN	F	7	11/12	0.75	0.49	103,125,136,138	0
5	MAN	A	6	11/12	0.76	0.41	107,126,136,139	0
5	MAN	I	4	11/12	0.78	0.23	121,127,136,144	0
9	MAN	J	4	11/12	0.78	0.29	113,122,131,140	0
5	NAG	I	2	14/15	0.79	0.23	52,86,103,119	0
10	BMA	M	3	11/12	0.79	0.37	117,124,133,134	0
9	MAN	J	6	11/12	0.79	0.51	120,129,142,146	0
5	MAN	I	5	11/12	0.79	0.44	99,133,143,148	0
8	MAN	E	6	11/12	0.80	0.29	79,101,109,111	0
5	MAN	F	4	11/12	0.80	0.22	77,88,110,124	0
5	MAN	A	7	11/12	0.81	0.41	105,113,122,124	0
5	MAN	I	7	11/12	0.82	0.61	129,141,150,154	0
9	MAN	J	5	11/12	0.82	0.53	131,139,145,147	0
5	MAN	A	5	11/12	0.83	0.38	110,124,130,130	0
8	MAN	E	7	11/12	0.83	0.49	106,125,132,135	0
5	BMA	F	3	11/12	0.86	0.19	86,94,105,114	0
9	MAN	K	4	11/12	0.87	0.32	81,98,111,120	0
5	MAN	A	4	11/12	0.87	0.25	83,107,120,129	0
9	BMA	J	3	11/12	0.88	0.27	94,108,120,132	0
6	NAG	B	1	14/15	0.89	0.14	55,70,87,111	0
7	NAG	D	2	14/15	0.90	0.28	72,94,113,131	0
5	BMA	A	3	11/12	0.91	0.21	74,78,93,103	0
8	MAN	E	4	11/12	0.91	0.28	97,104,109,116	0
10	NAG	M	2	14/15	0.91	0.24	47,70,93,116	0
9	BMA	K	3	11/12	0.92	0.21	65,86,101,111	0
5	NAG	A	2	14/15	0.92	0.20	38,61,70,72	0
5	MAN	F	5	11/12	0.92	0.23	81,93,100,101	0
5	NAG	I	1	14/15	0.92	0.12	36,47,67,77	0
8	BMA	E	3	11/12	0.94	0.18	59,75,85,97	0
8	NAG	E	2	14/15	0.95	0.10	30,51,59,85	0
5	NAG	A	1	14/15	0.95	0.12	35,50,65,67	0
9	NAG	J	2	14/15	0.95	0.11	35,49,75,83	0
5	NAG	F	2	14/15	0.96	0.10	26,50,70,90	0
9	NAG	K	2	14/15	0.96	0.11	37,47,66,68	0

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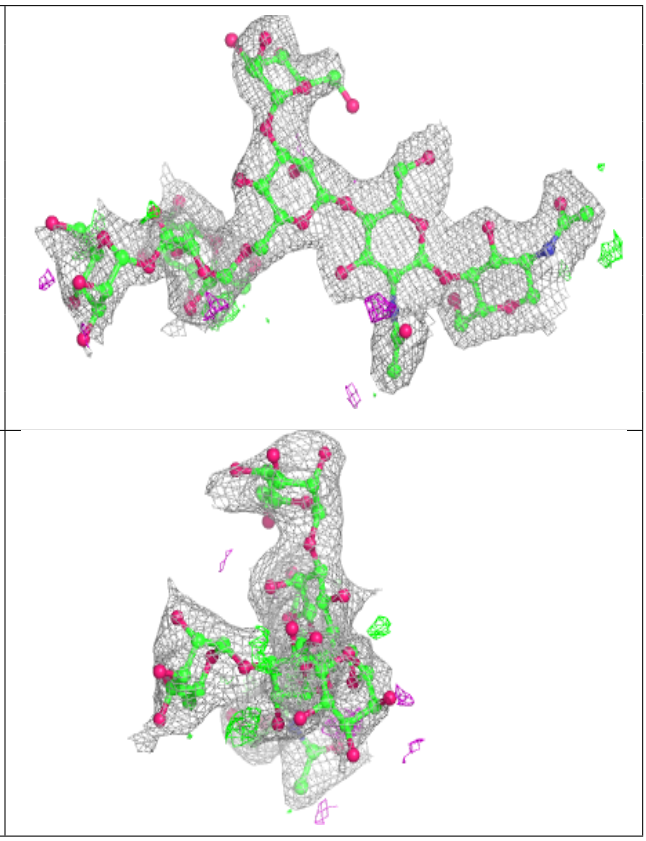
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	D	1	14/15	0.97	0.16	34,50,71,72	0
9	NAG	J	1	14/15	0.97	0.08	25,35,41,41	0
5	NAG	F	1	14/15	0.97	0.10	21,29,40,54	0
10	NAG	M	1	14/15	0.97	0.08	26,36,42,44	0
8	NAG	E	1	14/15	0.98	0.12	16,27,41,50	0
9	NAG	K	1	14/15	0.98	0.08	20,29,39,41	0

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.

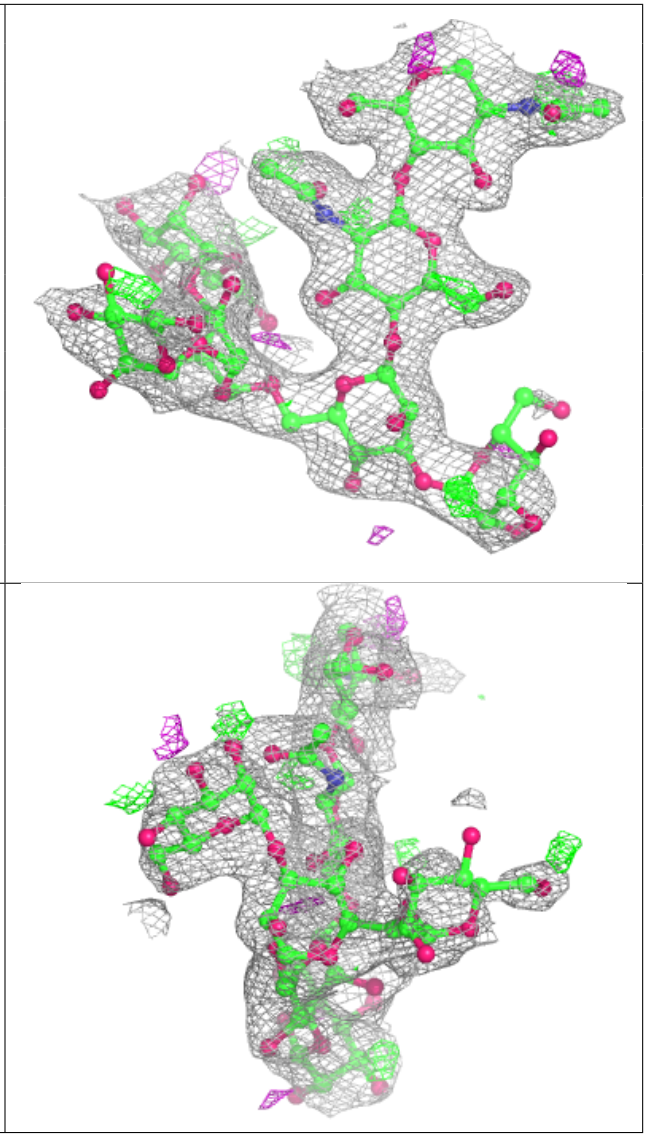
Electron density around Chain A:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



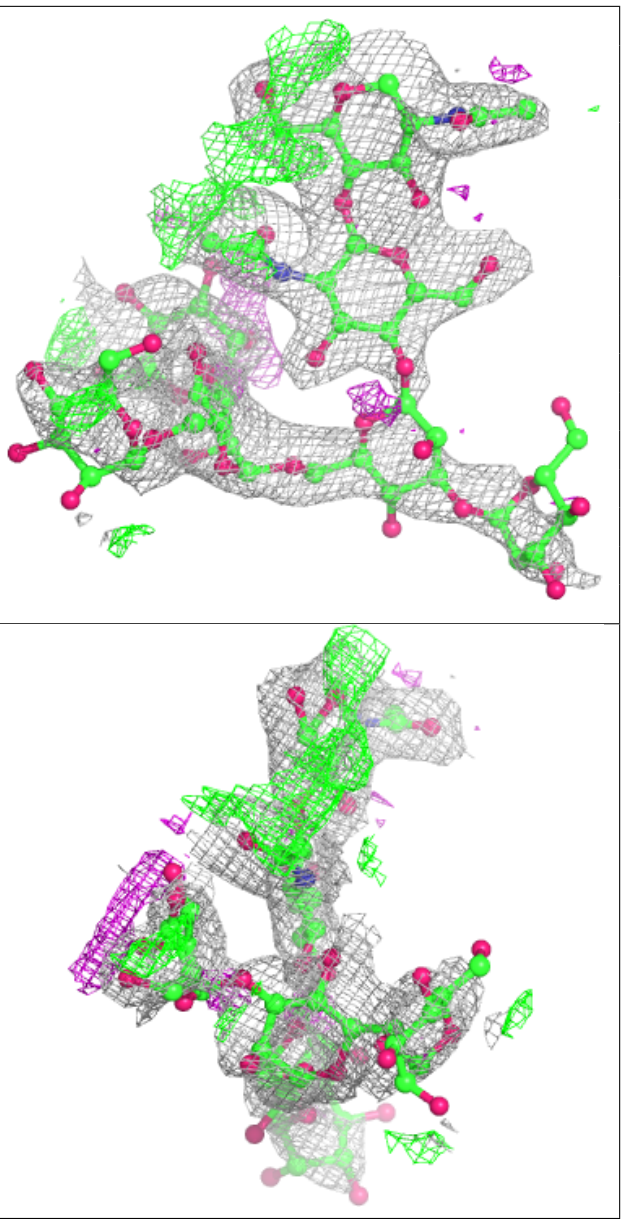
Electron density around Chain F:

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



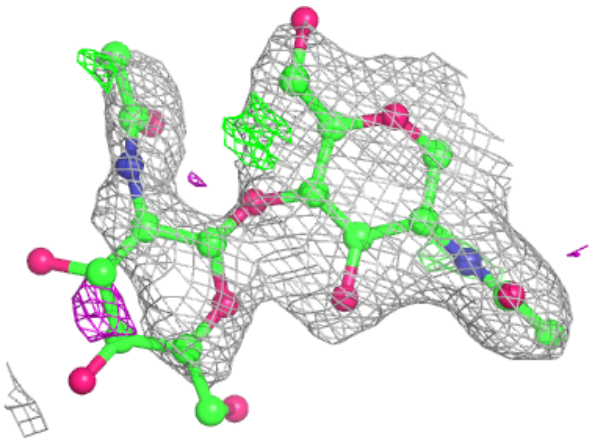
Electron density around Chain I:

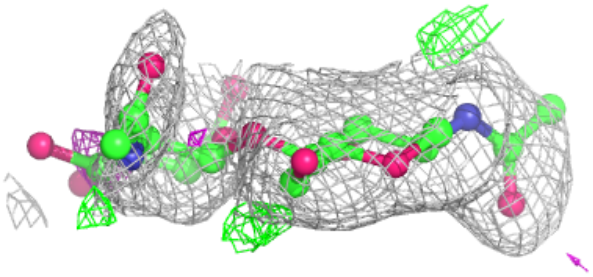
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

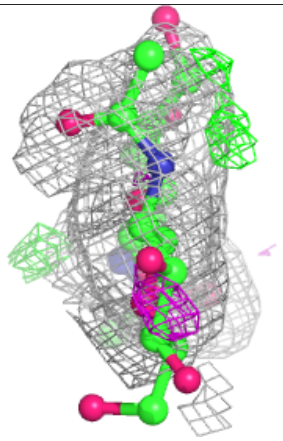


Electron density around Chain B:

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

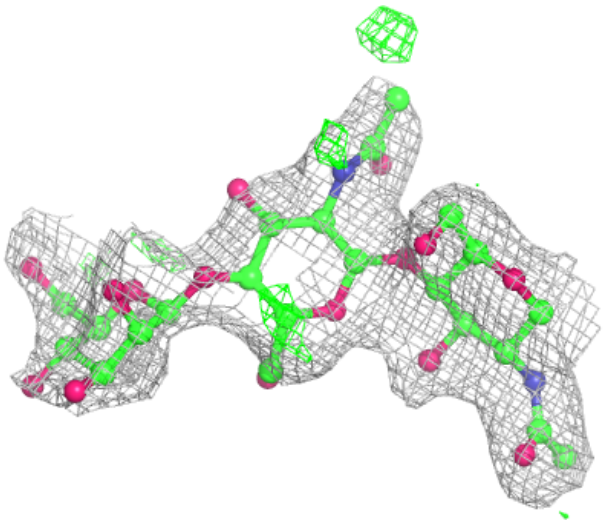


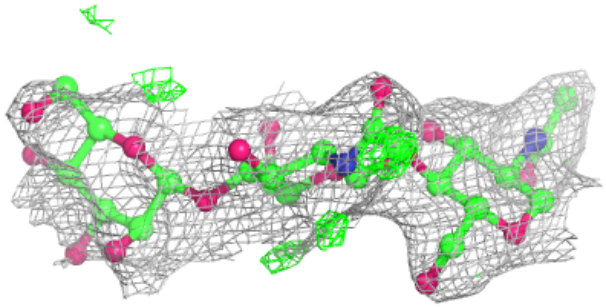


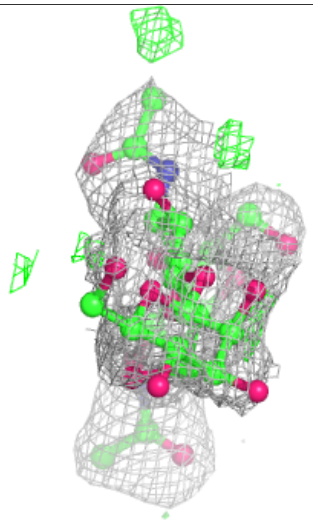


Electron density around Chain D:

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

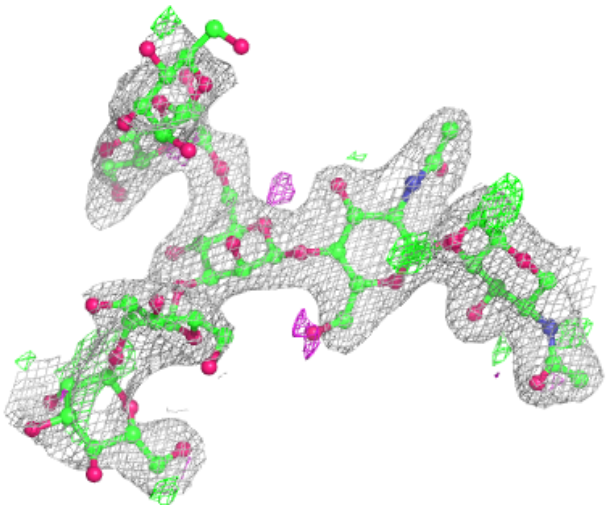


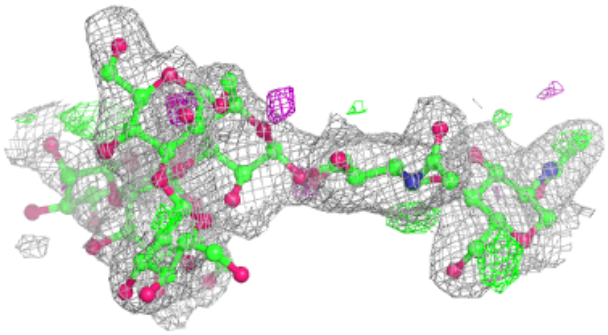


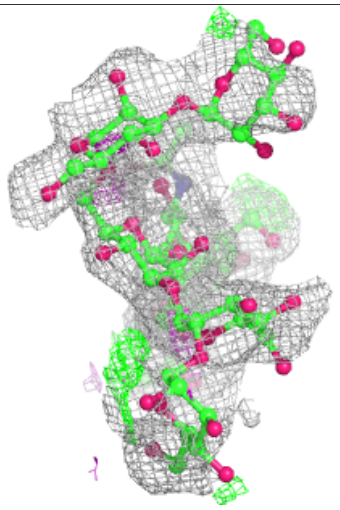


Electron density around Chain E:

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

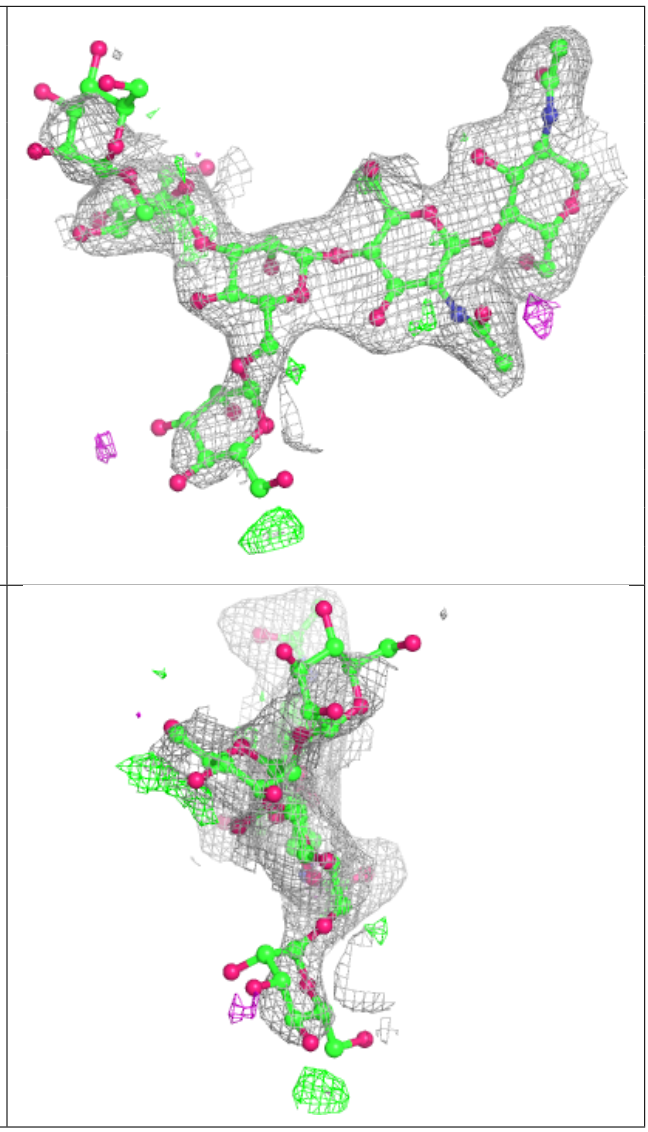






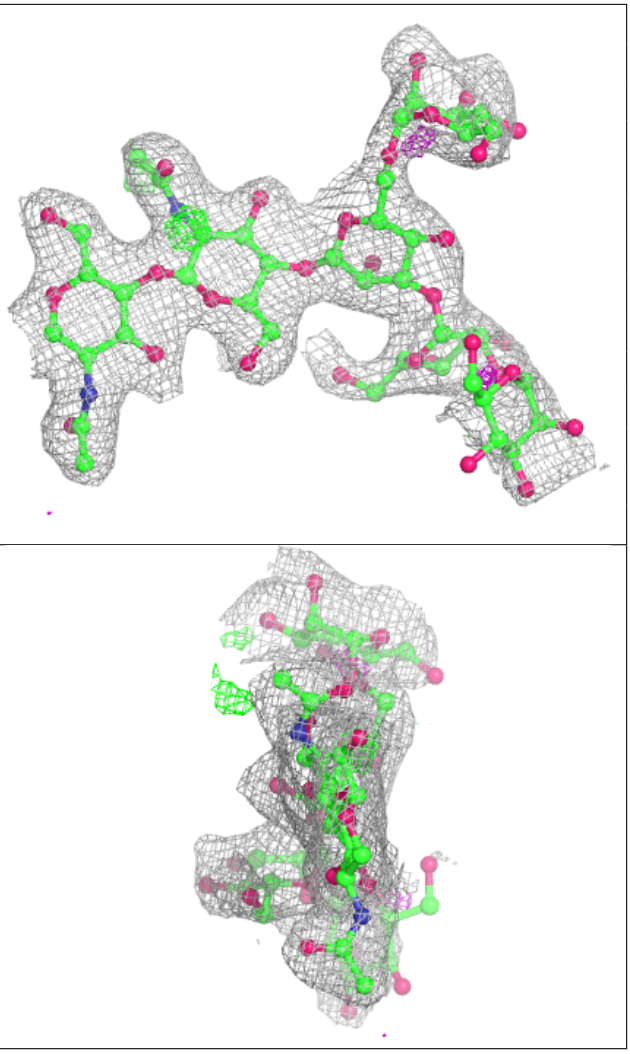
Electron density around Chain J:

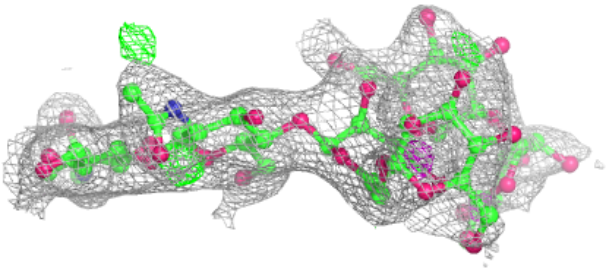
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

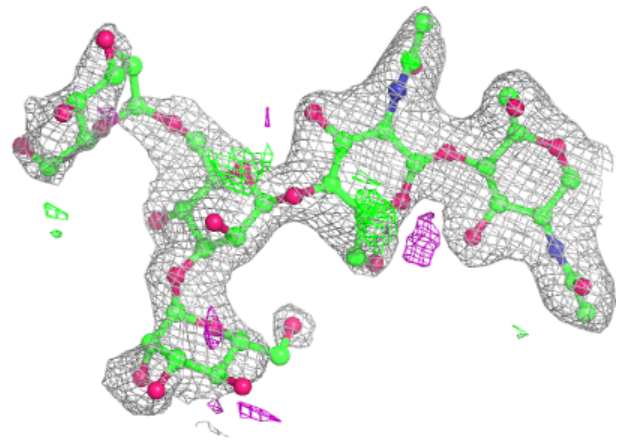
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

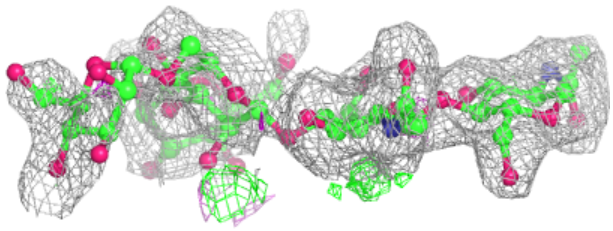


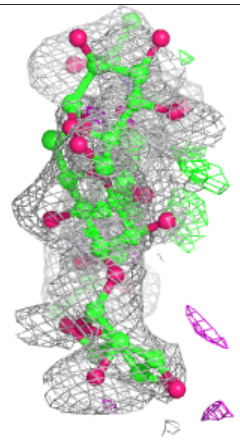


Electron density around Chain M:

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







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
11	NAG	G	1291	14/15	0.88	0.32	51,89,106,110	0
11	NAG	G	1446	14/15	0.91	0.21	60,84,91,92	0

6.5 Other polymers (i)

There are no such residues in this entry.