



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 03:08 PM UTC

PDB ID : 3EVJ / pdb_00003evj
Title : Intermediate structure of antithrombin bound to the natural pentasaccharide
Authors : Huntington, J.A.; Belzar, K.J.
Deposited on : 2008-10-13
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

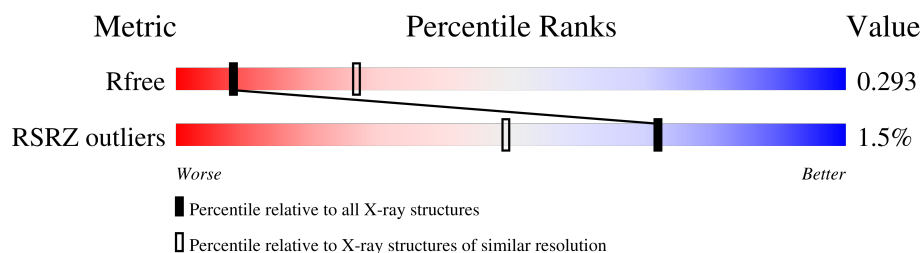
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

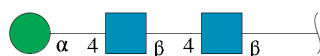
There are 7 unique types of molecules in this entry. The entry contains 6574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	404	Total	C	N	O	S	0	0	0
			3016	1922	498	579	17			
1	L	417	Total	C	N	O	S	0	0	0
			3148	2009	517	605	17			

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



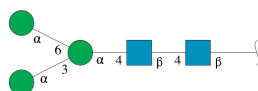
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	3	Total	C	N	O	0	0	0
			38	21	2	15			

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



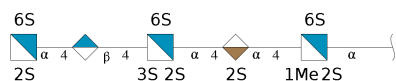
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



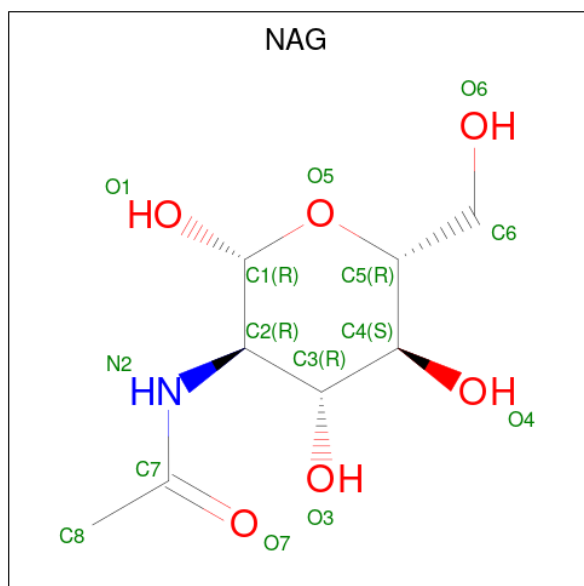
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			
5	F	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	I	1	Total	C	N	O	6	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	24	Total	O	0	0
			24	24		
7	L	21	Total	O	0	0
			21	21		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.85Å 87.06Å 92.38Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	63.24 – 3.00 63.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (63.24-3.00) 99.1 (63.24-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.289 0.235 , 0.293	Depositor DCC
R_{free} test set	1016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6574	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

22 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
2	NAG	A	1	1,2	14,14,15	0.66	0	17,19,21	1.02	1 (5%)
2	NAG	A	2	2	11,11,15	0.52	0	11,12,21	0.90	1 (9%)
2	MAN	A	3	2	11,11,12	0.61	0	15,15,17	0.43	0
3	NAG	B	1	1,3	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	B	2	3	14,14,15	0.58	0	17,19,21	0.63	0
3	NAG	C	1	1,3	14,14,15	0.77	0	17,19,21	1.18	2 (11%)
3	NAG	C	2	3	14,14,15	0.73	1 (7%)	17,19,21	0.61	0
4	NAG	D	1	1,4	14,14,15	0.67	0	17,19,21	0.63	0
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	0.68	0
4	MAN	D	3	4	11,11,12	0.70	0	15,15,17	0.81	1 (6%)
4	MAN	D	4	4	11,11,12	0.65	0	15,15,17	0.55	0
4	MAN	D	5	4	11,11,12	0.75	0	15,15,17	1.20	1 (6%)
5	ZDO	E	1	5	21,21,21	2.71	5 (23%)	26,32,32	1.38	3 (11%)
5	IDS	E	2	5	16,16,17	1.52	2 (12%)	16,24,26	0.82	1 (6%)
5	SUS	E	3	5	23,23,24	2.73	5 (21%)	26,36,38	1.43	3 (11%)
5	BDP	E	4	5	12,12,13	0.67	0	14,17,19	0.63	0
5	SGN	E	5	5	19,19,20	2.79	4 (21%)	23,29,31	1.39	3 (13%)
5	ZDO	F	1	5	21,21,21	2.69	5 (23%)	26,32,32	1.40	3 (11%)
5	IDS	F	2	5	16,16,17	1.51	2 (12%)	16,24,26	0.93	1 (6%)
5	SUS	F	3	5	23,23,24	2.75	5 (21%)	26,36,38	1.52	3 (11%)
5	BDP	F	4	5	12,12,13	0.68	0	14,17,19	0.77	0
5	SGN	F	5	5	19,19,20	2.79	4 (21%)	23,29,31	1.31	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/10/10/26	-
2	MAN	A	3	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	D	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	MAN	D	5	4	-	2/2/19/22	1/1/1/1
5	ZDO	E	1	5	-	8/13/33/33	0/1/1/1
5	IDS	E	2	5	-	0/9/26/29	0/1/1/1
5	SUS	E	3	5	-	7/16/33/36	0/1/1/1
5	BDP	E	4	5	-	0/4/21/24	0/1/1/1
5	SGN	E	5	5	-	1/11/28/31	0/1/1/1
5	ZDO	F	1	5	-	4/13/33/33	0/1/1/1
5	IDS	F	2	5	-	0/9/26/29	0/1/1/1
5	SUS	F	3	5	-	8/16/33/36	0/1/1/1
5	BDP	F	4	5	-	1/4/21/24	0/1/1/1
5	SGN	F	5	5	-	2/11/28/31	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	5	SGN	O2S-S1	7.42	1.50	1.42
5	F	3	SUS	O1S-S1	7.37	1.50	1.42
5	E	1	ZDO	OSB-S2	7.36	1.50	1.42
5	E	5	SGN	O2S-S1	7.35	1.50	1.42
5	E	3	SUS	O1S-S1	7.34	1.50	1.42

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	SUS	O1S-S1-O3S	-5.27	108.63	120.36
5	E	1	ZDO	OSA-S2-OSB	-5.00	109.24	120.36
5	F	1	ZDO	OSA-S2-OSB	-4.88	109.50	120.36
5	E	3	SUS	O1S-S1-O3S	-4.83	109.62	120.36
5	E	5	SGN	O1S-S1-O2S	-4.82	109.64	120.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	3	MAN	C1
4	D	3	MAN	C1

5 of 62 torsion outliers are listed below:

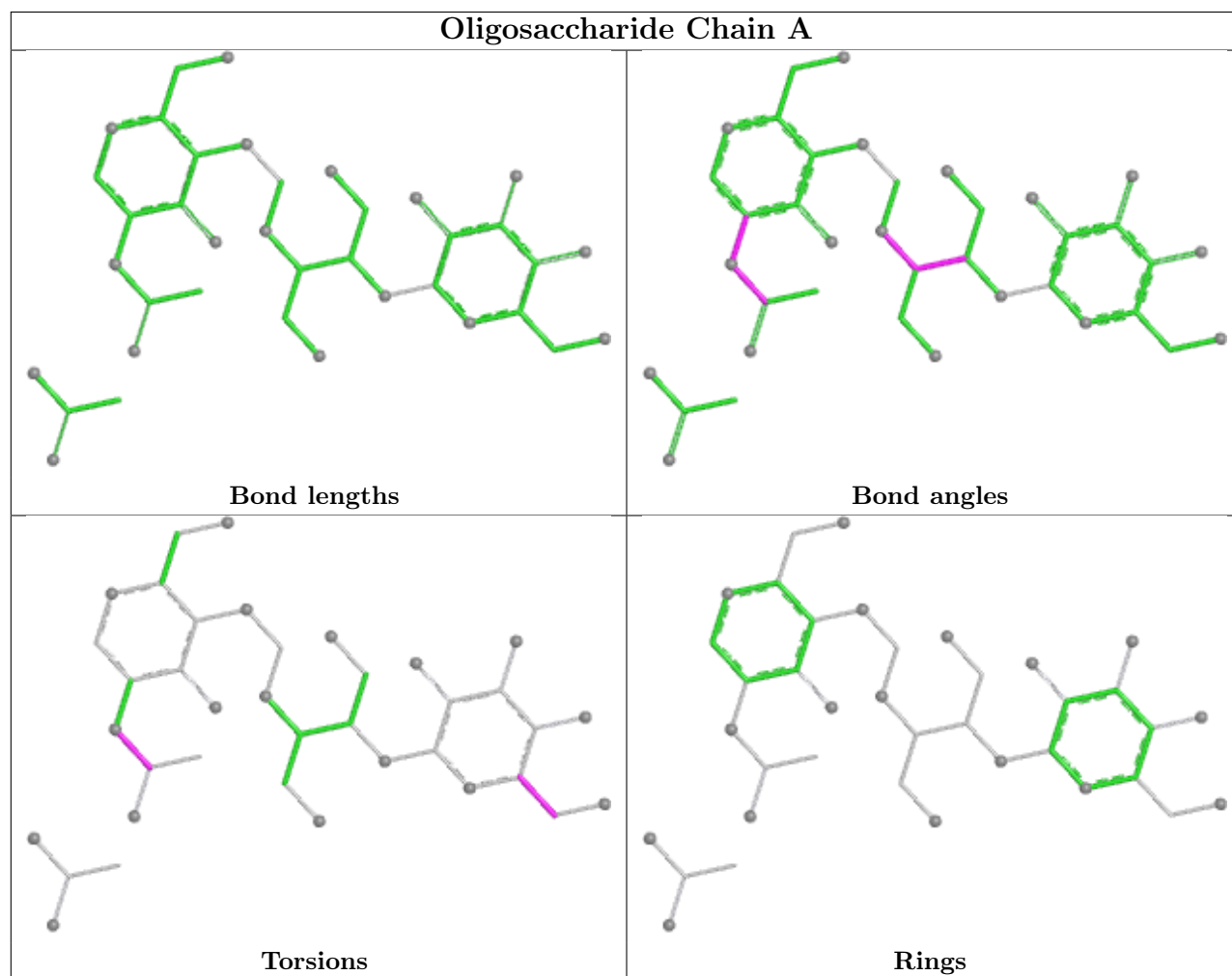
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
3	B	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2

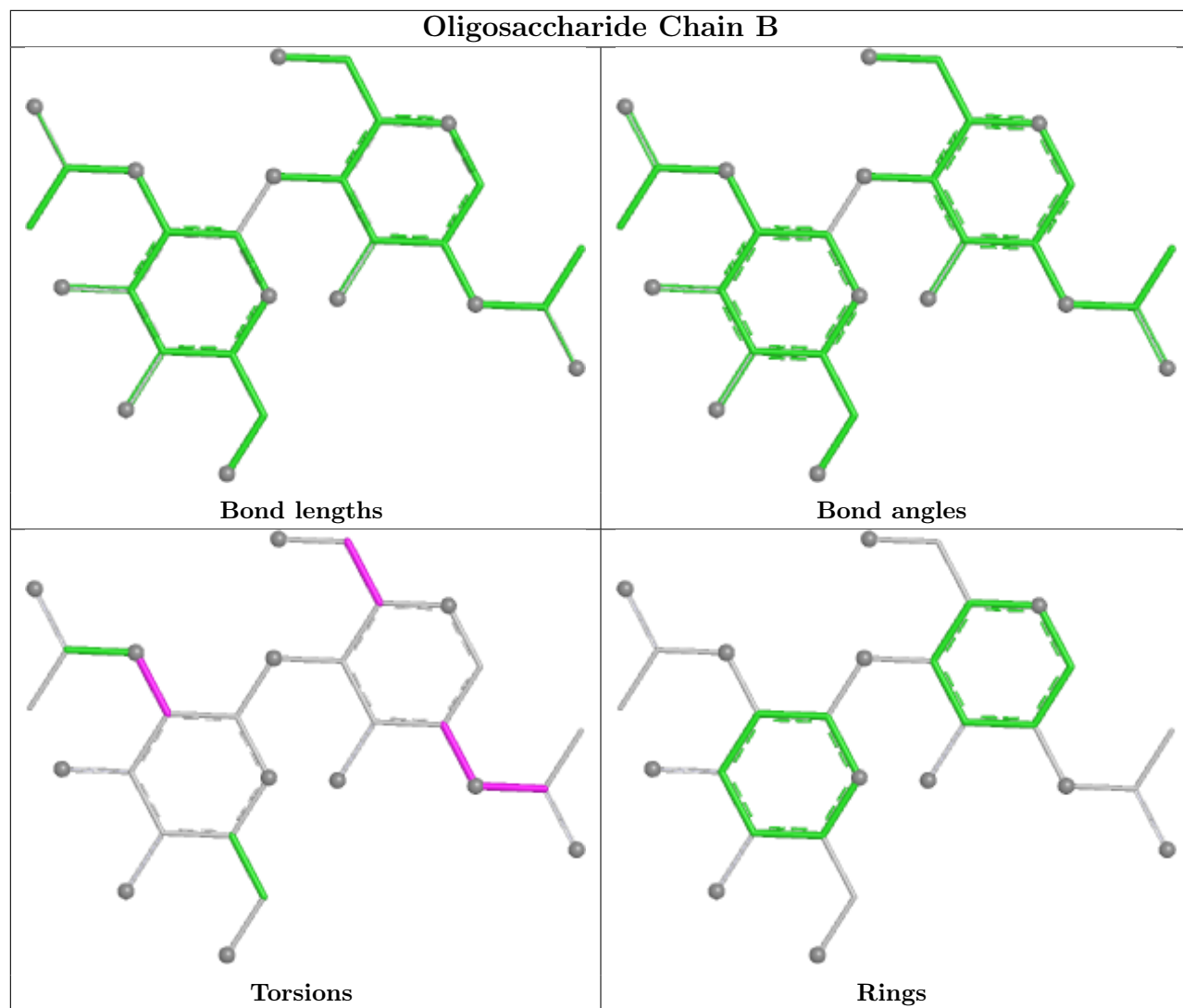
All (2) ring outliers are listed below:

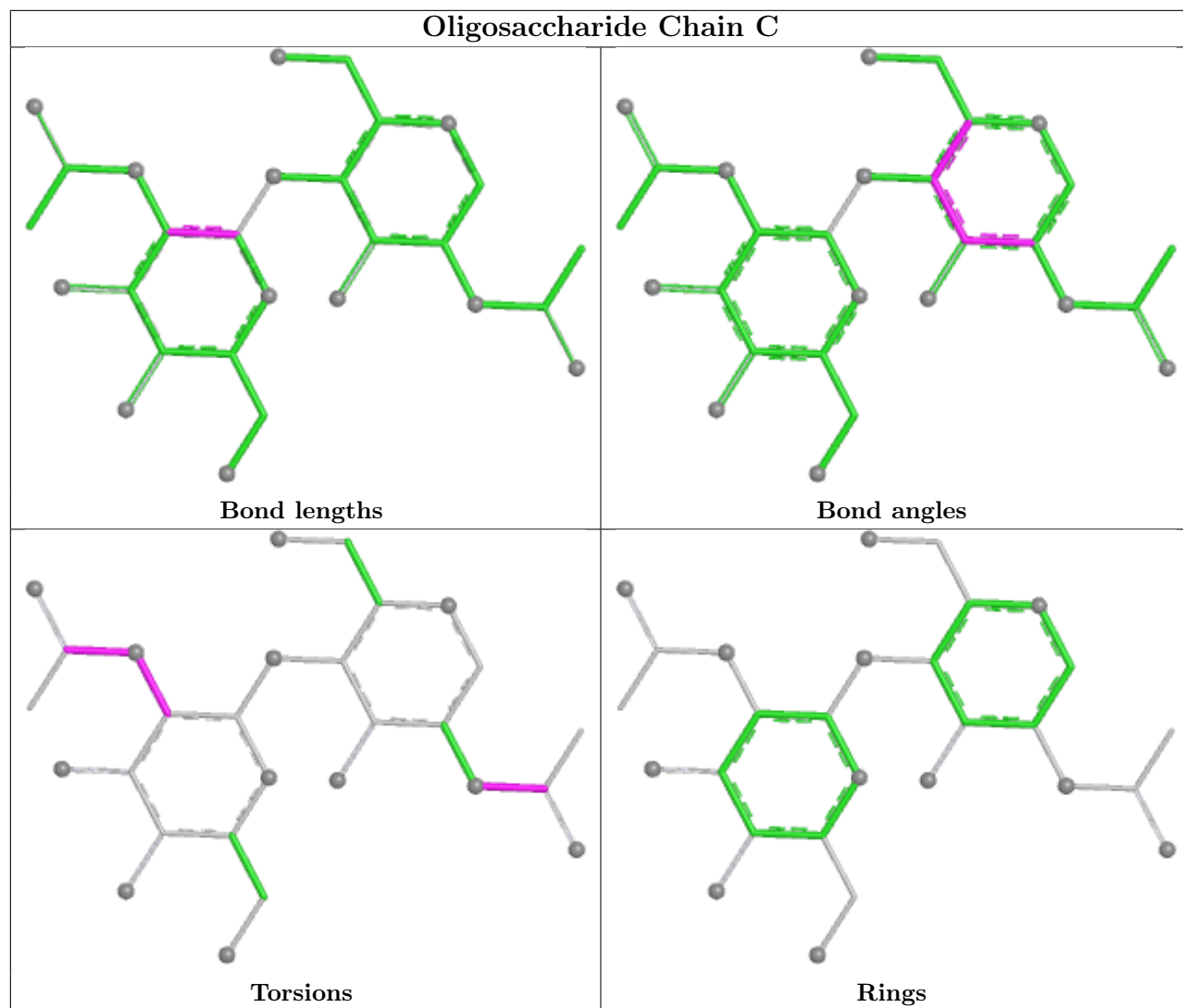
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	D	5	MAN	C1-C2-C3-C4-C5-O5

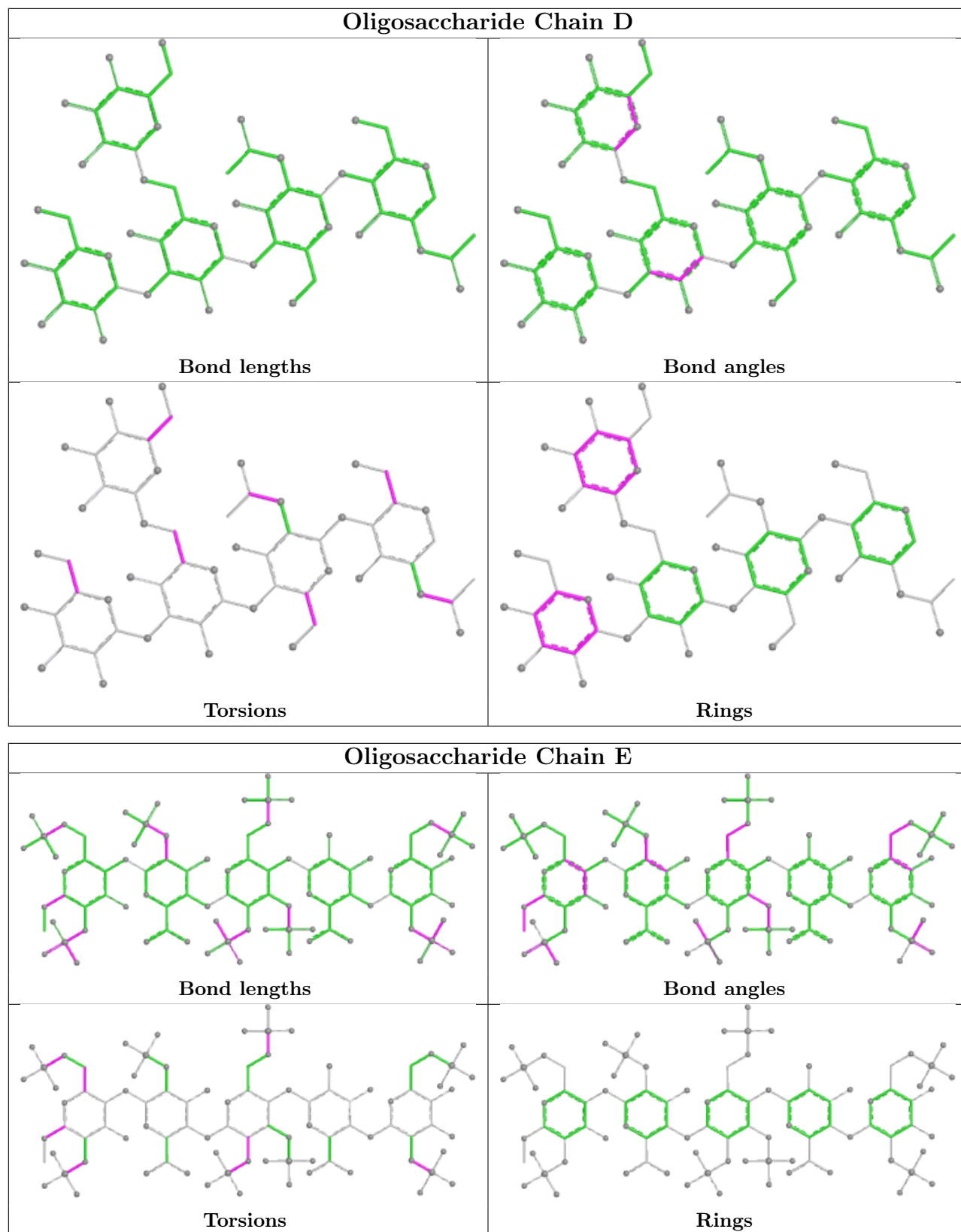
No monomer is involved in short contacts.

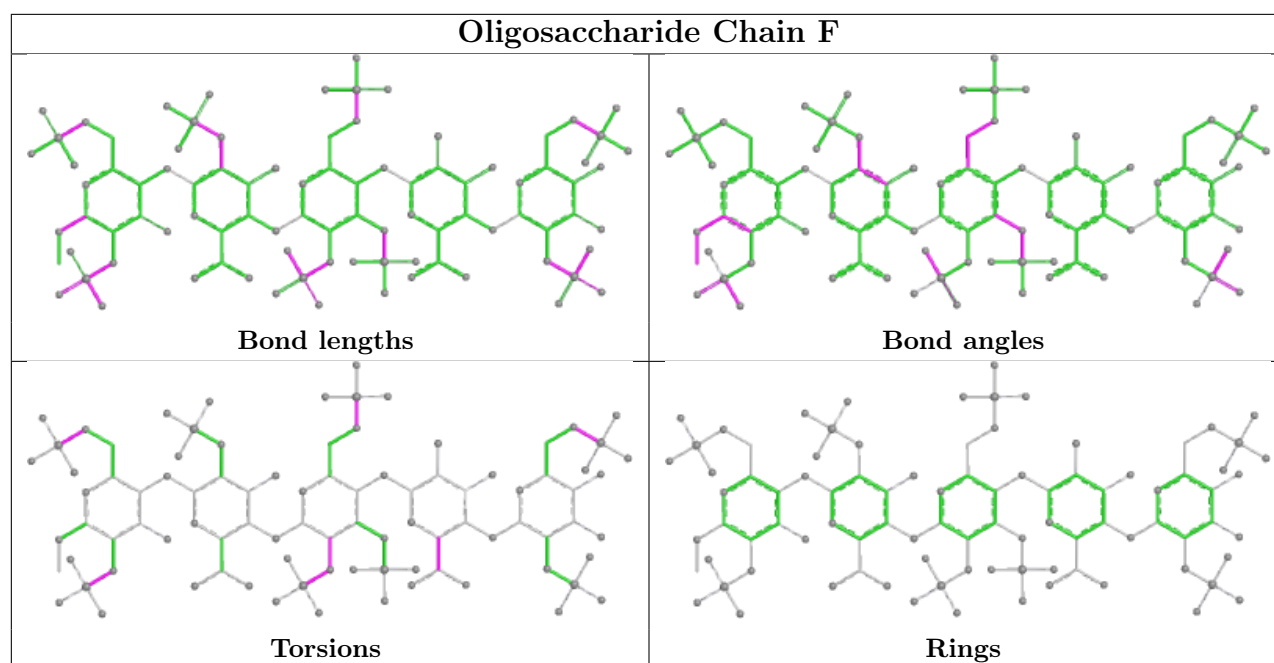
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











4.6 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	$\# Z > 2$
6	NAG	I	801	1	14,14,15	0.60	0	17,19,21	0.78	0
6	NAG	L	801	1	14,14,15	0.56	0	17,19,21	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	801	1	-	5/6/23/26	0/1/1/1
6	NAG	L	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	801	NAG	C8-C7-N2-C2
6	L	801	NAG	O7-C7-N2-C2
6	I	801	NAG	C1-C2-N2-C7
6	I	801	NAG	C3-C2-N2-C7
6	I	801	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	I	404/432 (93%)	0.28	5 (1%) 76 55	37, 65, 90, 100	0
1	L	417/432 (96%)	0.11	7 (1%) 69 45	33, 59, 90, 106	0
All	All	821/864 (95%)	0.19	12 (1%) 72 49	33, 62, 90, 106	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	94	ALA	3.8
1	I	179	ALA	2.6
1	L	16	PRO	2.6
1	I	8	CYS	2.3
1	L	95	CYS	2.3

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 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.

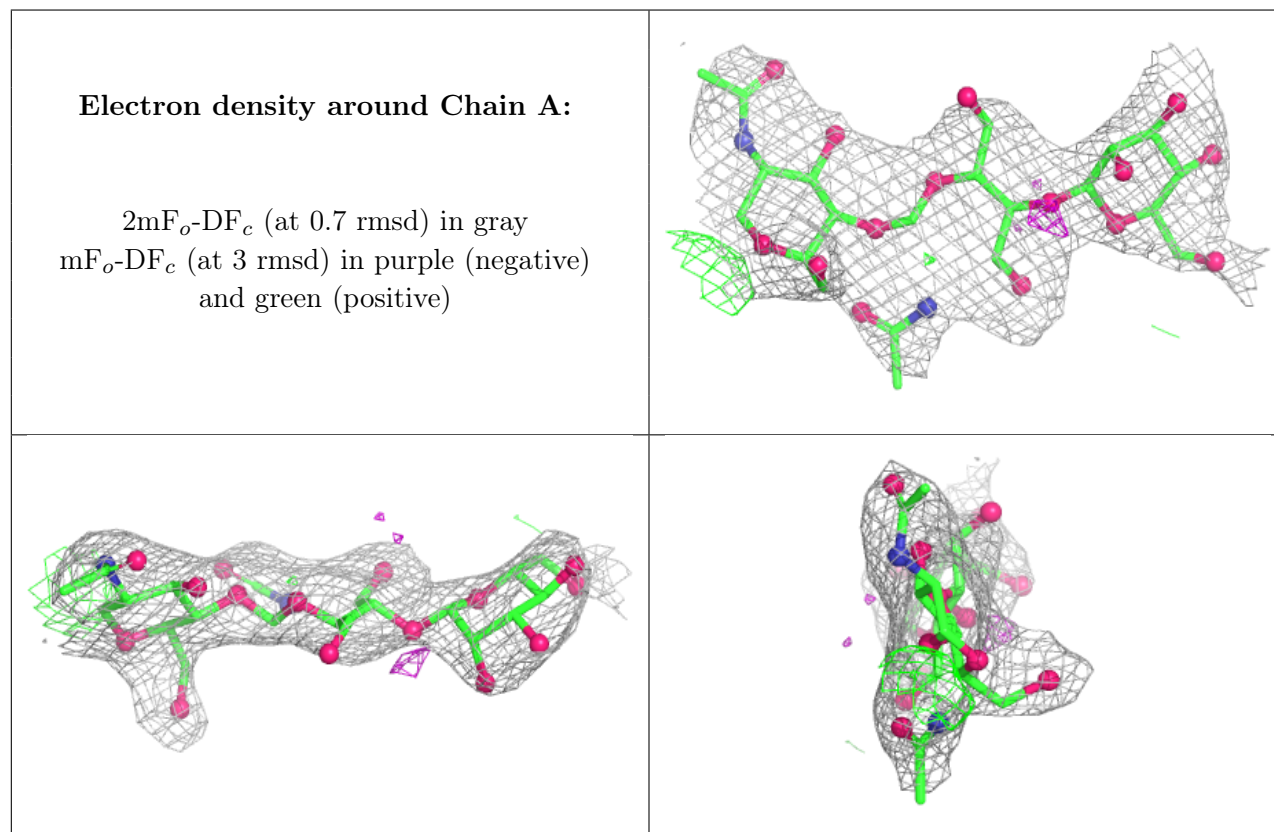
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	69,72,75,76	0
2	NAG	A	2	13/15	-	-	63,71,74,79	0
2	MAN	A	3	11/12	-	-	82,85,87,87	0
3	NAG	B	1	14/15	-	-	110,114,118,123	0
3	NAG	B	2	14/15	-	-	128,132,134,134	0

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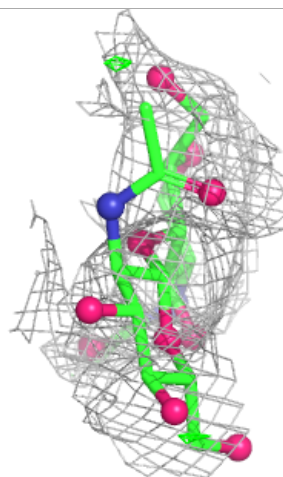
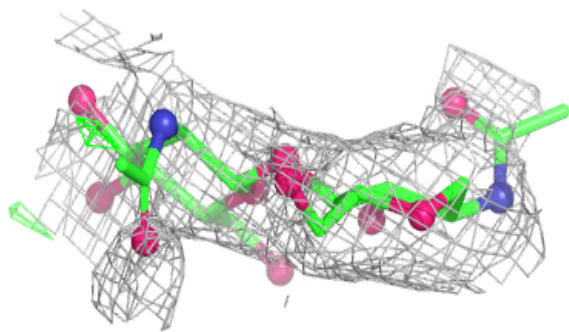
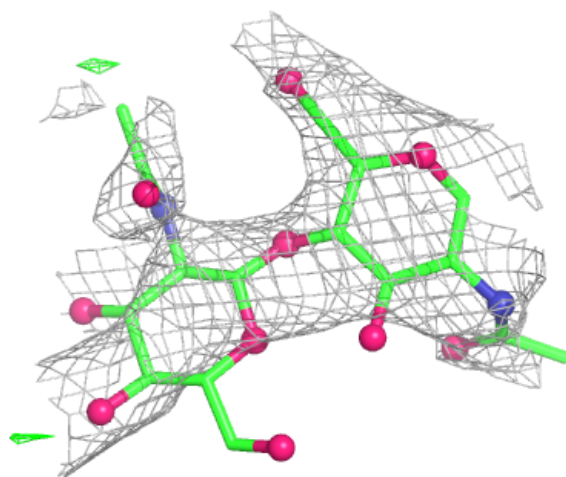
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	2	14/15	0.29	0.20	68,74,77,79	0
4	NAG	D	1	14/15	0.67	0.14	64,67,68,71	0
3	NAG	C	2	14/15	0.82	0.18	87,90,92,92	0
3	NAG	C	1	14/15	0.84	0.13	63,71,75,82	0
4	MAN	D	3	11/12	-	-	79,81,85,89	0
4	MAN	D	4	11/12	-	-	76,81,83,84	0
4	MAN	D	5	11/12	-	-	90,91,92,92	0
5	ZDO	E	1	21/21	-	-	103,104,110,110	0
5	IDS	E	2	16/17	-	-	101,108,116,116	0
5	SUS	E	3	23/24	-	-	87,92,101,102	0
5	BDP	E	4	12/13	-	-	88,91,94,96	0
5	SGN	E	5	19/20	-	-	76,90,98,99	0
5	ZDO	F	1	21/21	-	-	86,90,99,101	0
5	IDS	F	2	16/17	-	-	97,101,103,104	0
5	SUS	F	3	23/24	-	-	97,104,112,113	0
5	BDP	F	4	12/13	-	-	92,94,96,98	0
5	SGN	F	5	19/20	-	-	96,100,110,110	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.



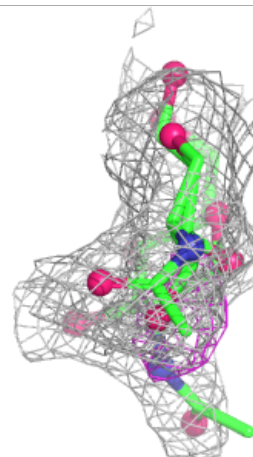
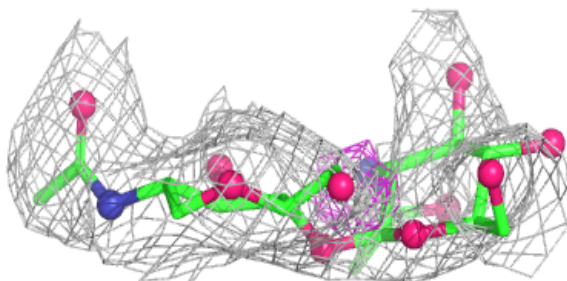
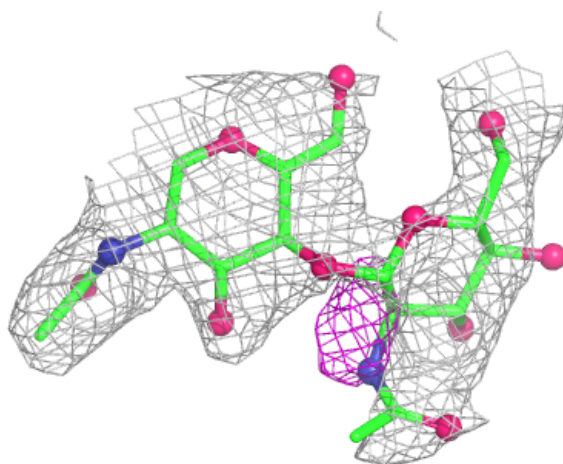
Electron density around Chain B:

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



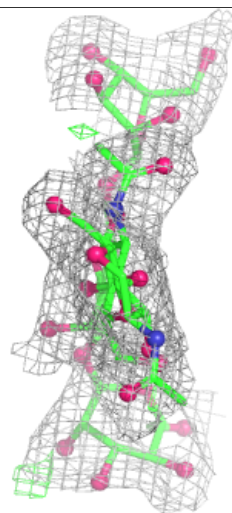
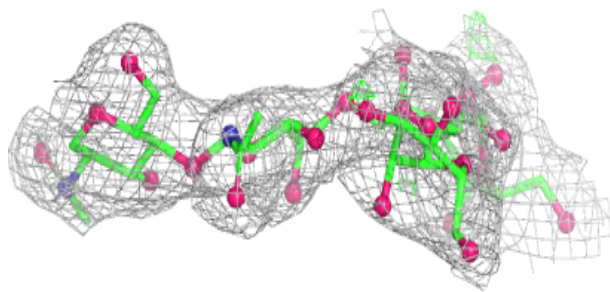
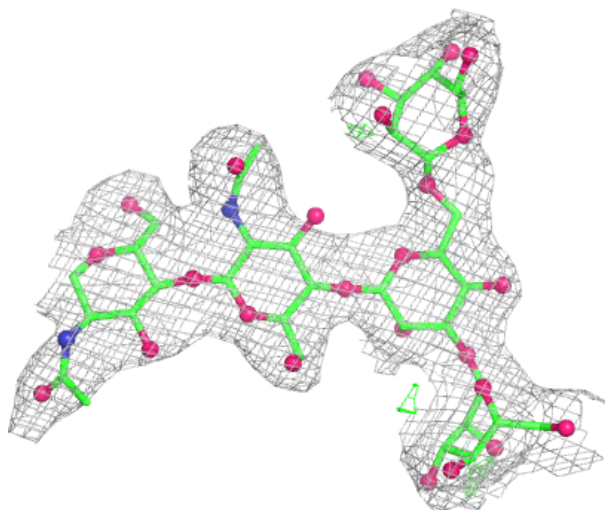
Electron density around Chain C:

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



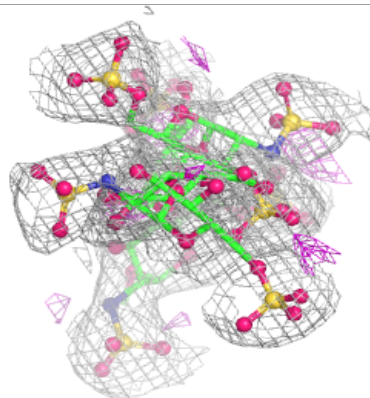
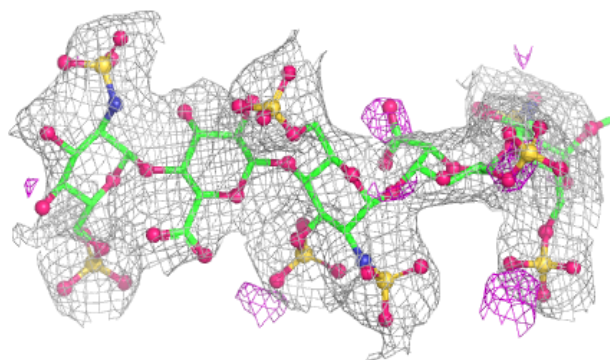
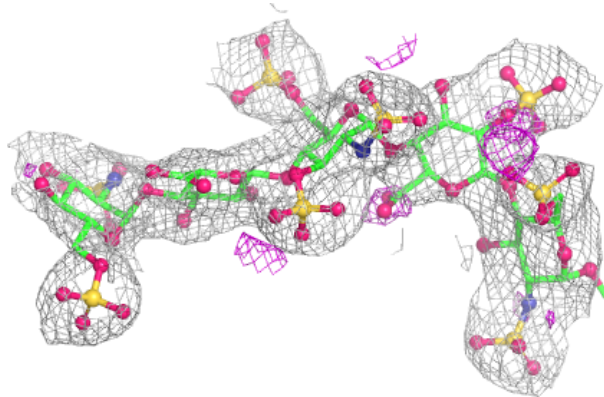
Electron density around Chain D:

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

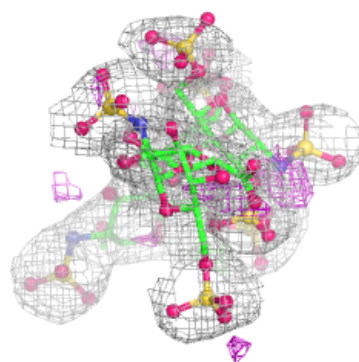
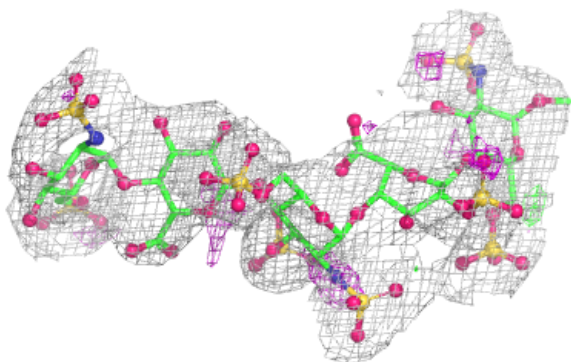
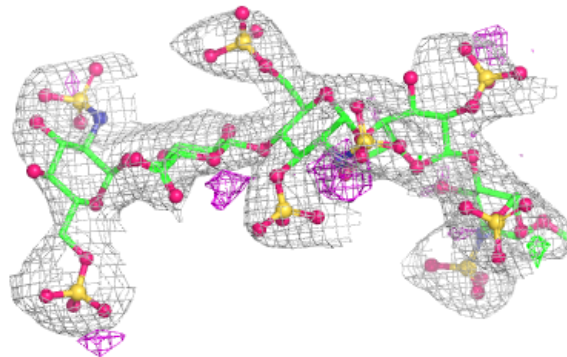


Electron density around Chain E:

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

**Electron density around Chain F:**

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



5.4 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($\text{\AA}^2$)	Q<0.9
6	NAG	I	801	14/15	0.55	0.15	105,107,108,109	6
6	NAG	L	801	14/15	0.86	0.10	80,81,83,83	0

5.5 Other polymers [i](#)

There are no such residues in this entry.