



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:46 AM UTC

PDB ID : 2WR0 / pdb_00002wr0
Title : Structures of influenza H2 Hemagglutinins
Authors : Liu, J.; Stevens, D.; Haire, L.; Coombs, P.; Russell, R.; Gamblin, S.; Skehel, J.
Deposited on : 2009-08-28
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	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

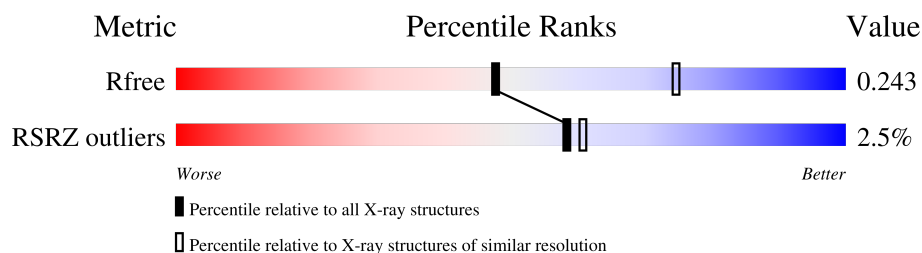
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

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
3	BMA	E	4	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12269 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3882	2436	671	753	22			
1	B	491	Total	C	N	O	S	0	0	0
			3893	2445	672	754	22			
1	C	486	Total	C	N	O	S	0	0	0
			3858	2424	666	746	22			

- Molecule 2 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
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-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
3	E	4	Total	C	N	O	0	0	1
			40	23	2	15			

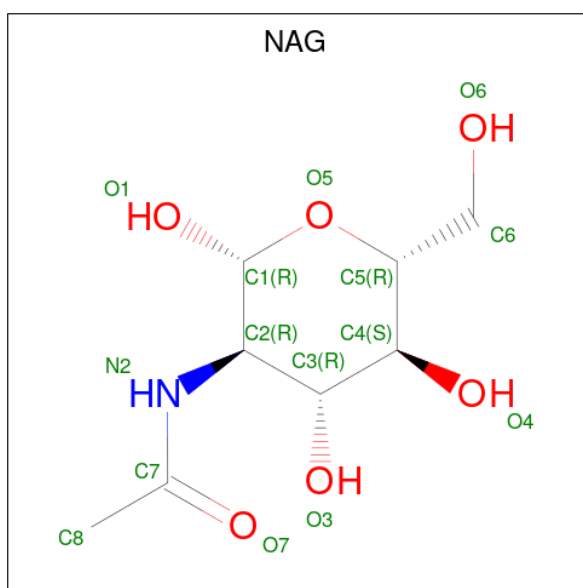
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	154	Total	O	0	0
			154	154		
6	B	160	Total	O	0	0
			160	160		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	162	Total 162	O 162	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.27Å 140.52Å 198.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.45 19.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-2.45) 99.6 (19.99-2.45)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.44Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.256 0.199 , 0.243	Depositor DCC
R_{free} test set	3590 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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](#)

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4.3.3 RNA [i](#)

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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](#)

Of 10 monosaccharides modelled in this entry, 9 were used for Mogul analysis.

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	D	1	2	14,14,15	0.55	0	17,19,21	1.43	2 (11%)
2	NAG	D	2	2	14,14,15	0.72	0	17,19,21	1.38	3 (17%)
3	NAG	E	1	3	14,14,15	0.52	0	17,19,21	1.61	4 (23%)
3	NAG	E	2	3	14,14,15	0.69	0	17,19,21	0.88	0
3	BMA	E	3	3	11,11,12	0.60	0	15,15,17	0.39	0
4	NAG	F	1	4	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	0.80	0
4	BMA	F	3	4	11,11,12	0.66	0	15,15,17	0.52	0
4	MAN	F	4	4	11,11,12	0.76	0	15,15,17	0.74	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
2	NAG	D	1	2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3	-	5/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C8-C7-N2	3.56	122.02	116.12
2	D	1	NAG	O5-C1-C2	-3.54	105.81	111.29
3	E	1	NAG	C2-N2-C7	3.42	127.48	122.90
2	D	1	NAG	C3-C4-C5	3.14	115.92	110.23
3	E	1	NAG	O7-C7-C8	-2.76	117.13	122.05
2	D	2	NAG	C2-N2-C7	-2.60	119.41	122.90
2	D	2	NAG	C4-C3-C2	-2.28	107.68	111.02
3	E	1	NAG	C4-C3-C2	2.18	114.22	111.02
2	D	2	NAG	O5-C1-C2	-2.07	108.10	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

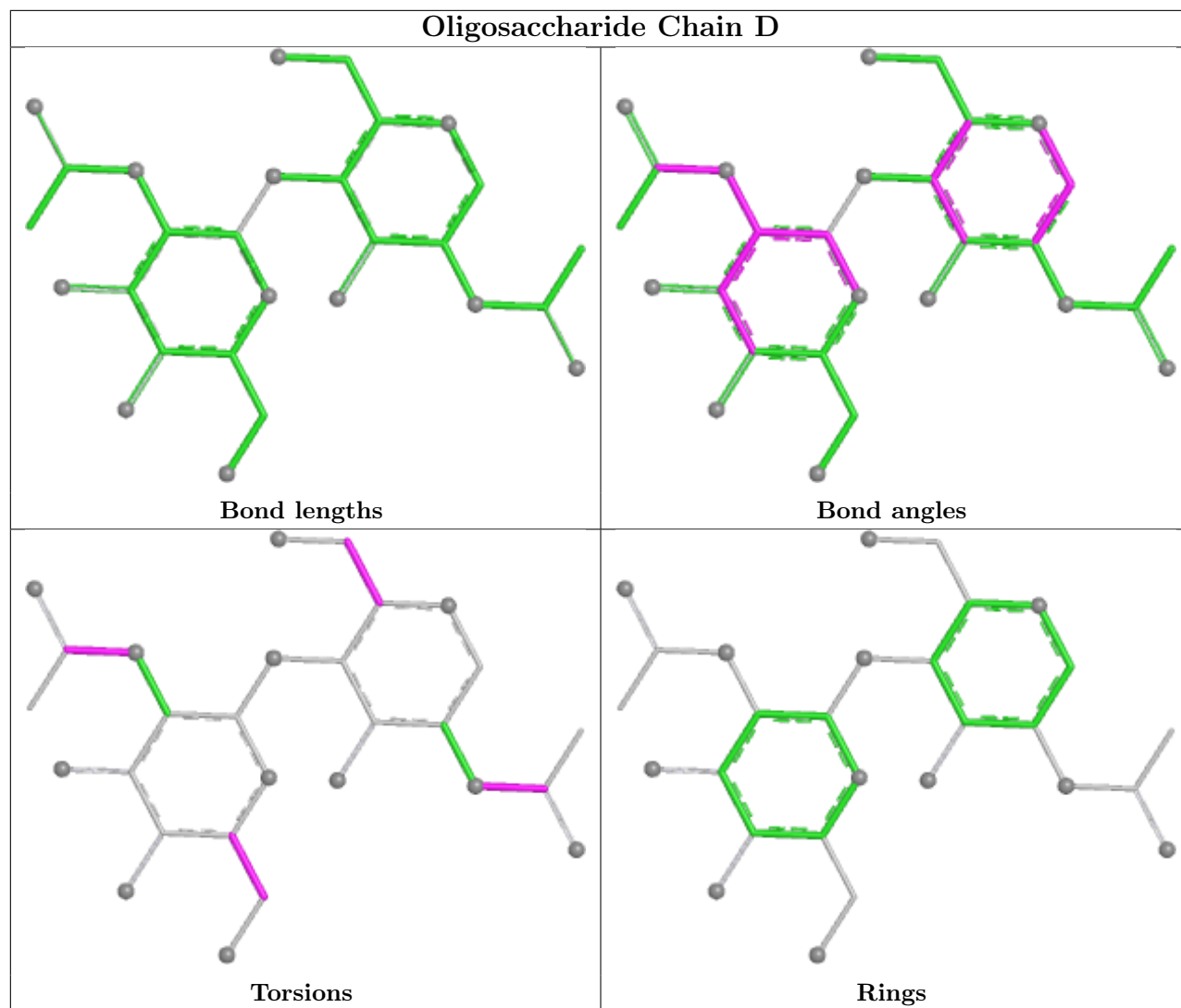
All (25) torsion outliers are listed below:

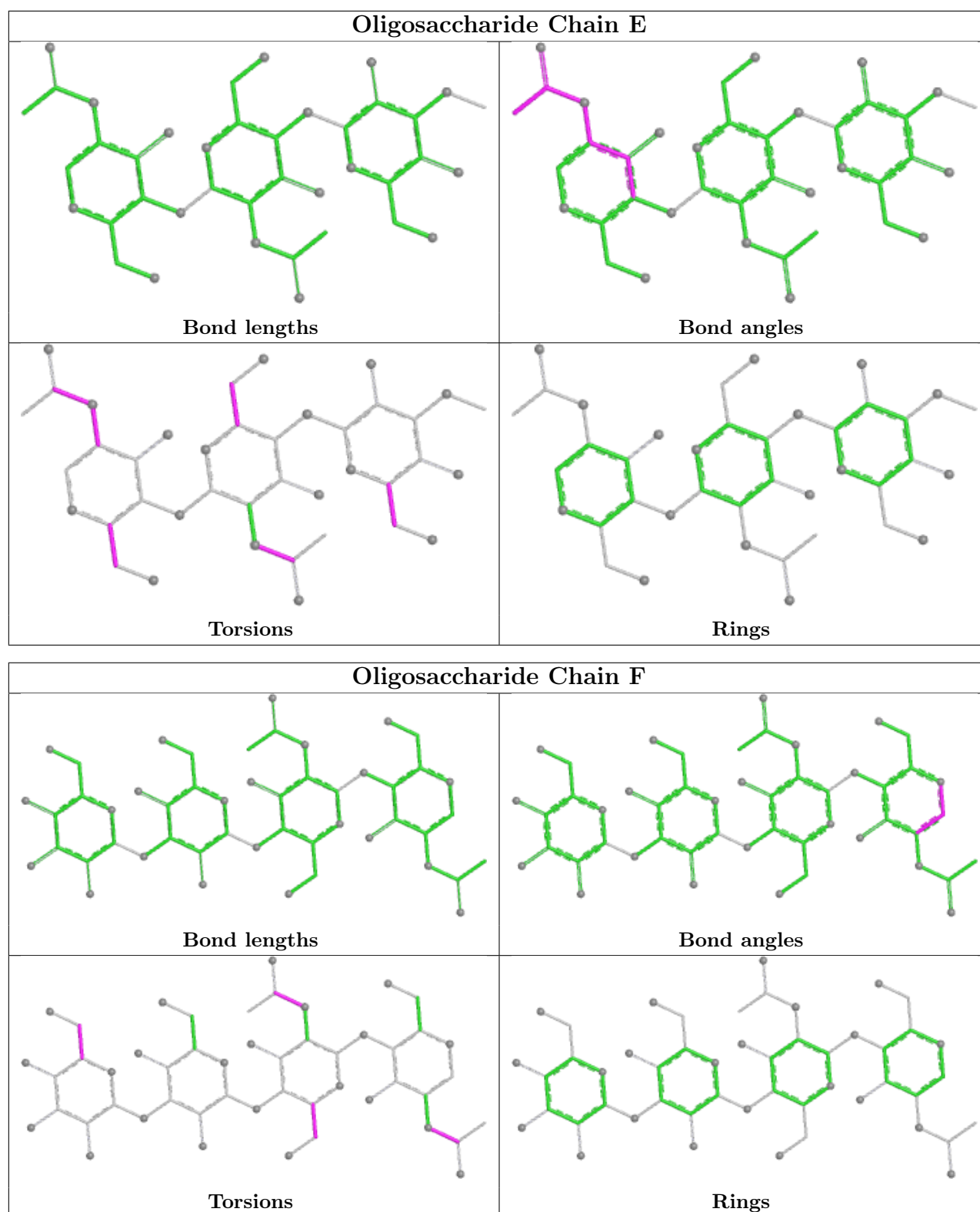
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	F	4	MAN	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	F	2	NAG	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.





4.6 Ligand geometry [i](#)

3 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
5	NAG	A	1500	-	14,14,15	0.59	0	17,19,21	0.99	2 (11%)
5	NAG	C	1497	-	14,14,15	0.55	0	17,19,21	1.13	2 (11%)
5	NAG	A	1499	-	14,14,15	0.54	0	17,19,21	1.22	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
5	NAG	A	1500	-	-	5/6/23/26	0/1/1/1
5	NAG	C	1497	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1499	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1499	NAG	O5-C1-C2	3.39	116.53	111.29
5	A	1500	NAG	C4-C3-C2	2.33	114.44	111.02
5	C	1497	NAG	O5-C1-C2	-2.29	107.74	111.29
5	A	1499	NAG	C1-O5-C5	2.28	115.25	112.19
5	C	1497	NAG	C3-C4-C5	2.26	114.34	110.23
5	A	1500	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1499	NAG	C1-C2-N2-C7
5	A	1499	NAG	C8-C7-N2-C2
5	A	1499	NAG	O7-C7-N2-C2
5	A	1500	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	A	1500	NAG	C8-C7-N2-C2
5	A	1500	NAG	O7-C7-N2-C2
5	C	1497	NAG	O5-C5-C6-O6
5	A	1500	NAG	O5-C5-C6-O6
5	C	1497	NAG	C4-C5-C6-O6
5	A	1500	NAG	C4-C5-C6-O6
5	A	1499	NAG	O5-C5-C6-O6

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 ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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	490/509 (96%)	-0.16	12 (2%) 59 62	21, 45, 92, 175	1 (0%)
1	B	491/509 (96%)	-0.24	12 (2%) 59 62	26, 44, 82, 159	0
1	C	486/509 (95%)	-0.16	12 (2%) 58 61	28, 46, 79, 131	0
All	All	1467/1527 (96%)	-0.19	36 (2%) 58 61	21, 45, 84, 175	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	6.5
1	C	113	THR	5.7
1	C	459	VAL	4.2
1	A	498	ALA	4.0
1	C	361	SER	3.9
1	B	141	LEU	3.8
1	A	495	SER	3.7
1	B	277	CYS	3.7
1	A	459	VAL	3.6
1	A	497	ALA	3.5
1	C	262	ARG	3.5
1	C	197	VAL	3.5
1	A	262	ARG	3.4
1	B	497	ALA	3.2
1	A	113	THR	3.1
1	C	75	LEU	2.9
1	B	114	HIS	2.9
1	B	498	ALA	2.8
1	B	262	ARG	2.8
1	C	324	PRO	2.8
1	B	75	LEU	2.7
1	B	113	THR	2.7
1	C	494	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	495	SER	2.6
1	B	494	GLU	2.5
1	B	459	VAL	2.5
1	A	464	ASN	2.4
1	C	389	ASN	2.4
1	A	453	MET	2.3
1	C	277	CYS	2.3
1	B	495	SER	2.2
1	C	74	LEU	2.2
1	A	195	GLN	2.2
1	A	73	ARG	2.0
1	B	492	GLU	2.0
1	A	277	CYS	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

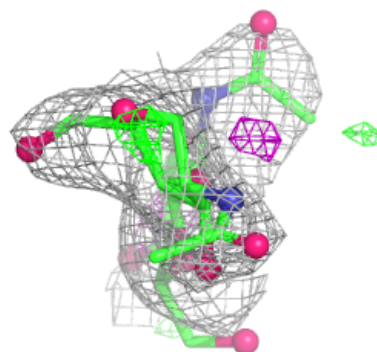
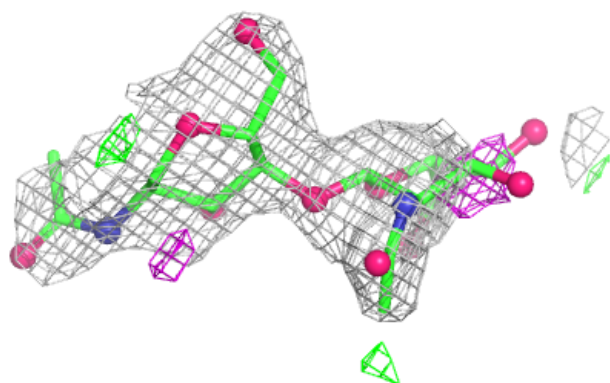
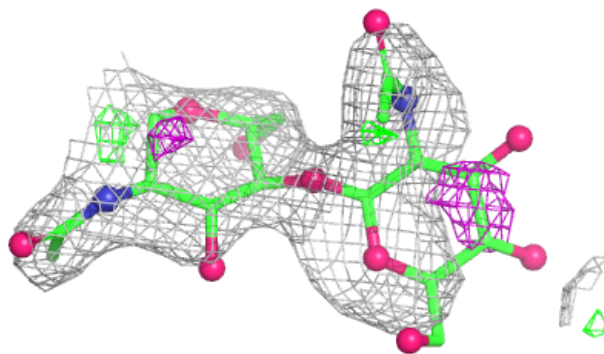
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	BMA	E	4	1/12	-0.33	0.47	129,129,129,129	0
3	BMA	E	3	11/12	0.42	0.14	129,129,129,129	0
3	NAG	E	1	14/15	0.46	0.23	127,128,129,129	0
2	NAG	D	2	14/15	0.47	0.16	101,102,102,102	0
3	NAG	E	2	14/15	0.47	0.19	127,128,129,129	0
4	BMA	F	3	11/12	0.55	0.13	82,83,83,83	0
4	MAN	F	4	11/12	0.64	0.13	83,83,83,83	0
2	NAG	D	1	14/15	0.80	0.16	100,101,101,101	0
4	NAG	F	1	14/15	0.80	0.15	83,83,84,84	0
4	NAG	F	2	14/15	0.83	0.11	82,82,83,83	0

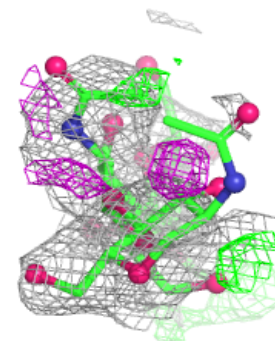
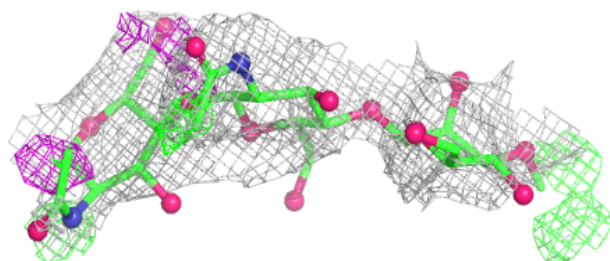
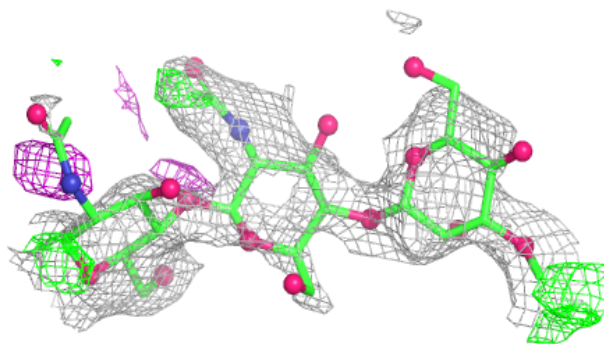
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

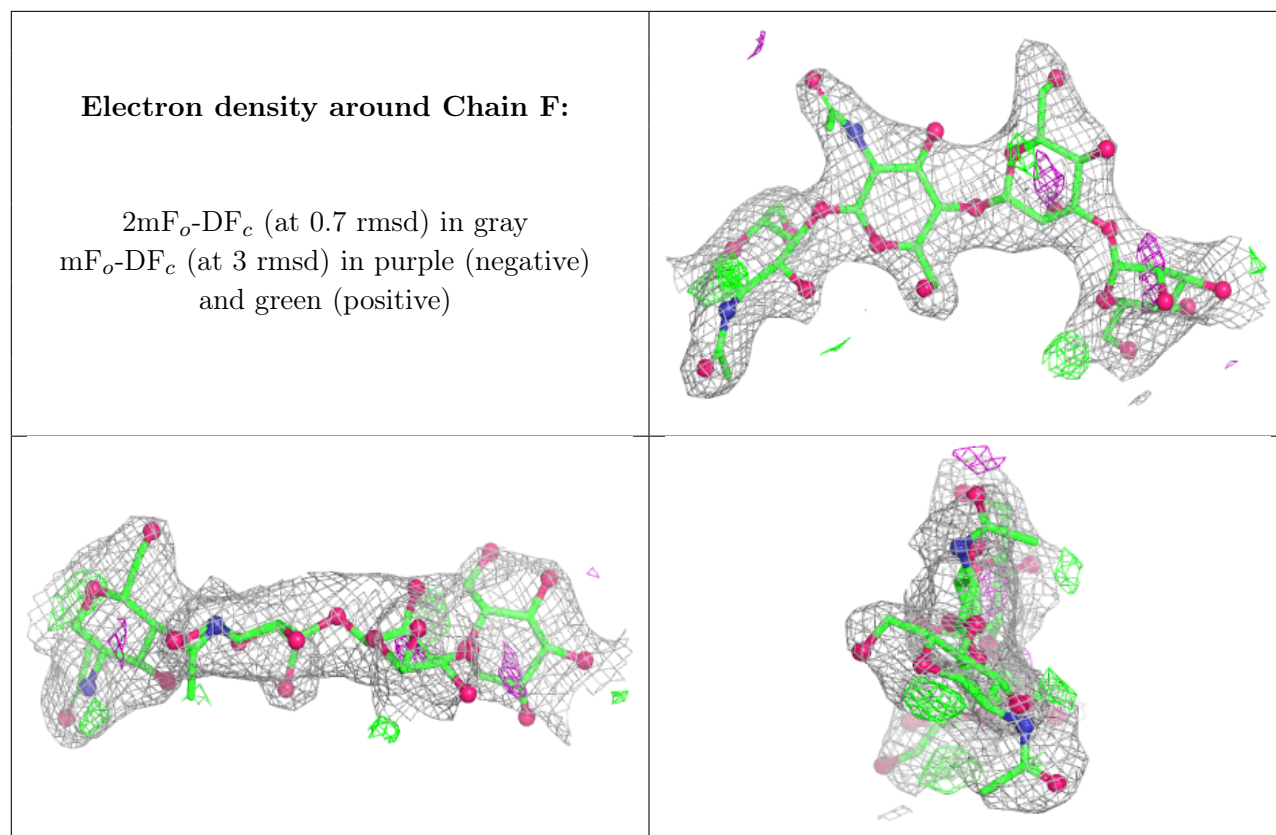
Electron density around Chain D:

$2mF_o-DF_c$ (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)





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
5	NAG	A	1499	14/15	0.57	0.17	149,152,153,153	0
5	NAG	A	1500	14/15	0.78	0.13	58,60,61,61	0
5	NAG	C	1497	14/15	0.86	0.10	63,65,65,65	0

5.5 Other polymers [i](#)

There are no such residues in this entry.