



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 03:28 AM UTC

PDB ID : 4CVU / pdb_00004cvu
Title : Structure of Fungal beta-mannosidase from Glycoside Hydrolase Family 2 of *Trichoderma harzianum*
Authors : Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.
Deposited on : 2014-03-31
Resolution : 1.90 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

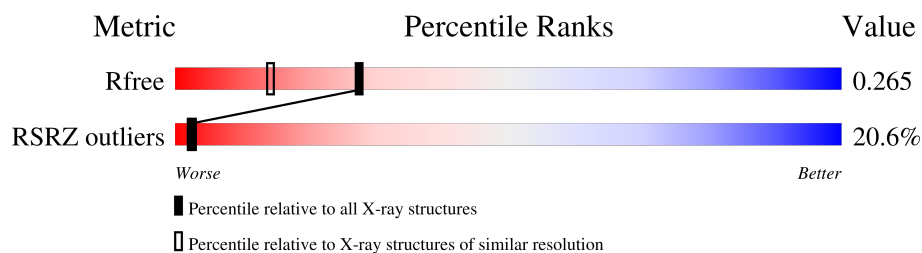
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

2 Entry composition [i](#)

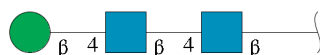
There are 13 unique types of molecules in this entry. The entry contains 8456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-MANNOSIDASE.

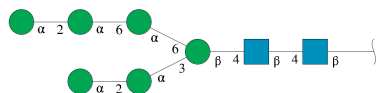
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	913	7241	4645	1208	1371	17	0	6	0

- Molecule 2 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			
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.

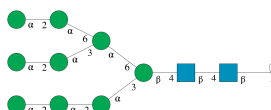


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	94	52	2	40	0	0	0

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

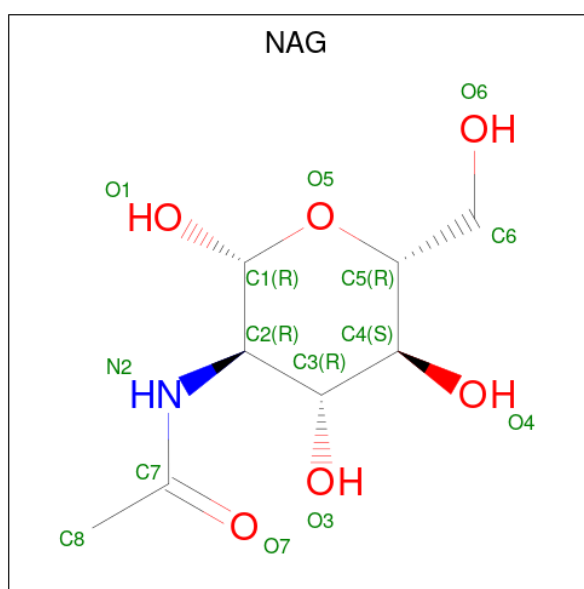
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
5	E	11	Total	C	N	O	0	0	0
			127	70	2	55			

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

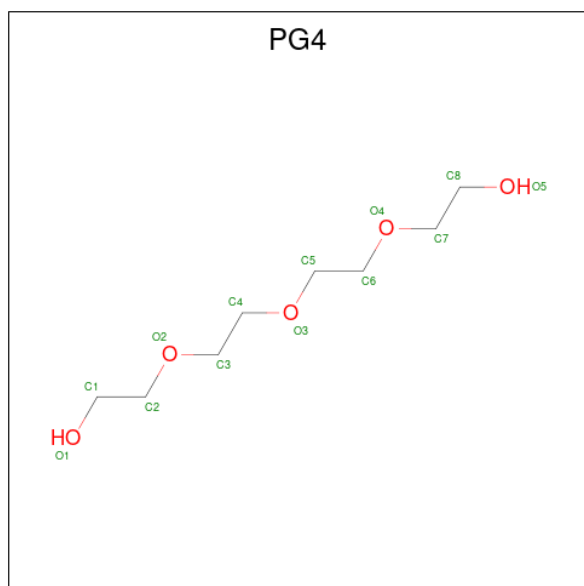
- Molecule 7 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	Cd	0	0
			17	17		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

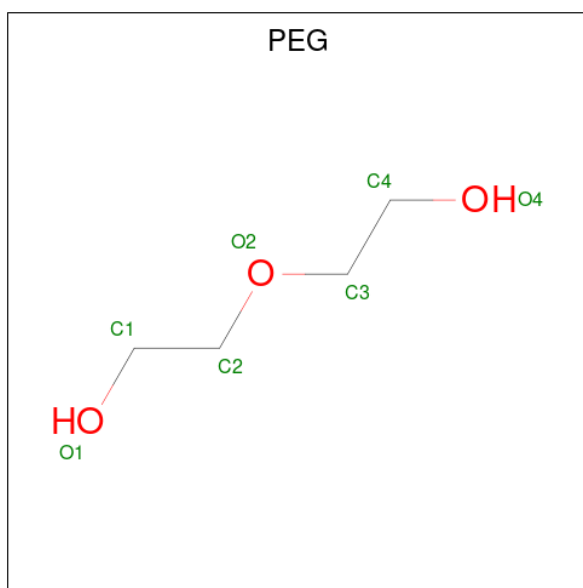
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	Na	0	0
			6	6		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		

- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Cl	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	741	Total	O	0	0
			741	741		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.46Å 166.46Å 121.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.70 – 1.90 117.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (117.70-1.90) 98.8 (117.70-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.234 , 0.263 0.239 , 0.265	Depositor DCC
R_{free} test set	6641 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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](#)

28 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	B	1	1,2	14,14,15	0.64	0	17,19,21	1.16	2 (11%)
2	NAG	B	2	2	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
2	BMA	B	3	2	11,11,12	0.50	0	15,15,17	0.66	0
3	NAG	C	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.90	0
3	NAG	C	2	3	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
3	BMA	C	3	3	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
3	MAN	C	4	3	11,11,12	0.60	0	15,15,17	2.05	3 (20%)
3	MAN	C	5	3	11,11,12	0.74	0	15,15,17	1.34	2 (13%)
3	MAN	C	6	3	11,11,12	0.66	0	15,15,17	0.86	1 (6%)
3	MAN	C	7	3	11,11,12	0.61	0	15,15,17	0.81	0
3	MAN	C	8	3	11,11,12	0.51	0	15,15,17	0.94	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
4	NAG	D	2	4	14,14,15	0.73	0	17,19,21	1.19	2 (11%)
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	1.03	1 (6%)
4	MAN	D	4	4	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
4	MAN	D	5	4	11,11,12	0.57	0	15,15,17	0.90	0
4	MAN	D	6	4	11,11,12	0.93	0	13,15,17	1.92	2 (15%)
5	NAG	E	1	1,5	14,14,15	0.67	0	17,19,21	1.12	2 (11%)
5	MAN	E	10	5	11,11,12	0.80	1 (9%)	15,15,17	0.78	0
5	MAN	E	11	5	11,11,12	0.63	0	15,15,17	0.72	1 (6%)
5	NAG	E	2	5	14,14,15	0.78	0	17,19,21	0.96	1 (5%)
5	BMA	E	3	5	11,11,12	0.51	0	15,15,17	0.83	1 (6%)
5	MAN	E	4	5	11,11,12	0.57	0	15,15,17	1.09	1 (6%)
5	MAN	E	5	5	11,11,12	0.99	0	15,15,17	1.04	1 (6%)
5	MAN	E	6	5	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
5	MAN	E	7	5	11,11,12	1.34	1 (9%)	15,15,17	3.01	2 (13%)
5	MAN	E	8	5	11,11,12	0.73	0	15,15,17	1.34	3 (20%)
5	MAN	E	9	5	11,11,12	0.70	0	15,15,17	1.22	1 (6%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	1/2/18/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	E	10	5	-	0/2/19/22	0/1/1/1
5	MAN	E	11	5	-	0/2/19/22	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	2/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1
5	MAN	E	8	5	-	0/2/19/22	0/1/1/1
5	MAN	E	9	5	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	MAN	O3-C3	-3.82	1.33	1.43
5	E	10	MAN	O5-C5	-2.27	1.39	1.43
3	C	1	NAG	C1-C2	2.27	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	MAN	O3-C3-C2	10.92	132.35	110.05
3	C	4	MAN	C1-O5-C5	5.93	120.14	112.19
4	D	6	MAN	C3-C4-C5	5.22	115.22	109.99
4	D	6	MAN	C1-C2-C3	-3.76	100.55	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	O5-C5-C4	3.48	119.30	110.83
3	C	2	NAG	C2-N2-C7	3.37	127.42	122.90
5	E	9	MAN	C1-O5-C5	2.96	116.15	112.19
3	C	6	MAN	C1-O5-C5	2.96	116.15	112.19
3	C	5	MAN	C1-C2-C3	2.92	113.89	109.64
3	C	8	MAN	C1-O5-C5	2.90	116.08	112.19
4	D	4	MAN	O2-C2-C3	-2.73	104.49	110.15
5	E	1	NAG	C1-O5-C5	2.65	115.73	112.19
5	E	8	MAN	C3-C4-C5	2.61	114.97	110.23
5	E	6	MAN	C2-C3-C4	-2.60	106.30	110.86
3	C	2	NAG	C8-C7-N2	2.57	120.38	116.12
3	C	3	BMA	O3-C3-C4	-2.55	104.36	110.38
2	B	1	NAG	C1-O5-C5	2.52	115.56	112.19
4	D	3	BMA	O4-C4-C3	-2.50	104.49	110.38
4	D	2	NAG	C3-C4-C5	-2.46	105.78	110.23
5	E	5	MAN	C1-O5-C5	2.41	115.42	112.19
4	D	1	NAG	C1-O5-C5	2.32	115.30	112.19
5	E	2	NAG	O7-C7-C8	-2.31	117.94	122.05
5	E	1	NAG	O5-C1-C2	-2.29	107.75	111.29
5	E	11	MAN	C1-O5-C5	2.26	115.22	112.19
5	E	8	MAN	C1-C2-C3	-2.20	106.44	109.64
5	E	4	MAN	O4-C4-C5	2.18	114.70	109.32
2	B	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	C	5	MAN	O2-C2-C1	-2.10	104.41	109.22
5	E	8	MAN	O4-C4-C3	-2.10	105.42	110.38
5	E	7	MAN	C1-O5-C5	2.08	114.98	112.19
5	E	3	BMA	O6-C6-C5	-2.08	104.25	111.33
3	C	4	MAN	O5-C5-C6	-2.06	103.66	107.66
4	D	2	NAG	O7-C7-C8	-2.03	118.44	122.05
2	B	1	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
5	E	6	MAN	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
5	E	6	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6

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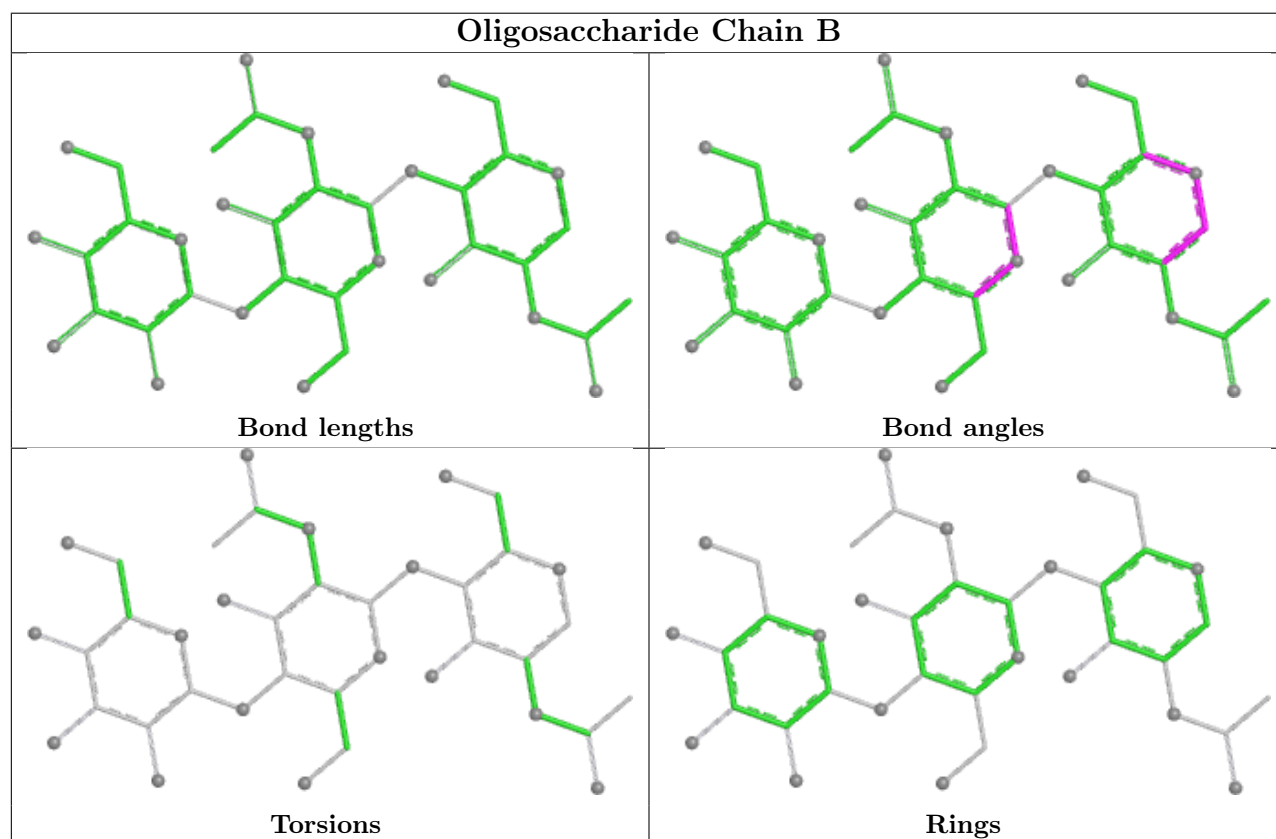
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Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
5	E	9	MAN	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6

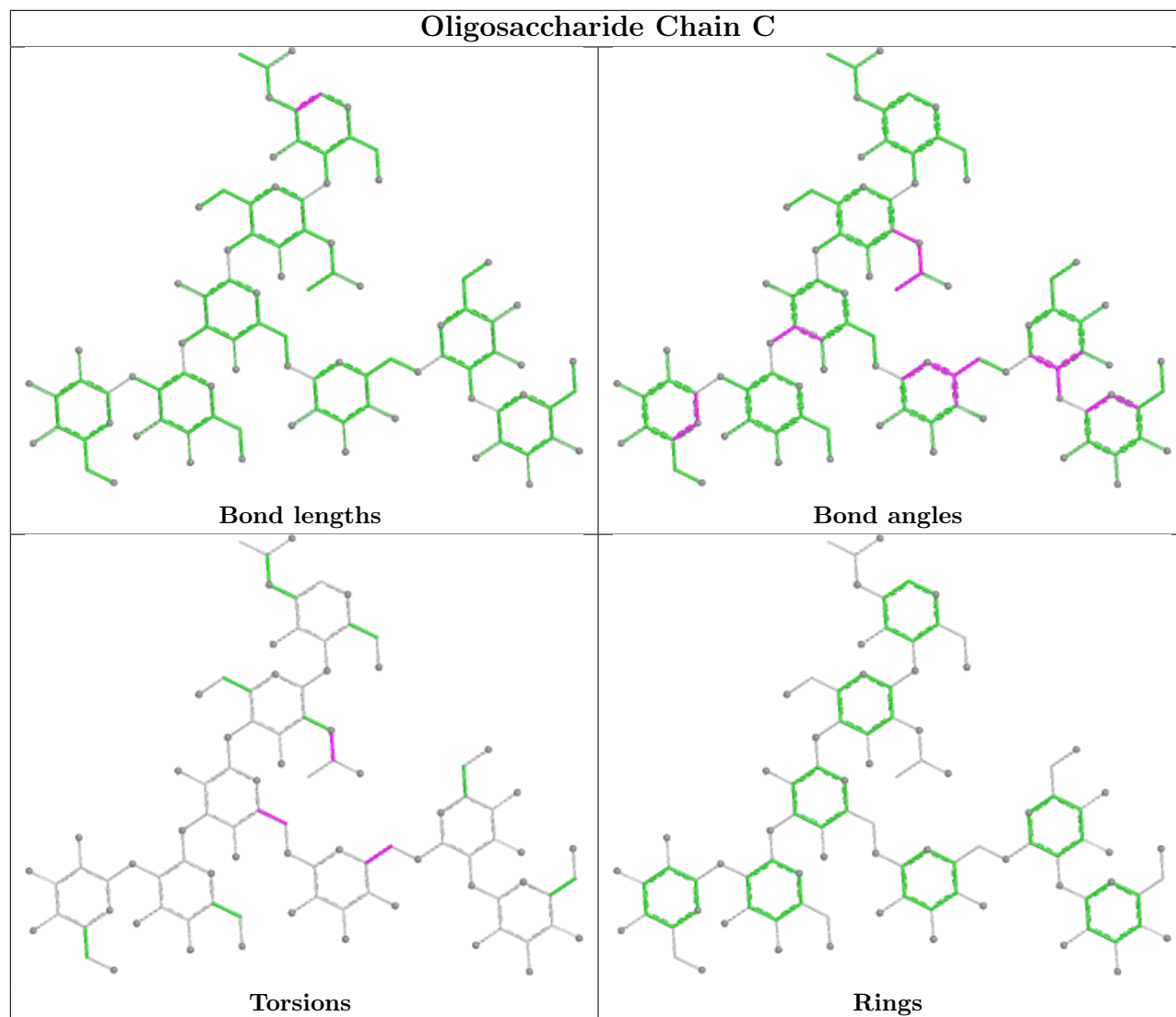
There are no ring outliers.

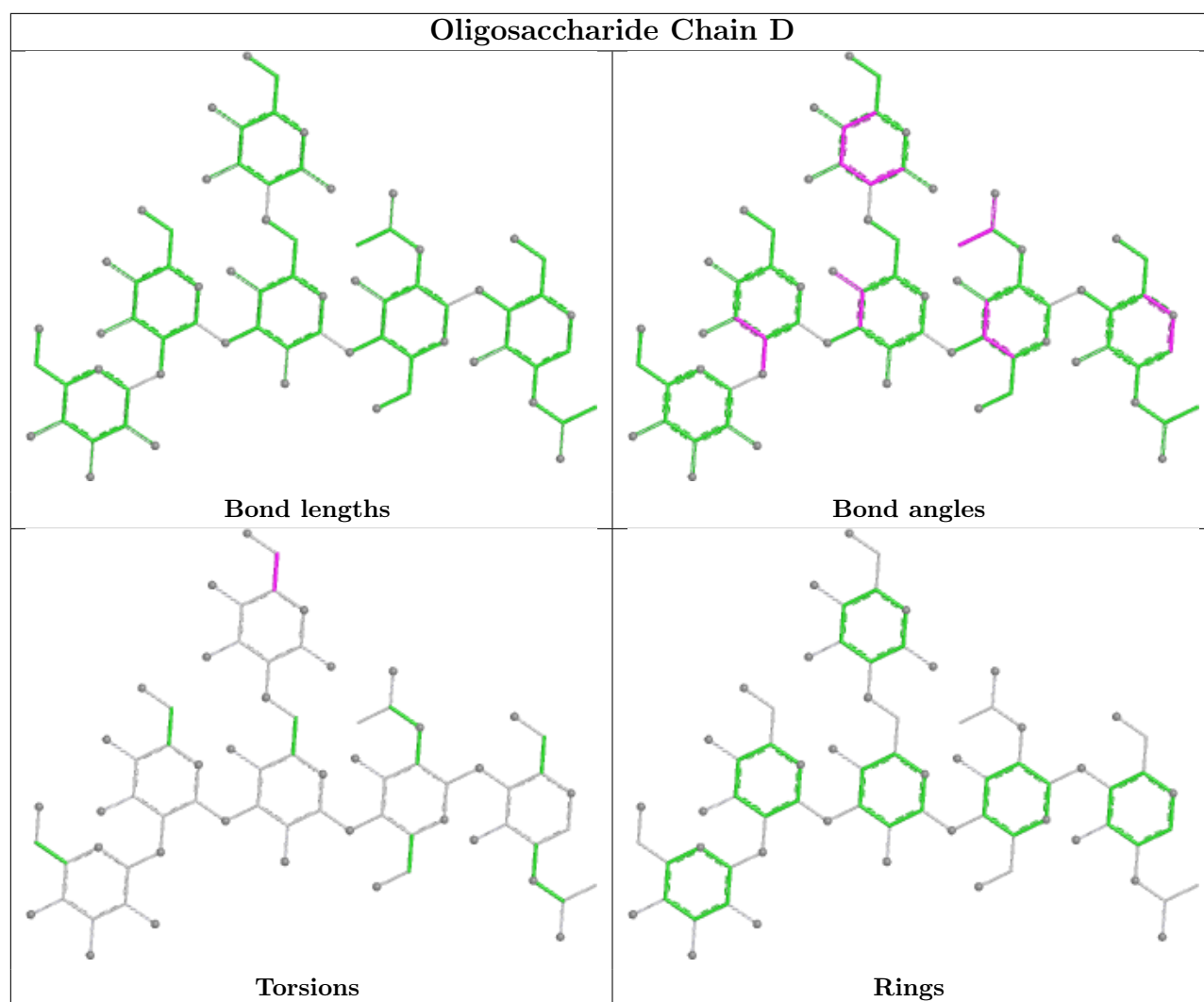
No monomer is involved in short contacts.

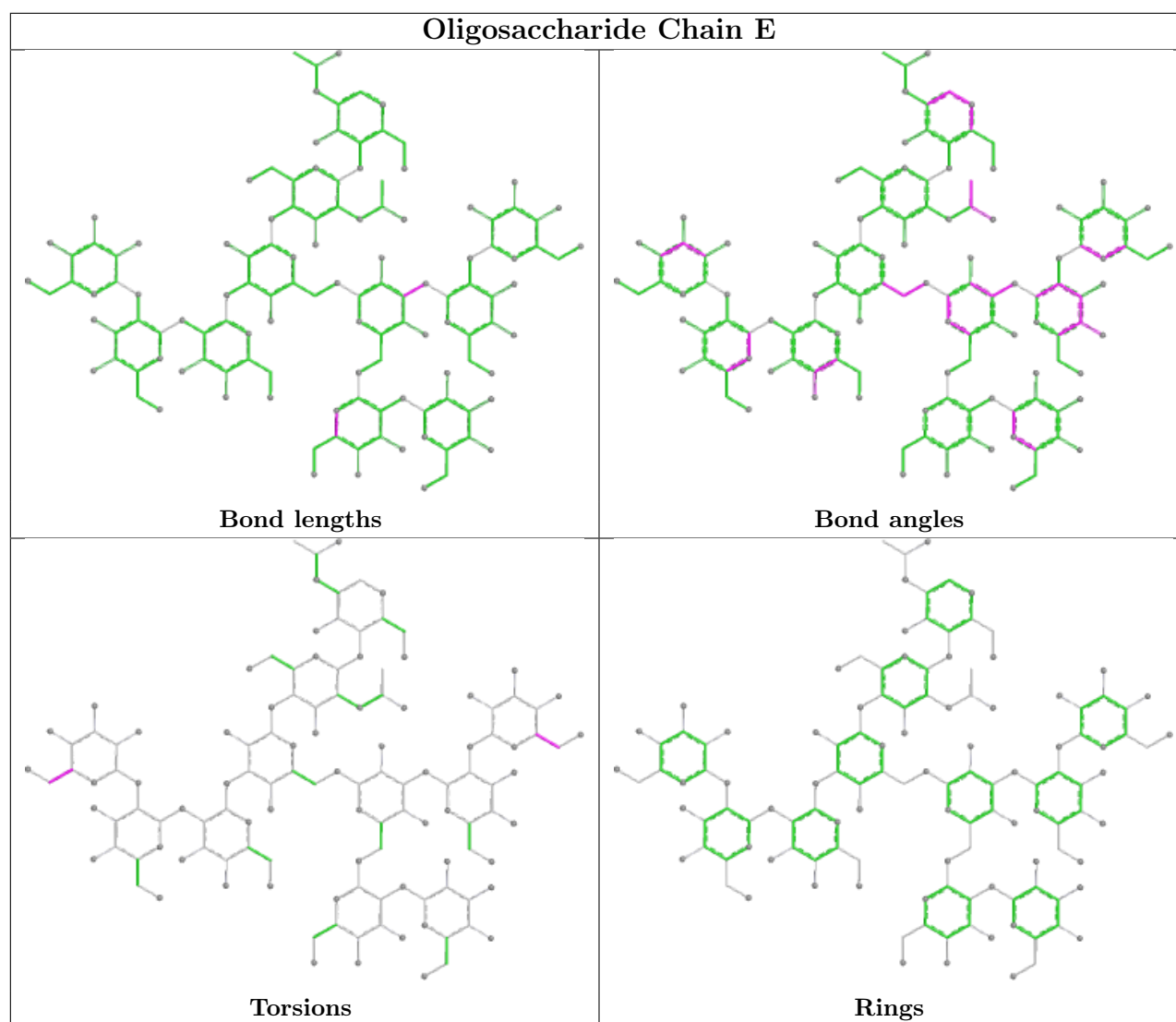
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain C







4.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 25 are monoatomic - leaving 9 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	$\# Z > 2$
6	NAG	A	1005	1	14,14,15	0.44	0	17,19,21	1.39	2 (11%)
6	NAG	A	1006	1	14,14,15	0.56	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PG4	A	1030	-	11,11,12	0.55	0	10,10,11	0.43	0
6	NAG	A	1001	1	14,14,15	0.96	1 (7%)	17,19,21	1.24	1 (5%)
6	NAG	A	1007	1	14,14,15	0.52	0	17,19,21	1.09	1 (5%)
6	NAG	A	1004	1	14,14,15	0.48	0	17,19,21	1.13	1 (5%)
10	PEG	A	1031	-	6,6,6	0.53	0	5,5,5	0.28	0
6	NAG	A	1003	1	14,14,15	0.94	1 (7%)	17,19,21	1.38	1 (5%)
6	NAG	A	1002	-	14,14,15	0.66	0	19,19,21	2.21	7 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
9	PG4	A	1030	-	-	4/9/9/10	-
6	NAG	A	1001	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
10	PEG	A	1031	-	-	3/4/4/4	-
6	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1002	-	-	4/6/22/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	NAG	C1-C2	2.06	1.55	1.52
6	A	1001	NAG	O5-C1	-2.04	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	NAG	C8-C7-N2	5.25	124.83	116.12
6	A	1003	NAG	C1-O5-C5	4.72	118.51	112.19
6	A	1002	NAG	C2-N2-C7	4.36	128.75	122.90
6	A	1004	NAG	C1-O5-C5	3.56	116.95	112.19
6	A	1001	NAG	C1-O5-C5	3.28	116.58	112.19
6	A	1002	NAG	C3-C2-N2	3.25	115.75	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1005	NAG	C1-O5-C5	2.84	116.00	112.19
6	A	1002	NAG	C3-C4-C5	2.84	114.39	110.76
6	A	1005	NAG	O5-C1-C2	-2.56	107.34	111.29
6	A	1002	NAG	O7-C7-C8	-2.54	117.53	122.05
6	A	1002	NAG	O7-C7-N2	-2.46	117.64	121.98
6	A	1006	NAG	C1-O5-C5	2.45	115.47	112.19
6	A	1007	NAG	O7-C7-C8	-2.08	118.34	122.05
6	A	1002	NAG	O5-C1-C2	-2.02	107.49	109.52

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1005	NAG	O5-C5-C6-O6
6	A	1005	NAG	C4-C5-C6-O6
6	A	1002	NAG	C8-C7-N2-C2
6	A	1002	NAG	O7-C7-N2-C2
6	A	1004	NAG	O5-C5-C6-O6
10	A	1031	PEG	O2-C3-C4-O4
9	A	1030	PG4	O2-C3-C4-O3
6	A	1006	NAG	C4-C5-C6-O6
6	A	1004	NAG	C4-C5-C6-O6
6	A	1006	NAG	O5-C5-C6-O6
6	A	1002	NAG	C1-C2-N2-C7
10	A	1031	PEG	O1-C1-C2-O2
10	A	1031	PEG	C4-C3-O2-C2
6	A	1002	NAG	O5-C5-C6-O6
9	A	1030	PG4	C3-C4-O3-C5
6	A	1001	NAG	C1-C2-N2-C7
9	A	1030	PG4	C5-C6-O4-C7
9	A	1030	PG4	O4-C7-C8-O5

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

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	913/942 (96%)	1.29	188 (20%) 2 2	22, 45, 69, 105	7 (0%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	5.7
1	A	277	ALA	5.3
1	A	749	THR	5.1
1	A	333	ALA	5.1
1	A	265	PRO	5.1
1	A	843	PHE	5.1
1	A	839	LYS	4.9
1	A	751	ASN	4.9
1	A	306	ASP	4.8
1	A	838	SER	4.7
1	A	837	SER	4.7
1	A	267	HIS	4.6
1	A	559	TYR	4.5
1	A	840	THR	4.5
1	A	276	ASP	4.4
1	A	223	GLY	4.4
1	A	96	GLY	4.2
1	A	103	ILE	4.2
1	A	26	GLY	4.2
1	A	332	SER	4.2
1	A	842	THR	4.1
1	A	268	ALA	4.0
1	A	168	ALA	3.9
1	A	752	GLU	3.9
1	A	746	TRP	3.8
1	A	102	ASP	3.8
1	A	841	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLN	3.8
1	A	262	GLY	3.7
1	A	266	LYS	3.7
1	A	836	ALA	3.7
1	A	241	PHE	3.7
1	A	880	THR	3.7
1	A	142	ALA	3.7
1	A	336	LYS	3.7
1	A	748	TYR	3.6
1	A	805	THR	3.6
1	A	104	ALA	3.6
1	A	144	ALA	3.6
1	A	100	HIS	3.5
1	A	339	ILE	3.5
1	A	501	ALA	3.5
1	A	430	ASP	3.4
1	A	305	ILE	3.4
1	A	307	ALA	3.4
1	A	563	SER	3.4
1	A	906	LEU	3.4
1	A	505	THR	3.4
1	A	795	VAL	3.4
1	A	101	SER	3.3
1	A	846	HIS	3.3
1	A	220	LEU	3.3
1	A	881	ALA	3.3
1	A	264	LEU	3.2
1	A	818	SER	3.2
1	A	308	HIS	3.2
1	A	141	SER	3.2
1	A	326	ILE	3.1
1	A	459	ASP	3.1
1	A	783	ASN	3.1
1	A	893	ALA	3.1
1	A	829	HIS	3.1
1	A	273	ILE	3.0
1	A	272	VAL	3.0
1	A	765	VAL	3.0
1	A	794	ASN	3.0
1	A	121	CYS	3.0
1	A	564	GLY	3.0
1	A	340	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	865[A]	HIS	3.0
1	A	222	LYS	3.0
1	A	297[A]	MET	3.0
1	A	217	ILE	3.0
1	A	320	ASN	3.0
1	A	812	LEU	3.0
1	A	361	ALA	3.0
1	A	94	ILE	3.0
1	A	774	VAL	2.9
1	A	285	TYR	2.9
1	A	97	LEU	2.9
1	A	284	LEU	2.9
1	A	831	LYS	2.9
1	A	170	ASP	2.9
1	A	304	THR	2.9
1	A	334	GLY	2.9
1	A	911	LYS	2.9
1	A	226	LEU	2.9
1	A	909	GLY	2.9
1	A	796	GLY	2.9
1	A	275[A]	THR	2.8
1	A	337	THR	2.8
1	A	98	SER	2.8
1	A	325	ASN	2.8
1	A	808	ILE	2.8
1	A	781	ILE	2.8
1	A	937	TRP	2.8
1	A	335	SER	2.8
1	A	835	ALA	2.8
1	A	215	GLY	2.8
1	A	260	PHE	2.7
1	A	777	LYS	2.7
1	A	451	ASP	2.7
1	A	338	PRO	2.7
1	A	37	LYS	2.7
1	A	99	LYS	2.7
1	A	722	TYR	2.7
1	A	771	LEU	2.7
1	A	331	SER	2.7
1	A	894	GLY	2.7
1	A	261	LEU	2.7
1	A	806	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	573	TYR	2.6
1	A	380	HIS	2.6
1	A	118	VAL	2.6
1	A	330	VAL	2.6
1	A	552	VAL	2.6
1	A	910	GLU	2.6
1	A	271	SER	2.6
1	A	343	GLN	2.6
1	A	807	ASN	2.6
1	A	583	THR	2.6
1	A	323	LEU	2.5
1	A	940	THR	2.5
1	A	809	GLN	2.5
1	A	291	GLY	2.5
1	A	834	ASN	2.5
1	A	311	LYS	2.5
1	A	233	ILE	2.5
1	A	810	SER	2.5
1	A	844	THR	2.5
1	A	303	VAL	2.5
1	A	764	PRO	2.5
1	A	228	SER	2.4
1	A	572	PHE	2.4
1	A	750	ALA	2.4
1	A	654	ARG	2.4
1	A	120	PHE	2.3
1	A	238	LYS	2.3
1	A	29	SER	2.3
1	A	489	GLU	2.3
1	A	147	LYS	2.3
1	A	578	SER	2.3
1	A	850	LEU	2.3
1	A	368	THR	2.3
1	A	908	PRO	2.3
1	A	30	ILE	2.3
1	A	804	ILE	2.3
1	A	918	LEU	2.3
1	A	181	TYR	2.2
1	A	763	GLU	2.2
1	A	780	PRO	2.2
1	A	221	SER	2.2
1	A	263	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	33	LEU	2.2
1	A	363	ILE	2.2
1	A	814	ILE	2.2
1	A	309	LYS	2.2
1	A	832	LEU	2.2
1	A	939	LEU	2.2
1	A	930	GLN	2.2
1	A	289	LEU	2.2
1	A	171	GLU	2.1
1	A	591	PHE	2.1
1	A	547	ASP	2.1
1	A	660	ASP	2.1
1	A	286	SER	2.1
1	A	68	GLY	2.1
1	A	126	GLY	2.1
1	A	550	LEU	2.1
1	A	545	GLU	2.1
1	A	293	THR	2.1
1	A	342	SER	2.1
1	A	146	CYS	2.1
1	A	776	LEU	2.1
1	A	28	ALA	2.1
1	A	571	ASP	2.1
1	A	145	SER	2.1
1	A	782	ALA	2.1
1	A	288	LYS	2.0
1	A	830	GLY	2.0
1	A	151	VAL	2.0
1	A	253	VAL	2.0
1	A	341	VAL	2.0
1	A	931	VAL	2.0
1	A	870	LYS	2.0
1	A	392	PRO	2.0
1	A	125[A]	VAL	2.0
1	A	139	VAL	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

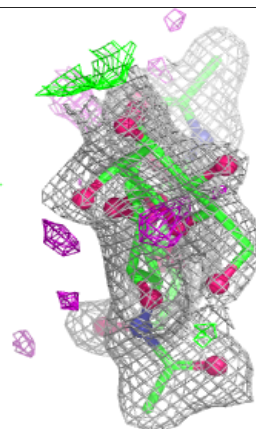
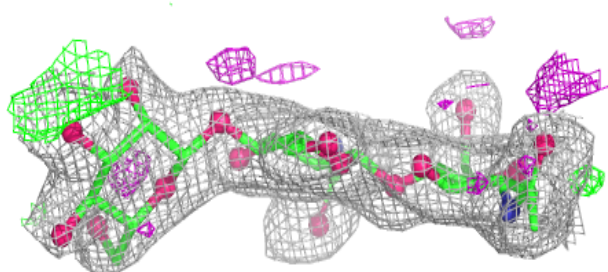
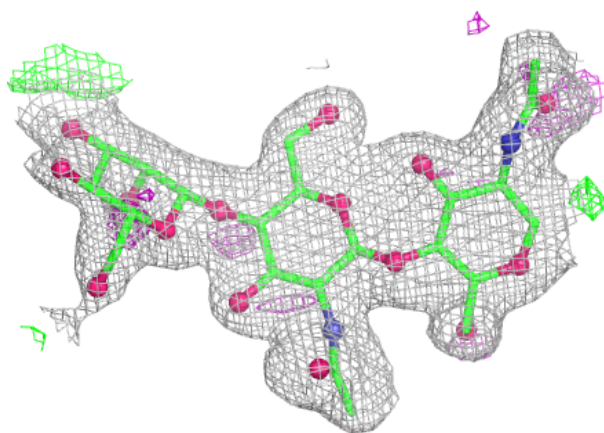
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	6	11/12	0.71	0.17	65,66,68,70	0
3	MAN	C	4	11/12	0.76	0.19	63,65,67,68	0
5	MAN	E	6	11/12	0.81	0.16	52,57,61,65	0
2	BMA	B	3	11/12	0.82	0.16	54,57,59,62	0
3	MAN	C	8	11/12	0.82	0.16	57,61,64,69	0
3	MAN	C	6	11/12	0.84	0.16	52,60,62,64	0
3	BMA	C	3	11/12	0.85	0.14	50,55,57,59	0
3	MAN	C	7	11/12	0.86	0.13	57,60,64,64	0
3	NAG	C	2	14/15	0.86	0.15	44,48,53,54	0
3	NAG	C	1	14/15	0.87	0.15	40,43,47,49	0
3	MAN	C	5	11/12	0.88	0.12	51,60,62,64	0
5	MAN	E	9	11/12	0.88	0.14	51,53,54,56	0
2	NAG	B	2	14/15	0.90	0.12	46,50,51,52	0
4	NAG	D	2	14/15	0.90	0.14	44,48,50,58	0
5	MAN	E	8	11/12	0.90	0.14	48,55,62,63	0
4	BMA	D	3	11/12	0.90	0.12	48,51,55,58	0
5	MAN	E	11	11/12	0.90	0.14	49,51,52,52	0
5	MAN	E	5	11/12	0.91	0.13	45,48,53,57	0
4	MAN	D	4	11/12	0.91	0.12	43,46,47,48	0
5	MAN	E	7	11/12	0.91	0.13	47,51,53,53	0
4	MAN	D	5	11/12	0.92	0.11	43,47,53,56	0
2	NAG	B	1	14/15	0.92	0.11	35,38,42,45	0
5	BMA	E	3	11/12	0.93	0.12	43,45,50,50	0
5	MAN	E	4	11/12	0.93	0.12	43,44,47,48	0
4	NAG	D	1	14/15	0.93	0.11	44,46,47,47	0
5	NAG	E	2	14/15	0.93	0.13	41,44,47,48	0
5	MAN	E	10	11/12	0.94	0.12	46,50,52,53	0
5	NAG	E	1	14/15	0.94	0.10	42,45,51,51	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.

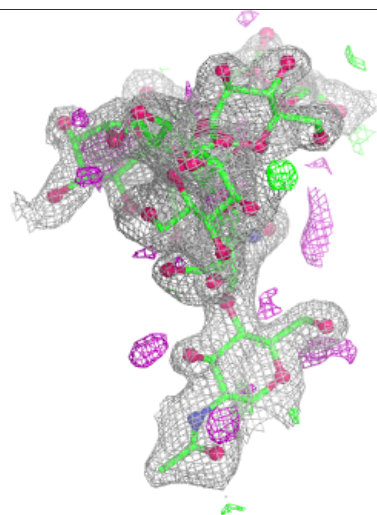
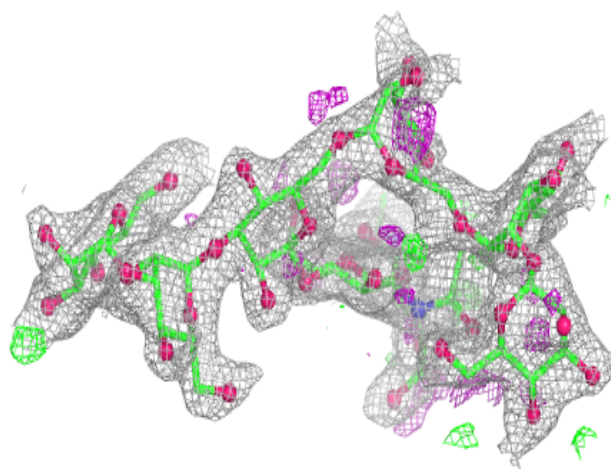
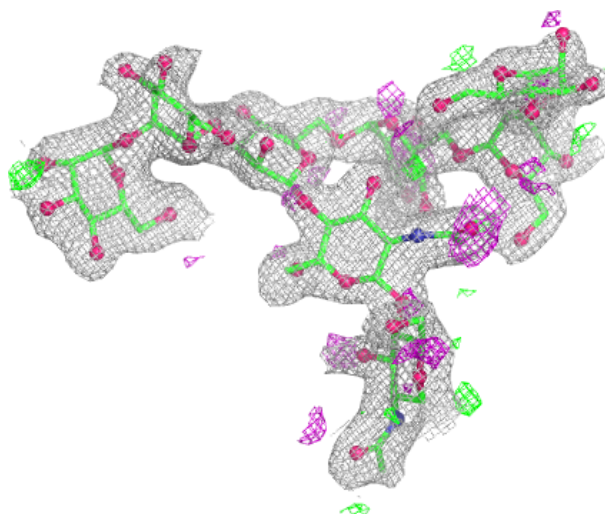
Electron density around Chain B:

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



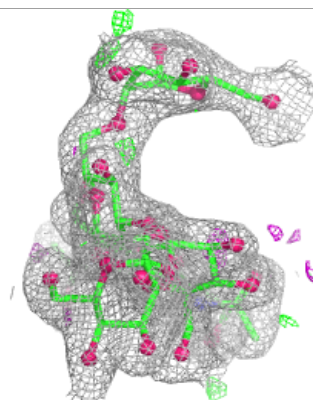
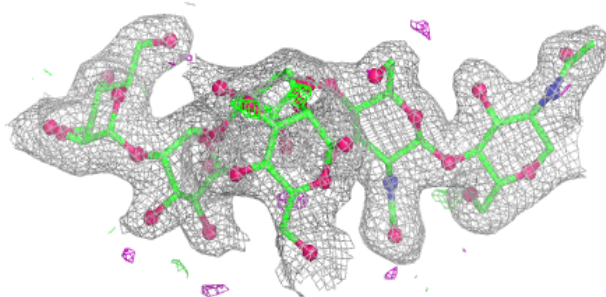
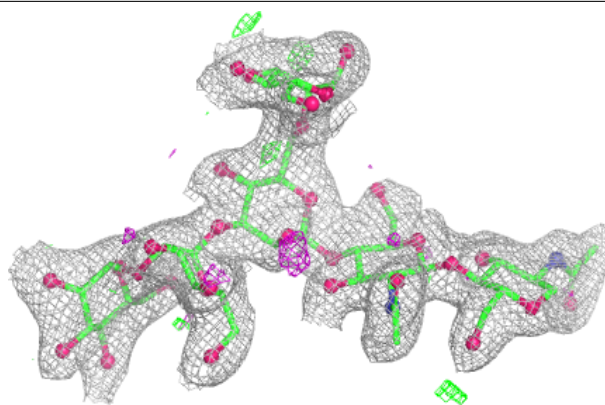
Electron density around Chain C:

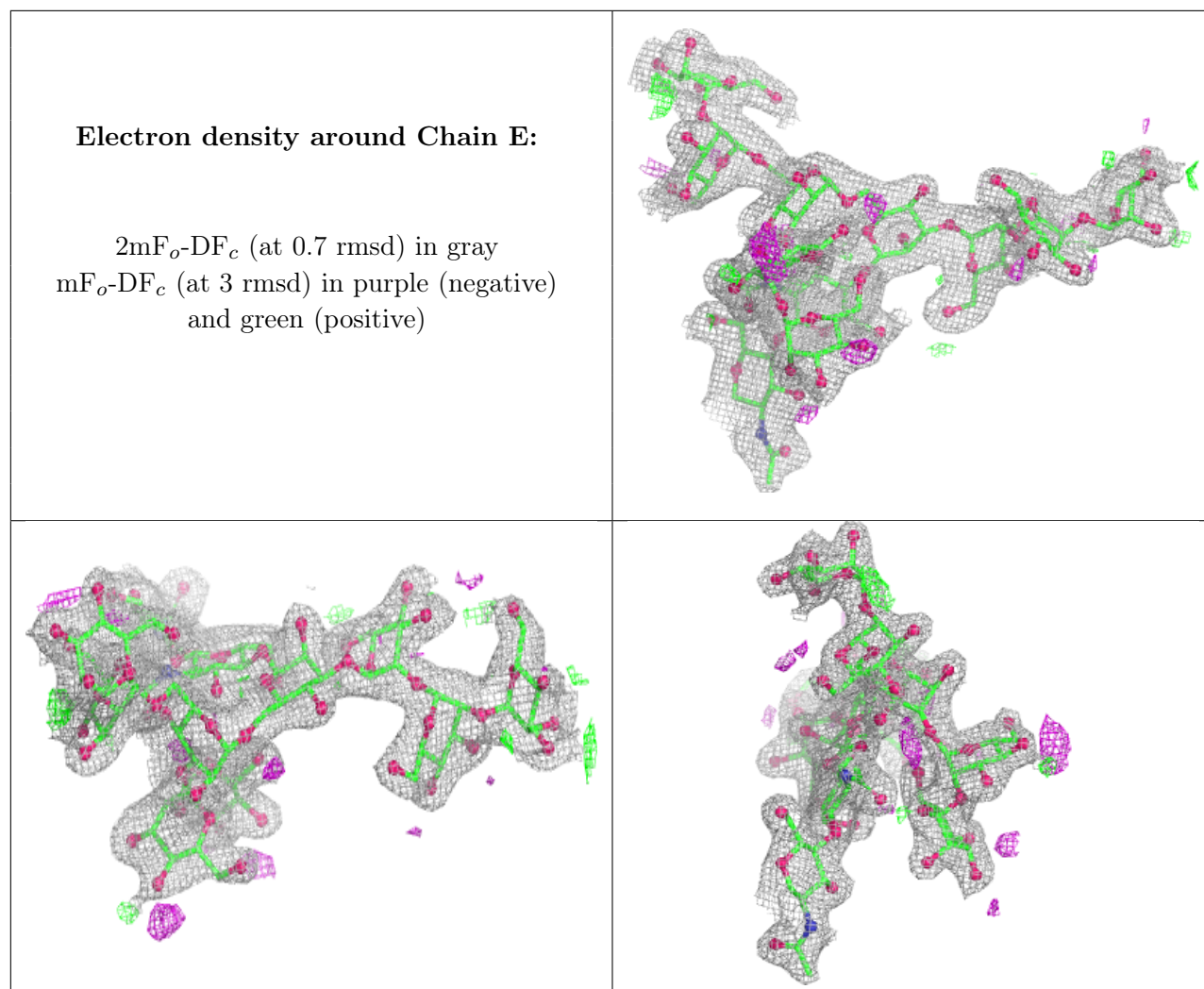
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
7	CD	A	1021	1/1	0.55	0.29	125,125,125,125	1
8	NA	A	1025	1/1	0.73	0.40	54,54,54,54	0
6	NAG	A	1002	14/15	0.76	0.19	67,73,78,80	0
6	NAG	A	1006	14/15	0.81	0.14	54,59,68,70	0
6	NAG	A	1005	14/15	0.83	0.15	56,60,63,68	0
9	PG4	A	1030	12/13	0.83	0.22	57,61,66,66	0
10	PEG	A	1031	7/7	0.83	0.20	58,60,62,64	0
6	NAG	A	1004	14/15	0.88	0.13	54,59,64,67	0
6	NAG	A	1001	14/15	0.91	0.12	46,51,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NA	A	1028	1/1	0.91	0.24	40,40,40,40	0
6	NAG	A	1007	14/15	0.91	0.11	40,43,46,47	0
6	NAG	A	1003	14/15	0.91	0.12	39,44,48,48	0
7	CD	A	1012	1/1	0.92	0.12	72,72,72,72	0
7	CD	A	1014	1/1	0.93	0.20	76,76,76,76	0
12	CL	A	1033	1/1	0.94	0.23	49,49,49,49	0
7	CD	A	1020	1/1	0.95	0.17	77,77,77,77	0
8	NA	A	1026	1/1	0.95	0.28	48,48,48,48	0
8	NA	A	1027	1/1	0.95	0.20	30,30,30,30	0
7	CD	A	1019	1/1	0.95	0.09	80,80,80,80	0
7	CD	A	1022	1/1	0.95	0.21	87,87,87,87	1
7	CD	A	1023	1/1	0.95	0.35	44,44,44,44	0
7	CD	A	1024	1/1	0.95	0.52	44,44,44,44	0
8	NA	A	1034	1/1	0.96	0.26	37,37,37,37	0
7	CD	A	1010	1/1	0.96	0.17	58,58,58,58	0
7	CD	A	1011	1/1	0.96	0.07	50,50,50,50	0
8	NA	A	1029	1/1	0.96	0.17	33,33,33,33	0
7	CD	A	1018	1/1	0.97	0.14	74,74,74,74	0
7	CD	A	1013	1/1	0.97	0.08	52,52,52,52	0
7	CD	A	1009	1/1	0.97	0.07	43,43,43,43	0
11	CA	A	1032	1/1	0.97	0.08	54,54,54,54	0
7	CD	A	1017	1/1	0.97	0.18	81,81,81,81	0
7	CD	A	1008	1/1	0.98	0.05	39,39,39,39	0
7	CD	A	1015	1/1	0.98	0.06	51,51,51,51	0
7	CD	A	1016	1/1	0.98	0.10	59,59,59,59	0

5.5 Other polymers

There are no such residues in this entry.