



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2022 – 12:15 am GMT

PDB ID : 4CVU  
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)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

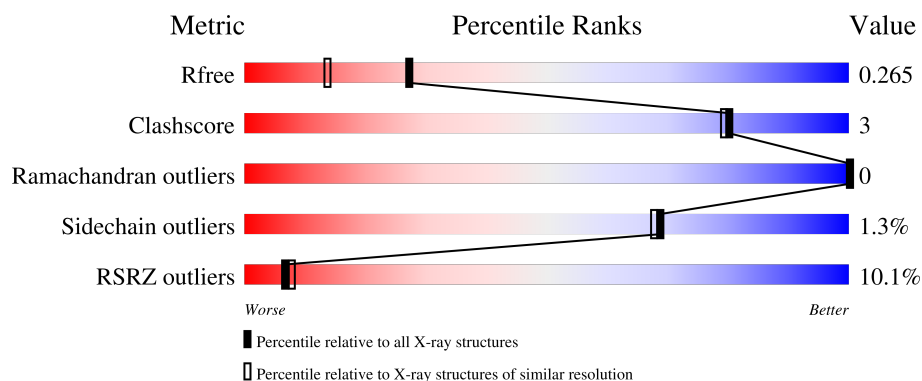
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	942	<div> <div>10%</div> <div>90%</div> <div>6%</div> </div>
2	B	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	C	8	<div> <div>12%</div> <div>62%</div> <div>25%</div> </div>
4	D	6	<div> <div>100%</div> </div>
5	E	11	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

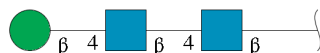
There are 13 unique types of molecules in this entry. The entry contains 8456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

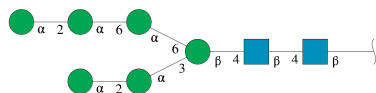
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	913	7241	4645	1208	1371	17	0	6	0

- 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.

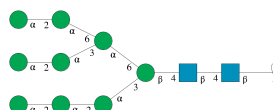


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	94	52	2	40	0	0	0

- 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.

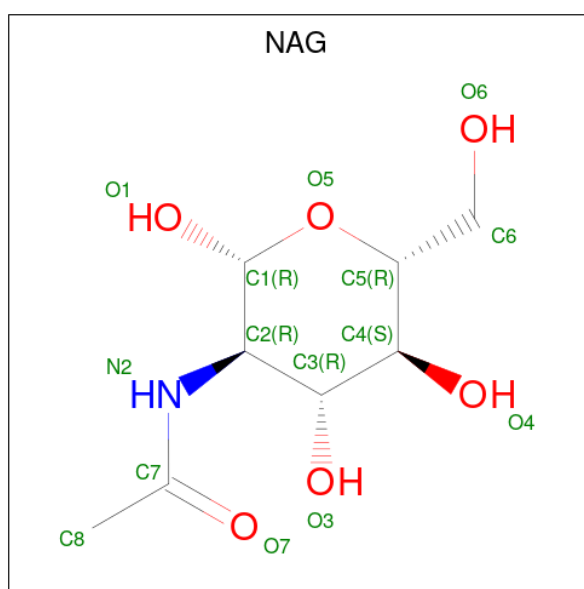
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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 (three-letter code: 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		

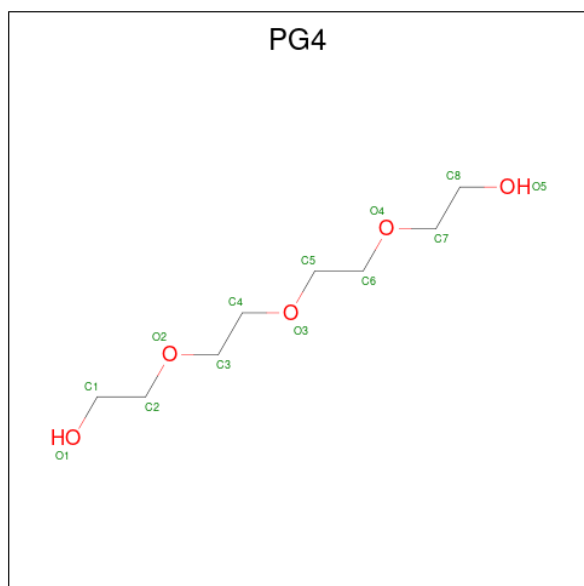
- Molecule 7 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

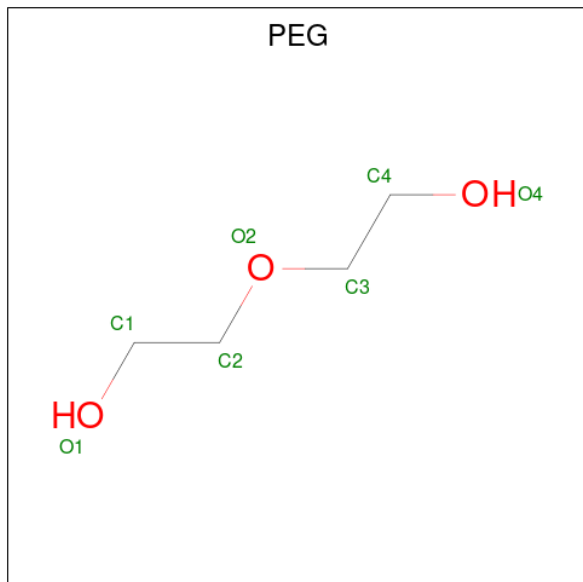
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	Na	0	0
			6	6		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

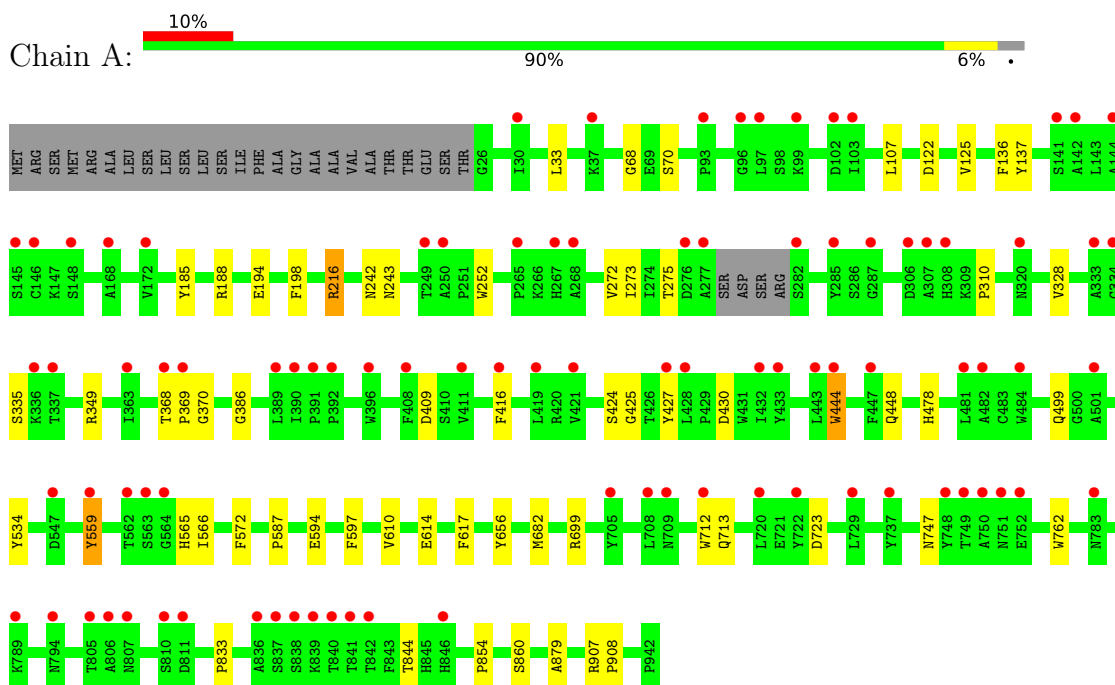
- Molecule 13 is water.

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

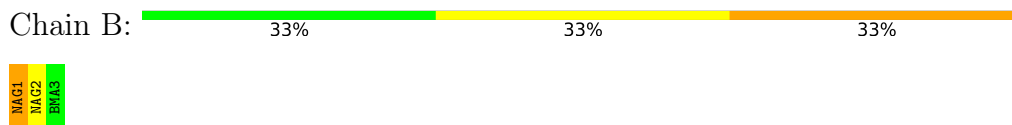
### 3 Residue-property plots

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.

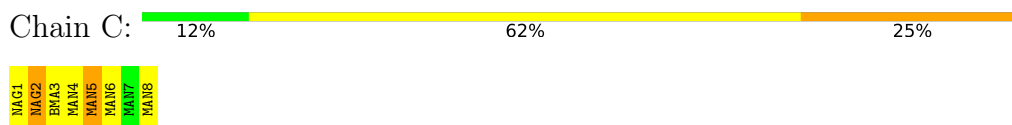
#### • Molecule 1: BETA-MANNOSIDASE



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



#### • Molecule 3: 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



- Molecule 4:  $\alpha$ -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

Chain D:

100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 5:  $\alpha$ -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

Chain E:

100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10  
MAN11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.46Å 166.46Å 121.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.70 – 1.90 48.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (117.70-1.90) 98.8 (48.30-1.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	6636 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CD, BMA, MAN, CA, CL, PG4, NA, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.67	0/7479	0.72	4/10243 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	723	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	409	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	723	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	188	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	SER	Peptide

### 5.2 Too-close contacts

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	A	7241	0	6832	39	0
2	B	39	0	34	1	0
3	C	94	0	79	1	0
4	D	72	0	61	0	0
5	E	127	0	105	0	0
6	A	98	0	90	0	0
7	A	17	0	0	0	0
8	A	6	0	0	0	0
9	A	12	0	15	0	0
10	A	7	0	10	0	0
11	A	1	0	0	0	0
12	A	1	0	0	1	0
13	A	741	0	0	7	0
All	All	8456	0	7226	40	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.

All (40) 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)
3:C:2:NAG:H81	3:C:5:MAN:O6	1.81	0.80
1:A:194:GLU:HG3	1:A:425:GLY:HA2	1.67	0.75
1:A:597:PHE:HB2	1:A:682:MET:CE	2.26	0.66
1:A:565:HIS:NE2	12:A:1033:CL:CL	2.58	0.65
1:A:597:PHE:HB2	1:A:682:MET:HE1	1.80	0.64
1:A:844:THR:O	13:A:1101:HOH:O	2.16	0.62
1:A:879:ALA:O	1:A:908:PRO:HA	2.03	0.58
1:A:656:TYR:CE1	1:A:854:PRO:HG2	2.41	0.55
1:A:444:TRP:CD1	1:A:444:TRP:C	2.80	0.54
1:A:860:SER:OG	13:A:1102:HOH:O	2.18	0.53
1:A:272:VAL:HG12	1:A:328:VAL:HG22	1.91	0.52
1:A:617:PHE:CD1	2:B:1:NAG:H82	2.45	0.51
1:A:107:LEU:O	1:A:136:PHE:HA	2.11	0.51
1:A:243:ASN:HD21	1:A:534:TYR:H	1.57	0.51
1:A:610[A]:VAL:CG1	1:A:614:GLU:HB2	2.42	0.50
1:A:572:PHE:CD1	1:A:587:PRO:HD3	2.46	0.49
1:A:597:PHE:HB2	1:A:682:MET:HE2	1.96	0.48
1:A:194:GLU:HG3	1:A:425:GLY:CA	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:CD	13:A:1179:HOH:O	2.53	0.47
1:A:335:SER:CB	13:A:1333:HOH:O	2.63	0.47
1:A:185:TYR:HB2	1:A:198:PHE:HB3	1.98	0.46
1:A:747:ASN:ND2	13:A:1111:HOH:O	2.39	0.46
1:A:242:ASN:O	1:A:243:ASN:HB2	2.16	0.45
1:A:430:ASP:OD1	1:A:478:HIS:CE1	2.69	0.45
1:A:427:TYR:CE2	1:A:448:GLN:HG2	2.51	0.45
1:A:713:GLN:OE1	1:A:713:GLN:N	2.46	0.45
1:A:762:TRP:CE3	1:A:833:PRO:HB3	2.53	0.44
1:A:125[A]:VAL:HG12	1:A:137:TYR:HB3	1.99	0.44
1:A:860:SER:CB	13:A:1102:HOH:O	2.65	0.43
1:A:273:ILE:HG22	1:A:275[B]:THR:HG23	2.01	0.42
1:A:368:THR:HA	1:A:369:PRO:HD3	1.87	0.42
1:A:33:LEU:HG	1:A:216:ARG:HA	2.01	0.42
1:A:252:TRP:CD1	1:A:310:PRO:HG2	2.55	0.42
1:A:559:TYR:CD1	1:A:559:TYR:N	2.86	0.42
1:A:370:GLY:HA3	1:A:566:ILE:O	2.20	0.41
1:A:444:TRP:C	1:A:444:TRP:HD1	2.22	0.41
1:A:386:GLY:HA2	1:A:416:PHE:CD2	2.55	0.41
1:A:610[A]:VAL:HG13	1:A:614:GLU:HB2	2.02	0.41
1:A:68:GLY:HA3	13:A:1718:HOH:O	2.20	0.41
1:A:243:ASN:HD21	1:A:534:TYR:N	2.19	0.40

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	A	915/942 (97%)	891 (97%)	24 (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	A	777/811 (96%)	766 (99%)	11 (1%)	67 65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	122	ASP
1	A	216	ARG
1	A	349[A]	ARG
1	A	349[B]	ARG
1	A	444	TRP
1	A	499	GLN
1	A	559	TYR
1	A	699	ARG
1	A	712	TRP
1	A	907	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	243	ASN

### 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

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	2,1	14,14,15	0.65	0	17,19,21	1.16	1 (5%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
2	BMA	B	3	2	11,11,12	0.52	0	15,15,17	0.76	0
3	NAG	C	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	0.90	0
3	NAG	C	2	3	14,14,15	0.66	0	17,19,21	1.30	2 (11%)
3	BMA	C	3	3	11,11,12	0.78	0	15,15,17	1.10	2 (13%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	2.07	3 (20%)
3	MAN	C	5	3	11,11,12	0.77	0	15,15,17	1.50	2 (13%)
3	MAN	C	6	3	11,11,12	0.68	0	15,15,17	0.87	1 (6%)
3	MAN	C	7	3	11,11,12	0.62	0	15,15,17	0.87	0
3	MAN	C	8	3	11,11,12	0.53	0	15,15,17	1.04	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.52	0	17,19,21	1.00	1 (5%)
4	NAG	D	2	4	14,14,15	0.74	0	17,19,21	1.21	1 (5%)
4	BMA	D	3	4	11,11,12	0.59	0	15,15,17	1.10	1 (6%)
4	MAN	D	4	4	11,11,12	0.63	0	15,15,17	1.27	2 (13%)
4	MAN	D	5	4	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
4	MAN	D	6	4	11,11,12	0.95	0	13,15,17	2.05	2 (15%)
5	NAG	E	1	5,1	14,14,15	0.69	0	17,19,21	1.10	2 (11%)
5	MAN	E	10	5	11,11,12	0.78	1 (9%)	15,15,17	0.87	0
5	MAN	E	11	5	11,11,12	0.65	0	15,15,17	0.72	1 (6%)
5	NAG	E	2	5	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
5	BMA	E	3	5	11,11,12	0.53	0	15,15,17	0.87	1 (6%)
5	MAN	E	4	5	11,11,12	0.58	0	15,15,17	1.12	2 (13%)
5	MAN	E	5	5	11,11,12	1.02	1 (9%)	15,15,17	1.11	2 (13%)
5	MAN	E	6	5	11,11,12	0.62	0	15,15,17	1.12	1 (6%)
5	MAN	E	7	5	11,11,12	1.40	1 (9%)	15,15,17	3.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	E	8	5	11,11,12	0.75	0	15,15,17	1.52	4 (26%)
5	MAN	E	9	5	11,11,12	0.71	0	15,15,17	1.34	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	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	-	1/2/19/22	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	4,1	-	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	5,1	-	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	MAN	O3-C3	-4.02	1.33	1.43
5	E	10	MAN	O5-C5	-2.19	1.39	1.43
3	C	1	NAG	C1-C2	2.07	1.55	1.52
5	E	5	MAN	O5-C1	-2.02	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	MAN	O3-C3-C2	11.67	132.35	109.99
3	C	4	MAN	C1-O5-C5	5.86	120.14	112.19
4	D	6	MAN	C3-C4-C5	5.27	115.22	109.97
4	D	6	MAN	C1-C2-C3	-4.50	100.55	110.91
3	C	4	MAN	O5-C5-C4	3.48	119.30	110.83
3	C	5	MAN	C1-C2-C3	3.44	113.89	109.67
3	C	2	NAG	C2-N2-C7	3.17	127.42	122.90
5	E	8	MAN	O5-C1-C2	3.06	115.49	110.77
5	E	9	MAN	C1-O5-C5	2.92	116.15	112.19
3	C	6	MAN	C1-O5-C5	2.92	116.15	112.19
3	C	8	MAN	C1-O5-C5	2.87	116.08	112.19
4	D	4	MAN	O2-C2-C3	-2.82	104.49	110.14
5	E	6	MAN	C2-C3-C4	-2.66	106.30	110.89
5	E	8	MAN	C3-C4-C5	2.65	114.97	110.24
5	E	8	MAN	C1-C2-C3	-2.63	106.44	109.67
5	E	1	NAG	C1-O5-C5	2.61	115.73	112.19
3	C	3	BMA	O3-C3-C4	-2.59	104.36	110.35
4	D	3	BMA	O4-C4-C3	-2.53	104.49	110.35
3	C	2	NAG	C8-C7-N2	2.53	120.38	116.10
4	D	2	NAG	C3-C4-C5	-2.50	105.78	110.24
2	B	1	NAG	C1-O5-C5	2.48	115.56	112.19
5	E	5	MAN	C1-O5-C5	2.38	115.42	112.19
3	C	5	MAN	O2-C2-C1	-2.32	104.41	109.15
4	D	1	NAG	C1-O5-C5	2.29	115.30	112.19
3	C	4	MAN	O5-C5-C6	-2.26	103.66	107.20
5	E	1	NAG	O5-C1-C2	-2.24	107.75	111.29
5	E	11	MAN	C1-O5-C5	2.24	115.22	112.19
5	E	2	NAG	O7-C7-C8	-2.22	117.94	122.06
4	D	5	MAN	O5-C5-C6	2.21	110.67	107.20
5	E	4	MAN	O4-C4-C5	2.18	114.70	109.30
5	E	8	MAN	O4-C4-C3	-2.13	105.42	110.35
2	B	2	NAG	C1-O5-C5	2.12	115.07	112.19
5	E	5	MAN	C6-C5-C4	-2.07	108.15	113.00
5	E	7	MAN	C1-O5-C5	2.06	114.98	112.19
5	E	3	BMA	O6-C6-C5	-2.05	104.25	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	MAN	C1-C2-C3	-2.04	107.16	109.67
3	C	3	BMA	O4-C4-C3	-2.01	105.70	110.35
5	E	4	MAN	O2-C2-C1	-2.00	105.06	109.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

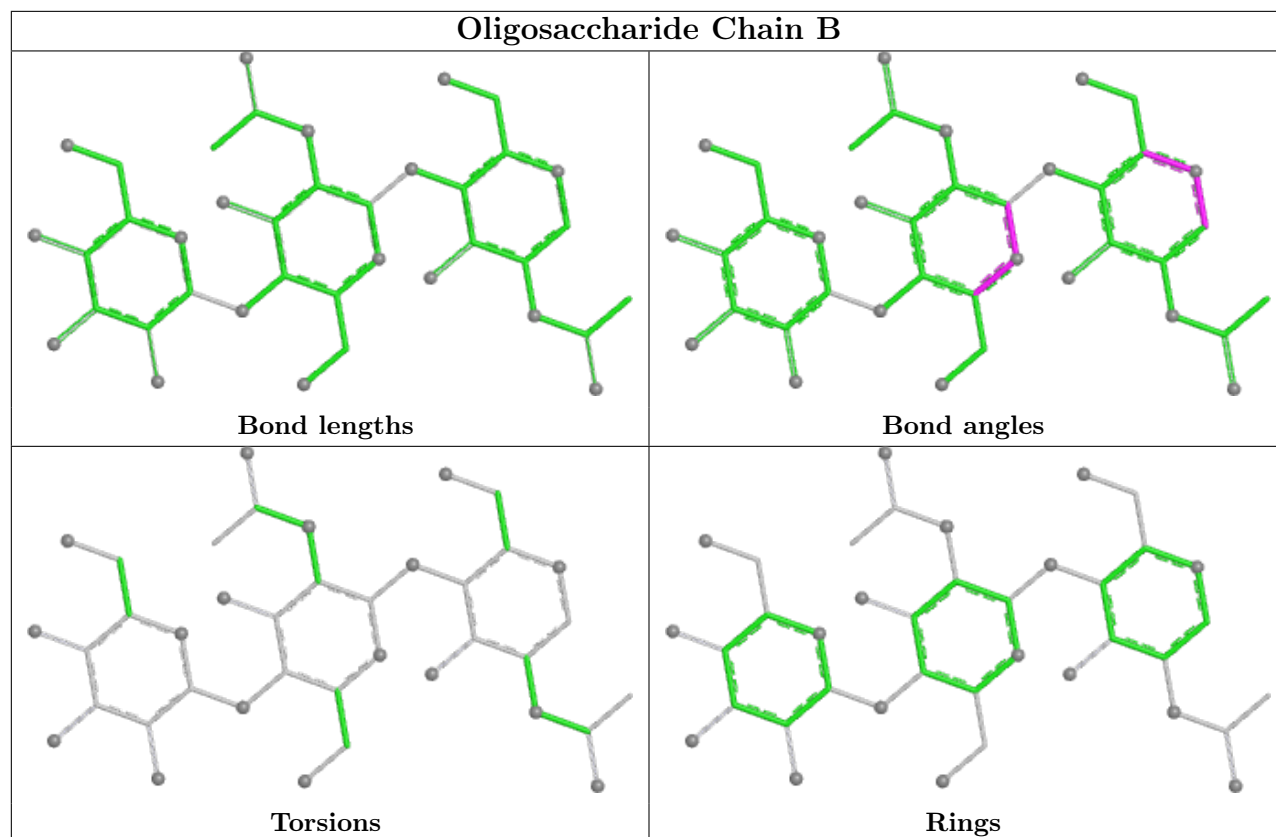
Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
5	E	6	MAN	O5-C5-C6-O6
5	E	6	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
5	E	9	MAN	C4-C5-C6-O6

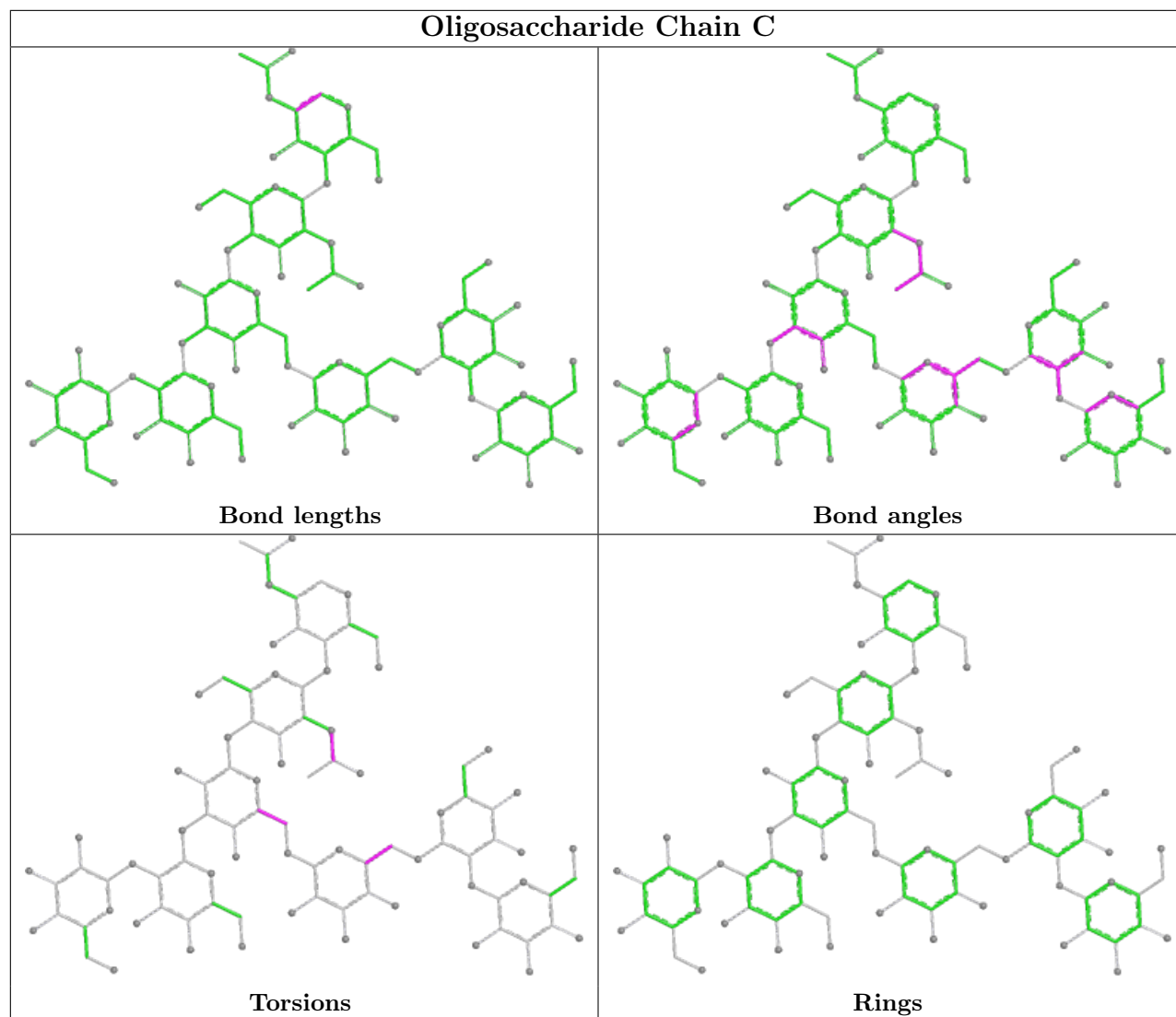
There are no ring outliers.

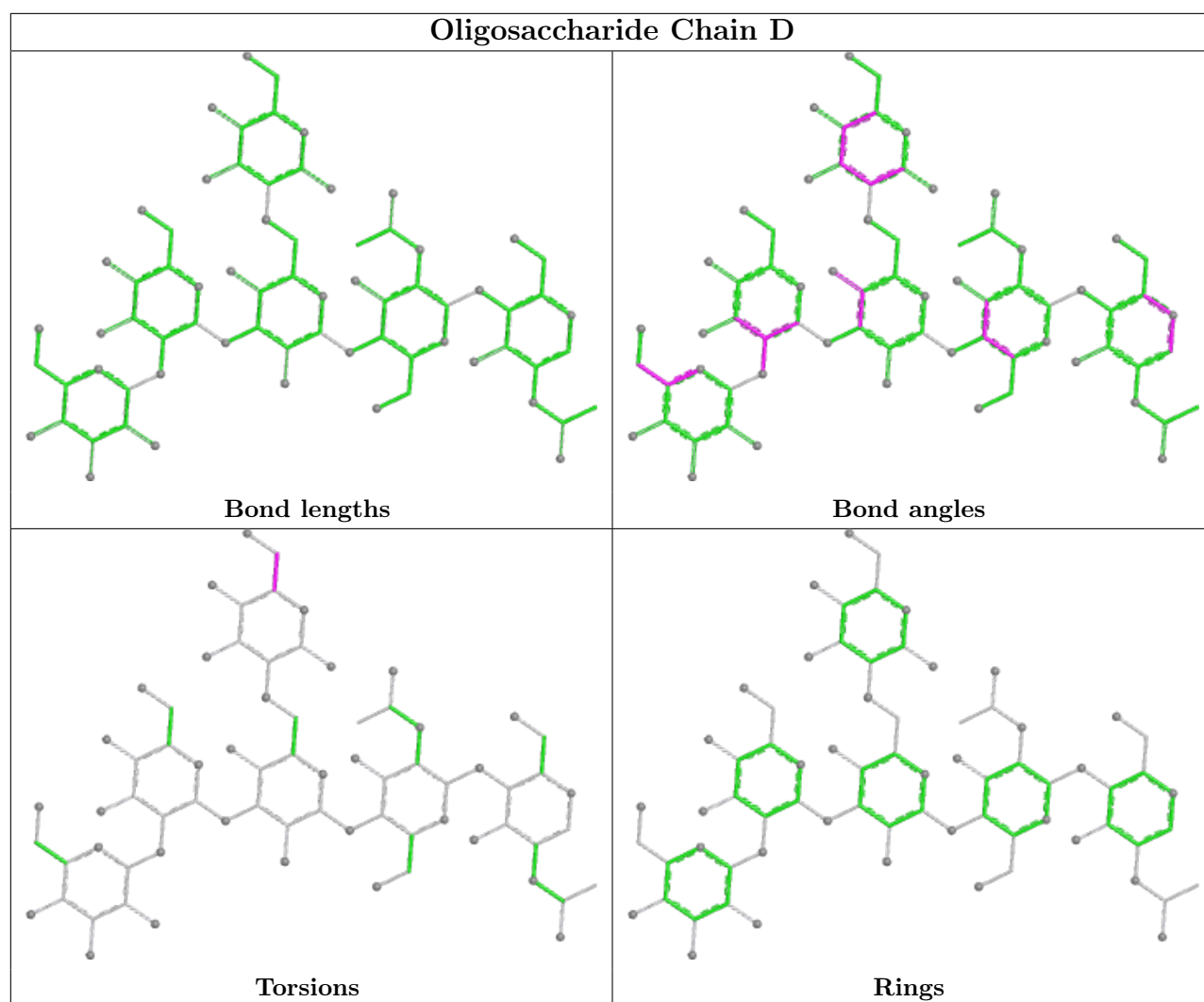
3 monomers are involved in 2 short contacts:

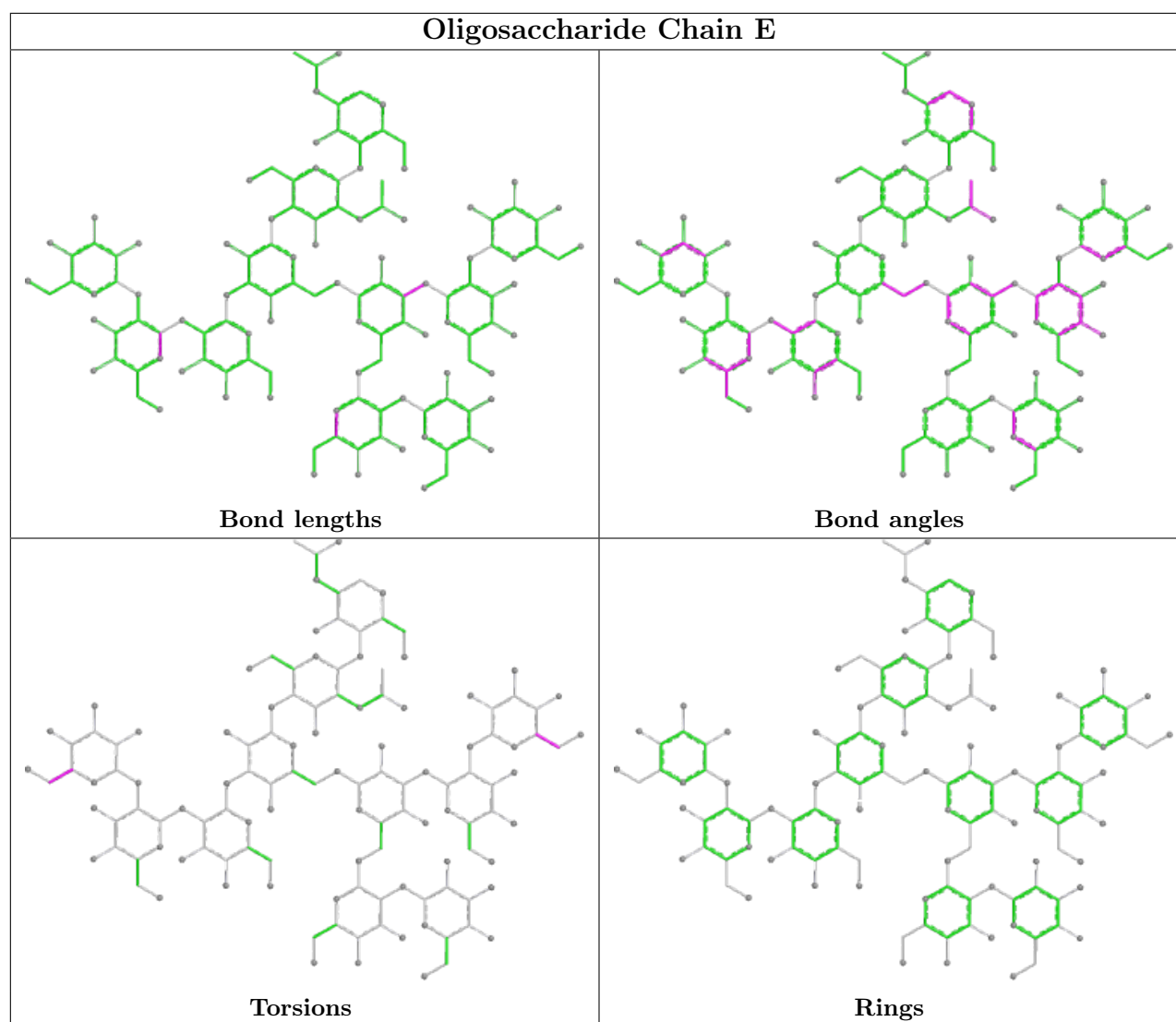
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
3	C	5	MAN	1	0
3	C	2	NAG	1	0

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









## 5.6 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	1006	1	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
9	PG4	A	1030	-	11,11,12	0.54	0	10,10,11	0.44	0
10	PEG	A	1031	-	6,6,6	0.53	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1002	-	14,14,15	0.66	0	19,19,21	2.14	7 (36%)
6	NAG	A	1003	1	14,14,15	0.93	1 (7%)	17,19,21	1.36	1 (5%)
6	NAG	A	1005	1	14,14,15	0.44	0	17,19,21	1.44	3 (17%)
6	NAG	A	1007	1	14,14,15	0.50	0	17,19,21	1.08	0
6	NAG	A	1001	1	14,14,15	0.96	1 (7%)	17,19,21	1.22	1 (5%)
6	NAG	A	1004	1	14,14,15	0.48	0	17,19,21	1.12	1 (5%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	NAG	O5-C1	-2.16	1.40	1.43
6	A	1003	NAG	O5-C1	-2.03	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	5.15	124.83	116.10
6	A	1003	NAG	C1-O5-C5	4.66	118.51	112.19
6	A	1002	NAG	C2-N2-C7	4.10	128.75	122.90
6	A	1004	NAG	C1-O5-C5	3.51	116.95	112.19
6	A	1001	NAG	C1-O5-C5	3.24	116.58	112.19
6	A	1002	NAG	C3-C2-N2	3.16	115.75	110.86
6	A	1005	NAG	C1-O5-C5	2.81	116.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	NAG	C3-C4-C5	2.79	114.39	110.77
6	A	1005	NAG	O5-C5-C6	2.52	111.16	107.20
6	A	1005	NAG	O5-C1-C2	-2.50	107.34	111.29
6	A	1002	NAG	O7-C7-C8	-2.43	117.53	122.06
6	A	1006	NAG	C1-O5-C5	2.42	115.47	112.19
6	A	1002	NAG	O7-C7-N2	-2.35	117.64	121.95
6	A	1002	NAG	O5-C1-C2	-2.02	107.49	109.52

There are no chirality outliers.

All (17) 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
9	A	1030	PG4	O2-C3-C4-O3
10	A	1031	PEG	O2-C3-C4-O4
6	A	1006	NAG	C4-C5-C6-O6
6	A	1004	NAG	C4-C5-C6-O6
6	A	1006	NAG	O5-C5-C6-O6
10	A	1031	PEG	O1-C1-C2-O2
10	A	1031	PEG	C4-C3-O2-C2
6	A	1002	NAG	C1-C2-N2-C7
6	A	1002	NAG	O5-C5-C6-O6
9	A	1030	PG4	C3-C4-O3-C5
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.

## 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 ⓘ

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	913/942 (96%)	0.57	92 (10%) 7 8	28, 45, 69, 105	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	749	THR	6.6
1	A	334	GLY	6.5
1	A	839	LYS	6.0
1	A	750	ALA	5.4
1	A	751	ASN	5.1
1	A	838	SER	5.0
1	A	389	LEU	4.7
1	A	419	LEU	4.5
1	A	421	VAL	4.4
1	A	267	HIS	4.4
1	A	428	LEU	4.4
1	A	563	SER	4.4
1	A	443	LEU	4.1
1	A	168	ALA	4.1
1	A	432	ILE	4.0
1	A	708	LEU	3.9
1	A	811	ASP	3.9
1	A	265	PRO	3.8
1	A	306	ASP	3.7
1	A	268	ALA	3.5
1	A	807	ASN	3.5
1	A	840	THR	3.4
1	A	810	SER	3.4
1	A	392	PRO	3.3
1	A	411	VAL	3.3
1	A	396	TRP	3.2
1	A	336	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	752	GLU	3.2
1	A	146	CYS	3.2
1	A	308	HIS	3.2
1	A	390	ILE	3.1
1	A	337	THR	3.1
1	A	564	GLY	3.1
1	A	805	THR	3.1
1	A	276	ASP	3.0
1	A	148	SER	3.0
1	A	103	ILE	3.0
1	A	748	TYR	2.9
1	A	722	TYR	2.8
1	A	391	PRO	2.8
1	A	481	LEU	2.8
1	A	93	PRO	2.8
1	A	96	GLY	2.8
1	A	737	TYR	2.7
1	A	37	LYS	2.6
1	A	141	SER	2.6
1	A	333	ALA	2.6
1	A	720	LEU	2.6
1	A	427	TYR	2.6
1	A	142	ALA	2.6
1	A	250	ALA	2.5
1	A	559	TYR	2.5
1	A	836	ALA	2.5
1	A	484	TRP	2.5
1	A	562	THR	2.5
1	A	363	ILE	2.5
1	A	277	ALA	2.5
1	A	794	ASN	2.5
1	A	285	TYR	2.5
1	A	145	SER	2.4
1	A	841	THR	2.4
1	A	842	THR	2.4
1	A	287	GLY	2.4
1	A	712	TRP	2.4
1	A	99	LYS	2.4
1	A	307	ALA	2.3
1	A	705	TYR	2.3
1	A	547	ASP	2.3
1	A	433	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	837	SER	2.3
1	A	447	PHE	2.2
1	A	30	ILE	2.2
1	A	282	SER	2.2
1	A	416	PHE	2.2
1	A	846	HIS	2.2
1	A	729	LEU	2.2
1	A	709	ASN	2.2
1	A	97	LEU	2.2
1	A	320	ASN	2.2
1	A	249	THR	2.1
1	A	144	ALA	2.1
1	A	408	PHE	2.1
1	A	783	ASN	2.1
1	A	482	ALA	2.1
1	A	806	ALA	2.1
1	A	789	LYS	2.1
1	A	172	VAL	2.1
1	A	501	ALA	2.1
1	A	444	TRP	2.0
1	A	102	ASP	2.0
1	A	369	PRO	2.0
1	A	368	THR	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MAN	C	4	11/12	0.69	0.40	63,65,67,68	0
4	MAN	D	6	11/12	0.76	0.21	65,66,68,70	0
3	NAG	C	2	14/15	0.83	0.19	44,48,53,54	0
5	MAN	E	7	11/12	0.83	0.17	47,51,53,53	0
3	MAN	C	8	11/12	0.84	0.20	57,61,64,69	0

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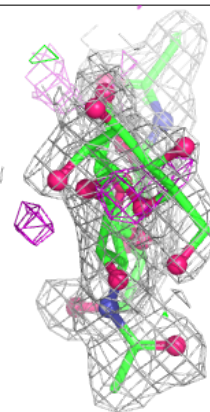
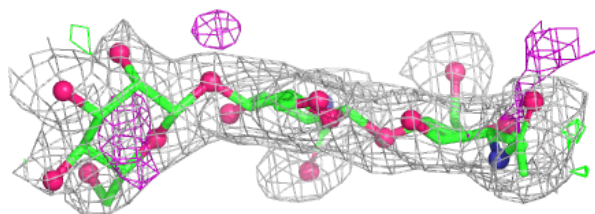
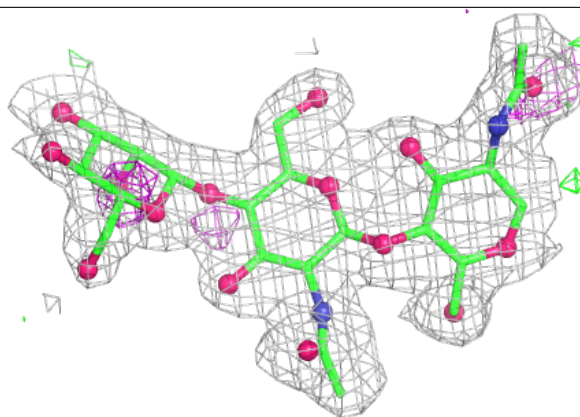
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	C	6	11/12	0.85	0.25	52,60,62,64	0
5	MAN	E	6	11/12	0.85	0.19	52,57,61,65	0
2	BMA	B	3	11/12	0.85	0.31	54,57,59,62	0
4	NAG	D	2	14/15	0.88	0.14	44,48,50,58	0
3	NAG	C	1	14/15	0.88	0.15	40,43,47,49	0
3	BMA	C	3	11/12	0.89	0.23	50,55,57,59	0
3	MAN	C	5	11/12	0.89	0.23	51,60,62,64	0
4	BMA	D	3	11/12	0.90	0.18	48,51,55,58	0
5	MAN	E	8	11/12	0.90	0.15	48,55,62,63	0
5	MAN	E	9	11/12	0.90	0.16	51,53,54,56	0
4	MAN	D	5	11/12	0.91	0.16	43,47,53,56	0
3	MAN	C	7	11/12	0.91	0.25	57,60,64,64	0
4	MAN	D	4	11/12	0.91	0.13	43,46,47,48	0
5	MAN	E	11	11/12	0.91	0.11	49,51,52,52	0
5	MAN	E	4	11/12	0.92	0.10	43,44,47,48	0
4	NAG	D	1	14/15	0.92	0.14	44,46,47,47	0
5	NAG	E	2	14/15	0.93	0.11	41,44,47,48	0
2	NAG	B	2	14/15	0.93	0.16	46,50,51,52	0
5	MAN	E	5	11/12	0.93	0.16	45,48,53,57	0
5	MAN	E	10	11/12	0.93	0.12	46,50,52,53	0
2	NAG	B	1	14/15	0.93	0.12	35,38,42,45	0
5	NAG	E	1	14/15	0.94	0.11	42,45,51,51	0
5	BMA	E	3	11/12	0.95	0.12	43,45,50,50	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.

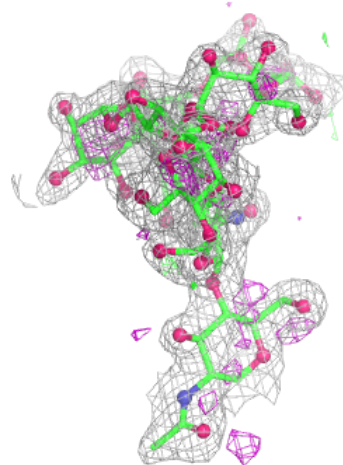
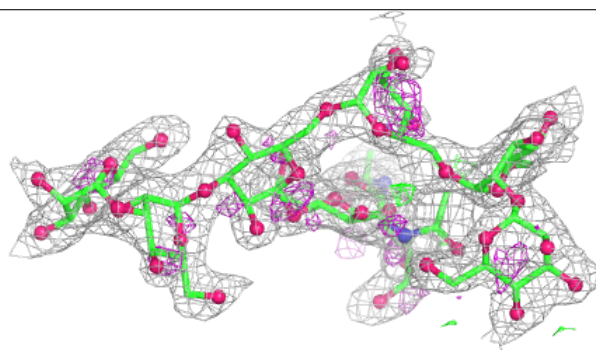
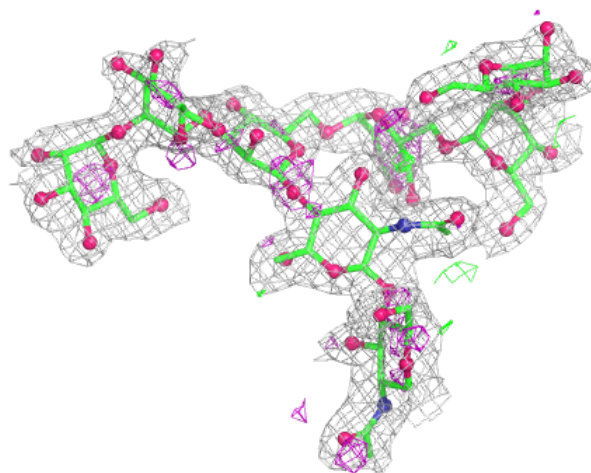
**Electron density around Chain B:**

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



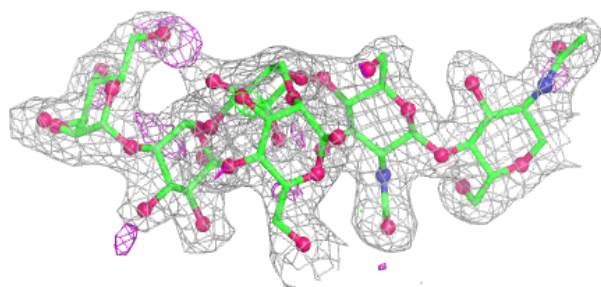
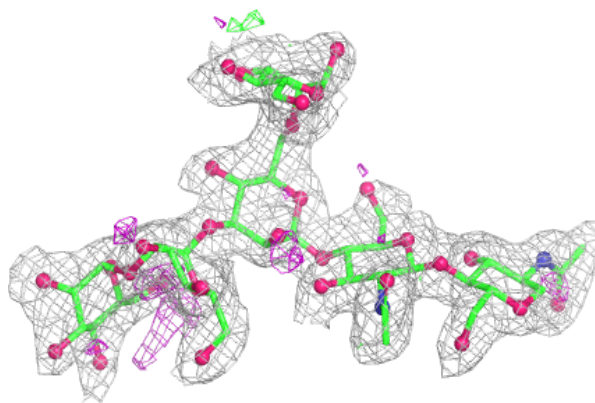
**Electron density around Chain C:**

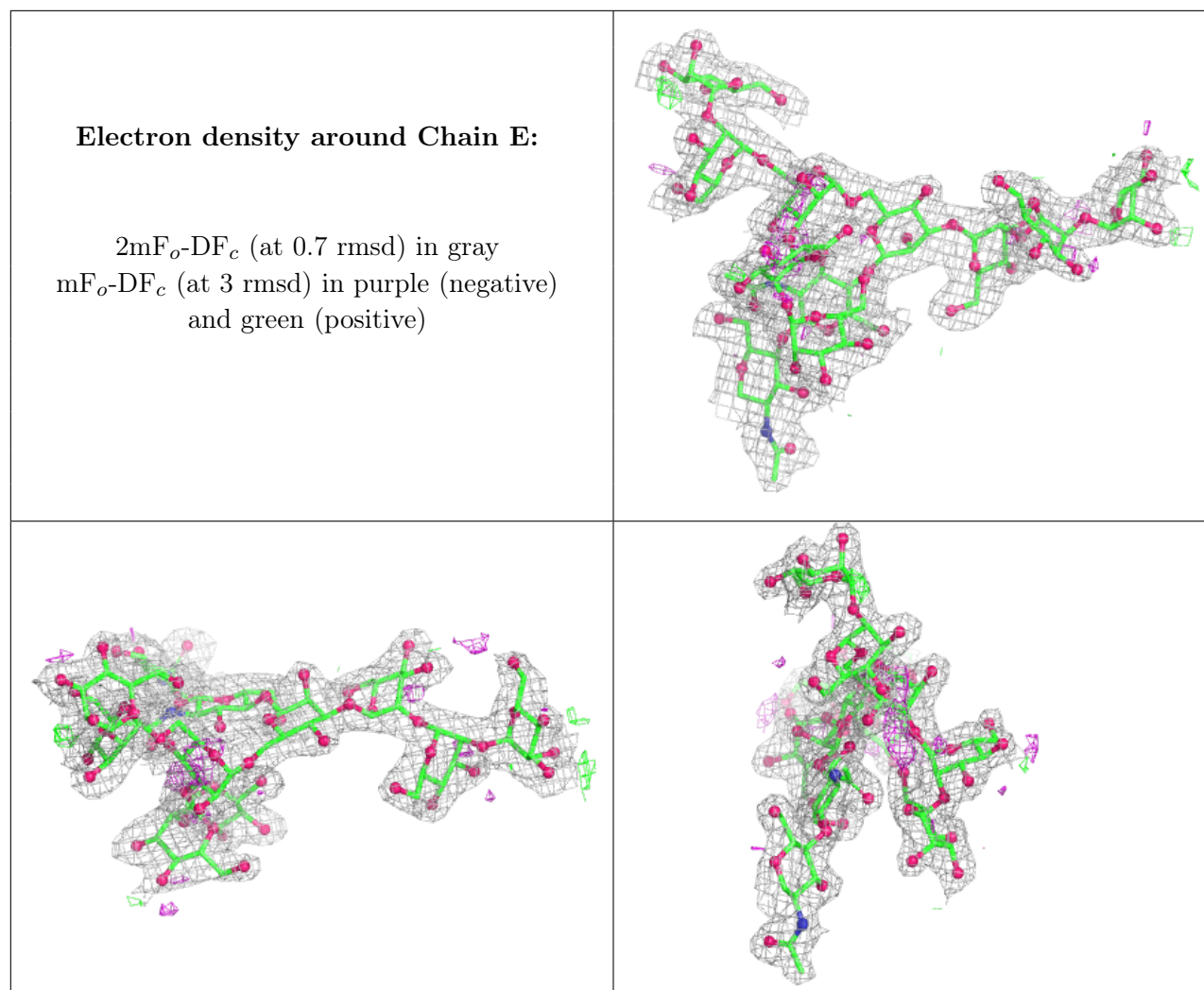
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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, 95<sup>th</sup> 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	0.67	0.21	125,125,125,125	1
8	NA	A	1025	1/1	0.68	0.28	54,54,54,54	0
9	PG4	A	1030	12/13	0.81	0.17	57,61,66,66	0
10	PEG	A	1031	7/7	0.81	0.18	58,60,62,64	0
6	NAG	A	1005	14/15	0.82	0.29	56,60,63,68	0
6	NAG	A	1002	14/15	0.84	0.28	67,73,78,80	0
6	NAG	A	1006	14/15	0.86	0.27	54,59,68,70	0
6	NAG	A	1004	14/15	0.89	0.13	54,59,64,67	0
6	NAG	A	1007	14/15	0.90	0.16	40,43,46,47	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	0.90	0.17	40,40,40,40	0
12	CL	A	1033	1/1	0.91	0.16	49,49,49,49	0
8	NA	A	1027	1/1	0.92	0.27	30,30,30,30	0
7	CD	A	1012	1/1	0.92	0.06	72,72,72,72	0
6	NAG	A	1001	14/15	0.92	0.18	46,51,55,57	0
7	CD	A	1023	1/1	0.92	0.37	44,44,44,44	0
6	NAG	A	1003	14/15	0.92	0.13	39,44,48,48	0
7	CD	A	1014	1/1	0.94	0.07	76,76,76,76	0
7	CD	A	1019	1/1	0.94	0.04	80,80,80,80	0
7	CD	A	1024	1/1	0.94	0.57	44,44,44,44	0
11	CA	A	1032	1/1	0.95	0.08	54,54,54,54	0
8	NA	A	1026	1/1	0.95	0.27	48,48,48,48	0
7	CD	A	1022	1/1	0.96	0.16	87,87,87,87	1
8	NA	A	1029	1/1	0.96	0.19	33,33,33,33	0
7	CD	A	1020	1/1	0.96	0.09	77,77,77,77	0
7	CD	A	1013	1/1	0.97	0.08	52,52,52,52	0
8	NA	A	1034	1/1	0.97	0.31	37,37,37,37	0
7	CD	A	1018	1/1	0.97	0.05	74,74,74,74	0
7	CD	A	1011	1/1	0.98	0.06	50,50,50,50	0
7	CD	A	1015	1/1	0.98	0.09	51,51,51,51	0
7	CD	A	1016	1/1	0.98	0.05	59,59,59,59	0
7	CD	A	1009	1/1	0.98	0.08	43,43,43,43	0
7	CD	A	1010	1/1	0.98	0.09	58,58,58,58	0
7	CD	A	1017	1/1	0.99	0.08	81,81,81,81	0
7	CD	A	1008	1/1	0.99	0.10	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.