



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2025 – 10:06 PM JST

PDB ID : 9L3P / pdb\_00009l3p  
Title : Crystal structure of endo-processive xyloglucanase Xeg5A E285A from *Aspergillus oryzae* with GLLX/L  
Authors : Nakamichi, Y.; Shimada, N.; Watanabe, M.; Fujii, T.; Matsuzawa, T.  
Deposited on : 2024-12-19  
Resolution : 2.34 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](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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

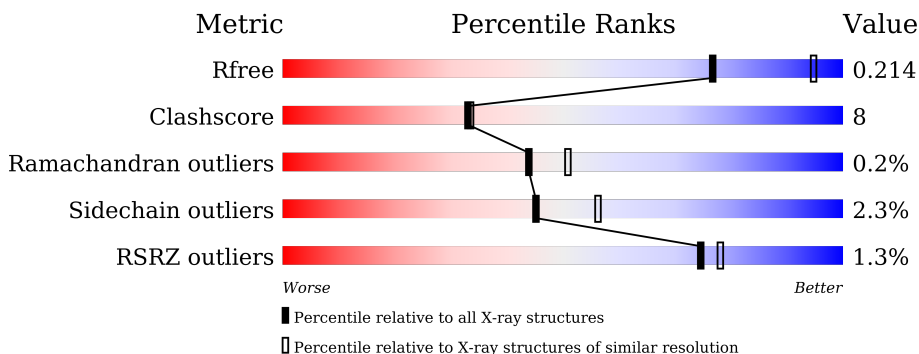
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	648	<div> <div></div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	5	<div> <div>20%</div> <div>80%</div> </div>
3	C	6	<div> <div>83%</div> <div>17%</div> </div>
4	D	9	<div> <div>44%</div> <div>44%</div> <div>11%</div> </div>
5	E	3	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4671 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 Glycoside hydrolase superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	3	0
			4328	2755	707	859	7			

There are 97 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-70	MET	-	initiating methionine	UNP I8IVP5
A	-69	ARG	-	expression tag	UNP I8IVP5
A	-68	PHE	-	expression tag	UNP I8IVP5
A	-67	PRO	-	expression tag	UNP I8IVP5
A	-66	SER	-	expression tag	UNP I8IVP5
A	-65	ILE	-	expression tag	UNP I8IVP5
A	-64	PHE	-	expression tag	UNP I8IVP5
A	-63	THR	-	expression tag	UNP I8IVP5
A	-62	ALA	-	expression tag	UNP I8IVP5
A	-61	VAL	-	expression tag	UNP I8IVP5
A	-60	LEU	-	expression tag	UNP I8IVP5
A	-59	PHE	-	expression tag	UNP I8IVP5
A	-58	ALA	-	expression tag	UNP I8IVP5
A	-57	ALA	-	expression tag	UNP I8IVP5
A	-56	SER	-	expression tag	UNP I8IVP5
A	-55	SER	-	expression tag	UNP I8IVP5
A	-54	ALA	-	expression tag	UNP I8IVP5
A	-53	LEU	-	expression tag	UNP I8IVP5
A	-52	ALA	-	expression tag	UNP I8IVP5
A	-51	ALA	-	expression tag	UNP I8IVP5
A	-50	PRO	-	expression tag	UNP I8IVP5
A	-49	VAL	-	expression tag	UNP I8IVP5
A	-48	ASN	-	expression tag	UNP I8IVP5
A	-47	THR	-	expression tag	UNP I8IVP5
A	-46	THR	-	expression tag	UNP I8IVP5
A	-45	THR	-	expression tag	UNP I8IVP5
A	-44	GLU	-	expression tag	UNP I8IVP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	ASP	-	expression tag	UNP I8IVP5
A	-42	GLU	-	expression tag	UNP I8IVP5
A	-41	THR	-	expression tag	UNP I8IVP5
A	-40	ALA	-	expression tag	UNP I8IVP5
A	-39	GLN	-	expression tag	UNP I8IVP5
A	-38	ILE	-	expression tag	UNP I8IVP5
A	-37	PRO	-	expression tag	UNP I8IVP5
A	-36	ALA	-	expression tag	UNP I8IVP5
A	-35	GLU	-	expression tag	UNP I8IVP5
A	-34	ALA	-	expression tag	UNP I8IVP5
A	-33	VAL	-	expression tag	UNP I8IVP5
A	-32	ILE	-	expression tag	UNP I8IVP5
A	-31	GLY	-	expression tag	UNP I8IVP5
A	-30	TYR	-	expression tag	UNP I8IVP5
A	-29	SER	-	expression tag	UNP I8IVP5
A	-28	ASP	-	expression tag	UNP I8IVP5
A	-27	LEU	-	expression tag	UNP I8IVP5
A	-26	GLU	-	expression tag	UNP I8IVP5
A	-25	GLY	-	expression tag	UNP I8IVP5
A	-24	ASP	-	expression tag	UNP I8IVP5
A	-23	PHE	-	expression tag	UNP I8IVP5
A	-22	ASP	-	expression tag	UNP I8IVP5
A	-21	VAL	-	expression tag	UNP I8IVP5
A	-20	ALA	-	expression tag	UNP I8IVP5
A	-19	VAL	-	expression tag	UNP I8IVP5
A	-18	LEU	-	expression tag	UNP I8IVP5
A	-17	PRO	-	expression tag	UNP I8IVP5
A	-16	PHE	-	expression tag	UNP I8IVP5
A	-15	SER	-	expression tag	UNP I8IVP5
A	-14	ASN	-	expression tag	UNP I8IVP5
A	-13	SER	-	expression tag	UNP I8IVP5
A	-12	THR	-	expression tag	UNP I8IVP5
A	-11	ASN	-	expression tag	UNP I8IVP5
A	-10	ASN	-	expression tag	UNP I8IVP5
A	-9	GLY	-	expression tag	UNP I8IVP5
A	-8	LEU	-	expression tag	UNP I8IVP5
A	-7	LEU	-	expression tag	UNP I8IVP5
A	-6	PHE	-	expression tag	UNP I8IVP5
A	-5	ILE	-	expression tag	UNP I8IVP5
A	-4	ASN	-	expression tag	UNP I8IVP5
A	-3	THR	-	expression tag	UNP I8IVP5
A	-2	THR	-	expression tag	UNP I8IVP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ILE	-	expression tag	UNP I8IVP5
A	0	ALA	-	expression tag	UNP I8IVP5
A	1	SER	-	expression tag	UNP I8IVP5
A	2	ILE	-	expression tag	UNP I8IVP5
A	3	ALA	-	expression tag	UNP I8IVP5
A	4	ALA	-	expression tag	UNP I8IVP5
A	5	LYS	-	expression tag	UNP I8IVP5
A	6	GLU	-	expression tag	UNP I8IVP5
A	7	GLU	-	expression tag	UNP I8IVP5
A	8	GLY	-	expression tag	UNP I8IVP5
A	9	VAL	-	expression tag	UNP I8IVP5
A	10	SER	-	expression tag	UNP I8IVP5
A	11	LEU	-	expression tag	UNP I8IVP5
A	12	GLU	-	expression tag	UNP I8IVP5
A	13	LYS	-	expression tag	UNP I8IVP5
A	14	ARG	-	expression tag	UNP I8IVP5
A	15	GLU	-	expression tag	UNP I8IVP5
A	16	ALA	-	expression tag	UNP I8IVP5
A	17	GLU	-	expression tag	UNP I8IVP5
A	285	ALA	GLU	engineered mutation	UNP I8IVP5
A	570	VAL	-	expression tag	UNP I8IVP5
A	571	ASP	-	expression tag	UNP I8IVP5
A	572	HIS	-	expression tag	UNP I8IVP5
A	573	HIS	-	expression tag	UNP I8IVP5
A	574	HIS	-	expression tag	UNP I8IVP5
A	575	HIS	-	expression tag	UNP I8IVP5
A	576	HIS	-	expression tag	UNP I8IVP5
A	577	HIS	-	expression tag	UNP I8IVP5

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



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

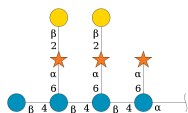
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(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
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]alpha-D-glucopyranose.



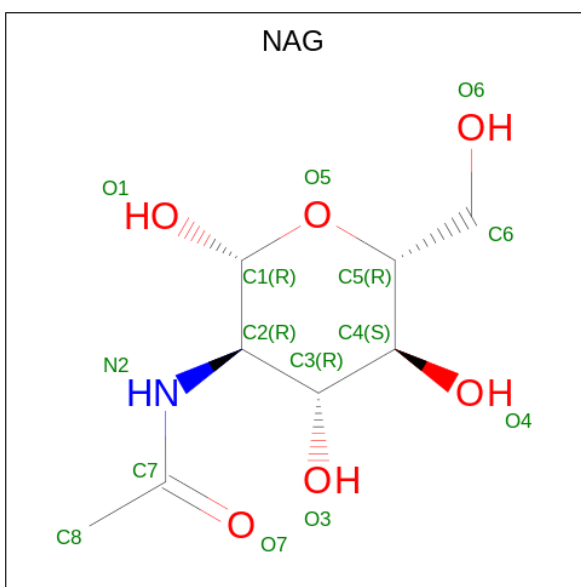
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	9	Total	C	O		0	0	0
			94	51	43				

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose.



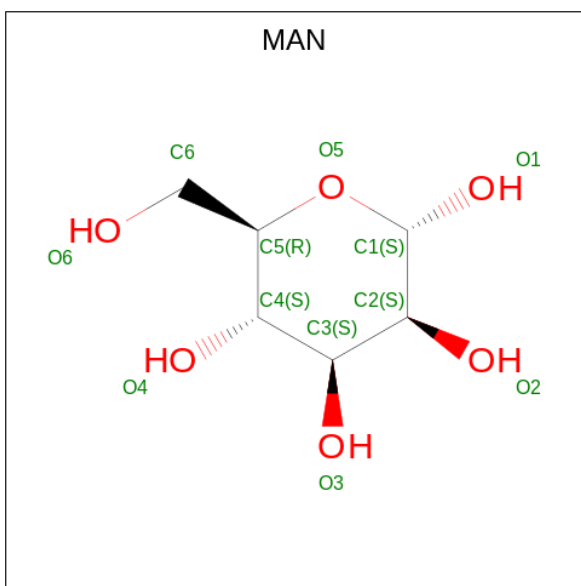
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	O		0	0	0
			32	17	15				

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

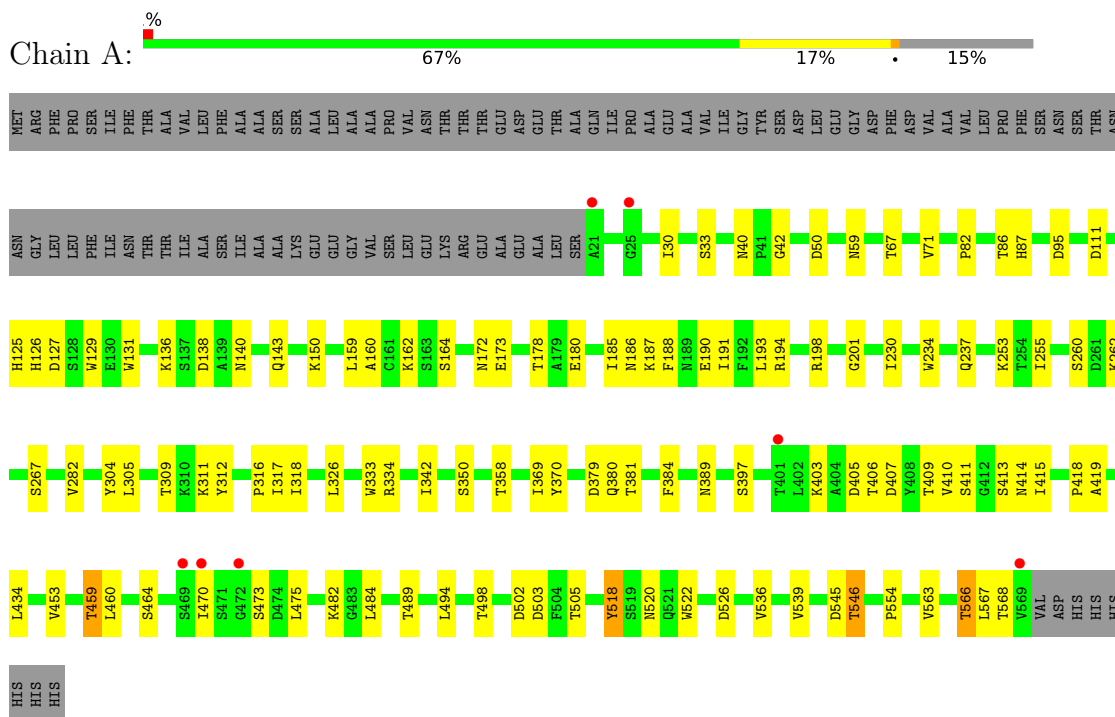
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	45	Total 45	O 45	0	0

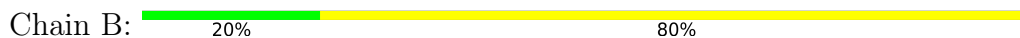
### 3 Residue-property plots

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.

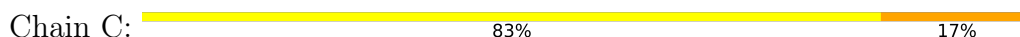
- Molecule 1: Glycoside hydrolase superfamily



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



- Molecule 3: alpha-D-mannopyranose-(1-2)-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



MAN1
MAN2
MAN3
MAN4
MAN5
MAN6

- Molecule 4: beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]alpha-D-glucopyranose

Chain D:  44% 44% 11%

GLC1
BGC2
BGC3
XYA4
GAL5
BGC6
XYA7
GAL8
XYA9

- Molecule 5: beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose

Chain E:  33% 67%

BGC1
XYA2
GAL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.60Å 116.46Å 105.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.79 – 2.34 37.79 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.79-2.34) 99.4 (37.79-2.34)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.206 , 0.215 0.207 , 0.214	Depositor DCC
$R_{free}$ test set	1573 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.38	0/4449	0.58	0/6090

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4328	0	4112	69	0
2	B	61	0	52	0	0
3	C	72	0	61	1	0
4	D	94	0	78	2	0
5	E	32	0	28	0	0
6	A	28	0	26	0	0
7	A	11	0	10	0	0
8	A	45	0	0	0	0
All	All	4671	0	4367	69	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 8.

The worst 5 of 69 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)
1:A:539:VAL:HG11	1:A:567:LEU:HD23	1.61	0.80
1:A:470:ILE:HG12	1:A:475:LEU:HD13	1.67	0.77
1:A:403:LYS:HG2	1:A:406:THR:HB	1.67	0.75
1:A:460:LEU:HG	1:A:563:VAL:HG21	1.76	0.68
1:A:379:ASP:OD1	1:A:419:ALA:N	2.32	0.63

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	550/648 (85%)	513 (93%)	36 (6%)	1 (0%)	44 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	TYR

### 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	483/560 (86%)	471 (98%)	12 (2%)	42 53

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	THR
1	A	473	SER
1	A	566	THR
1	A	536	VAL
1	A	260	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	126	HIS
1	A	140	ASN
1	A	528	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

23 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	0.63	1 (7%)	17,19,21	0.75	0
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	0.67	0
2	BMA	B	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.21	1 (6%)
2	MAN	B	4	2	11,11,12	1.58	3 (27%)	15,15,17	1.72	3 (20%)
2	MAN	B	5	2	11,11,12	1.79	2 (18%)	15,15,17	1.43	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	3,1	14,14,15	0.74	1 (7%)	17,19,21	0.57	0
3	NAG	C	2	3	14,14,15	0.95	1 (7%)	17,19,21	0.84	0
3	BMA	C	3	3	11,11,12	1.29	1 (9%)	15,15,17	1.15	1 (6%)
3	MAN	C	4	3	11,11,12	1.15	1 (9%)	15,15,17	1.46	2 (13%)
3	MAN	C	5	3	11,11,12	1.02	1 (9%)	15,15,17	1.24	2 (13%)
3	MAN	C	6	3	11,11,12	1.78	3 (27%)	15,15,17	1.12	0
4	GLC	D	1	4	12,12,12	0.37	0	17,17,17	0.64	0
4	BGC	D	2	4	11,11,12	0.34	0	15,15,17	0.48	0
4	BGC	D	3	4	11,11,12	0.25	0	15,15,17	0.58	0
4	XYS	D	4	4	9,9,10	1.96	2 (22%)	10,12,14	2.28	4 (40%)
4	GAL	D	5	4	11,11,12	0.88	0	15,15,17	1.28	1 (6%)
4	BGC	D	6	4	11,11,12	0.66	0	15,15,17	1.14	1 (6%)
4	XYS	D	7	4	9,9,10	0.39	0	10,12,14	1.07	0
4	GAL	D	8	4	11,11,12	0.87	0	15,15,17	1.01	0
4	XYS	D	9	4	9,9,10	1.96	2 (22%)	10,12,14	1.65	3 (30%)
5	BGC	E	1	5	12,12,12	0.33	0	17,17,17	0.31	0
5	XYS	E	2	5	9,9,10	2.13	2 (22%)	10,12,14	1.87	3 (30%)
5	GAL	E	3	5	11,11,12	1.47	2 (18%)	15,15,17	1.40	3 (20%)

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	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	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
4	GLC	D	1	4	-	2/2/22/22	0/1/1/1
4	BGC	D	2	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	D	3	4	-	2/2/19/22	0/1/1/1
4	XYS	D	4	4	-	-	0/1/1/1
4	GAL	D	5	4	-	0/2/19/22	0/1/1/1
4	BGC	D	6	4	-	2/2/19/22	0/1/1/1
4	XYS	D	7	4	-	-	0/1/1/1
4	GAL	D	8	4	-	2/2/19/22	0/1/1/1
4	XYS	D	9	4	-	-	0/1/1/1
5	BGC	E	1	5	-	2/2/22/22	0/1/1/1
5	XYS	E	2	5	-	-	0/1/1/1
5	GAL	E	3	5	-	0/2/19/22	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	XYS	O5-C1	4.74	1.52	1.42
2	B	5	MAN	C2-C3	4.24	1.58	1.52
4	D	4	XYS	O5-C1	4.20	1.51	1.42
3	C	6	MAN	C2-C3	3.67	1.57	1.52
4	D	9	XYS	O5-C1	3.65	1.50	1.42

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	4.75	118.63	112.19
4	D	4	XYS	C5-O5-C1	4.60	118.60	111.52
4	D	4	XYS	O2-C2-C1	-4.02	100.94	109.15
4	D	6	BGC	C1-C2-C3	3.94	114.50	109.67
4	D	5	GAL	C1-C2-C3	3.61	114.10	109.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

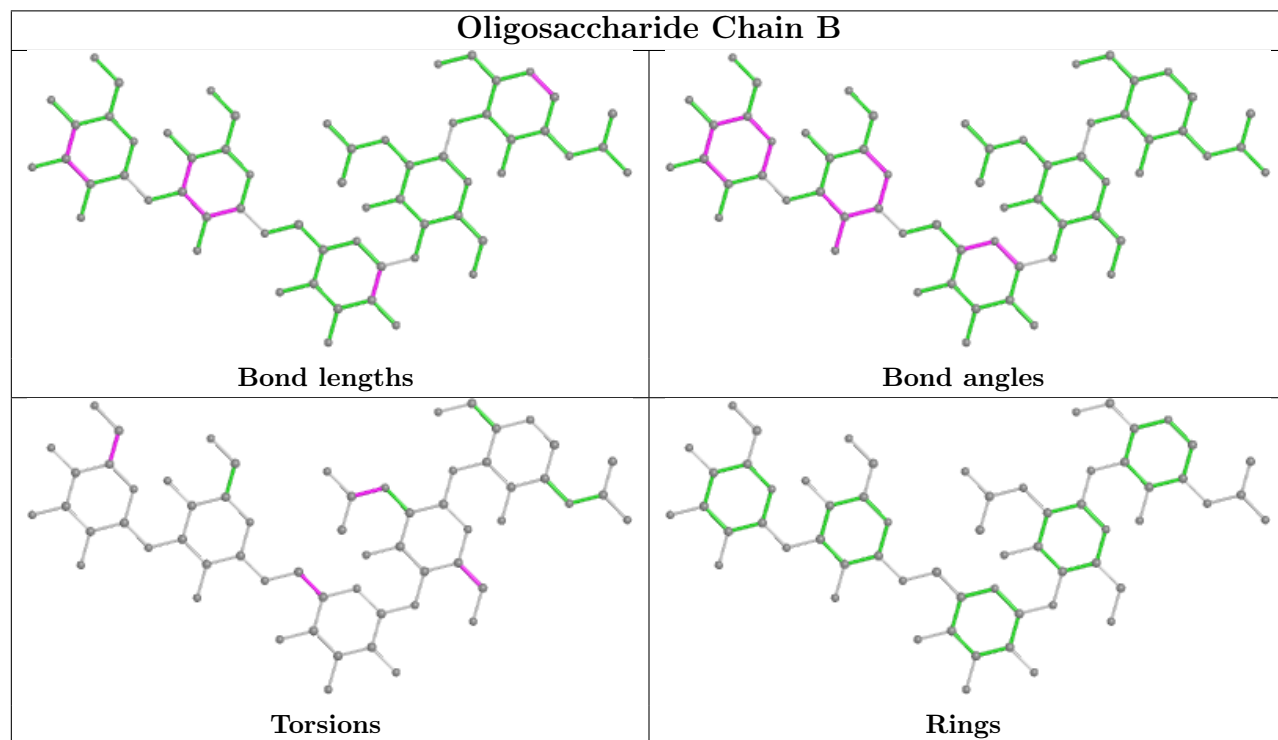
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	6	BGC	O5-C5-C6-O6
4	D	8	GAL	C4-C5-C6-O6
4	D	2	BGC	O5-C5-C6-O6

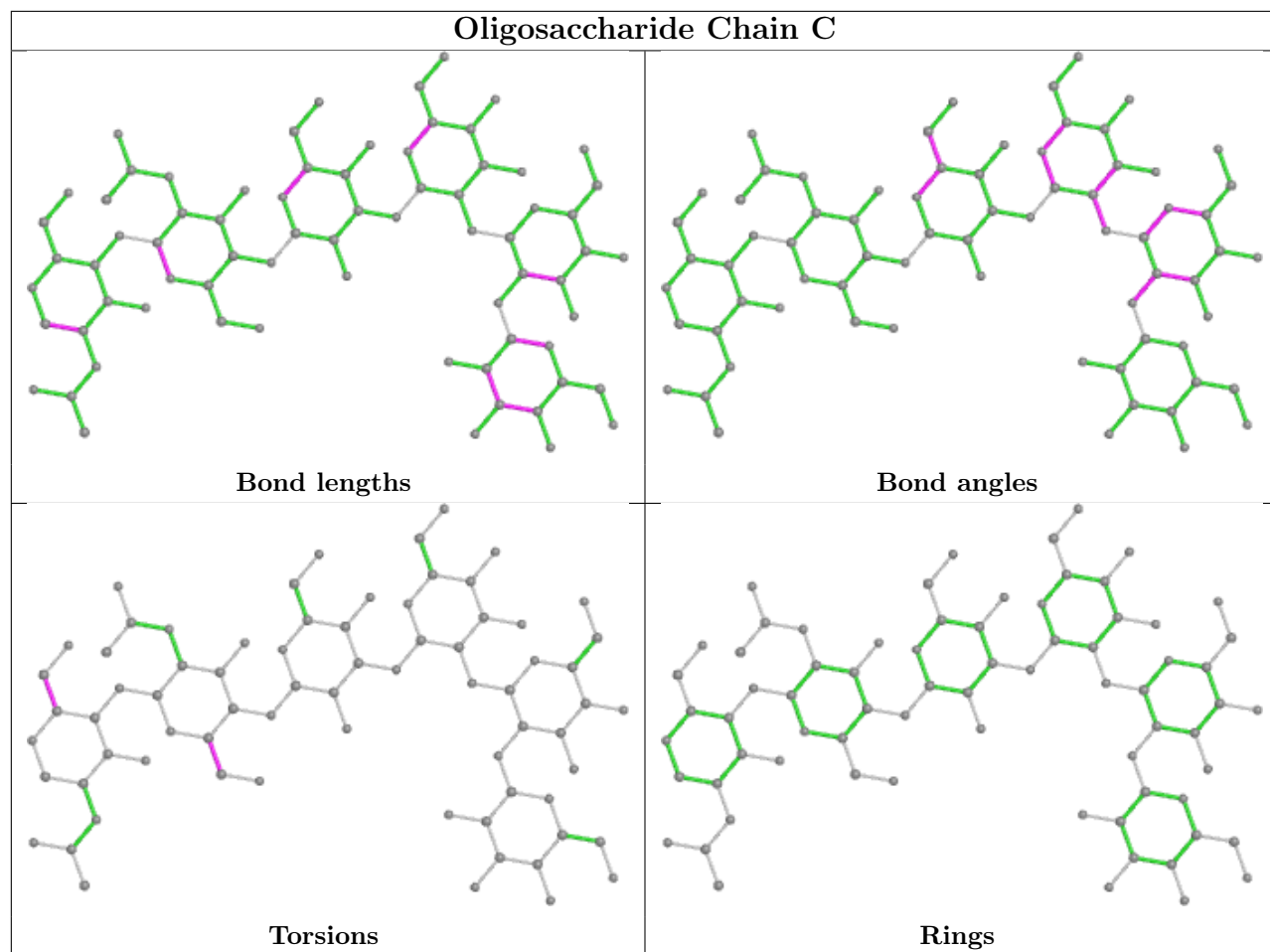
There are no ring outliers.

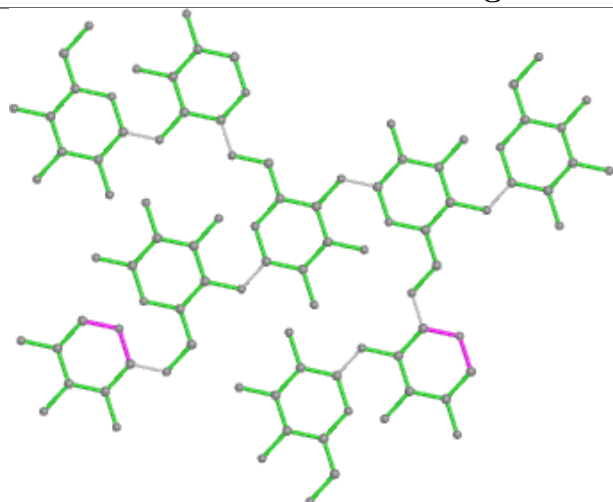
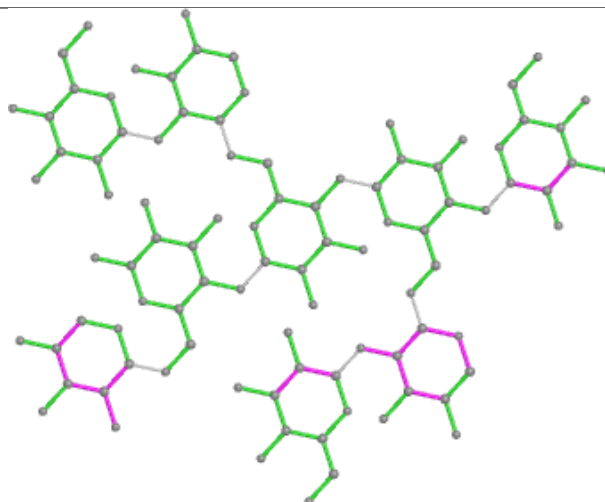
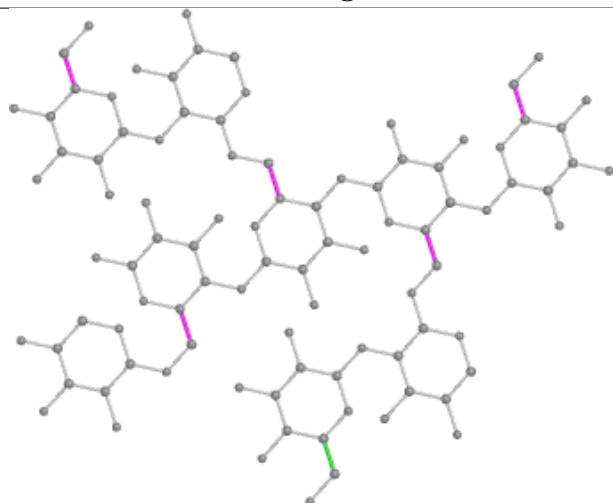
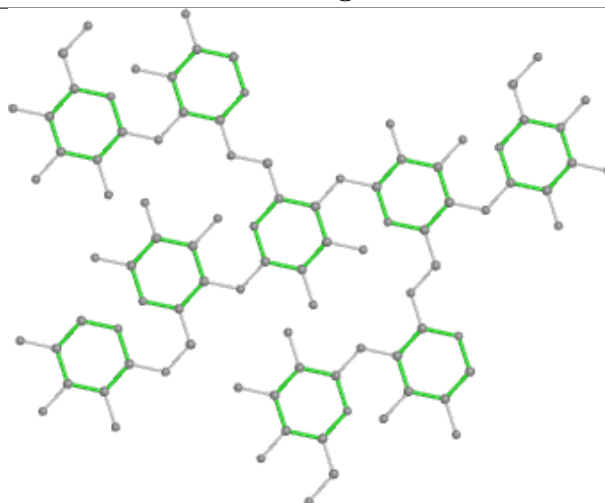
3 monomers are involved in 3 short contacts:

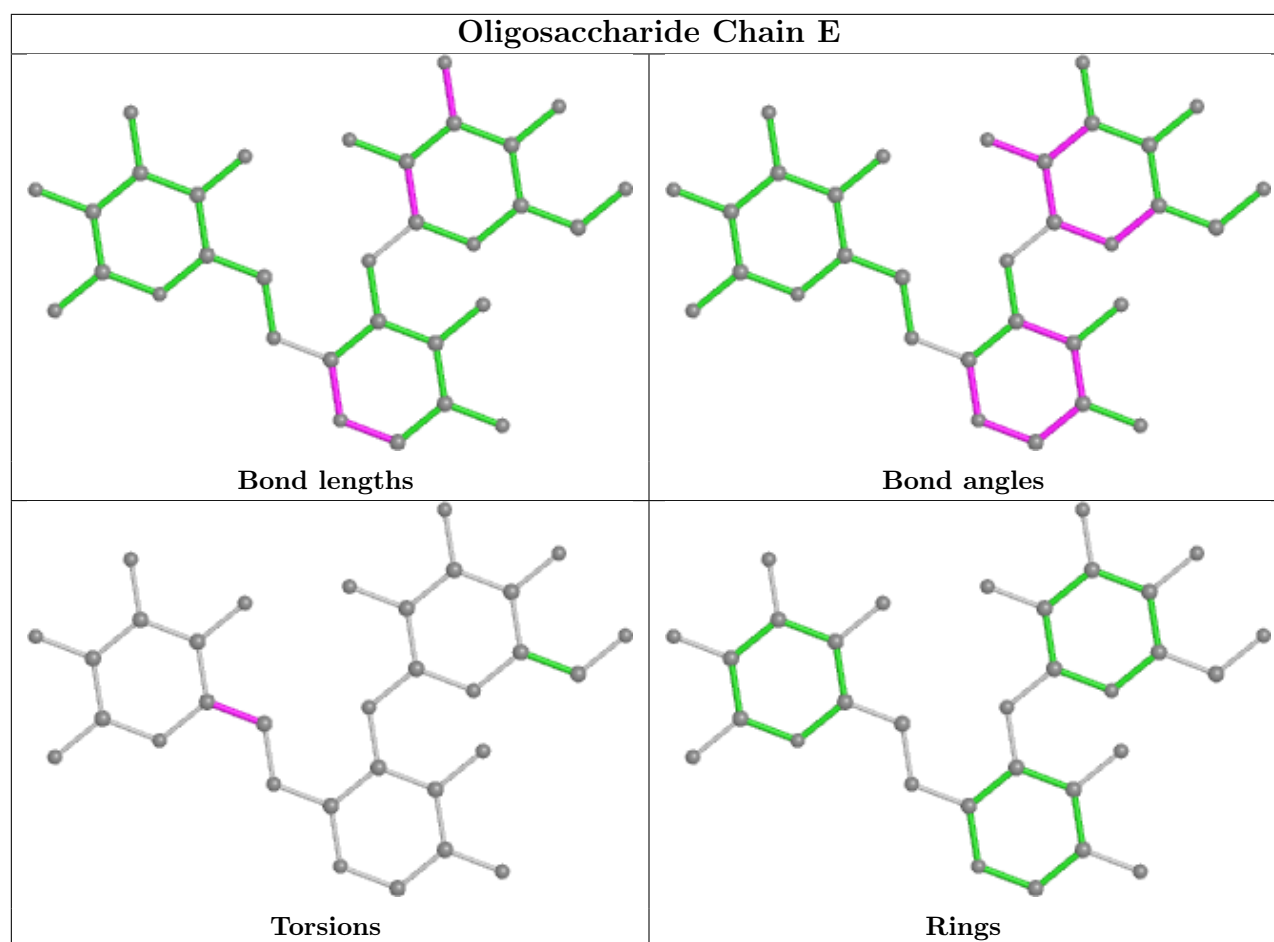
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	1	0
4	D	4	XYS	1	0
4	D	1	GLC	1	0

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





**Oligosaccharide Chain D****Bond lengths****Bond angles****Torsions****Rings**



## 5.6 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	$\# Z  > 2$
6	NAG	A	601	1	14,14,15	0.51	0	17,19,21	0.50	0
7	MAN	A	603	1	11,11,12	0.19	0	15,15,17	0.52	0
6	NAG	A	602	1	14,14,15	0.81	1 (7%)	17,19,21	0.73	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	601	1	-	4/6/23/26	0/1/1/1
7	MAN	A	603	1	-	0/2/19/22	0/1/1/1
6	NAG	A	602	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	NAG	O5-C1	2.69	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	NAG	C1-O5-C5	2.21	115.18	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
6	A	601	NAG	C1-C2-N2-C7
6	A	602	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	549/648 (84%)	0.18	7 (1%) 74 78	25, 51, 74, 103	3 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	4.5
1	A	469	SER	3.4
1	A	470	ILE	3.0
1	A	472	GLY	2.4
1	A	25	GLY	2.3

### 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
2	BMA	B	3	11/12	0.53	0.14	85,89,95,102	0
4	BGC	D	6	11/12	0.59	0.17	69,79,83,88	0
4	XYS	D	9	9/10	0.69	0.22	49,57,60,61	9
4	GAL	D	8	11/12	0.70	0.18	61,73,75,79	11
5	BGC	E	1	12/12	0.70	0.14	68,76,81,82	0
5	GAL	E	3	11/12	0.70	0.19	62,68,69,73	11
4	GAL	D	5	11/12	0.73	0.16	58,59,63,65	11

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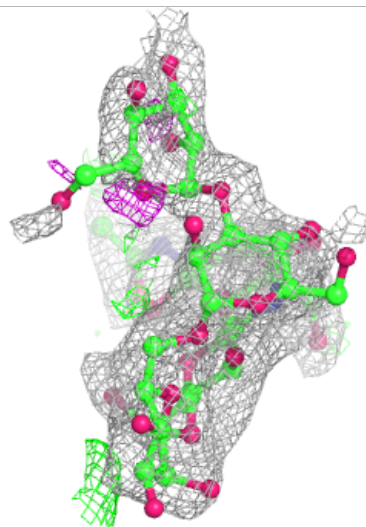
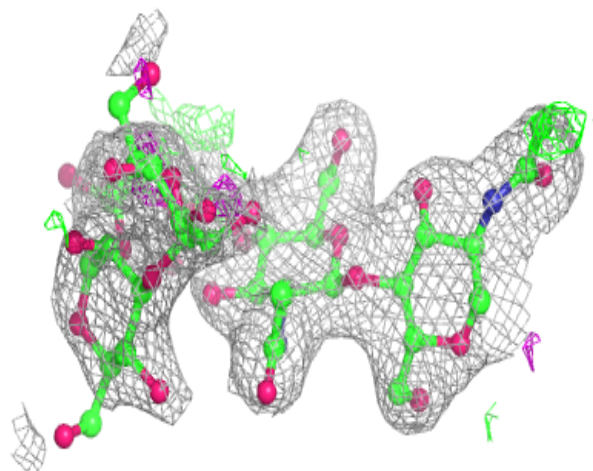
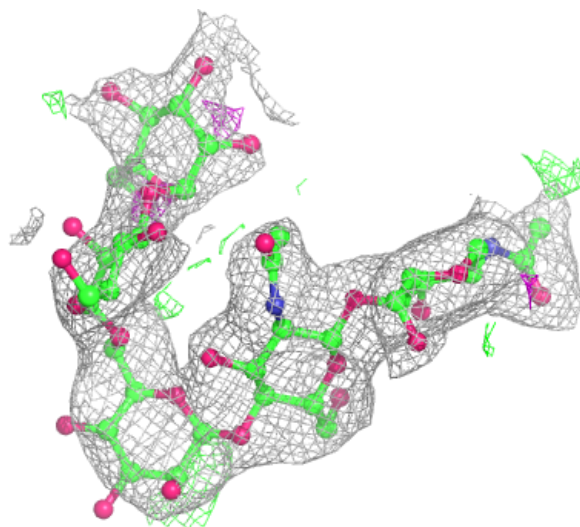
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	B	4	11/12	0.73	0.14	78,85,93,95	0
3	NAG	C	2	14/15	0.76	0.14	63,71,81,82	0
4	XYS	D	4	9/10	0.76	0.20	61,64,66,67	9
4	XYS	D	7	9/10	0.78	0.19	68,75,81,91	0
2	MAN	B	5	11/12	0.79	0.18	59,68,76,80	0
3	BMA	C	3	11/12	0.80	0.11	59,64,67,68	0
5	XYS	E	2	9/10	0.82	0.14	58,67,71,75	0
4	GLC	D	1	12/12	0.85	0.12	51,59,61,61	0
3	MAN	C	5	11/12	0.86	0.10	57,61,68,69	0
3	MAN	C	6	11/12	0.86	0.11	64,66,69,71	0
2	NAG	B	2	14/15	0.86	0.12	61,67,75,77	0
3	NAG	C	1	14/15	0.87	0.10	56,63,70,72	0
3	MAN	C	4	11/12	0.90	0.09	57,62,66,69	0
4	BGC	D	2	11/12	0.90	0.10	52,55,62,68	0
4	BGC	D	3	11/12	0.90	0.11	56,59,65,68	11
2	NAG	B	1	14/15	0.91	0.10	45,49,56,58	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.

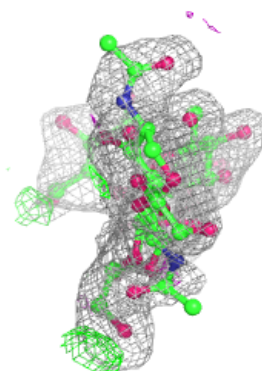
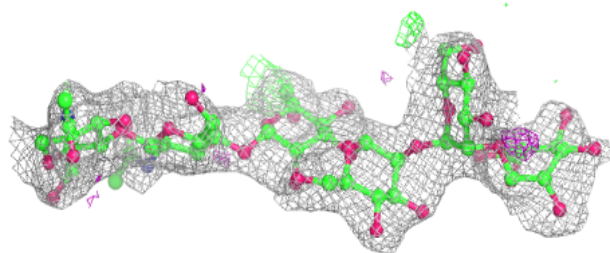
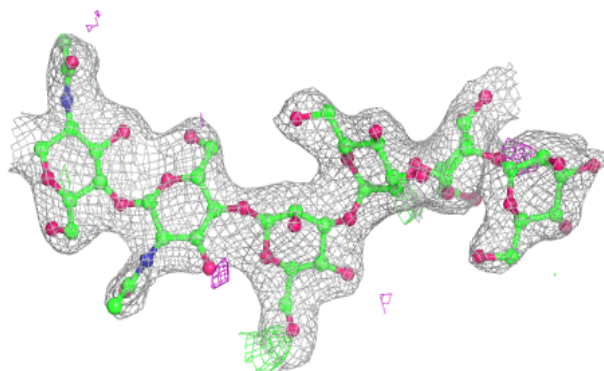
**Electron density around Chain B:**

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



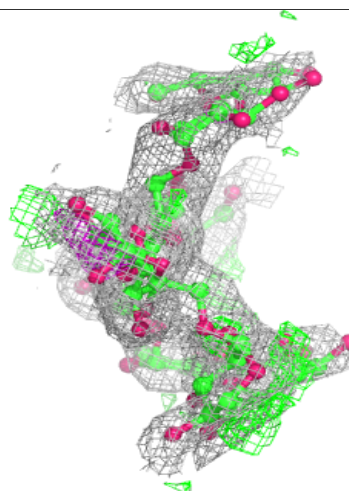
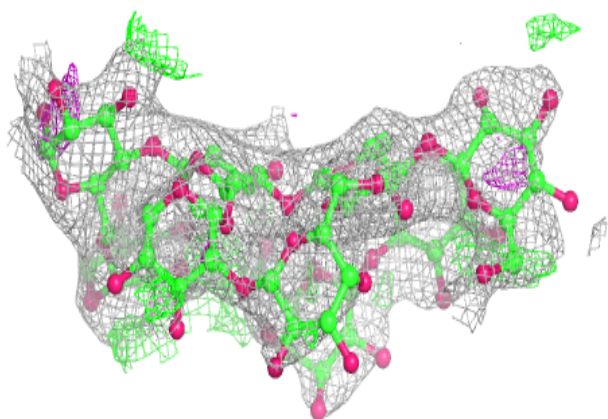
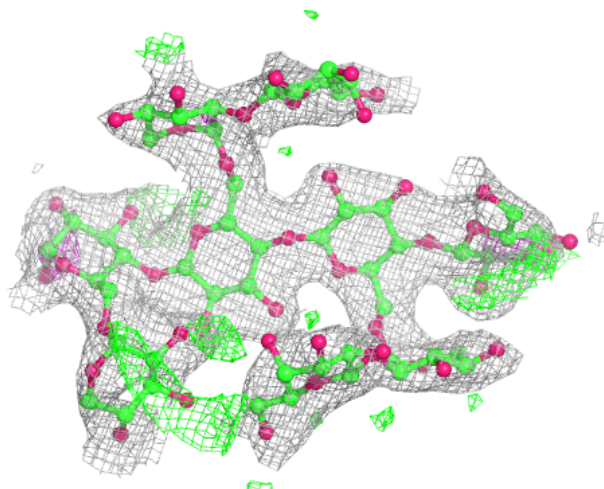
**Electron density around Chain C:**

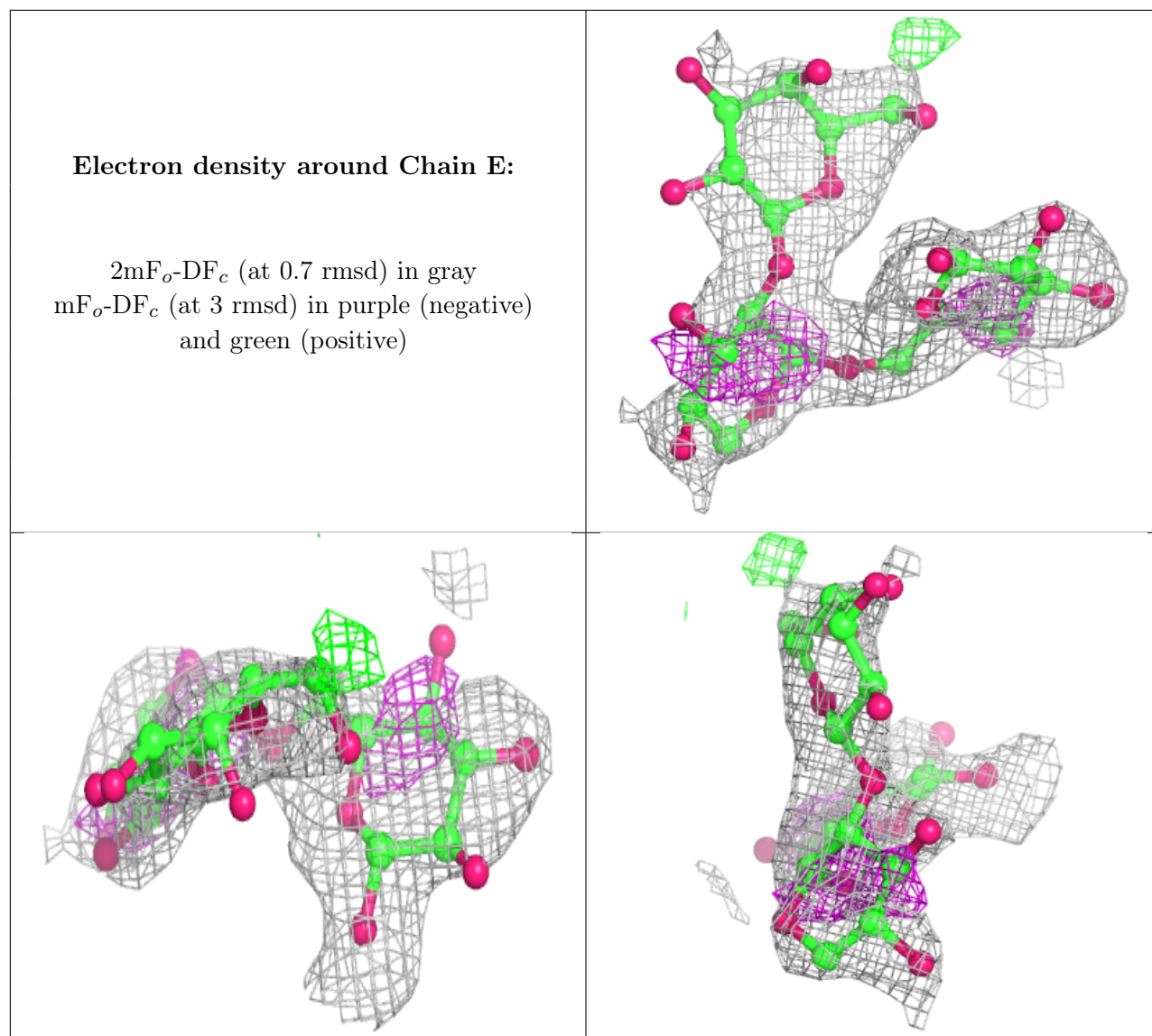
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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	MAN	A	603	11/12	0.44	0.17	75,88,96,99	0
6	NAG	A	601	14/15	0.74	0.14	77,79,83,84	0
6	NAG	A	602	14/15	0.78	0.12	60,67,75,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.