



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2024 – 11:27 PM EST

PDB ID : 1NHC  
Title : Structural insights into the processivity of endopolygalacturonase I from *Aspergillus niger*  
Authors : van Pouderoyen, G.; Snijder, H.J.; Benen, J.A.; Dijkstra, B.W.  
Deposited on : 2002-12-19  
Resolution : 1.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

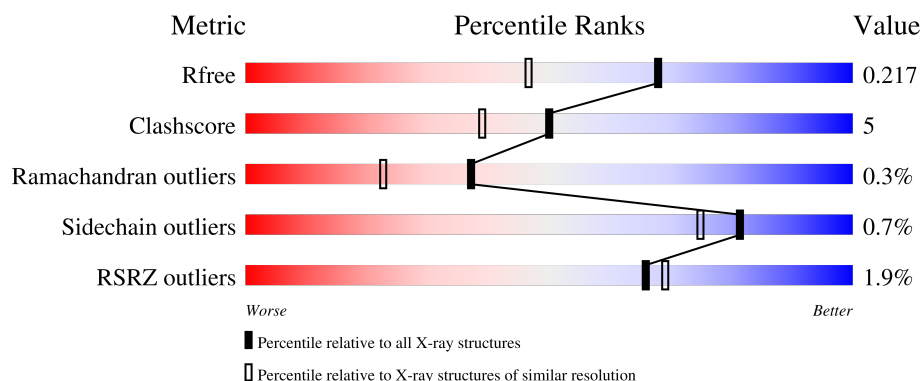
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	336	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
1	B	336	<div> <div>4%</div> <div>85%</div> <div>15%</div> </div>
1	C	336	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>
1	D	336	<div> <div>2%</div> <div>86%</div> <div>13%</div> </div>
1	E	336	<div> <div>%</div> <div>87%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	336	
2	G	2	
3	H	6	
4	I	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	I	3	X	-	-	-
7	GOL	B	405	-	-	X	-
7	GOL	D	405	-	-	X	-
7	GOL	E	408	-	-	X	-
7	GOL	F	405	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16429 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 Polygalacturonase I.

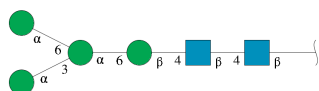
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	B	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	C	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	D	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	E	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	F	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			

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



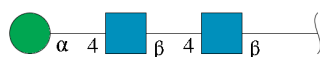
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



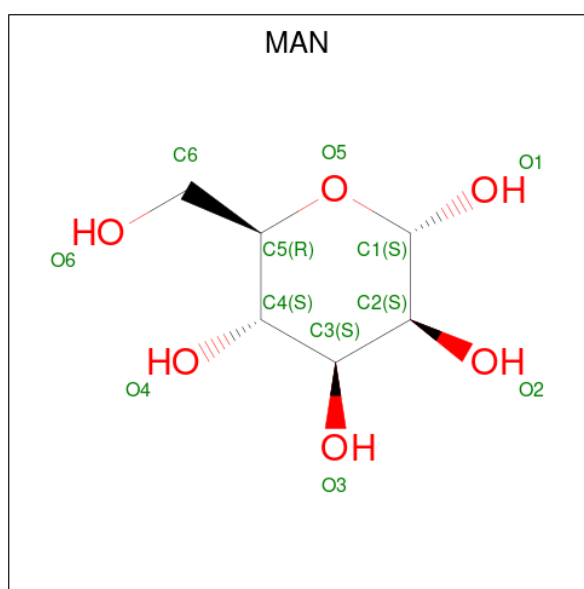
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



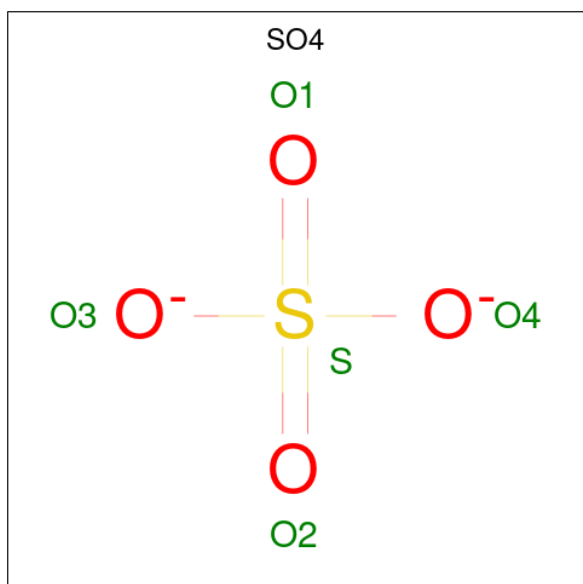
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



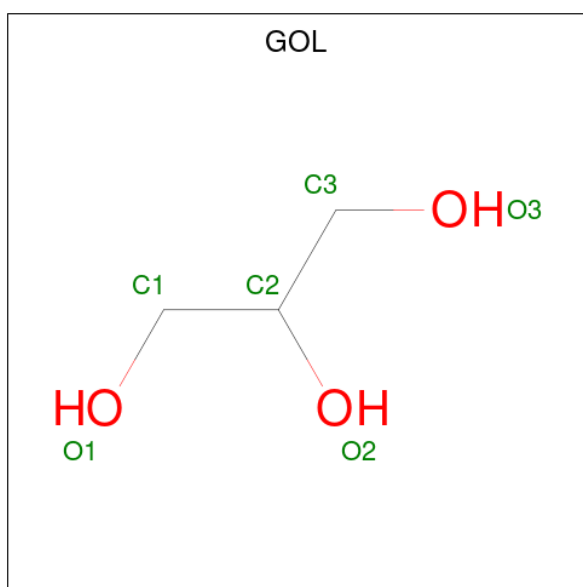
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

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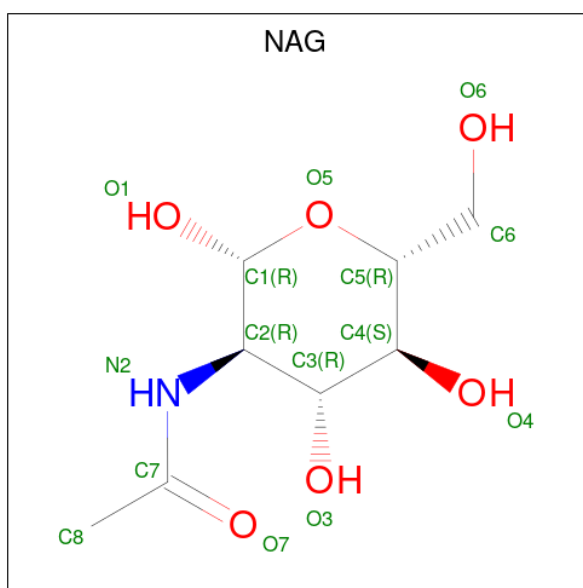
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	236	Total O 236 236	0	0

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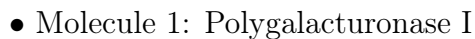


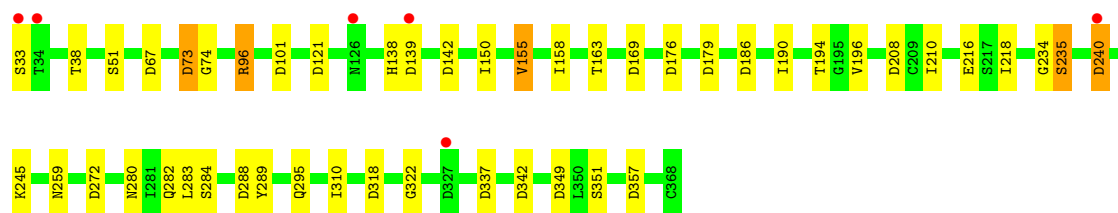
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	162	Total 162	O 162	0	0
9	C	258	Total 258	O 258	0	0
9	D	211	Total 211	O 211	0	0
9	E	252	Total 252	O 252	0	0
9	F	234	Total 234	O 234	0	0

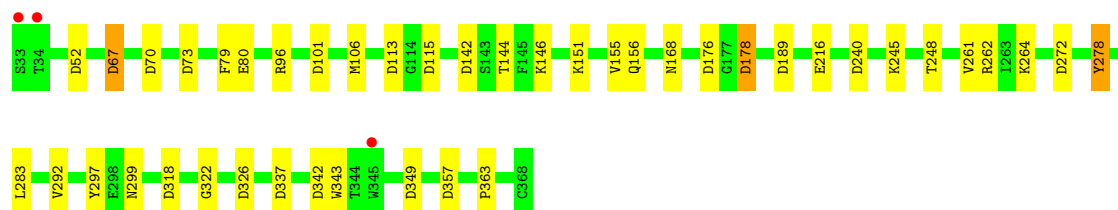
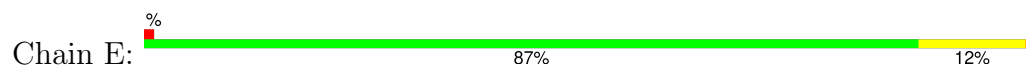


- Molecule 1: Polygalacturonase I

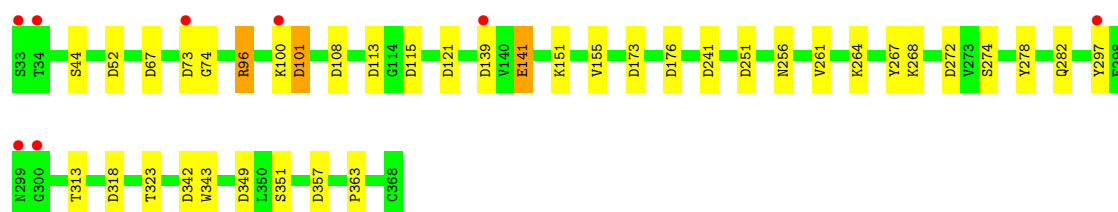
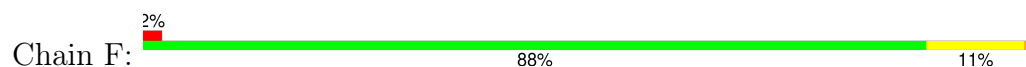




• Molecule 1: Polygalacturonase I



• Molecule 1: Polygalacturonase I



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



• Molecule 3: alpha-D-mannopyranose-(1-3)-[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



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



MAG1  
MAG2  
MAG3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.01Å 84.13Å 96.03Å 114.32° 98.00° 89.75°	Depositor
Resolution (Å)	35.81 – 1.70 35.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.81-1.70) 97.5 (35.81-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.175 , 0.209 0.185 , 0.217	Depositor DCC
$R_{free}$ test set	10409 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.055 for -h,k,-k-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: BMA, NAG, GOL, MAN, SO4

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	0.74	1/2482 (0.0%)	1.02	17/3374 (0.5%)
1	B	0.68	0/2482	1.01	18/3374 (0.5%)
1	C	0.73	0/2482	1.03	17/3374 (0.5%)
1	D	0.71	0/2482	1.03	17/3374 (0.5%)
1	E	0.73	1/2482 (0.0%)	0.98	16/3374 (0.5%)
1	F	0.75	0/2482	1.00	19/3374 (0.6%)
All	All	0.72	2/14892 (0.0%)	1.01	104/20244 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	TYR	CZ-OH	5.50	1.47	1.37
1	E	278	TYR	CZ-OH	5.17	1.46	1.37

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	CB-CG-OD2	8.71	126.14	118.30
1	D	357	ASP	CB-CG-OD2	8.37	125.83	118.30
1	D	176	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	342	ASP	CB-CG-OD2	8.09	125.58	118.30
1	D	186	ASP	CB-CG-OD2	7.98	125.48	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2444	0	2273	18	2
1	B	2444	0	2273	34	2
1	C	2444	0	2273	15	2
1	D	2444	0	2273	30	1
1	E	2444	0	2273	26	1
1	F	2444	0	2274	25	1
2	G	28	0	25	2	0
3	H	72	0	61	1	0
4	I	39	0	34	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
5	C	22	0	20	0	0
5	D	22	0	20	0	0
5	E	22	0	20	0	0
5	F	11	0	10	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	20	0	0	0	0
6	D	10	0	0	0	0
6	E	20	0	0	0	0
6	F	10	0	0	0	0
7	A	6	0	8	1	0
7	B	6	0	8	6	0
7	D	6	0	8	5	1
7	E	6	0	8	8	0
7	F	6	0	8	5	0
8	C	14	0	13	0	0
8	E	14	0	13	0	0
8	F	14	0	13	4	0
9	A	236	0	0	9	1
9	B	162	0	0	3	0
9	C	258	0	0	4	0
9	D	211	0	0	6	0
9	E	252	0	0	5	1
9	F	234	0	0	4	0
All	All	16429	0	13948	151	6

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 5.

The worst 5 of 151 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:B:96:ARG:NH2	7:B:405:GOL:H12	1.23	1.46
1:B:96:ARG:NH2	7:B:405:GOL:C1	1.98	1.26
1:F:100:LYS:HG2	1:F:141:GLU:OE2	1.50	1.12
1:D:284:SER:HB3	1:F:282:GLN:HE22	1.18	1.06
1:A:261:VAL:HG22	9:A:686:HOH:O	1.55	1.04

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASP:OD2	1:C:337:ASP:OD2[1_646]	1.79	0.41
9:A:687:HOH:O	9:E:725:HOH:O[1_554]	1.94	0.26
1:F:100:LYS:CE	7:D:405:GOL:O2[1_455]	1.97	0.23
1:A:337:ASP:OD2	1:E:178:ASP:OD2[1_554]	2.11	0.09
1:B:327:ASP:OD2	1:C:298:GLU:OE2[1_646]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	37	23
1	B	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	37	23
1	C	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	37	23
1	D	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	37	23
1	E	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	37	23
1	F	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	37	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2004/2016 (99%)	1886 (94%)	112 (6%)	6 (0%)	37	23

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	155	VAL
1	A	155	VAL
1	B	155	VAL
1	D	155	VAL
1	C	155	VAL

### 5.3.2 Protein sidechains ⓘ

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	278/278 (100%)	276 (99%)	2 (1%)	81	75
1	B	278/278 (100%)	277 (100%)	1 (0%)	89	85
1	C	278/278 (100%)	276 (99%)	2 (1%)	81	75
1	D	278/278 (100%)	275 (99%)	3 (1%)	70	60
1	E	278/278 (100%)	277 (100%)	1 (0%)	89	85
1	F	278/278 (100%)	275 (99%)	3 (1%)	70	60
All	All	1668/1668 (100%)	1656 (99%)	12 (1%)	81	75

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

Mol	Chain	Res	Type
1	D	351	SER
1	E	70	ASP
1	F	351	SER
1	F	141	GLU
1	C	337	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	282	GLN
1	E	168	ASN
1	F	299	ASN
1	F	282	GLN
1	C	299	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 ⓘ

11 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	G	1	2,1	14,14,15	0.62	0	17,19,21	2.12	4 (23%)
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	2.68	5 (29%)
3	NAG	H	1	3,1	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
3	NAG	H	2	3	14,14,15	0.58	0	17,19,21	2.65	2 (11%)
3	BMA	H	3	3	11,11,12	0.88	1 (9%)	15,15,17	1.82	4 (26%)
3	MAN	H	4	3	11,11,12	0.65	0	15,15,17	1.25	2 (13%)
3	MAN	H	5	3	11,11,12	0.67	0	15,15,17	0.82	0
3	MAN	H	6	3	11,11,12	0.65	0	15,15,17	0.57	0
4	NAG	I	1	4,1	14,14,15	0.65	0	17,19,21	1.14	3 (17%)
4	NAG	I	2	4	14,14,15	0.56	0	17,19,21	2.57	4 (23%)
4	MAN	I	3	4	11,11,12	0.67	0	15,15,17	2.47	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	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	1/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	MAN	I	3	4	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	O5-C1	-2.34	1.39	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C1-O5-C5	7.22	121.87	112.19
3	H	2	NAG	C1-O5-C5	7.16	121.78	112.19
4	I	3	MAN	C1-O5-C5	7.04	121.62	112.19
3	H	2	NAG	O5-C1-C2	7.00	122.12	111.29
2	G	2	NAG	C1-O5-C5	6.66	121.12	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	3	MAN	C1

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	MAN	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2

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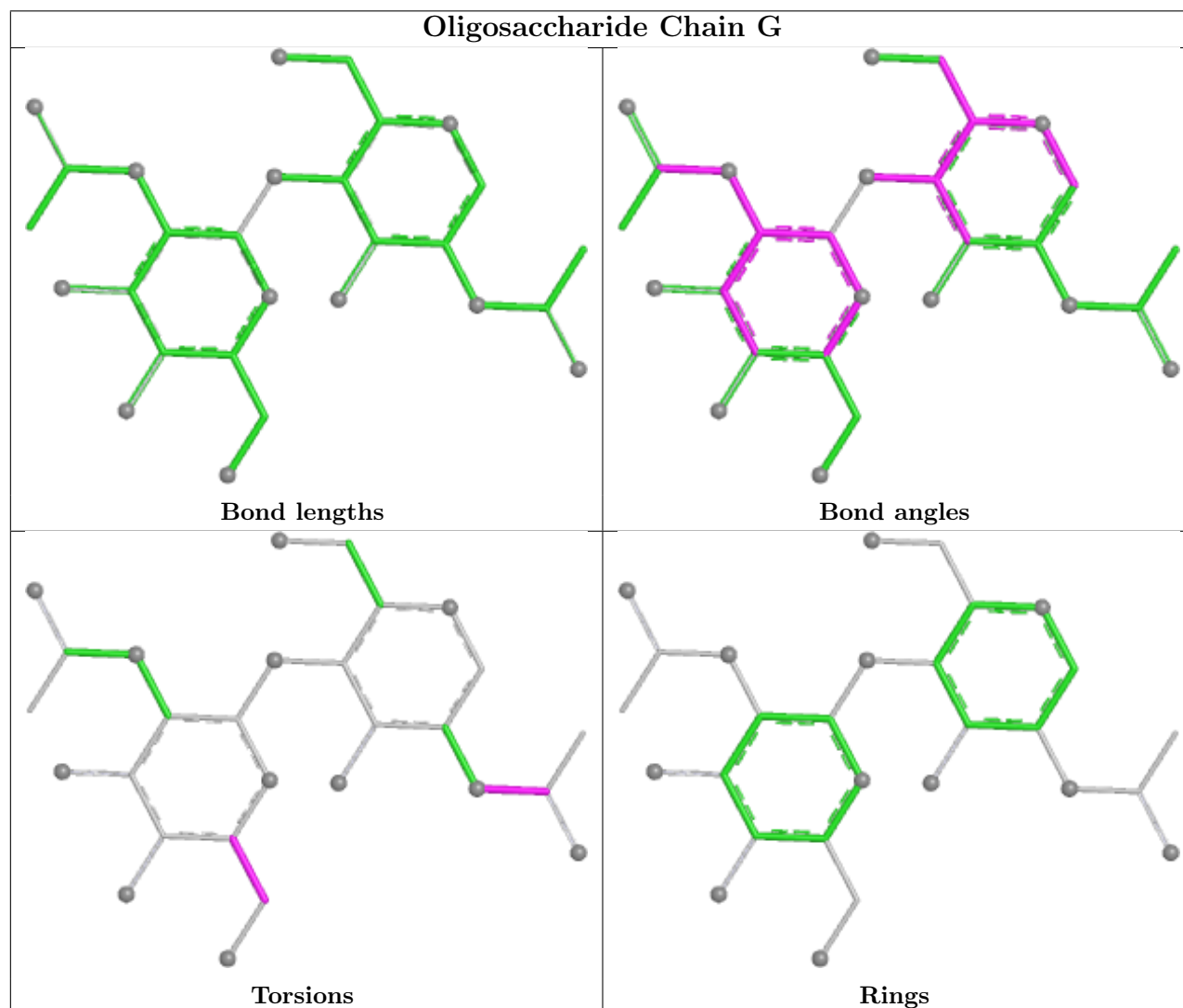
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O7-C7-N2-C2
4	I	2	NAG	O5-C5-C6-O6

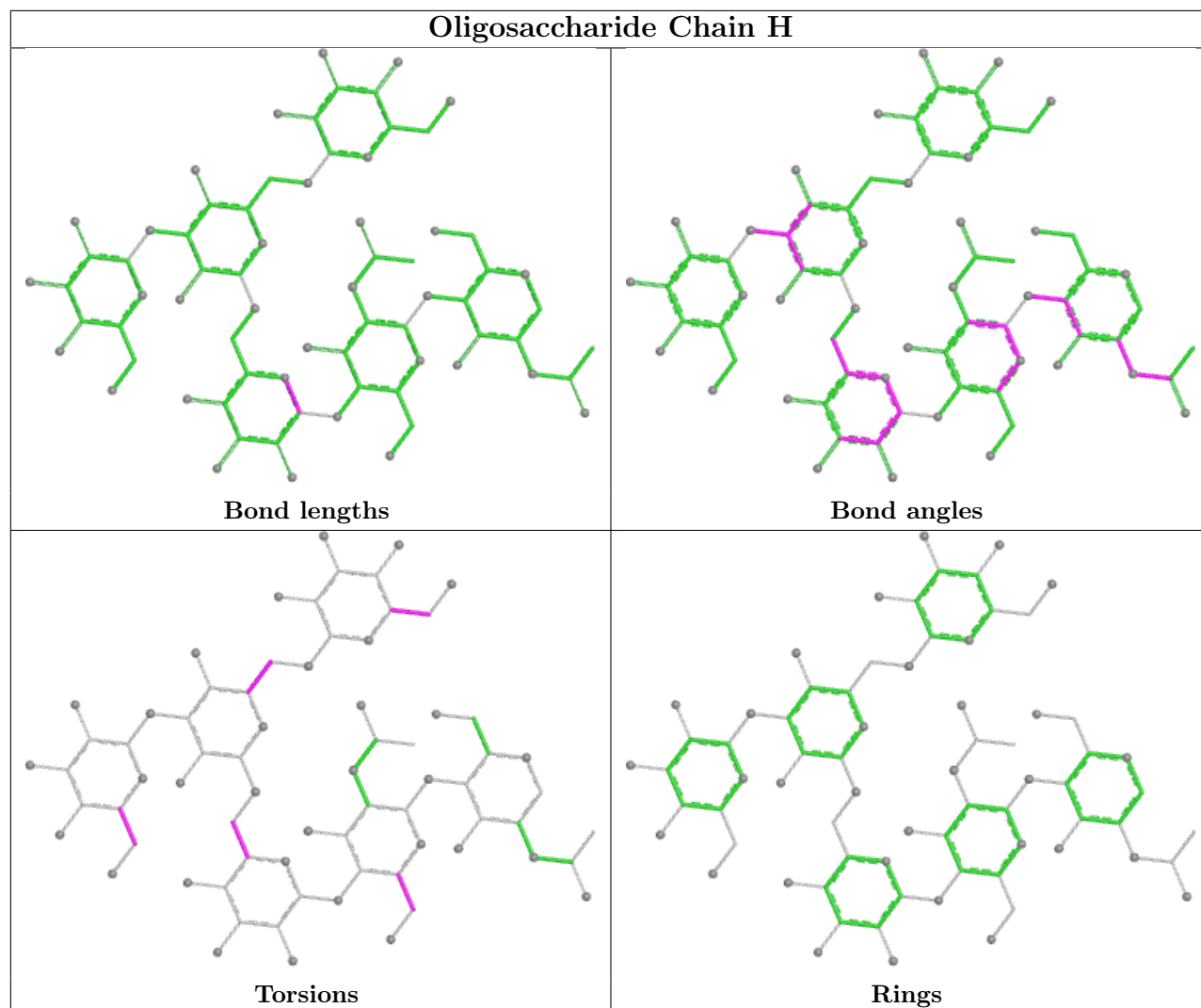
There are no ring outliers.

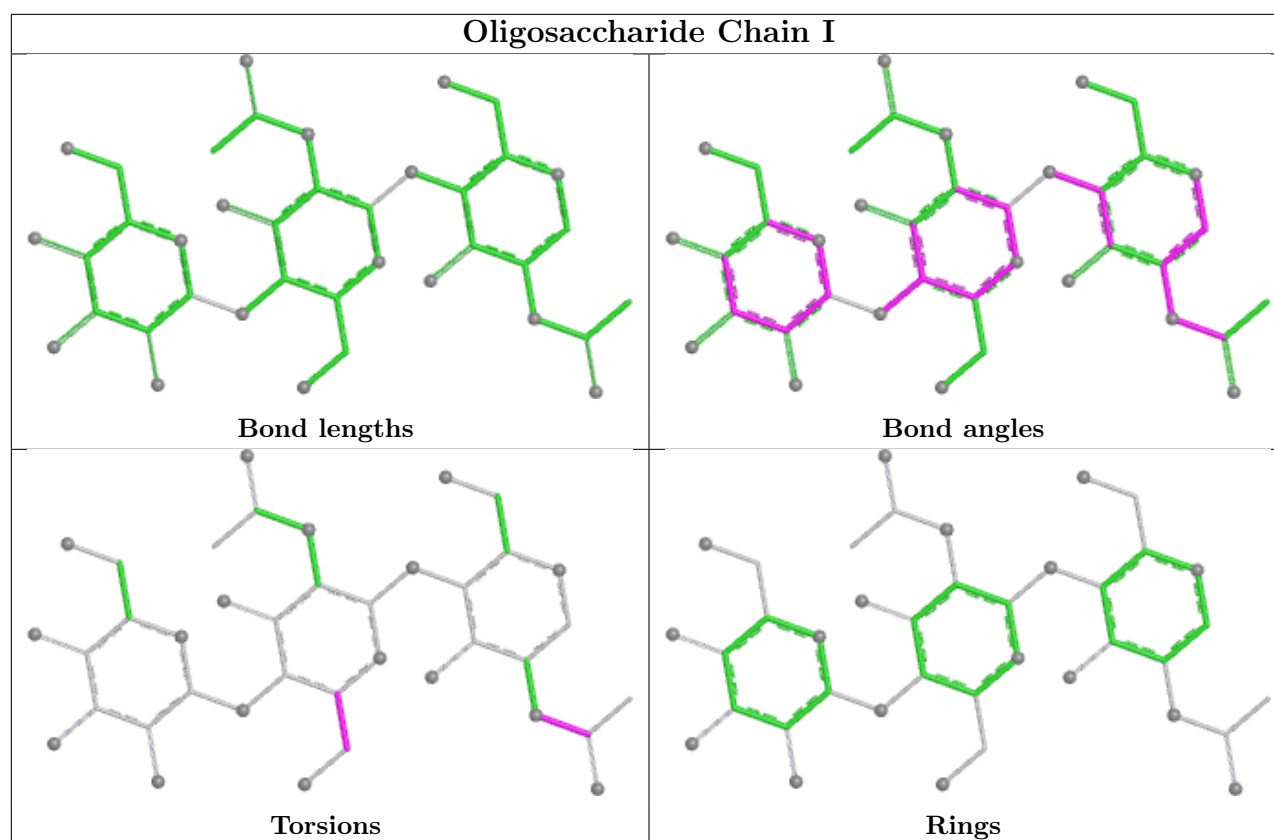
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	2	0
2	G	1	NAG	2	0
3	H	5	MAN	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](#)

35 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	SO4	F	403	-	4,4,4	0.43	0	6,6,6	0.42	0
5	MAN	E	401	1	11,11,12	0.57	0	15,15,17	0.94	0
6	SO4	C	404	-	4,4,4	0.26	0	6,6,6	0.66	0
6	SO4	C	406	-	4,4,4	0.34	0	6,6,6	0.61	0
7	GOL	A	405	-	5,5,5	0.42	0	5,5,5	0.44	0
7	GOL	B	405	-	5,5,5	0.37	0	5,5,5	0.80	0
6	SO4	B	404	-	4,4,4	0.48	0	6,6,6	0.36	0
6	SO4	E	404	-	4,4,4	0.27	0	6,6,6	0.42	0
7	GOL	D	405	-	5,5,5	0.59	0	5,5,5	2.64	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	F	401	1	11,11,12	0.76	0	15,15,17	0.93	0
6	SO4	D	404	-	4,4,4	0.43	0	6,6,6	0.47	0
6	SO4	C	405	-	4,4,4	0.45	0	6,6,6	0.46	0
8	NAG	E	403	1	14,14,15	0.67	0	17,19,21	0.97	0
8	NAG	C	403	1	14,14,15	0.50	0	17,19,21	0.73	0
6	SO4	D	403	-	4,4,4	0.19	0	6,6,6	0.60	0
7	GOL	F	405	-	5,5,5	0.49	0	5,5,5	0.36	0
7	GOL	E	408	-	5,5,5	0.19	0	5,5,5	0.72	0
6	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.50	0
6	SO4	F	404	-	4,4,4	0.77	0	6,6,6	0.72	0
8	NAG	F	402	1	14,14,15	1.13	3 (21%)	17,19,21	2.18	6 (35%)
6	SO4	B	403	-	4,4,4	0.32	0	6,6,6	0.25	0
5	MAN	D	401	1	11,11,12	0.79	1 (9%)	15,15,17	0.83	0
5	MAN	B	401	1	11,11,12	0.85	1 (9%)	15,15,17	0.88	0
5	MAN	A	401	1	11,11,12	0.90	1 (9%)	15,15,17	1.20	1 (6%)
6	SO4	A	403	-	4,4,4	0.26	0	6,6,6	0.74	0
6	SO4	E	405	-	4,4,4	0.44	0	6,6,6	0.64	0
6	SO4	E	406	-	4,4,4	0.73	0	6,6,6	0.43	0
5	MAN	E	402	1	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
5	MAN	A	402	1	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
6	SO4	E	407	-	4,4,4	0.16	0	6,6,6	0.49	0
5	MAN	D	402	1	11,11,12	0.92	2 (18%)	15,15,17	0.76	0
5	MAN	C	402	1	11,11,12	0.92	1 (9%)	15,15,17	0.89	0
5	MAN	B	402	1	11,11,12	0.70	0	15,15,17	1.06	1 (6%)
6	SO4	C	407	-	4,4,4	0.36	0	6,6,6	0.54	0
5	MAN	C	401	1	11,11,12	0.73	0	15,15,17	1.13	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
5	MAN	E	401	1	-	0/2/19/22	0/1/1/1
7	GOL	A	405	-	-	4/4/4/4	-
7	GOL	B	405	-	-	0/4/4/4	-
7	GOL	D	405	-	-	2/4/4/4	-
5	MAN	F	401	1	-	1/2/19/22	0/1/1/1
8	NAG	E	403	1	-	2/6/23/26	0/1/1/1
8	NAG	C	403	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	F	405	-	-	1/4/4/4	-
7	GOL	E	408	-	-	2/4/4/4	-
8	NAG	F	402	1	-	4/6/23/26	0/1/1/1
5	MAN	D	401	1	-	2/2/19/22	0/1/1/1
5	MAN	B	401	1	-	2/2/19/22	0/1/1/1
5	MAN	A	401	1	-	2/2/19/22	0/1/1/1
5	MAN	E	402	1	-	2/2/19/22	0/1/1/1
5	MAN	A	402	1	-	0/2/19/22	0/1/1/1
5	MAN	D	402	1	-	0/2/19/22	0/1/1/1
5	MAN	C	402	1	-	2/2/19/22	0/1/1/1
5	MAN	B	402	1	-	2/2/19/22	0/1/1/1
5	MAN	C	401	1	-	2/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	MAN	O5-C1	-2.25	1.39	1.43
8	F	402	NAG	O5-C1	-2.23	1.39	1.43
5	D	401	MAN	O5-C1	-2.23	1.39	1.43
5	C	402	MAN	O5-C1	-2.16	1.40	1.43
8	F	402	NAG	C3-C2	2.15	1.57	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	402	NAG	C2-N2-C7	-5.59	115.41	122.90
7	D	405	GOL	C3-C2-C1	4.46	128.16	111.80
8	F	402	NAG	C8-C7-N2	3.36	121.69	116.12
8	F	402	NAG	O7-C7-C8	-2.93	116.84	122.05
5	C	401	MAN	C1-C2-C3	2.83	113.77	109.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	GOL	O1-C1-C2-O2
7	A	405	GOL	O1-C1-C2-C3
7	A	405	GOL	C1-C2-C3-O3
7	E	408	GOL	C1-C2-C3-O3
5	B	402	MAN	O5-C5-C6-O6



There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	405	GOL	1	0
7	B	405	GOL	6	0
7	D	405	GOL	5	1
7	F	405	GOL	5	0
7	E	408	GOL	8	0
8	F	402	NAG	4	0

## 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	336/336 (100%)	0.03	6 (1%) 67 70	14, 22, 34, 50	0
1	B	336/336 (100%)	0.28	13 (3%) 44 47	15, 25, 42, 66	0
1	C	336/336 (100%)	-0.13	3 (0%) 81 83	13, 21, 33, 54	0
1	D	336/336 (100%)	0.02	6 (1%) 67 70	15, 22, 34, 52	0
1	E	336/336 (100%)	-0.09	3 (0%) 81 83	13, 21, 33, 63	0
1	F	336/336 (100%)	0.04	8 (2%) 59 62	14, 22, 35, 60	0
All	All	2016/2016 (100%)	0.03	39 (1%) 66 69	13, 22, 35, 66	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	THR	5.8
1	E	33	SER	5.4
1	F	33	SER	4.9
1	B	33	SER	4.1
1	E	34	THR	4.0

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

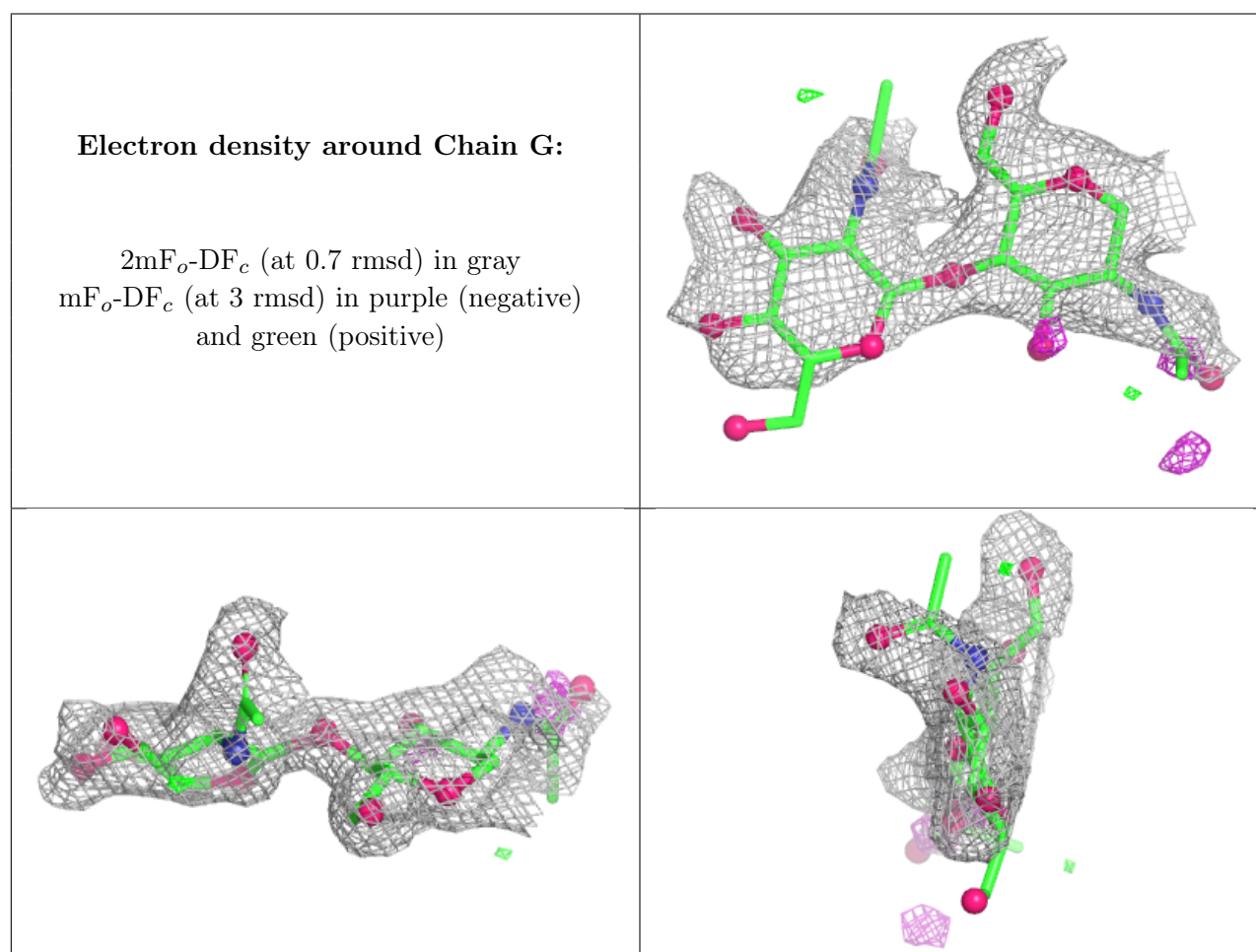
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

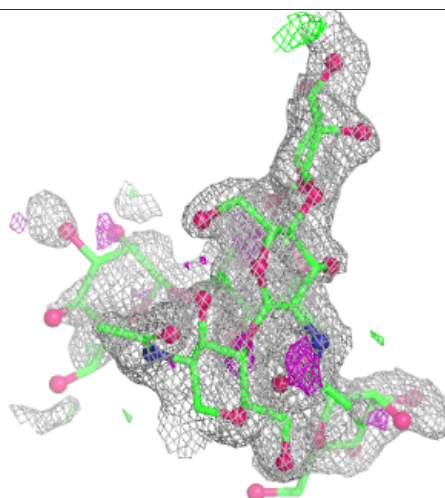
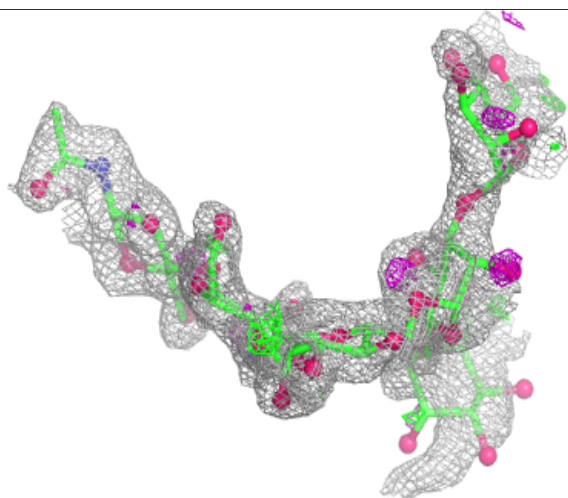
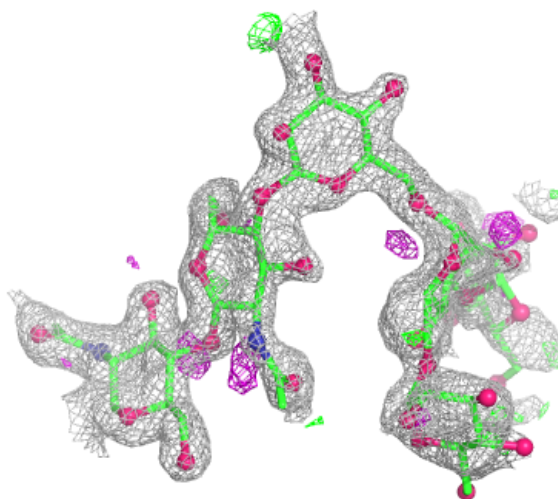
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	H	6	11/12	0.35	0.19	69,70,71,71	0
3	MAN	H	5	11/12	0.37	0.20	63,65,66,67	0
4	MAN	I	3	11/12	0.56	0.18	50,51,52,52	0
4	NAG	I	2	14/15	0.59	0.16	46,53,55,57	0
3	MAN	H	4	11/12	0.66	0.15	58,59,60,62	0
2	NAG	G	2	14/15	0.67	0.16	65,65,68,69	0
3	NAG	H	2	14/15	0.68	0.15	46,48,50,50	0
2	NAG	G	1	14/15	0.71	0.17	40,46,50,50	0
3	BMA	H	3	11/12	0.75	0.12	48,49,50,50	0
4	NAG	I	1	14/15	0.78	0.13	30,37,40,42	0
3	NAG	H	1	14/15	0.87	0.12	27,33,37,39	0

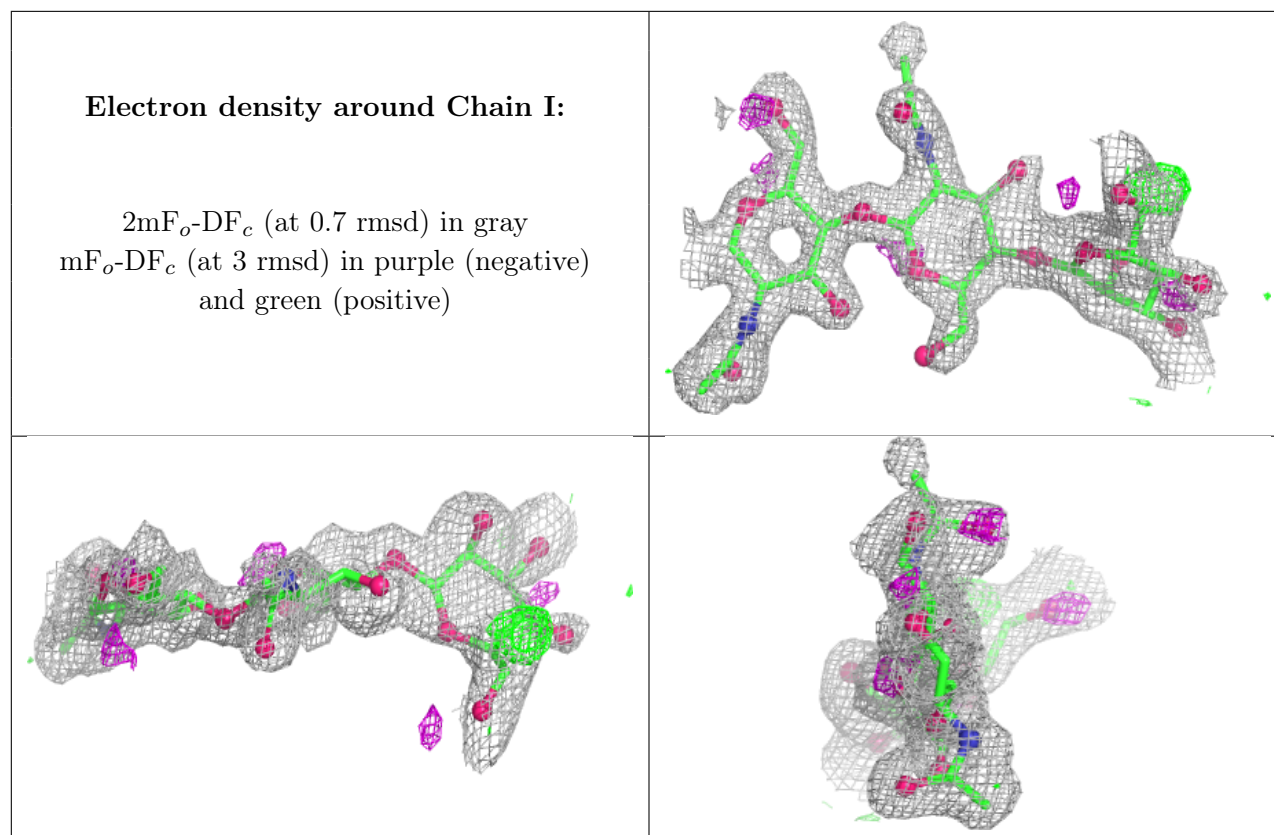
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain H:**

$2mF_o-DF_c$  (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	GOL	E	408	6/6	0.52	0.21	53,54,54,55	0
5	MAN	B	402	11/12	0.64	0.15	50,51,52,52	0
7	GOL	B	405	6/6	0.65	0.21	44,45,48,48	0
7	GOL	D	405	6/6	0.67	0.22	37,39,44,46	0
8	NAG	F	402	14/15	0.69	0.16	38,42,50,52	0
8	NAG	E	403	14/15	0.72	0.14	47,49,53,55	0
8	NAG	C	403	14/15	0.73	0.14	44,46,49,50	0
5	MAN	D	401	11/12	0.74	0.14	43,45,47,48	0
5	MAN	B	401	11/12	0.75	0.14	57,58,59,61	0
7	GOL	A	405	6/6	0.76	0.18	41,44,44,46	0
7	GOL	F	405	6/6	0.77	0.19	34,44,46,50	0
5	MAN	C	401	11/12	0.77	0.13	38,41,45,46	0
6	SO4	C	406	5/5	0.78	0.14	34,35,39,43	0
6	SO4	E	406	5/5	0.81	0.12	34,37,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	401	11/12	0.82	0.11	42,45,48,51	0
5	MAN	A	402	11/12	0.84	0.12	33,36,39,40	0
5	MAN	E	401	11/12	0.84	0.11	36,39,42,43	0
5	MAN	E	402	11/12	0.85	0.11	36,40,43,47	0
5	MAN	F	401	11/12	0.86	0.10	33,35,37,38	0
5	MAN	C	402	11/12	0.88	0.10	32,37,40,42	0
6	SO4	D	404	5/5	0.89	0.10	36,37,39,40	0
6	SO4	B	403	5/5	0.89	0.10	48,51,52,52	0
5	MAN	D	402	11/12	0.90	0.09	23,27,31,31	0
6	SO4	A	404	5/5	0.91	0.13	30,35,37,39	0
6	SO4	B	404	5/5	0.92	0.09	35,35,37,39	0
6	SO4	F	404	5/5	0.92	0.13	30,30,36,37	0
6	SO4	D	403	5/5	0.97	0.09	28,30,31,33	0
6	SO4	E	407	5/5	0.97	0.08	28,29,31,34	0
6	SO4	F	403	5/5	0.97	0.11	29,30,32,33	0
6	SO4	C	407	5/5	0.97	0.07	26,29,32,32	0
6	SO4	A	403	5/5	0.98	0.07	26,26,27,32	0
6	SO4	C	404	5/5	0.98	0.06	24,25,25,26	0
6	SO4	E	404	5/5	0.98	0.07	22,24,26,28	0
6	SO4	C	405	5/5	0.99	0.04	15,16,17,18	0
6	SO4	E	405	5/5	0.99	0.03	16,16,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.