



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 09:30 AM BST

PDB ID : 5XBZ  
Title : Crystal structure of GH family 81 beta-1,3-glucanase from *Rhizomucor miehei* complexed with laminaripentaose  
Authors : Yang, S.; Qin, Z.; Zhou, P.; Yan, Q.; Jiang, Z.  
Deposited on : 2017-03-21  
Resolution : 2.70 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

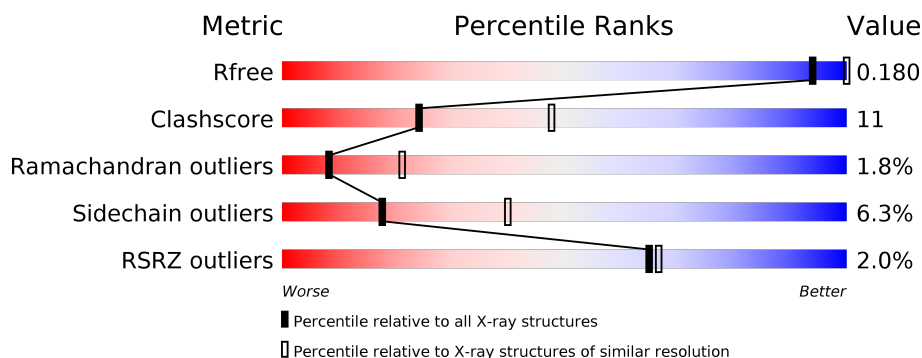
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



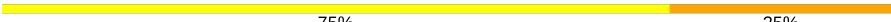

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	796	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	796	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>•</div> <div>11%</div> </div> </div>
2	C	5	<div> <div></div> <div>40%</div> <div>60%</div> </div>
2	F	5	<div> <div></div> <div>80%</div> <div>20%</div> </div>
2	G	5	<div> <div></div> <div>100%</div> </div>
3	D	4	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	4	 75%25%
4	E	3	 33%67%

## 2 Entry composition [i](#)

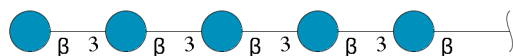
There are 5 unique types of molecules in this entry. The entry contains 11705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endo-beta-1,3-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	1	0
			5614	3594	934	1073	13			
1	B	705	Total	C	N	O	S	0	2	0
			5568	3567	929	1059	13			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



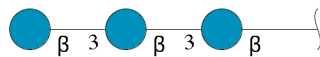
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	F	5	Total	C	O	0	0	0
			56	30	26			
2	G	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	0	0	0
			45	24	21			
3	H	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.




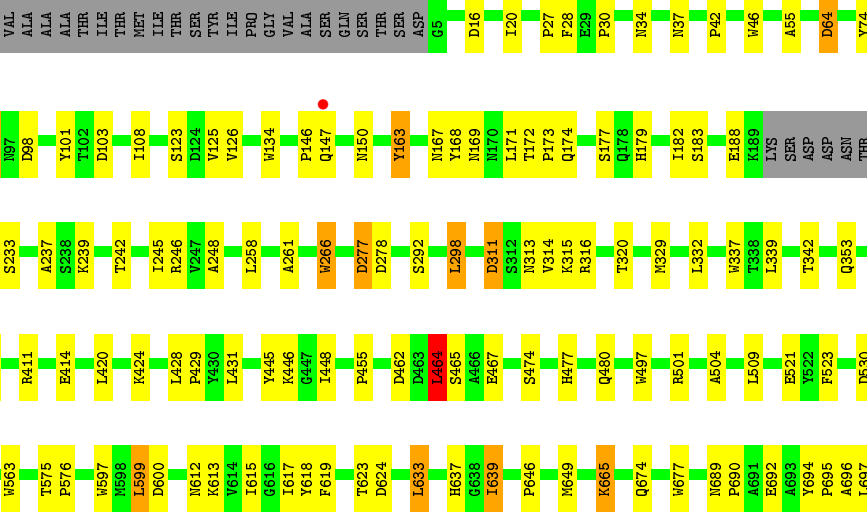
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	89	Total	O	0	0
			89	89		

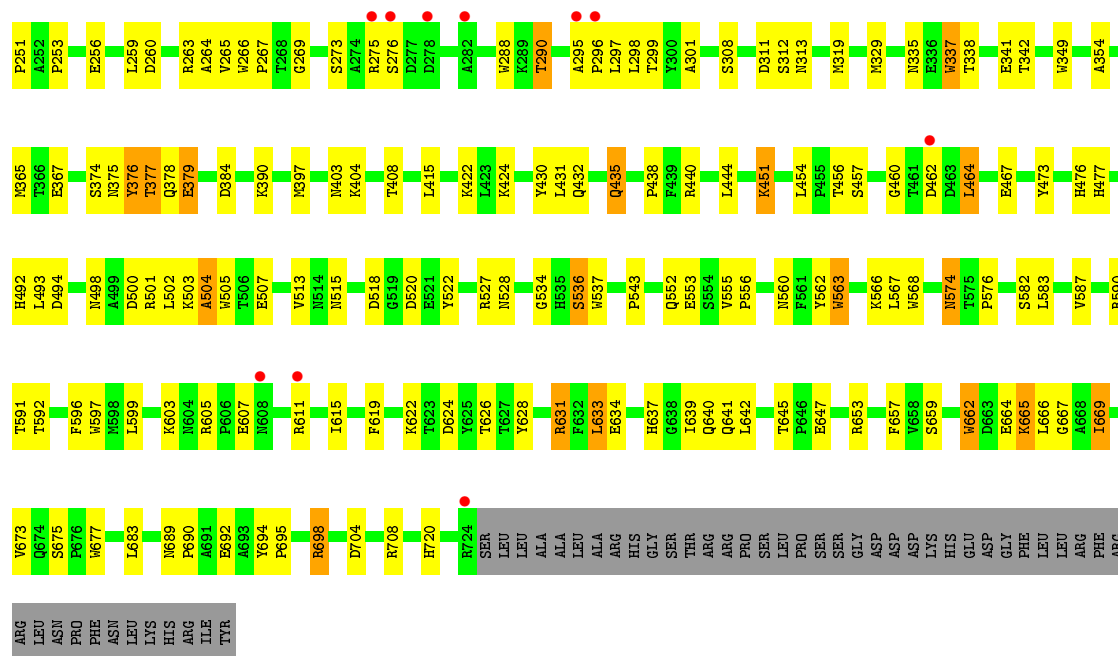
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain A: 



Residue	State	Percentage
W69	Green	70%
R228	Green	70%
S92	Green	70%
Y93	Green	70%
T96	Green	70%
I97	Green	70%
D98	Green	70%
Y101	Green	70%
T102	Green	70%
D103	Green	70%
I108	Green	70%
S123	Green	70%
D124	Green	70%
V125	Green	70%
V126	Green	70%
W134	Green	70%
P146	Green	70%
Q147	Green	70%
M150	Green	70%
Y163	Green	70%
M167	Green	70%
Y168	Green	70%
M169	Green	70%
N170	Green	70%
L171	Green	70%
T172	Green	70%
P173	Green	70%
Q174	Green	70%
E29	Green	70%
P30	Green	70%
S177	Green	70%
Q178	Green	70%
H179	Green	70%
I182	Green	70%
S183	Green	70%
E188	Green	70%
K189	Green	70%
LYS	Green	70%
SER	Green	70%
ASP	Green	70%
ASN	Green	70%
THR	Green	70%
SER	Green	70%
T197	Green	70%
M207	Green	70%
D222	Green	70%
K223	Green	70%
K382	Green	70%
Y386	Green	70%
K390	Green	70%
R411	Green	70%
E414	Green	70%
L420	Green	70%
K424	Green	70%
L428	Green	70%
P429	Green	70%
Y430	Green	70%
L431	Green	70%
Y445	Green	70%
K446	Green	70%
G447	Green	70%
L448	Green	70%
P455	Green	70%
D462	Green	70%
K463	Green	70%
L464	Green	70%
S465	Green	70%
A466	Green	70%
E467	Green	70%
S474	Green	70%
H477	Green	70%
Q480	Green	70%
H497	Green	70%
R501	Green	70%
A504	Green	70%
P690	Green	70%
A691	Green	70%
E692	Green	70%
A693	Green	70%
Y694	Green	70%
P695	Green	70%
A696	Green	70%
L697	Green	70%
K698	Green	70%
K699	Green	70%
V700	Green	70%
D704	Green	70%
Y710	Green	70%
D551	Yellow	17%
S554	Yellow	17%
V555	Yellow	17%
P556	Yellow	17%
W563	Yellow	17%
T575	Yellow	17%
P576	Yellow	17%
W597	Yellow	17%
M598	Yellow	17%
L599	Yellow	17%
D600	Yellow	17%
M612	Yellow	17%
K613	Yellow	17%
V614	Yellow	17%
T615	Yellow	17%
G616	Yellow	17%
P617	Yellow	17%
V618	Yellow	17%
P619	Yellow	17%
T623	Yellow	17%
D624	Yellow	17%
L633	Yellow	17%
H637	Yellow	17%
G638	Yellow	17%
T639	Yellow	17%
P646	Yellow	17%
M649	Yellow	17%
PHE	Yellow	17%
K665	Yellow	17%
Q674	Yellow	17%
W677	Yellow	17%
M689	Yellow	17%
P690	Yellow	17%
A691	Yellow	17%
E692	Yellow	17%
A693	Yellow	17%
Y694	Yellow	17%
P695	Yellow	17%
A696	Yellow	17%
L697	Yellow	17%
K698	Yellow	17%
K699	Yellow	17%
V700	Yellow	17%
D704	Yellow	17%
Y710	Yellow	17%
R718	Orange	11%
F719	Orange	11%
H720	Orange	11%
F721	Orange	11%
PHE	Orange	11%
ARG	Orange	11%
ARG	Orange	11%
SER	Orange	11%
LEU	Orange	11%
LEU	Orange	11%
ALA	Orange	11%
ALA	Orange	11%
LEU	Orange	11%
ALA	Orange	11%
ARG	Orange	11%
GLY	Orange	11%

- [illegible]

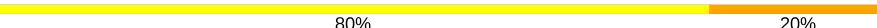


- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain C:  40% 60%



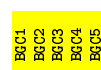
- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain F:  80% 20%



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain G:  100%

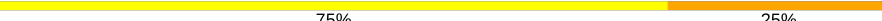


- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain D:  100%



- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain H:  75% 25%

BGC1  
BGC2  
BGC3  
BGC4

- Molecule 4: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain E:  33% 67%

BGC1  
BGC2  
BGC3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.92Å 96.96Å 127.64Å 90.00° 93.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.70) 98.9 (47.63-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.174 , 0.190 0.177 , 0.180	Depositor DCC
$R_{free}$ test set	1765 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: BGC

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	8/5776 (0.1%)	0.81	6/7890 (0.1%)
1	B	0.65	10/5731 (0.2%)	0.75	1/7826 (0.0%)
All	All	0.70	18/11507 (0.2%)	0.78	7/15716 (0.0%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TRP	CD2-CE2	6.30	1.49	1.41
1	A	266	TRP	CD2-CE2	6.13	1.48	1.41
1	B	505	TRP	CD2-CE2	6.11	1.48	1.41
1	A	563	TRP	CD2-CE2	5.85	1.48	1.41
1	B	349	TRP	CD2-CE2	5.67	1.48	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	LEU	CA-CB-CG	7.08	131.59	115.30
1	A	64	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	464	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	176	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	16	ASP	CB-CG-OD1	5.31	123.08	118.30

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	5614	0	5399	97	0
1	B	5568	0	5348	148	0
2	C	56	0	48	3	0
2	F	56	0	48	1	0
2	G	56	0	48	1	0
3	D	45	0	39	0	0
3	H	45	0	39	1	0
4	E	34	0	30	0	0
5	A	142	0	0	12	0
5	B	89	0	0	6	0
All	All	11705	0	10999	246	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 11.

The worst 5 of 246 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:574:ASN:OD1	1:B:576:PRO:HD2	1.25	1.26
1:B:698:ARG:HG2	1:B:698:ARG:HH21	1.15	1.04
1:A:101:TYR:CZ	5:A:901:HOH:O	2.16	0.94
1:B:430:TYR:CD1	1:B:435:GLN:HG2	2.03	0.94
1:B:503:LYS:O	1:B:507:GLU:HG3	1.69	0.92

There are no symmetry-related clashes.

## 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	707/796 (89%)	654 (92%)	47 (7%)	6 (1%)	19 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	701/796 (88%)	611 (87%)	71 (10%)	19 (3%)	5	12
All	All	1408/1592 (88%)	1265 (90%)	118 (8%)	25 (2%)	8	21

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	376	TYR
1	B	498	ASN
1	A	188	GLU
1	A	544	ASP
1	B	182	ILE

### 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	599/685 (87%)	568 (95%)	31 (5%)	23	49
1	B	591/685 (86%)	546 (92%)	45 (8%)	13	30
All	All	1190/1370 (87%)	1114 (94%)	76 (6%)	18	39

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	MET
1	B	207	MET
1	B	633	LEU
1	B	84	GLN
1	B	163	TYR

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

Mol	Chain	Res	Type
1	A	409	GLN
1	B	322	GLN

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Mol	Chain	Res	Type
1	A	689	ASN
1	A	169	ASN
1	B	140	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 ⓘ

26 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	BGC	C	1	2	12,12,12	0.91	0	17,17,17	1.25	3 (17%)
2	BGC	C	2	2	11,11,12	0.51	0	15,15,17	1.49	1 (6%)
2	BGC	C	3	2	11,11,12	0.71	0	15,15,17	3.09	7 (46%)
2	BGC	C	4	2	11,11,12	0.63	0	15,15,17	1.56	3 (20%)
2	BGC	C	5	2	11,11,12	0.66	0	15,15,17	1.85	3 (20%)
3	BGC	D	1	3	12,12,12	0.59	0	17,17,17	1.46	2 (11%)
3	BGC	D	2	3	11,11,12	0.43	0	15,15,17	2.06	3 (20%)
3	BGC	D	3	3	11,11,12	0.41	0	15,15,17	1.30	2 (13%)
3	BGC	D	4	3	11,11,12	0.64	0	15,15,17	2.72	5 (33%)
4	BGC	E	1	4	12,12,12	0.79	0	17,17,17	0.76	0
4	BGC	E	2	4	11,11,12	0.85	1 (9%)	15,15,17	1.77	3 (20%)
4	BGC	E	3	4	11,11,12	0.64	0	15,15,17	1.24	1 (6%)
2	BGC	F	1	2	12,12,12	0.58	0	17,17,17	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	F	2	2	11,11,12	0.44	0	15,15,17	1.16	1 (6%)
2	BGC	F	3	2	11,11,12	0.60	0	15,15,17	3.44	7 (46%)
2	BGC	F	4	2	11,11,12	0.78	0	15,15,17	1.42	2 (13%)
2	BGC	F	5	2	11,11,12	0.75	0	15,15,17	3.03	7 (46%)
2	BGC	G	1	2	12,12,12	0.90	0	17,17,17	1.94	4 (23%)
2	BGC	G	2	2	11,11,12	0.37	0	15,15,17	1.49	3 (20%)
2	BGC	G	3	2	11,11,12	0.38	0	15,15,17	1.00	0
2	BGC	G	4	2	11,11,12	0.33	0	15,15,17	1.42	2 (13%)
2	BGC	G	5	2	11,11,12	0.55	0	15,15,17	1.22	1 (6%)
3	BGC	H	1	3	12,12,12	0.54	0	17,17,17	1.40	3 (17%)
3	BGC	H	2	3	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
3	BGC	H	3	3	11,11,12	0.53	0	15,15,17	1.40	2 (13%)
3	BGC	H	4	3	11,11,12	0.58	0	15,15,17	1.64	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	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	BGC	C	5	2	-	2/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	1/2/19/22	0/1/1/1
4	BGC	E	1	4	-	0/2/22/22	0/1/1/1
4	BGC	E	2	4	-	0/2/19/22	0/1/1/1
4	BGC	E	3	4	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	F	3	2	-	2/2/19/22	0/1/1/1
2	BGC	F	4	2	-	0/2/19/22	0/1/1/1
2	BGC	F	5	2	-	2/2/19/22	0/1/1/1
2	BGC	G	1	2	-	1/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	0/2/19/22	0/1/1/1
2	BGC	G	4	2	-	0/2/19/22	0/1/1/1
2	BGC	G	5	2	-	0/2/19/22	0/1/1/1
3	BGC	H	1	3	-	2/2/22/22	0/1/1/1
3	BGC	H	2	3	-	0/2/19/22	0/1/1/1
3	BGC	H	3	3	-	2/2/19/22	0/1/1/1
3	BGC	H	4	3	-	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)
4	E	2	BGC	C2-C3	2.08	1.55	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	BGC	C1-O5-C5	9.24	124.72	112.19
2	F	3	BGC	C1-O5-C5	7.88	122.86	112.19
2	C	3	BGC	C1-C2-C3	7.11	118.41	109.67
3	D	4	BGC	C1-O5-C5	7.08	121.78	112.19
2	F	3	BGC	C1-C2-C3	6.15	117.23	109.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	BGC	O5-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
3	H	1	BGC	C4-C5-C6-O6
2	C	5	BGC	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 5 short contacts:

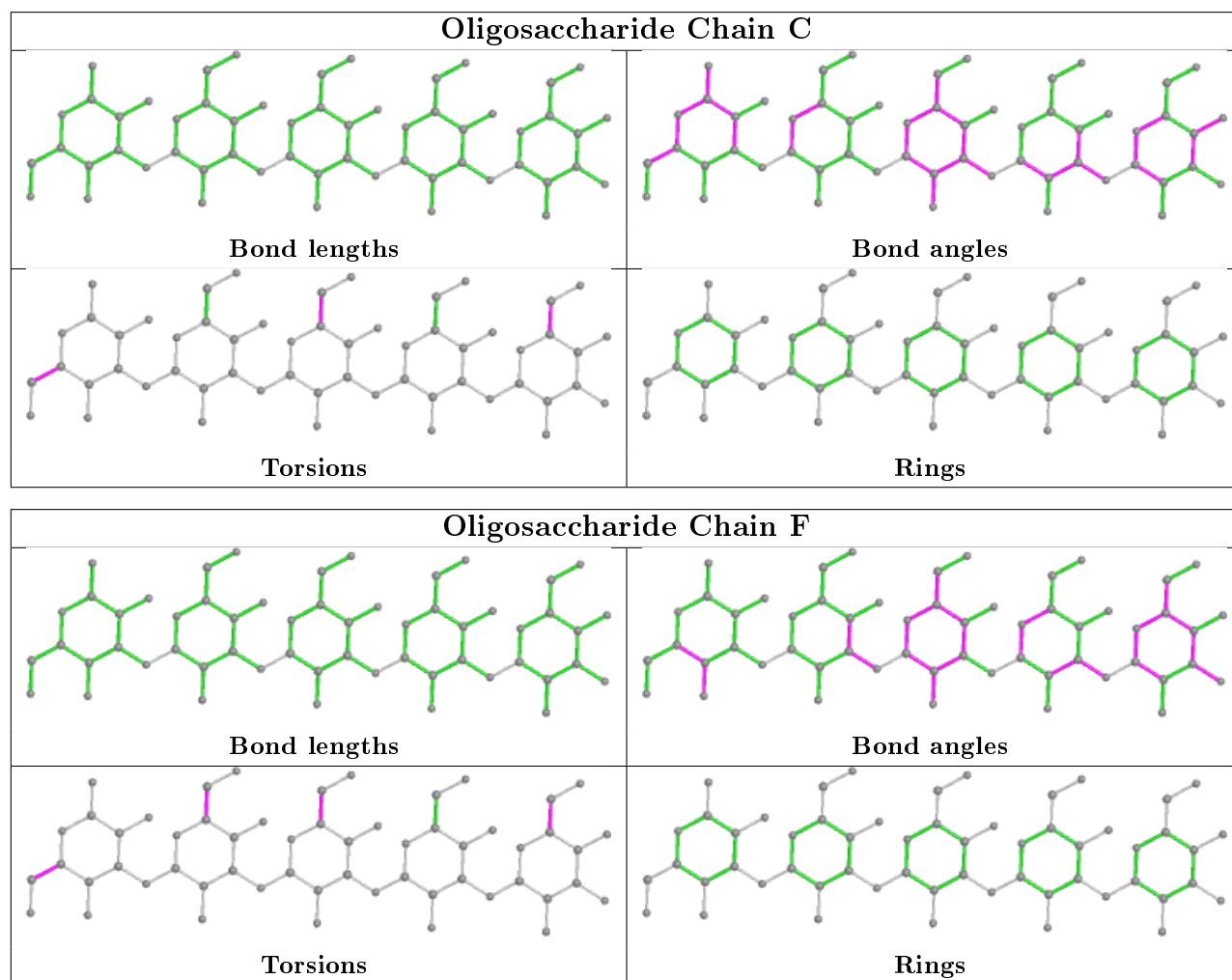
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	BGC	1	0
2	G	3	BGC	1	0
2	C	3	BGC	1	0

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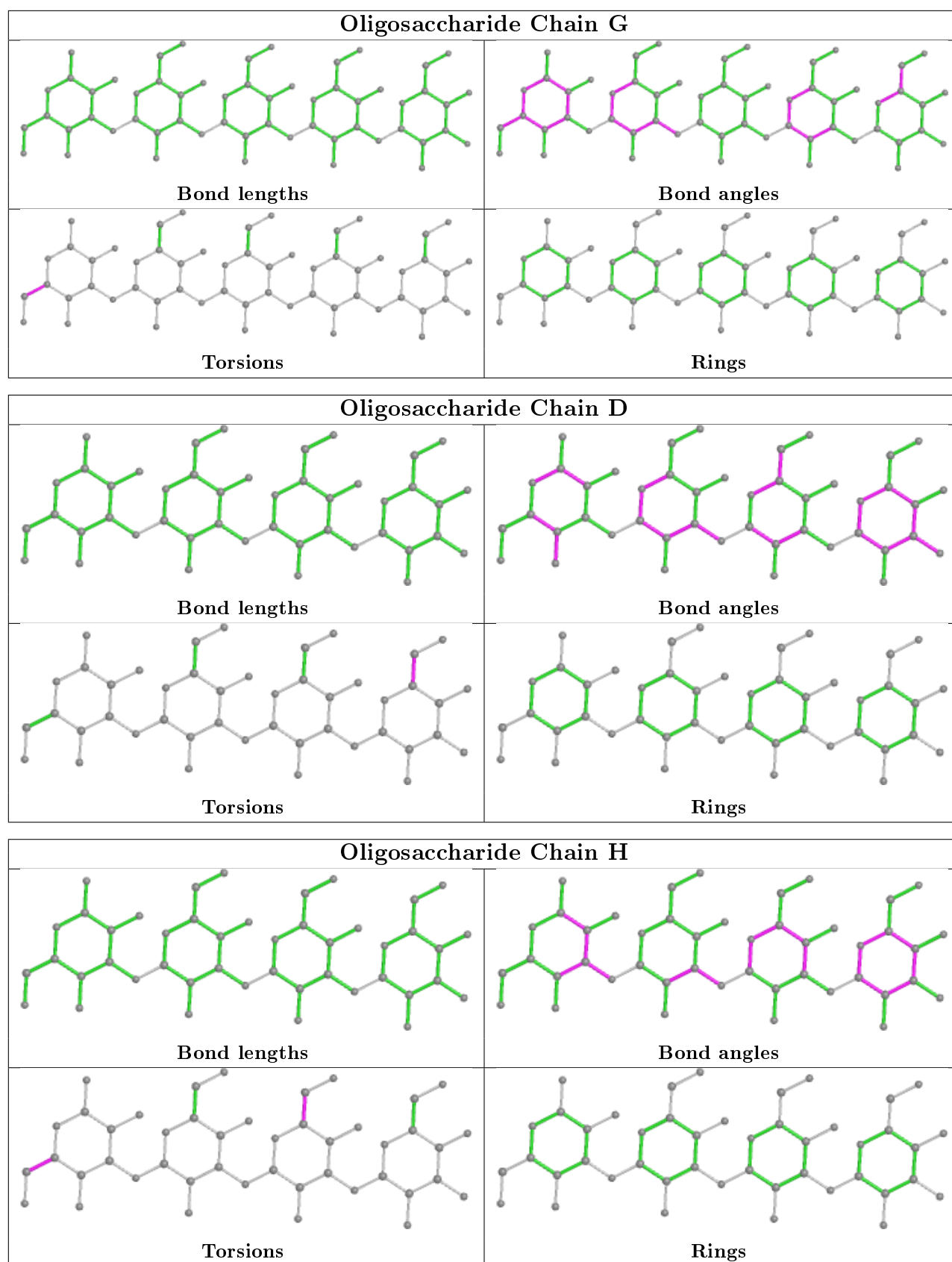
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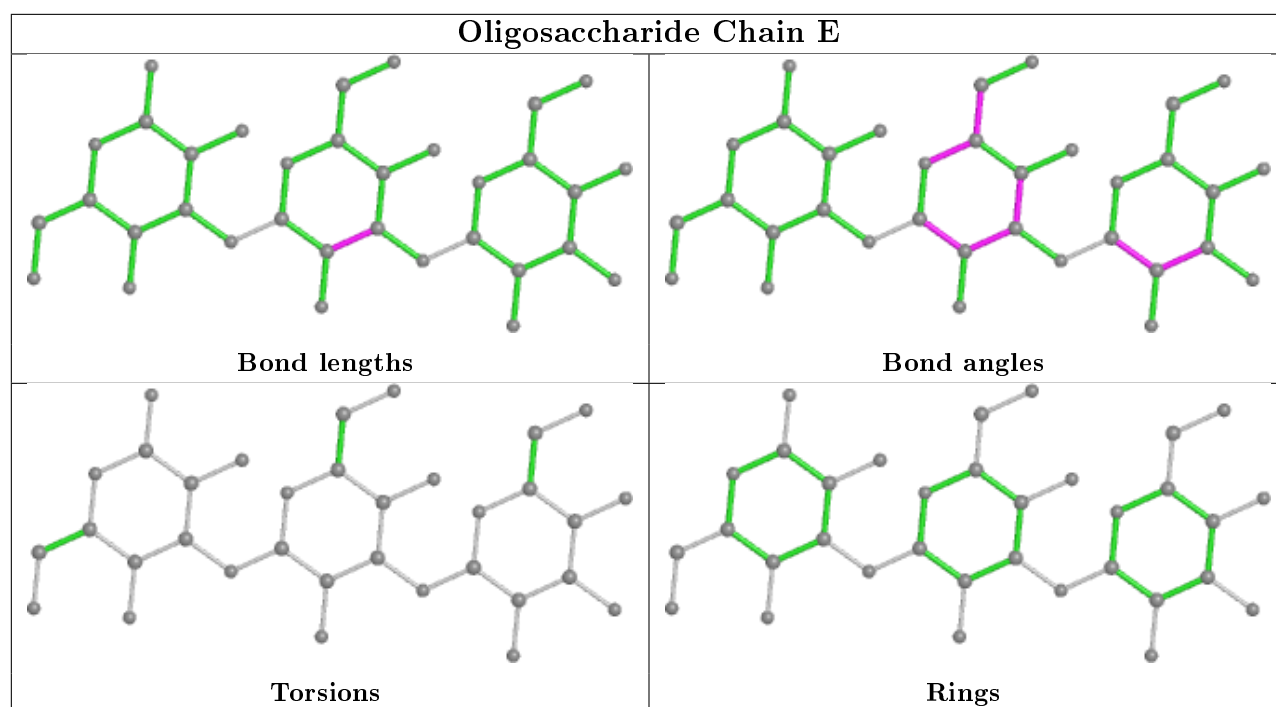
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	BGC	1	0
3	H	3	BGC	1	0
2	C	4	BGC	1	0

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](#)

There are no ligands in this entry.

## 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	710/796 (89%)	-0.63	4 (0%) 89 91	7, 15, 37, 82	0
1	B	705/796 (88%)	-0.02	24 (3%) 45 45	15, 36, 67, 87	0
All	All	1415/1592 (88%)	-0.32	28 (1%) 65 67	7, 25, 58, 87	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ASP	4.1
1	B	5	GLY	4.0
1	B	724	ARG	4.0
1	A	74	TYR	3.7
1	B	462	ASP	3.5

### 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	BGC	G	1	12/12	0.71	0.35	54,62,68,68	0
3	BGC	H	4	11/12	0.76	0.37	78,81,84,84	0
2	BGC	G	5	11/12	0.77	0.35	58,72,77,80	0
3	BGC	H	1	12/12	0.82	0.29	46,59,65,67	0
4	BGC	E	1	12/12	0.83	0.21	37,44,50,51	0

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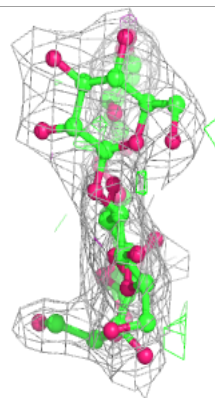
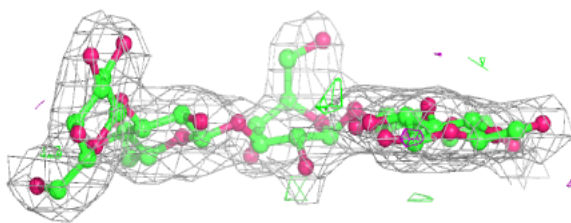
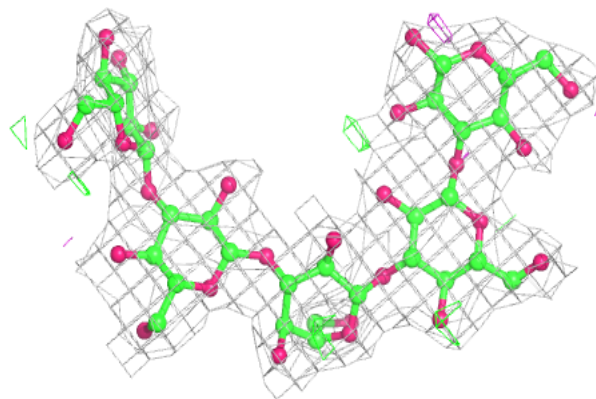
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	H	3	11/12	0.86	0.23	68,72,75,78	0
3	BGC	D	4	11/12	0.87	0.29	44,47,56,59	0
3	BGC	H	2	11/12	0.88	0.15	44,54,63,66	0
4	BGC	E	3	11/12	0.88	0.18	30,41,45,52	0
2	BGC	F	1	12/12	0.88	0.19	48,54,59,61	0
2	BGC	F	5	11/12	0.89	0.18	35,40,40,46	0
4	BGC	E	2	11/12	0.91	0.17	34,41,42,42	0
2	BGC	C	5	11/12	0.92	0.13	18,19,21,22	0
2	BGC	G	2	11/12	0.92	0.17	48,54,57,58	0
2	BGC	F	4	11/12	0.93	0.13	35,38,39,40	0
3	BGC	D	1	12/12	0.93	0.18	26,29,32,32	0
2	BGC	G	4	11/12	0.93	0.21	53,57,61,63	0
2	BGC	G	3	11/12	0.94	0.15	44,47,49,52	0
2	BGC	C	1	12/12	0.94	0.18	17,23,28,28	0
2	BGC	F	3	11/12	0.94	0.14	35,40,43,44	0
3	BGC	D	3	11/12	0.95	0.17	26,29,33,39	0
2	BGC	F	2	11/12	0.96	0.12	35,44,47,49	0
2	BGC	C	3	11/12	0.97	0.12	13,13,14,14	0
3	BGC	D	2	11/12	0.97	0.14	24,26,28,29	0
2	BGC	C	2	11/12	0.98	0.12	12,13,14,15	0
2	BGC	C	4	11/12	0.99	0.10	11,12,13,15	0

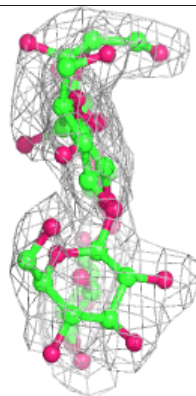
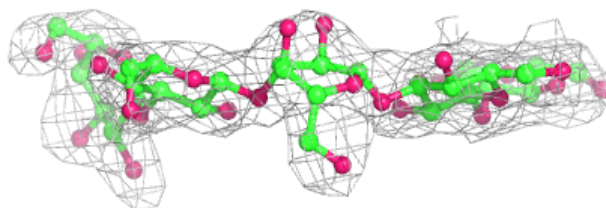
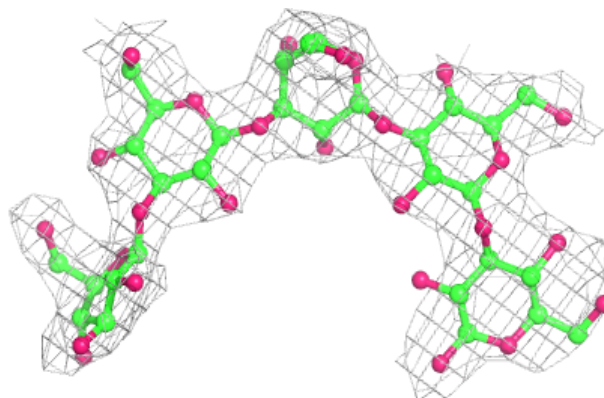
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

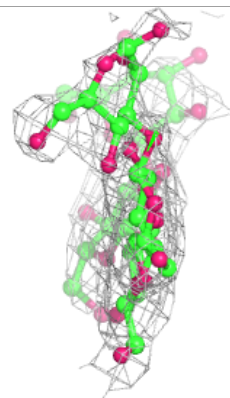
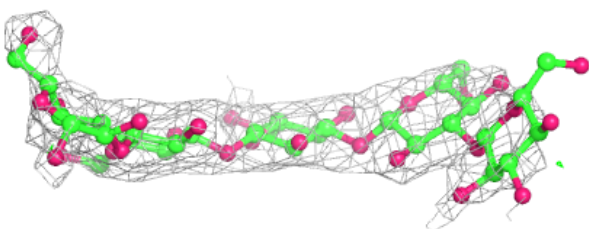
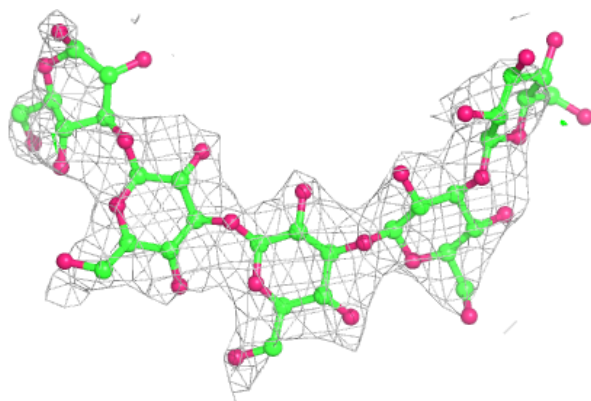
**Electron density around Chain F:**

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

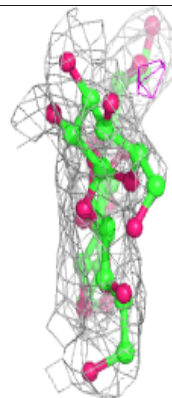
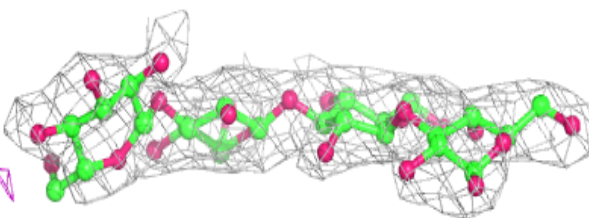
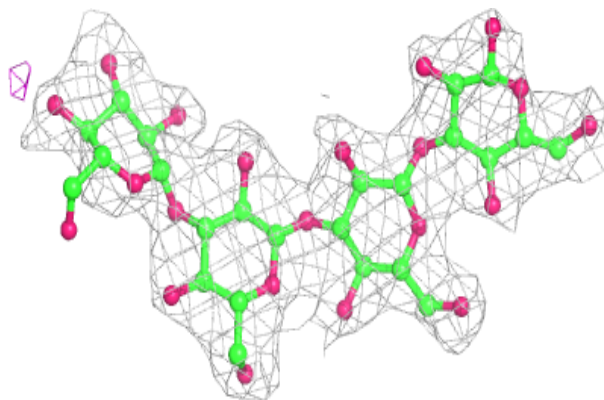


**Electron density around Chain G:**

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

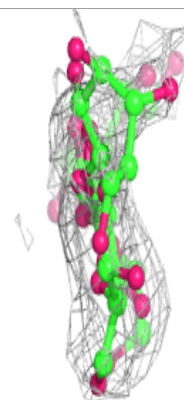
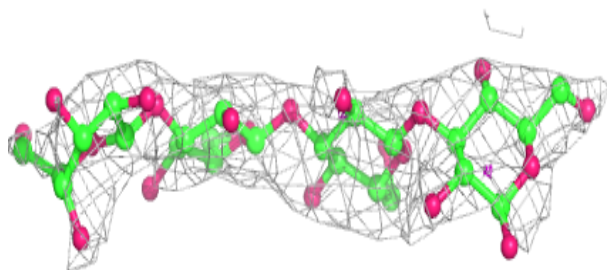
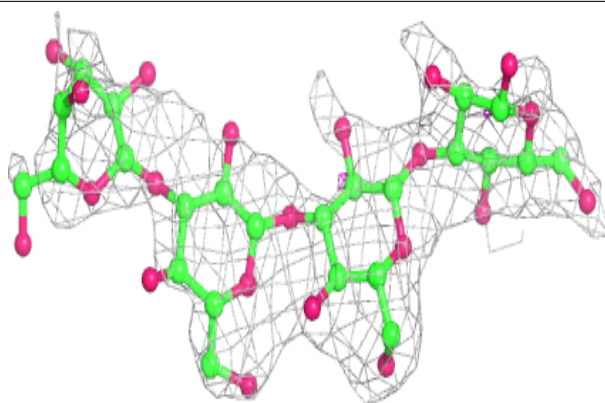
**Electron density around Chain D:**

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

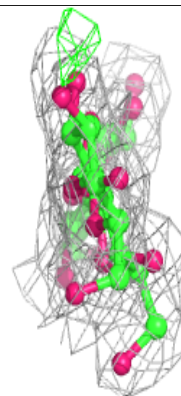
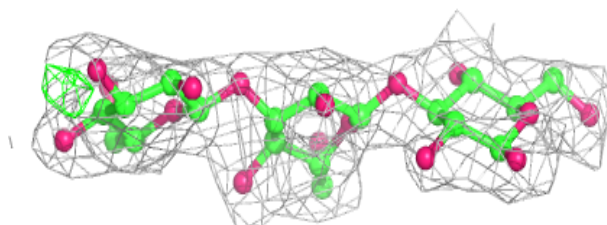
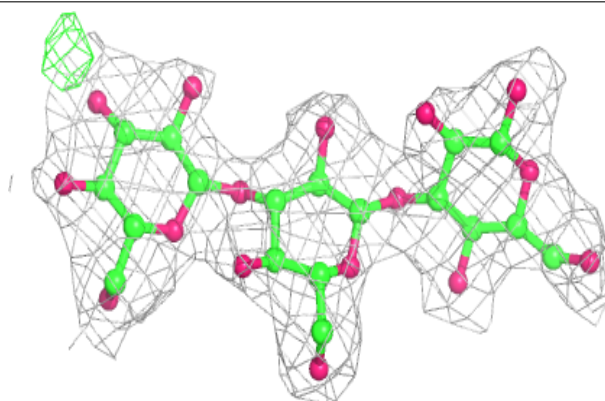


**Electron density around Chain H:**

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

**Electron density around Chain E:**

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



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.