



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 04:18 PM EDT

PDB ID : 5TKF  
Title : Neurospora crassa polysaccharide monooxygenase 2 high mannosylation  
Authors : O'Dell, W.B.; Meilleur, F.  
Deposited on : 2016-10-06  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

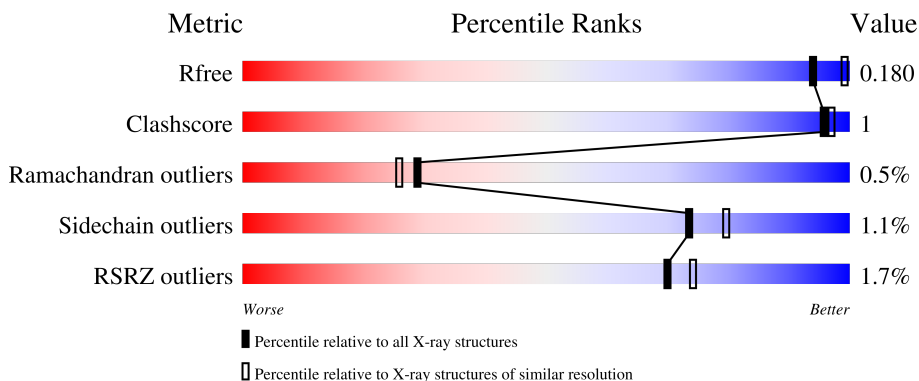
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



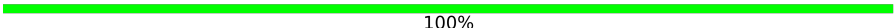

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	223	 96%
1	B	223	 98%
1	C	223	 97%
1	D	223	 96%
2	E	7	 29% 57% 14%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	G	4	 50% 25% 25%

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	G	4	-	-	-	X

## 2 Entry composition i

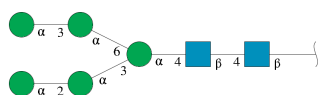
There are 8 unique types of molecules in this entry. The entry contains 14510 atoms, of which 6652 are hydrogens and 0 are deuteriums.

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 Lytic polysaccharide monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	223	Total 3299	C 1046	H 1625	N 283	O 336	S 9	0	12	0
1	B	223	Total 3302	C 1047	H 1632	N 283	O 331	S 9	0	10	0
1	C	223	Total 3261	C 1036	H 1607	N 280	O 329	S 9	0	5	0
1	D	223	Total 3297	C 1045	H 1628	N 283	O 332	S 9	0	10	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]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
			Total	C	H	N	O			
2	E	7	Total 156	C 46	H 73	N 2	O 35	0	0	0

- Molecule 3 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
			Total	C	H	N	O			
3	F	2	Total 55	C 16	H 27	N 2	O 10	0	0	0

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

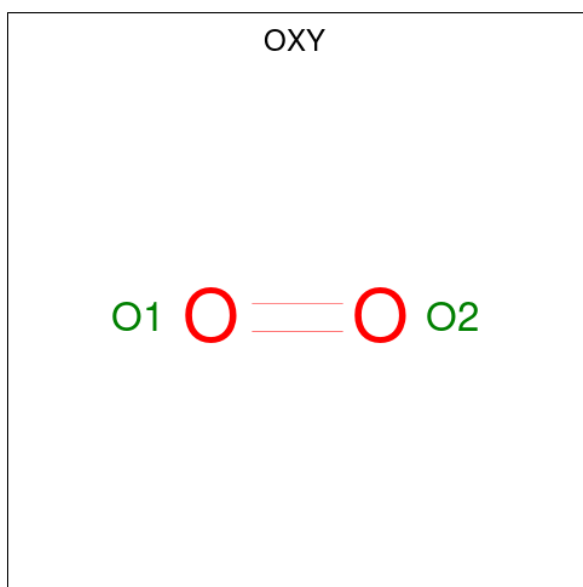


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	G	4	96	28	46	2	20	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

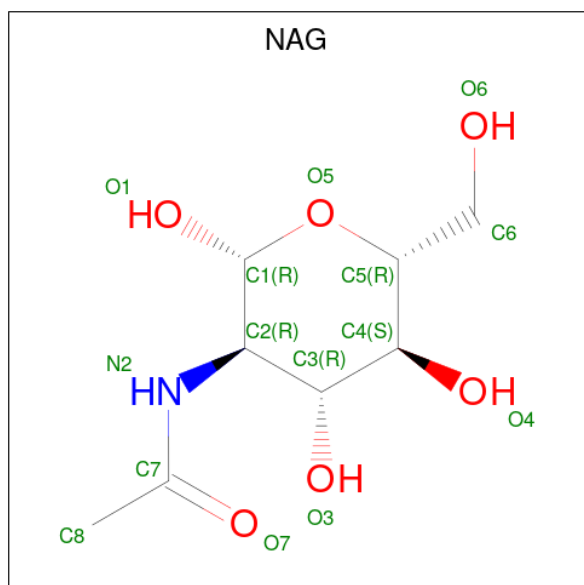
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	D	1	Total	Cu	0	0
			1	1		

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 2 2	0	0
6	D	1	Total O 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C H N O 28 8 14 1 5	0	0

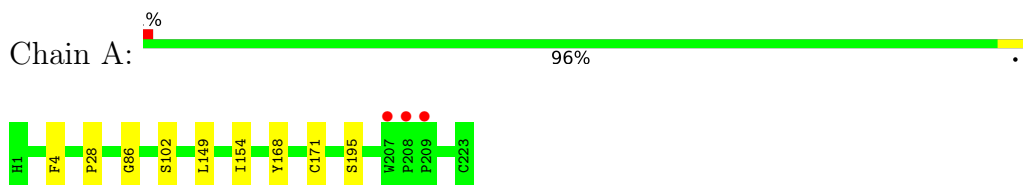
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	298	Total O 298 298	0	1
8	B	257	Total O 257 257	0	0
8	C	249	Total O 249 249	0	0
8	D	204	Total O 204 204	0	0

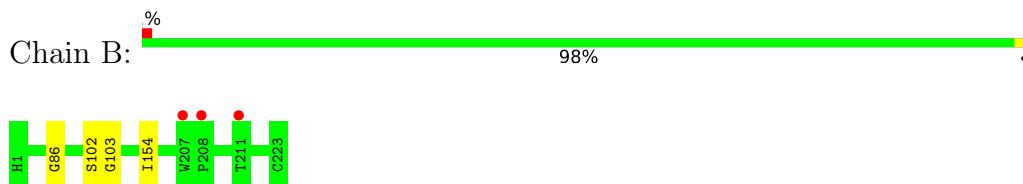
### 3 Residue-property plots [i](#)

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.

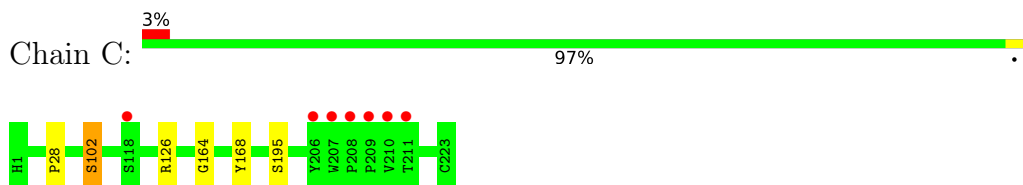
- Molecule 1: Lytic polysaccharide monooxygenase



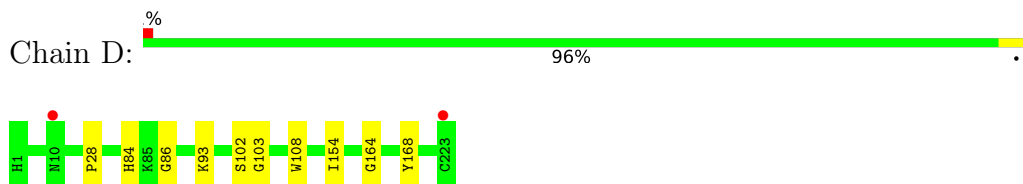
- Molecule 1: Lytic polysaccharide monooxygenase



- Molecule 1: Lytic polysaccharide monooxygenase



- Molecule 1: Lytic polysaccharide monooxygenase



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



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

Chain F:  100%

MAG1  
MAG2

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

Chain G:  50% 25% 25%

MAG1  
MAG2  
MAN3  
MAN4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.30Å 67.04Å 84.15Å 97.57° 97.61° 97.43°	Depositor
Resolution (Å)	40.31 – 2.10 40.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.31-2.10) 97.1 (40.31-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, $R_{free}$	0.142 , 0.177 0.146 , 0.180	Depositor DCC
$R_{free}$ test set	2000 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtrriage
Anisotropy	0.544	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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: OXY, CU, NAG, MAN

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	0.26	0/1758	0.47	0/2400
1	B	0.26	0/1741	0.49	0/2375
1	C	0.25	0/1708	0.46	0/2332
1	D	0.25	0/1743	0.48	0/2376
All	All	0.25	0/6950	0.48	0/9483

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	1674	1625	1578	3	0
1	B	1670	1632	1596	1	0
1	C	1654	1607	1590	5	0
1	D	1669	1628	1583	3	0
2	E	83	73	70	2	0
3	F	28	27	25	0	0
4	G	50	46	43	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	D	14	14	13	0	0
8	A	298	0	0	0	0
8	B	257	0	0	0	0
8	C	249	0	0	2	1
8	D	204	0	0	0	0
All	All	7858	6652	6498	15	1

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 1.

All (15) 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:C:102:SER:O	8:C:401:HOH:O	2.13	0.66
1:C:126:ARG:HD3	4:G:4:MAN:H3	1.80	0.61
2:E:1:NAG:H3	2:E:1:NAG:H83	1.82	0.61
1:C:126:ARG:HH11	4:G:4:MAN:C3	2.18	0.57
8:C:421:HOH:O	4:G:4:MAN:H2	2.11	0.51
1:D:28:PRO:HB3	1:D:168:TYR:CZ	2.52	0.45
1:A:28:PRO:HB3	1:A:168:TYR:CZ	2.52	0.44
1:A:86:GLY:HA3	1:A:154:ILE:O	2.18	0.43
1:C:126:ARG:NH1	4:G:4:MAN:O3	2.50	0.42
1:D:93[B]:LYS:HD3	1:D:108:TRP:CE2	2.55	0.42
1:B:86:GLY:HA3	1:B:154:ILE:O	2.20	0.41
1:A:149:LEU:O	1:A:171:CYS:HA	2.20	0.40
2:E:1:NAG:H3	2:E:1:NAG:C8	2.50	0.40
1:D:86:GLY:HA3	1:D:154:ILE:O	2.21	0.40
1:C:28:PRO:HB3	1:C:168:TYR:CZ	2.56	0.40

All (1) 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)
8:C:586:HOH:O	8:C:619:HOH:O[1_455]	2.08	0.12

## 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	233/223 (104%)	224 (96%)	9 (4%)	0	100	100
1	B	231/223 (104%)	222 (96%)	7 (3%)	2 (1%)	17	12
1	C	226/223 (101%)	213 (94%)	12 (5%)	1 (0%)	34	32
1	D	231/223 (104%)	222 (96%)	6 (3%)	3 (1%)	12	7
All	All	921/892 (103%)	881 (96%)	34 (4%)	6 (1%)	29	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103[A]	GLY
1	B	103[B]	GLY
1	D	103[A]	GLY
1	D	103[B]	GLY
1	C	164	GLY
1	D	164	GLY

### 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	190/178 (107%)	187 (98%)	3 (2%)	62	69
1	B	186/178 (104%)	184 (99%)	2 (1%)	73	79
1	C	183/178 (103%)	181 (99%)	2 (1%)	73	79
1	D	187/178 (105%)	184 (98%)	3 (2%)	62	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	746/712 (105%)	736 (99%)	10 (1%)	73 75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	102	SER
1	A	195	SER
1	B	102[A]	SER
1	B	102[B]	SER
1	C	102	SER
1	C	195	SER
1	D	84	HIS
1	D	102[A]	SER
1	D	102[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

13 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	E	1	1,2	14,14,15	0.24	0	17,19,21	1.24	2 (11%)
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.53	0
2	MAN	E	3	2	11,11,12	1.05	1 (9%)	15,15,17	1.07	2 (13%)
2	MAN	E	4	2	11,11,12	0.79	0	15,15,17	1.11	1 (6%)
2	MAN	E	5	2	11,11,12	1.07	0	15,15,17	1.07	1 (6%)
2	MAN	E	6	2	11,11,12	0.91	1 (9%)	15,15,17	1.11	2 (13%)
2	MAN	E	7	2	11,11,12	0.71	0	15,15,17	0.86	0
3	NAG	F	1	1,3	14,14,15	0.56	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	0.49	0
4	NAG	G	1	1,4	14,14,15	0.45	0	17,19,21	0.56	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.50	0
4	MAN	G	3	4	11,11,12	1.17	2 (18%)	15,15,17	1.58	4 (26%)
4	MAN	G	4	4	11,11,12	0.89	0	15,15,17	2.19	6 (40%)

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	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	MAN	O5-C5	2.61	1.48	1.43
2	E	6	MAN	C1-C2	2.29	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	MAN	C1-C2	2.14	1.57	1.52
4	G	3	MAN	C4-C5	2.01	1.57	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	4	MAN	C1-O5-C5	4.93	118.86	112.19
4	G	4	MAN	O2-C2-C1	4.41	118.17	109.15
2	E	1	NAG	C2-N2-C7	3.67	128.13	122.90
4	G	3	MAN	C3-C4-C5	2.91	115.43	110.24
2	E	4	MAN	O2-C2-C3	-2.88	104.37	110.14
4	G	3	MAN	O2-C2-C3	-2.72	104.69	110.14
4	G	3	MAN	C2-C3-C4	2.71	115.58	110.89
2	E	6	MAN	O2-C2-C3	-2.57	104.98	110.14
4	G	4	MAN	C1-C2-C3	2.49	112.73	109.67
2	E	3	MAN	C1-C2-C3	2.33	112.54	109.67
2	E	5	MAN	O2-C2-C3	-2.31	105.52	110.14
2	E	3	MAN	O2-C2-C3	-2.26	105.60	110.14
2	E	6	MAN	C1-O5-C5	2.25	115.24	112.19
4	G	3	MAN	C1-O5-C5	2.24	115.22	112.19
4	G	4	MAN	O5-C5-C6	2.16	110.59	107.20
4	G	4	MAN	O5-C1-C2	2.05	113.94	110.77
2	E	1	NAG	C1-C2-N2	2.03	113.96	110.49
4	G	4	MAN	C6-C5-C4	-2.01	108.29	113.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	4	MAN	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
4	G	3	MAN	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
2	E	6	MAN	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
4	G	3	MAN	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6

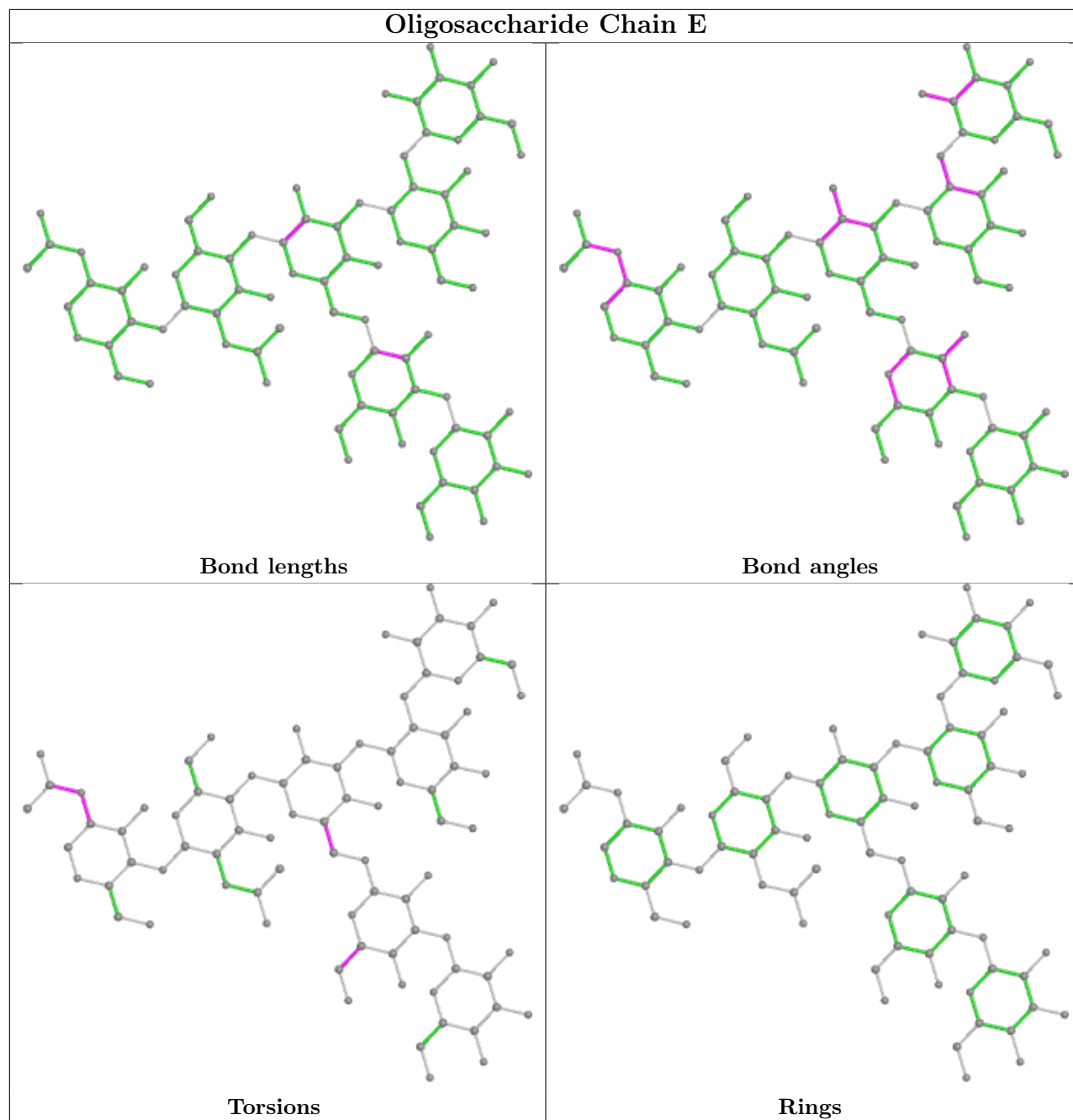
There are no ring outliers.

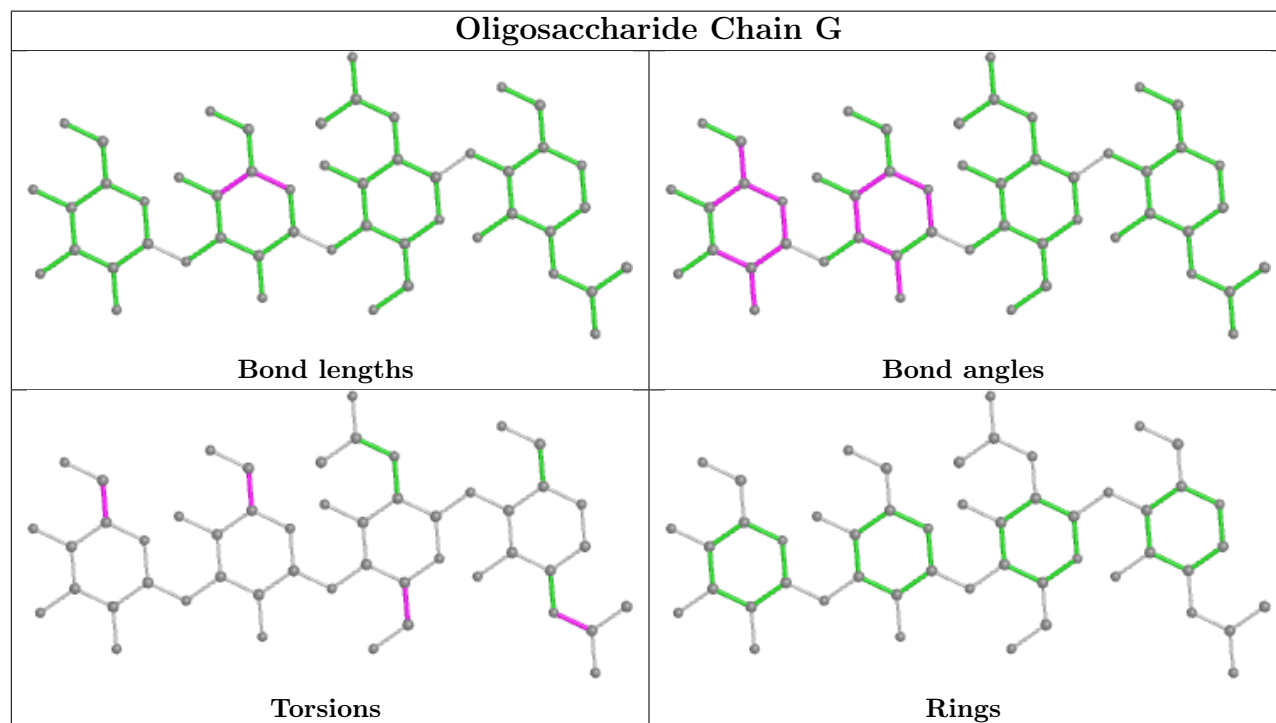
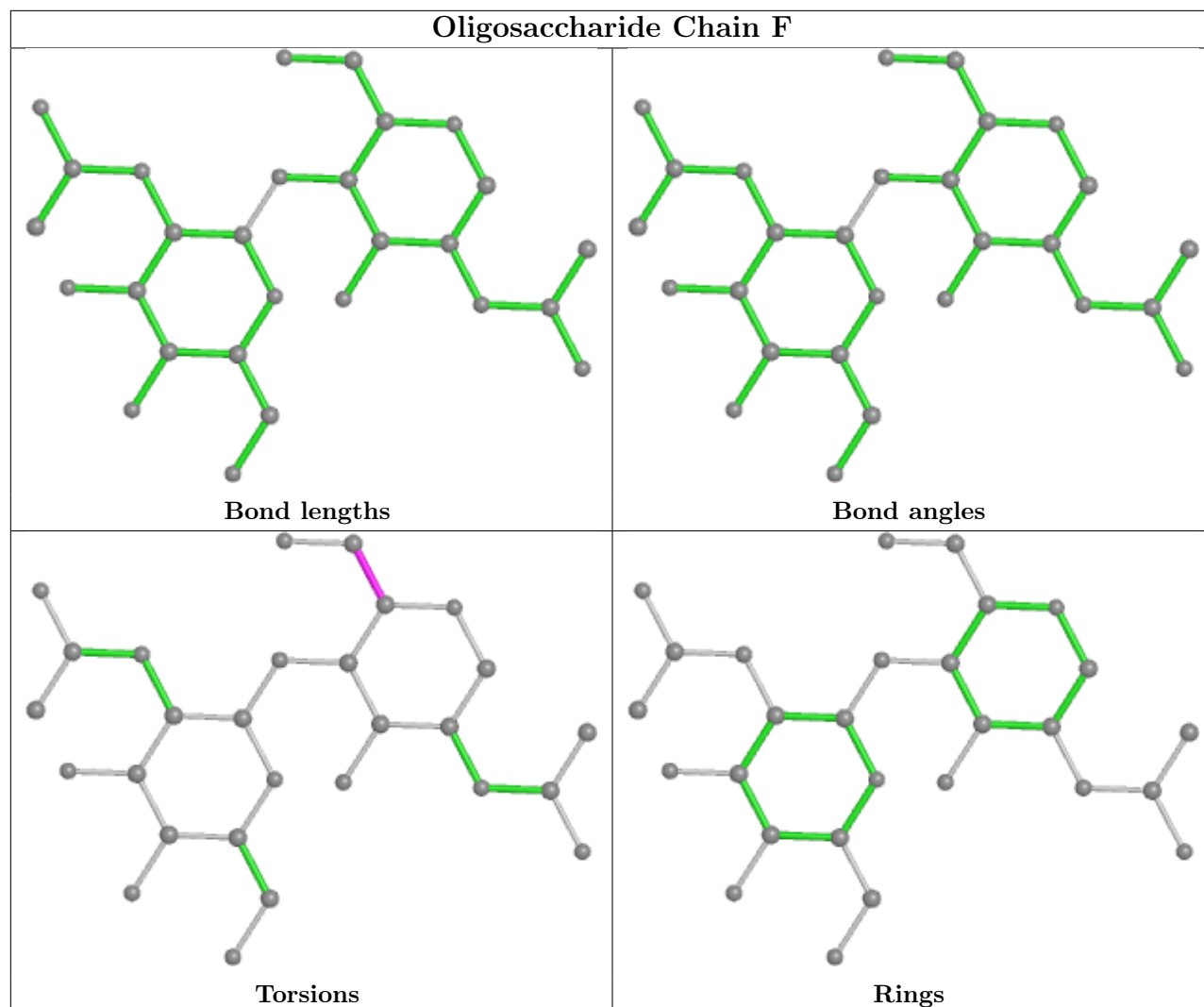
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
4	G	4	MAN	4	0

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







## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	OXY	D	303	-	1,1,1	0.12	0	-		
6	OXY	B	309	-	1,1,1	0.17	0	-		
7	NAG	D	301	1	14,14,15	0.27	0	17,19,21	0.38	0

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
7	NAG	D	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	223/223 (100%)	-0.44	3 (1%) 77 80	8, 14, 24, 59	0
1	B	223/223 (100%)	-0.27	3 (1%) 77 80	8, 15, 33, 66	0
1	C	223/223 (100%)	-0.36	7 (3%) 49 55	10, 19, 34, 66	0
1	D	223/223 (100%)	-0.10	2 (0%) 84 86	9, 21, 39, 49	0
All	All	892/892 (100%)	-0.29	15 (1%) 70 74	8, 17, 36, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	TRP	4.0
1	A	207	TRP	3.7
1	C	207	TRP	3.5
1	B	211	THR	3.1
1	D	223	CYS	3.0
1	C	211	THR	2.8
1	D	10	ASN	2.6
1	A	209	PRO	2.5
1	C	209	PRO	2.5
1	C	206	TYR	2.4
1	C	118	SER	2.4
1	B	208	PRO	2.3
1	C	208	PRO	2.2
1	C	210	VAL	2.1
1	A	208	PRO	2.1

### 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

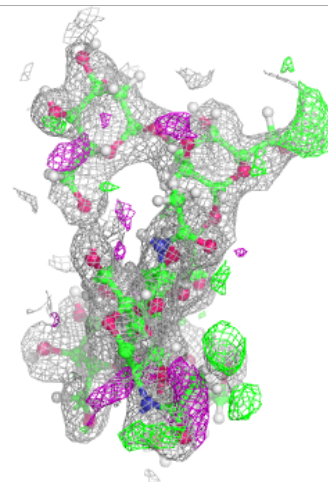
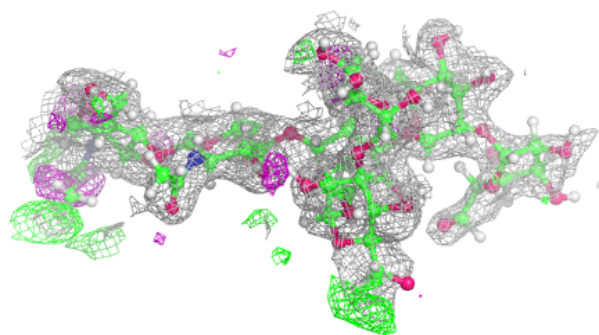
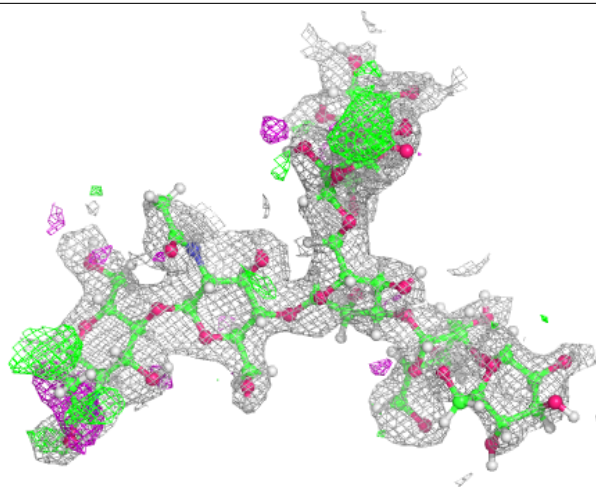
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	MAN	G	3	11/12	0.28	0.33	50,53,63,65	0
4	MAN	G	4	11/12	0.47	0.41	60,62,74,74	0
3	NAG	F	2	14/15	0.69	0.26	49,55,65,66	0
2	MAN	E	5	11/12	0.76	0.31	56,59,71,71	0
2	MAN	E	4	11/12	0.77	0.19	44,49,57,59	0
2	MAN	E	3	11/12	0.79	0.20	42,46,54,54	0
3	NAG	F	1	14/15	0.81	0.30	33,42,50,50	0
2	MAN	E	6	11/12	0.81	0.20	44,49,59,59	0
4	NAG	G	2	14/15	0.83	0.17	37,44,52,53	0
2	MAN	E	7	11/12	0.84	0.17	37,41,50,50	0
2	NAG	E	1	14/15	0.85	0.17	21,27,39,39	0
2	NAG	E	2	14/15	0.88	0.15	32,36,43,43	0
4	NAG	G	1	14/15	0.91	0.12	26,35,43,43	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.

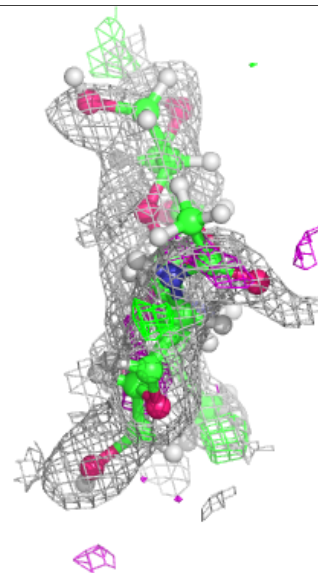
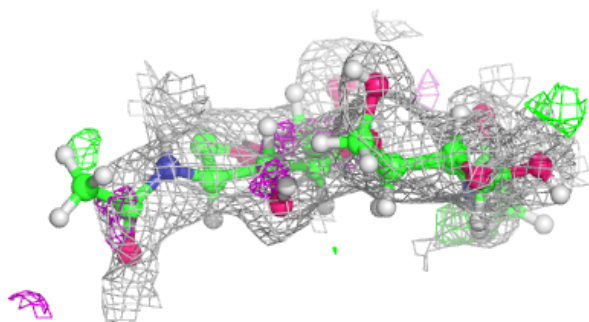
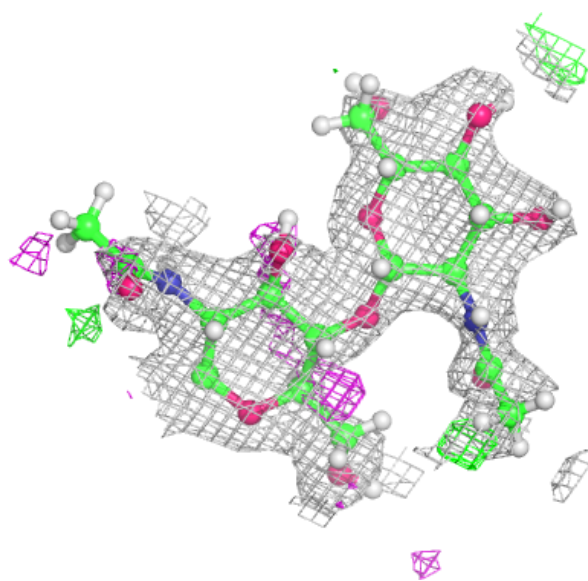
**Electron density around Chain E:**

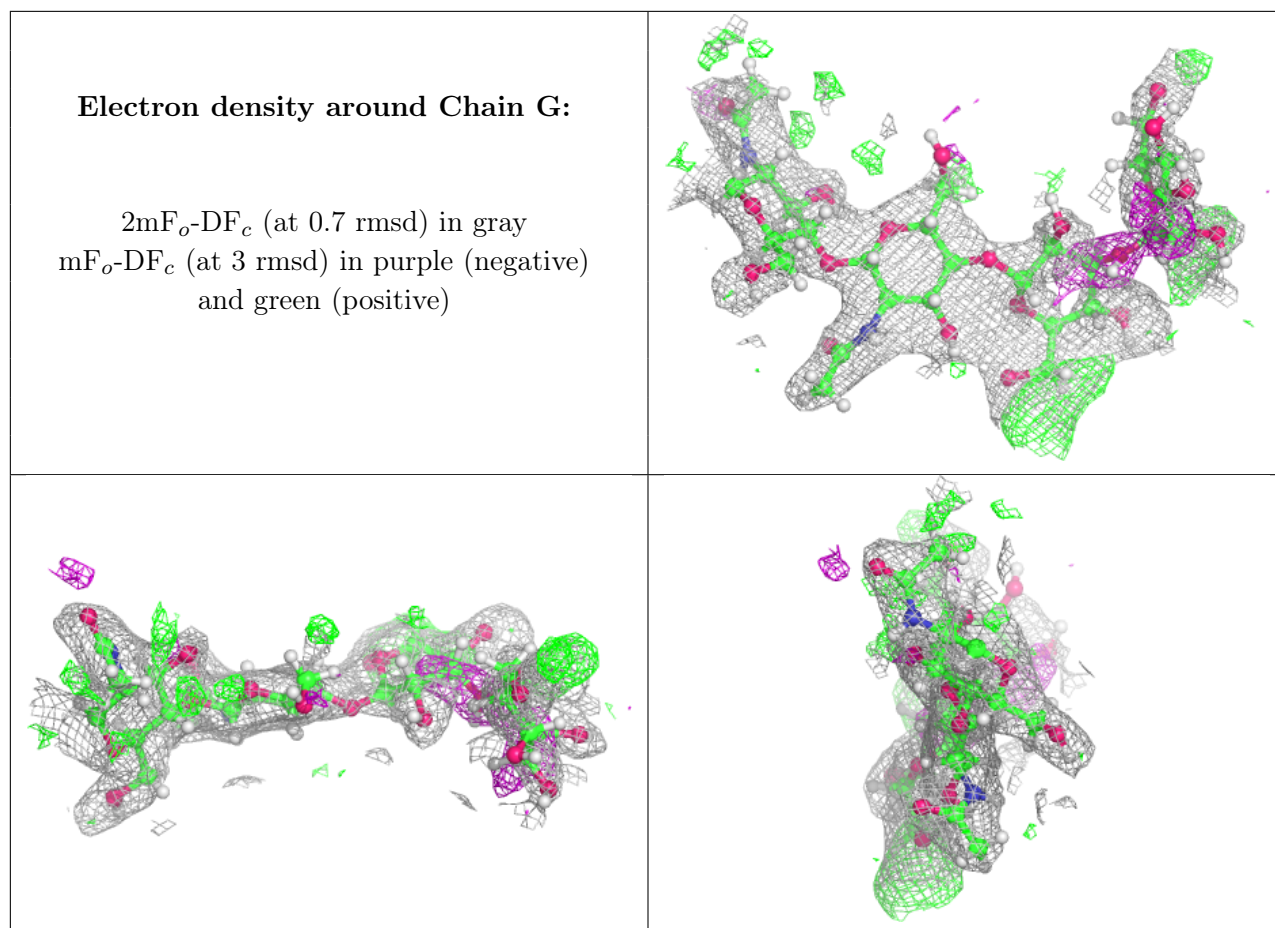
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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(Å <sup>2</sup> )	Q<0.9
6	OXY	D	303	2/2	0.85	0.34	41,41,41,41	2
7	NAG	D	301	14/15	0.86	0.30	30,40,49,49	0
6	OXY	B	309	2/2	0.90	0.29	41,41,41,41	2
5	CU	D	302	1/1	1.00	0.12	19,19,19,19	0
5	CU	A	308	1/1	1.00	0.09	11,11,11,11	0
5	CU	B	303	1/1	1.00	0.11	12,12,12,12	0
5	CU	C	305	1/1	1.00	0.10	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.