



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 23, 2020 – 02:14 PM JST

PDB ID : 7DFO  
Title : Crystal structure of glycoside hydrolase family 11 beta-xylanase from *Streptomyces olivaceoviridis* E-86 in complex with 4-O-methyl-alpha-D-glucuronopyranosyl xylo-tetraose  
Authors : Fujimoto, Z.; Kishine, N.; Kaneko, S.  
Deposited on : 2020-11-09  
Resolution : 2.00 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 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	:	2.16
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)	:	2.16

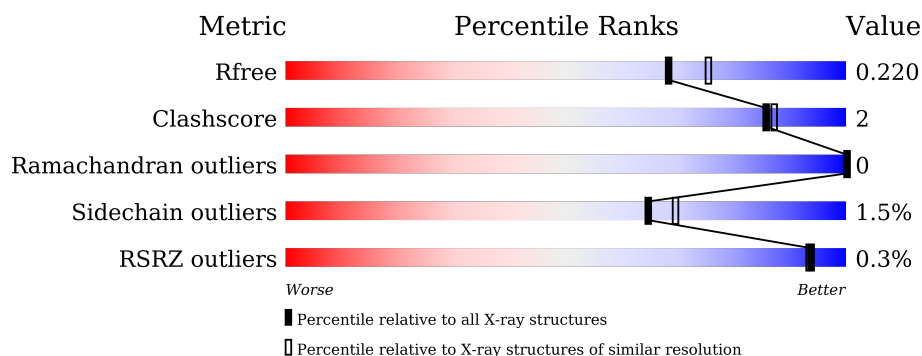
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>88%</span> <span>6%</span> <span>5%</span> </div> </div>
1	B	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>88%</span> <span>6%</span> <span>5%</span> </div> </div>
1	C	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>88%</span> <span>5%</span> <span>6%</span> </div> </div>
1	D	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>92%</span> <span>•</span> <span>5%</span> </div> </div>
1	E	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>88%</span> <span>7%</span> <span>5%</span> </div> </div>
1	F	205	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>90%</span> <span>5%</span> <span>5%</span> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	205	 89% 6% 5%
1	H	205	 86% 8% 5%
1	I	205	 88% 5% 5%
2	J	3	 100%
2	M	3	 100%
2	O	3	 67% 33%
2	P	3	 33% 33% 33%
3	K	5	 100%
3	N	5	 60% 40%
4	L	4	 100%
5	Q	2	 50% 50%

## 2 Entry composition

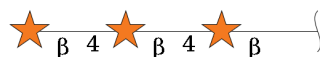
There are 8 unique types of molecules in this entry. The entry contains 14706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	1	0
			1503	944	254	301	4			
1	B	194	Total	C	N	O	S	0	2	0
			1511	949	256	302	4			
1	C	193	Total	C	N	O	S	0	0	0
			1494	939	252	299	4			
1	D	194	Total	C	N	O	S	0	0	0
			1499	942	253	300	4			
1	E	194	Total	C	N	O	S	0	1	0
			1503	944	254	301	4			
1	F	194	Total	C	N	O	S	0	1	0
			1505	945	256	300	4			
1	G	194	Total	C	N	O	S	0	2	0
			1509	947	257	301	4			
1	H	194	Total	C	N	O	S	0	1	0
			1502	944	253	301	4			
1	I	194	Total	C	N	O	S	0	1	0
			1504	944	256	300	4			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	J	3	Total	C	O	0	0	0
			28	15	13			
2	M	3	Total	C	O	0	0	0
			28	15	13			
2	O	3	Total	C	O	0	0	0
			28	15	13			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	P	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is an oligosaccharide called 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	K	5	Total	C	O	0	0	0
			50	27	23			
3	N	5	Total	C	O	0	0	0
			50	27	23			

- Molecule 4 is an oligosaccharide called 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	L	4	Total	C	O	0	0	0
			41	22	19			

- Molecule 5 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	Q	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	4	Total Cl 4 4	0	0
6	D	5	Total Cl 5 5	0	0
6	E	5	Total Cl 5 5	0	0
6	H	4	Total Cl 4 4	0	0
6	B	2	Total Cl 2 2	0	0
6	I	10	Total Cl 10 10	0	0
6	C	6	Total Cl 6 6	0	0
6	A	5	Total Cl 5 5	0	0
6	F	2	Total Cl 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	4	Total Na 4 4	0	0
7	E	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	I	4	Total Na 4 4	0	0
7	C	1	Total Na 1 1	0	0
7	A	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	117	Total O 117 117	0	0
8	B	88	Total O 88 88	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	101	Total 101	O 101	0	0
8	D	102	Total 102	O 102	0	0
8	E	100	Total 100	O 100	0	0
8	F	76	Total 76	O 76	0	0
8	G	73	Total 73	O 73	0	0
8	H	101	Total 101	O 101	0	0
8	I	90	Total 90	O 90	0	0

i

- Molecule 1: Endo-1,4-beta-xylanase



- Chain B:  88% 6% 5%

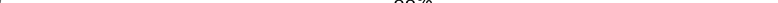


- Chain C:  88% 5% 6%



- Chain D:  92% • 5%




- Chain E:  88% 7% 5%



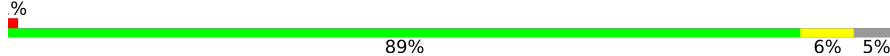
- Molecule 1: Endo-1,4-beta-xylanase



Chain F:  90% 5% 5%



- Molecule 1: Endo-1,4-beta-xylanase

Chain G:  89% 6% 5%




- Molecule 1: Endo-1,4-beta-xylanase

Chain H:  86% 8% 5%



- Molecule 1: Endo-1,4-beta-xylanase

Chain I:  88% 5% 5%



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain J:  100%



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain M:  100%



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain O:  67% 33%



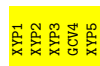
- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain P:  33% 33% 33%



- Molecule 3: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain K:  100%



- Molecule 3: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-[beta-D-xylopyranose-(1-4)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain N:  60% 40%



- Molecule 4: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain L:  100%



- Molecule 5: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain Q:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.71Å 142.71Å 72.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 2.00 47.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.06-2.00) 99.3 (47.02-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.165 , 0.218 0.172 , 0.220	Depositor DCC
$R_{free}$ test set	5434 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.187 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: XYP, NA, CL, GCV

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	0.66	0/1551	0.88	0/2113
1	B	0.67	0/1563	0.89	0/2128
1	C	0.68	0/1538	0.89	0/2095
1	D	0.68	0/1543	0.87	0/2102
1	E	0.65	0/1551	0.87	1/2113 (0.0%)
1	F	0.66	0/1554	0.86	0/2116
1	G	0.65	0/1563	0.85	0/2128
1	H	0.69	0/1550	0.88	0/2112
1	I	0.75	0/1554	0.88	0/2116
All	All	0.68	0/13967	0.87	1/19023 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	ARG	NE-CZ-NH1	5.23	122.92	120.30

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	1503	0	1373	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1511	0	1386	7	0
1	C	1494	0	1366	6	0
1	D	1499	0	1370	3	0
1	E	1503	0	1373	6	0
1	F	1505	0	1380	4	0
1	G	1509	0	1384	6	0
1	H	1502	0	1374	13	0
1	I	1504	0	1374	9	0
2	J	28	0	0	0	0
2	M	28	0	0	0	0
2	O	28	0	0	1	0
2	P	28	0	0	1	0
3	K	50	0	9	0	0
3	N	50	0	9	1	0
4	L	41	0	9	0	0
5	Q	19	0	0	1	0
6	A	5	0	0	0	0
6	B	2	0	0	0	0
6	C	6	0	0	1	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	2	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	10	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	4	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	I	4	0	0	0	0
8	A	117	0	0	0	0
8	B	88	0	0	1	0
8	C	101	0	0	1	0
8	D	102	0	0	0	0
8	E	100	0	0	0	0
8	F	76	0	0	0	0
8	G	73	0	0	0	0
8	H	101	0	0	0	0
8	I	90	0	0	0	0
All	All	14706	0	12407	59	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 2.

The worst 5 of 59 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:H:21[B]:THR:HG22	1:H:47:PHE:HB2	1.46	0.94
1:H:21[B]:THR:HG22	1:H:47:PHE:CB	2.06	0.85
1:D:128:GLU:O	1:D:131:LYS:HE2	2.02	0.60
1:G:113:THR:O	1:G:141:GLN:HG3	2.07	0.54
1:C:46:ASN:HD22	1:C:47:PHE:N	2.06	0.54

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	193/205 (94%)	188 (97%)	5 (3%)	0	100	100
1	B	194/205 (95%)	189 (97%)	5 (3%)	0	100	100
1	C	191/205 (93%)	185 (97%)	6 (3%)	0	100	100
1	D	192/205 (94%)	187 (97%)	5 (3%)	0	100	100
1	E	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
1	F	193/205 (94%)	189 (98%)	4 (2%)	0	100	100
1	G	194/205 (95%)	189 (97%)	5 (3%)	0	100	100
1	H	193/205 (94%)	188 (97%)	5 (3%)	0	100	100
1	I	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
All	All	1736/1845 (94%)	1687 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	157/165 (95%)	153 (98%)	4 (2%)	47	49
1	B	158/165 (96%)	155 (98%)	3 (2%)	57	61
1	C	156/165 (94%)	153 (98%)	3 (2%)	57	61
1	D	156/165 (94%)	156 (100%)	0	100	100
1	E	157/165 (95%)	155 (99%)	2 (1%)	69	74
1	F	157/165 (95%)	154 (98%)	3 (2%)	57	61
1	G	158/165 (96%)	156 (99%)	2 (1%)	69	74
1	H	157/165 (95%)	157 (100%)	0	100	100
1	I	157/165 (95%)	153 (98%)	4 (2%)	47	49
All	All	1413/1485 (95%)	1392 (98%)	21 (2%)	65	69

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	193	LEU
1	E	193	LEU
1	I	59	ARG
1	C	59	ARG
1	I	160	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	153	ASN
1	F	118	GLN
1	I	118	GLN
1	E	46	ASN
1	E	118	GLN

### 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 ⓘ

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	XYP	J	1	2	10,10,10	0.92	0	14,14,14	1.85	3 (21%)
2	XYP	J	2	2	9,9,10	0.89	0	10,12,14	2.32	5 (50%)
2	XYP	J	3	2	9,9,10	0.55	0	10,12,14	2.09	3 (30%)
3	XYP	K	1	3	10,10,10	0.65	0	14,14,14	1.91	4 (28%)
3	XYP	K	2	3	9,9,10	0.91	0	10,12,14	1.48	3 (30%)
3	XYP	K	3	3	9,9,10	0.63	0	10,12,14	2.16	4 (40%)
3	GCV	K	4	3	10,13,14	1.23	1 (10%)	11,18,20	1.68	2 (18%)
3	XYP	K	5	3	9,9,10	0.71	0	10,12,14	2.07	3 (30%)
4	XYP	L	1	4	10,10,10	1.22	1 (10%)	14,14,14	2.10	5 (35%)
4	XYP	L	2	4	9,9,10	1.04	0	10,12,14	1.07	1 (10%)
4	XYP	L	3	4	9,9,10	1.16	1 (11%)	10,12,14	1.76	4 (40%)
4	GCV	L	4	4	10,13,14	1.16	0	11,18,20	1.38	1 (9%)
2	XYP	M	1	2	10,10,10	0.71	0	14,14,14	1.88	3 (21%)
2	XYP	M	2	2	9,9,10	0.77	0	10,12,14	1.49	3 (30%)
2	XYP	M	3	2	9,9,10	0.74	0	10,12,14	2.01	3 (30%)
3	XYP	N	1	3	10,10,10	1.00	0	14,14,14	2.04	5 (35%)
3	XYP	N	2	3	9,9,10	0.77	0	10,12,14	1.66	3 (30%)
3	XYP	N	3	3	9,9,10	0.54	0	10,12,14	1.37	1 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GCV	N	4	3	10,13,14	1.09	0	11,18,20	1.87	4 (36%)
3	XYP	N	5	3	9,9,10	0.75	0	10,12,14	1.27	1 (10%)
2	XYP	O	1	2	10,10,10	1.02	0	14,14,14	2.07	6 (42%)
2	XYP	O	2	2	9,9,10	0.79	0	10,12,14	1.28	1 (10%)
2	XYP	O	3	2	9,9,10	0.85	0	10,12,14	2.13	3 (30%)
2	XYP	P	1	2	10,10,10	1.01	0	14,14,14	1.01	0
2	XYP	P	2	2	9,9,10	0.56	0	10,12,14	1.78	2 (20%)
2	XYP	P	3	2	9,9,10	0.67	0	10,12,14	1.64	3 (30%)
5	XYP	Q	1	5	10,10,10	0.81	0	14,14,14	1.74	4 (28%)
5	XYP	Q	2	5	9,9,10	1.54	2 (22%)	10,12,14	2.09	4 (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	XYP	J	1	2	-	-	0/1/1/1
2	XYP	J	2	2	-	-	0/1/1/1
2	XYP	J	3	2	-	-	0/1/1/1
3	XYP	K	1	3	-	-	0/1/1/1
3	XYP	K	2	3	-	-	0/1/1/1
3	XYP	K	3	3	-	-	0/1/1/1
3	GCV	K	4	3	-	1/2/23/26	0/1/1/1
3	XYP	K	5	3	-	-	0/1/1/1
4	XYP	L	1	4	-	-	0/1/1/1
4	XYP	L	2	4	-	-	0/1/1/1
4	XYP	L	3	4	-	-	0/1/1/1
4	GCV	L	4	4	-	1/2/23/26	0/1/1/1
2	XYP	M	1	2	-	-	0/1/1/1
2	XYP	M	2	2	-	-	0/1/1/1
2	XYP	M	3	2	-	-	0/1/1/1
3	XYP	N	1	3	-	-	0/1/1/1
3	XYP	N	2	3	-	-	0/1/1/1
3	XYP	N	3	3	-	-	0/1/1/1
3	GCV	N	4	3	-	0/2/23/26	0/1/1/1
3	XYP	N	5	3	-	-	0/1/1/1
2	XYP	O	1	2	-	-	0/1/1/1
2	XYP	O	2	2	-	-	0/1/1/1
2	XYP	O	3	2	-	-	0/1/1/1
2	XYP	P	1	2	-	-	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	P	2	2	-	-	0/1/1/1
2	XYP	P	3	2	-	-	0/1/1/1
5	XYP	Q	1	5	-	-	0/1/1/1
5	XYP	Q	2	5	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	2	XYP	C2-C3	2.87	1.56	1.52
5	Q	2	XYP	O2-C2	2.63	1.48	1.43
3	K	4	GCV	C2-C3	2.50	1.56	1.52
4	L	3	XYP	C2-C3	2.45	1.56	1.52
4	L	1	XYP	O1-C1	2.12	1.46	1.39

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	XYP	C5-C4-C3	5.04	115.86	109.67
2	J	3	XYP	C1-C2-C3	5.03	115.85	109.67
2	J	1	XYP	C4-C3-C2	4.68	119.00	110.89
2	J	2	XYP	O4-C4-C3	-4.58	100.96	110.14
2	O	1	XYP	C5-C4-C3	4.56	115.27	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	4	GCV	C3-C4-O4-C7
4	L	4	GCV	C5-C4-O4-C7

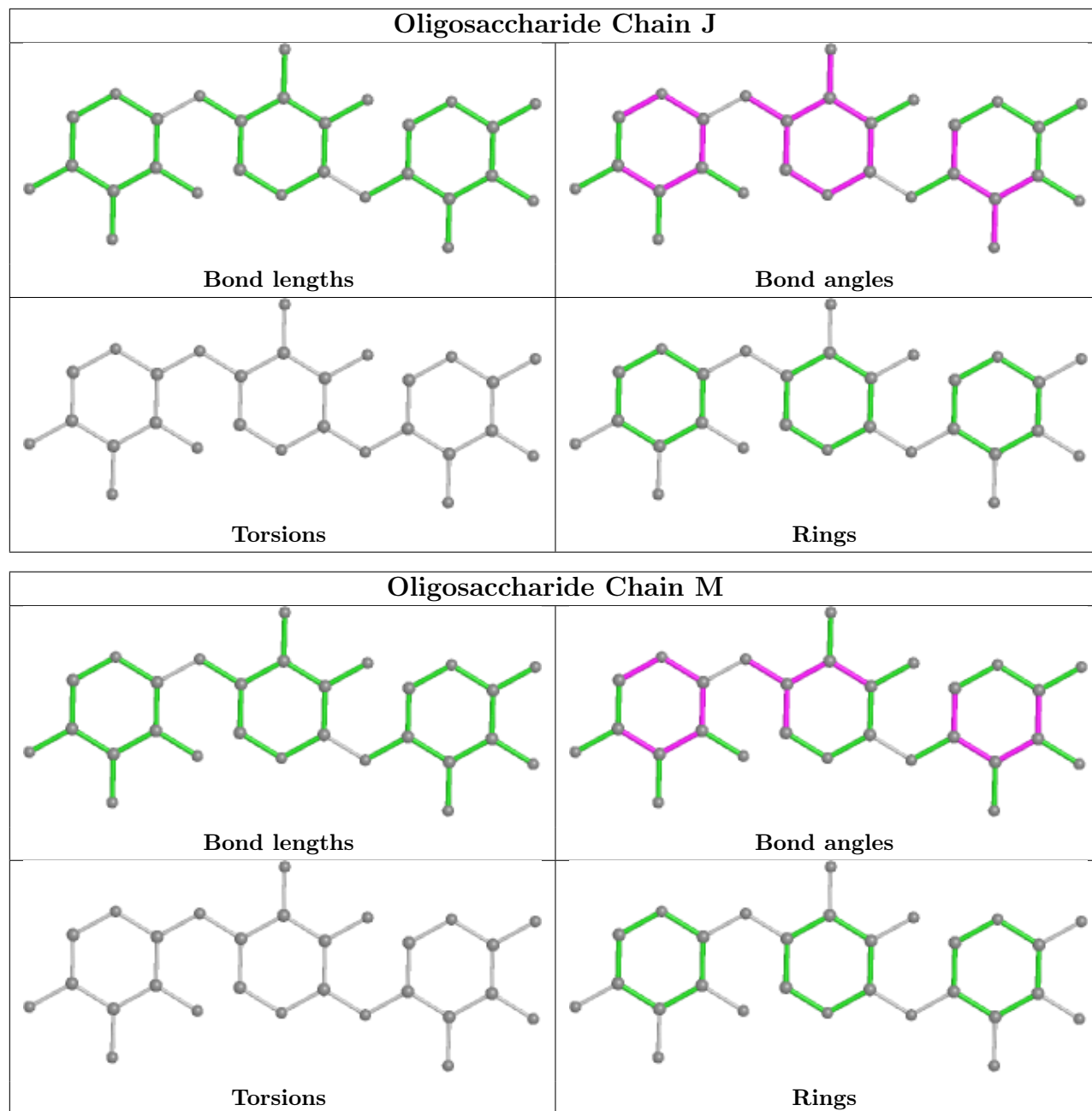
There are no ring outliers.

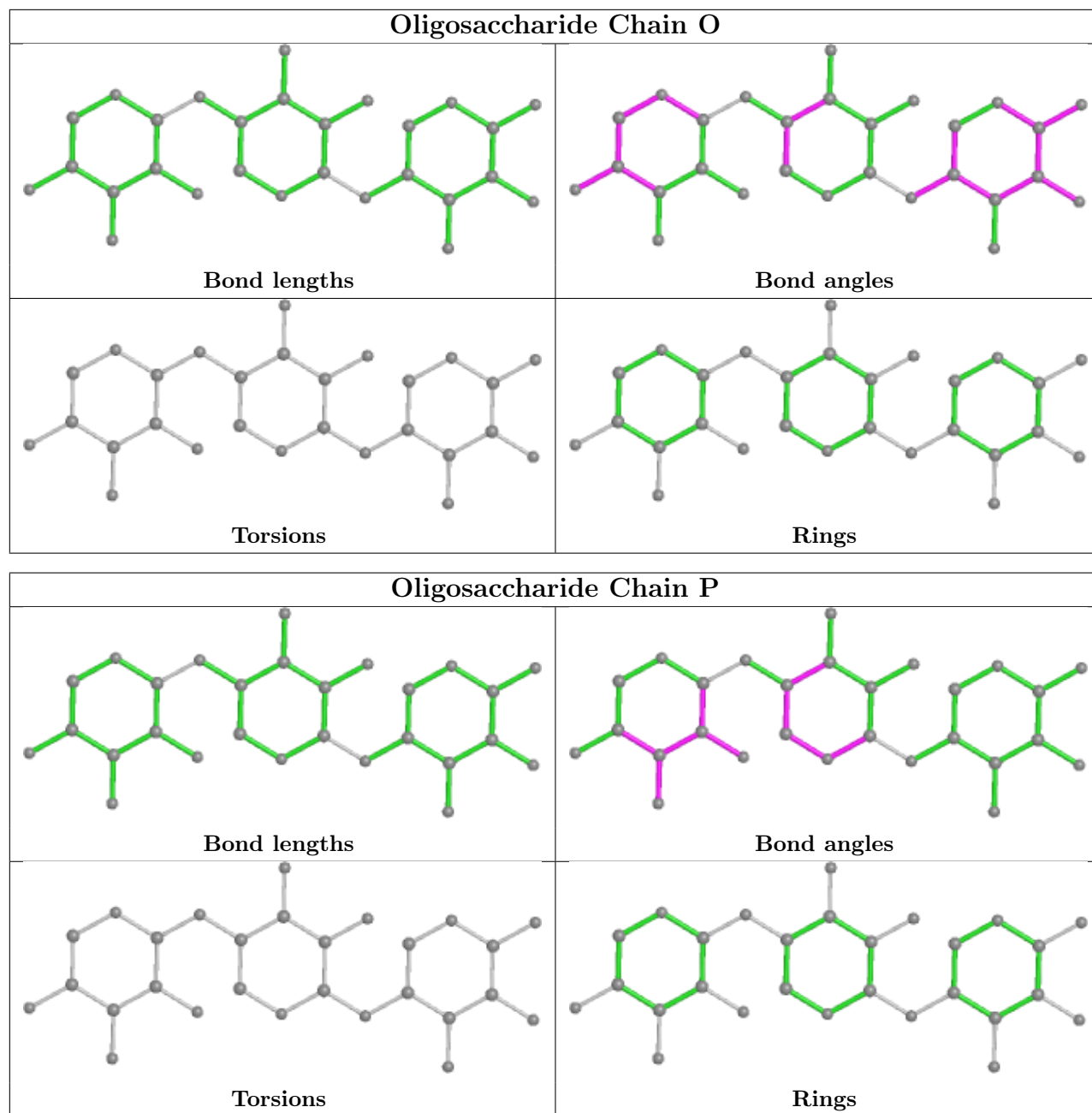
5 monomers are involved in 3 short contacts:

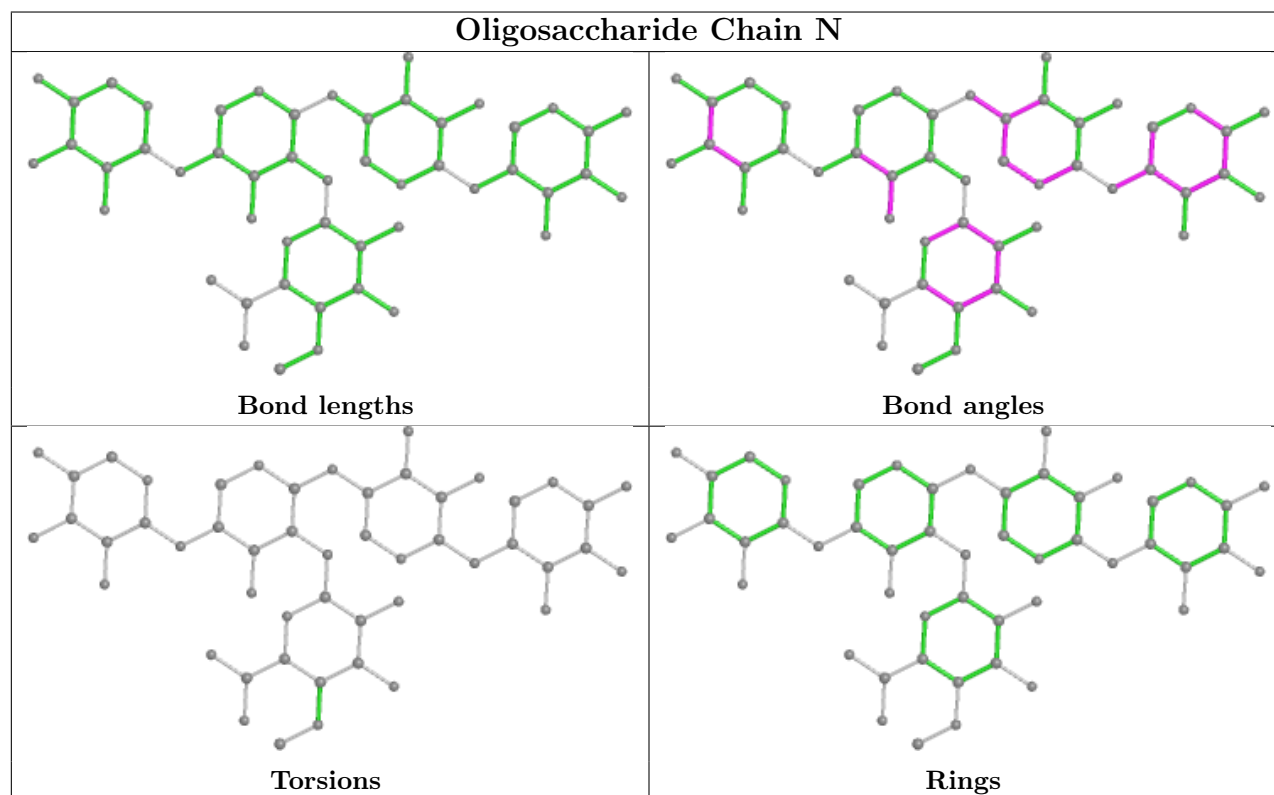
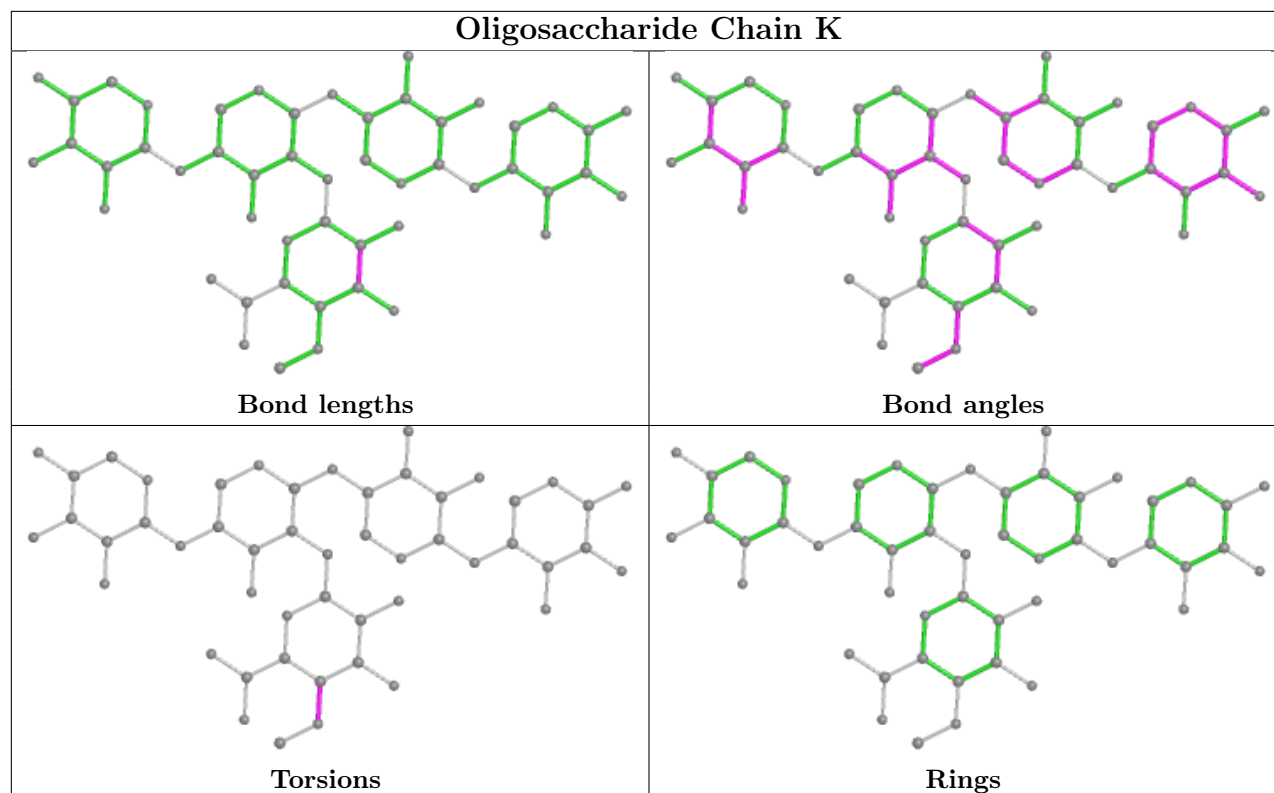
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	4	GCV	1	0
3	N	3	XYP	1	0
2	O	1	XYP	1	0
5	Q	1	XYP	1	0
2	P	3	XYP	1	0

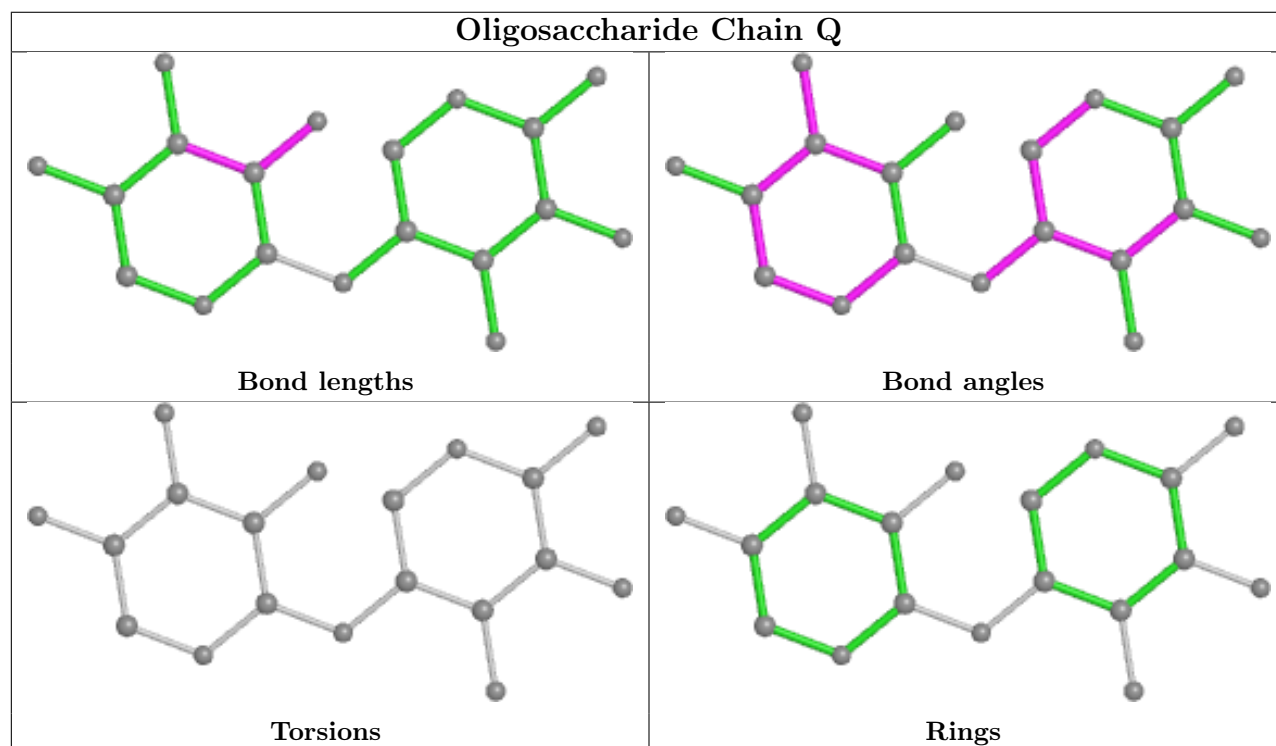
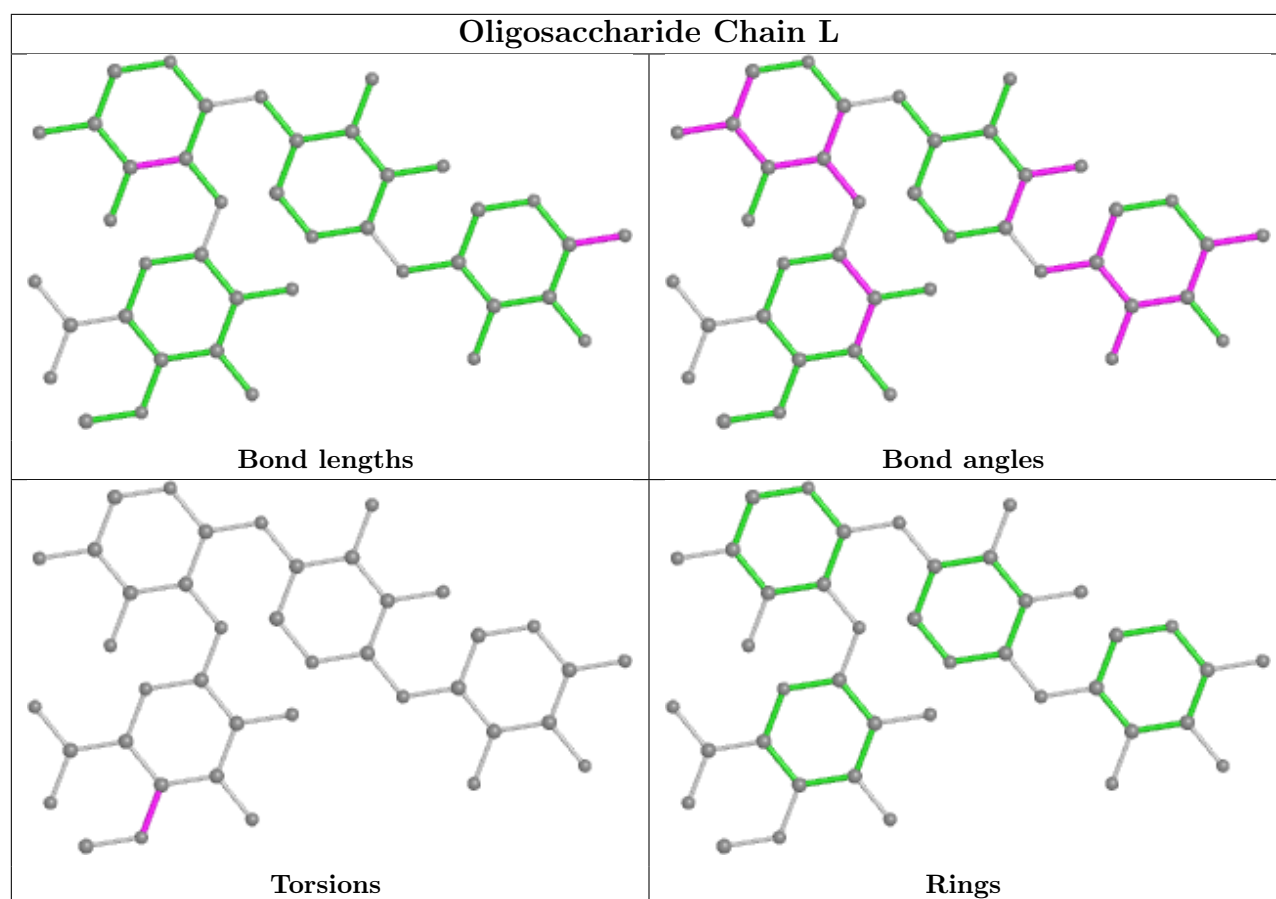
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry

Of 56 ligands modelled in this entry, 56 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	194/205 (94%)	-0.50	2 (1%) 82 81	22, 29, 46, 73	0
1	B	194/205 (94%)	-0.50	0 100 100	23, 33, 44, 61	0
1	C	193/205 (94%)	-0.54	0 100 100	23, 31, 46, 60	0
1	D	194/205 (94%)	-0.55	0 100 100	23, 30, 40, 57	0
1	E	194/205 (94%)	-0.55	1 (0%) 91 90	25, 33, 47, 64	0
1	F	194/205 (94%)	-0.44	0 100 100	28, 38, 50, 64	0
1	G	194/205 (94%)	-0.51	2 (1%) 82 81	26, 35, 48, 70	0
1	H	194/205 (94%)	-0.54	0 100 100	24, 32, 43, 57	0
1	I	194/205 (94%)	-0.54	0 100 100	24, 32, 43, 54	0
All	All	1745/1845 (94%)	-0.52	5 (0%) 94 93	22, 33, 46, 73	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	2.9
1	E	193	LEU	2.6
1	G	193	LEU	2.5
1	G	194	ALA	2.2
1	A	193	LEU	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

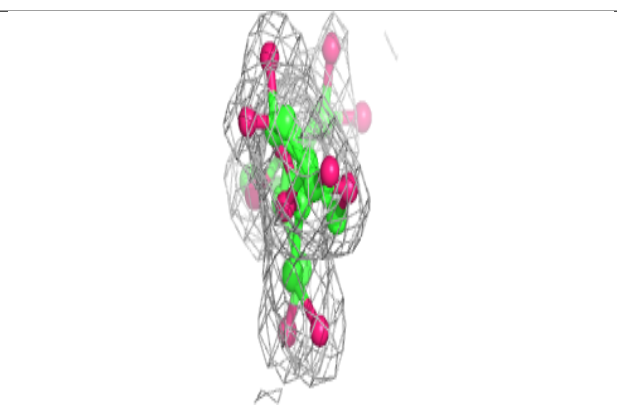
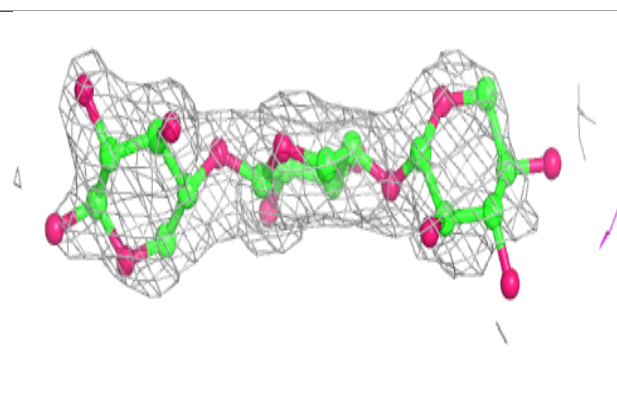
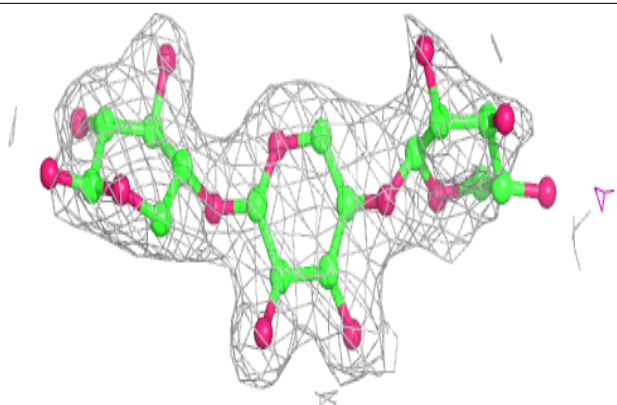
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GCV	L	4	13/14	0.72	0.27	63,76,82,83	0
2	XYP	P	3	9/10	0.74	0.30	68,82,88,95	0
3	XYP	N	5	9/10	0.77	0.27	72,78,83,83	0
3	GCV	K	4	13/14	0.77	0.24	65,76,82,84	0
5	XYP	Q	1	10/10	0.81	0.50	72,88,95,96	0
3	GCV	N	4	13/14	0.83	0.25	60,69,82,86	0
3	XYP	K	5	9/10	0.84	0.20	69,72,75,80	0
2	XYP	P	2	9/10	0.85	0.14	68,70,76,83	0
5	XYP	Q	2	9/10	0.85	0.24	39,55,64,65	0
2	XYP	J	3	9/10	0.87	0.18	62,73,78,88	0
2	XYP	M	3	9/10	0.88	0.16	59,68,72,75	0
4	XYP	L	3	9/10	0.89	0.12	40,50,60,63	0
4	XYP	L	1	10/10	0.89	0.20	36,46,55,55	0
2	XYP	M	1	10/10	0.90	0.17	51,58,62,68	0
2	XYP	P	1	10/10	0.91	0.17	50,59,63,67	0
2	XYP	O	3	9/10	0.91	0.11	50,56,61,67	0
2	XYP	O	1	10/10	0.92	0.20	44,49,57,58	0
3	XYP	N	1	10/10	0.93	0.20	38,48,54,55	0
2	XYP	J	1	10/10	0.93	0.13	40,51,61,66	0
2	XYP	J	2	9/10	0.94	0.09	33,41,44,48	0
3	XYP	N	3	9/10	0.94	0.09	41,47,55,56	0
3	XYP	K	3	9/10	0.95	0.08	38,46,53,54	0
2	XYP	M	2	9/10	0.95	0.10	32,43,49,54	0
3	XYP	K	2	9/10	0.95	0.10	26,27,31,31	0
2	XYP	O	2	9/10	0.96	0.09	32,40,44,45	0
3	XYP	N	2	9/10	0.96	0.09	32,34,37,40	0
3	XYP	K	1	10/10	0.96	0.18	37,47,50,57	0
4	XYP	L	2	9/10	0.96	0.07	27,34,37,38	0

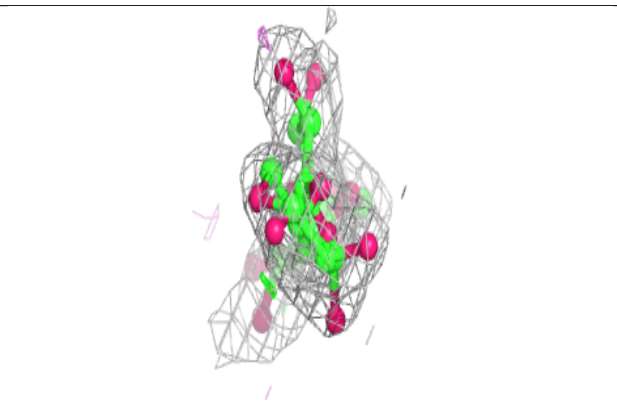
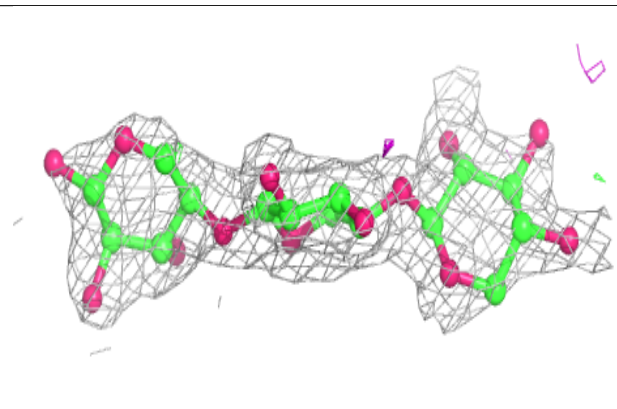
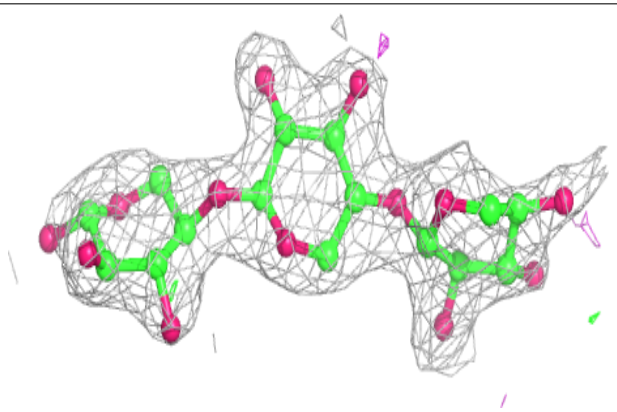
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain J:**

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

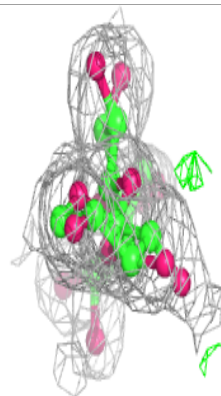
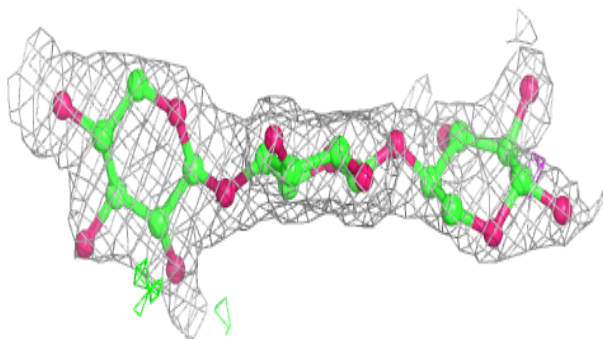
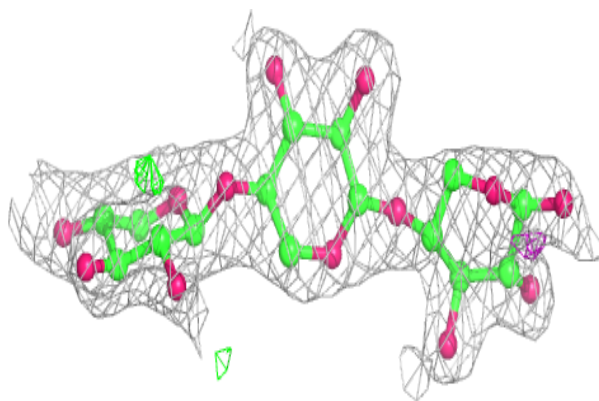
**Electron density around Chain M:**

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

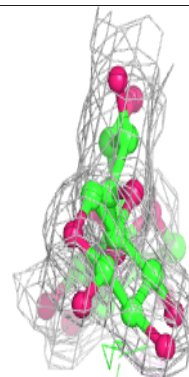
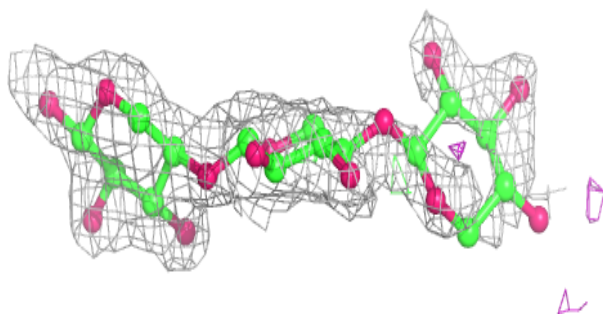
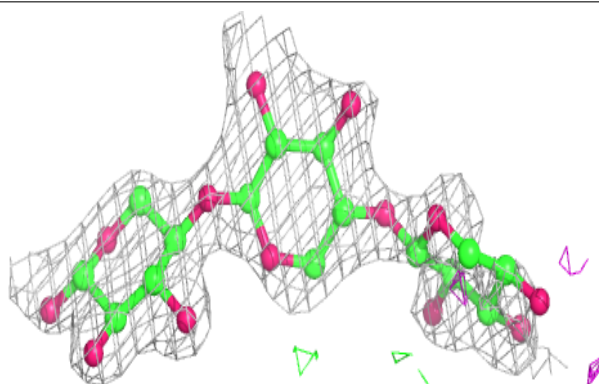


**Electron density around Chain O:**

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

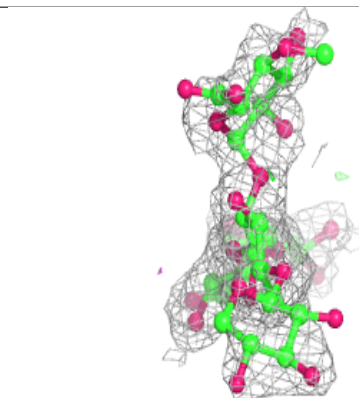
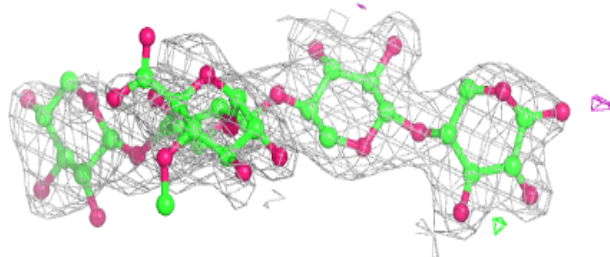
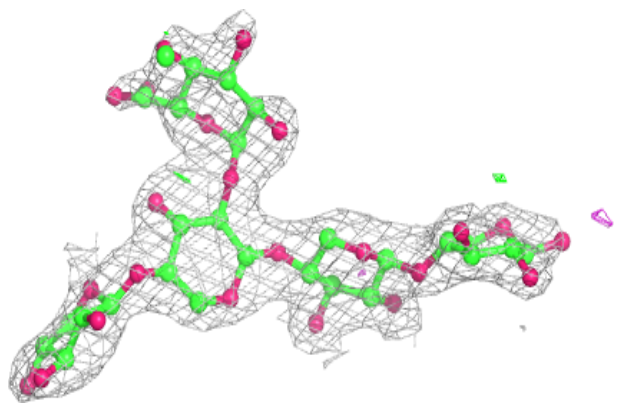
**Electron density around Chain P:**

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

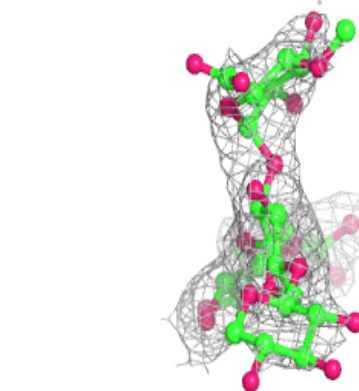
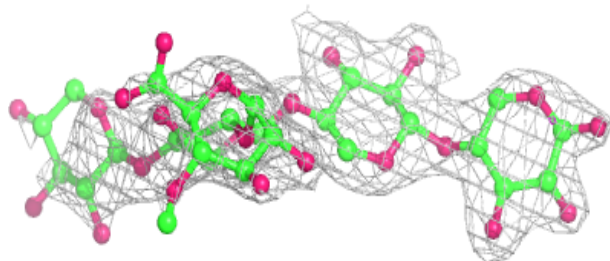
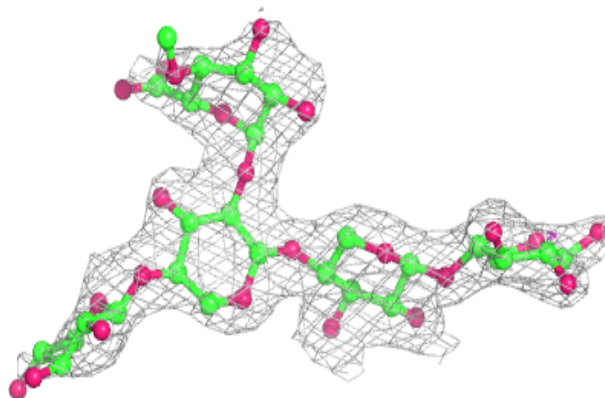


**Electron density around Chain K:**

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

**Electron density around Chain N:**

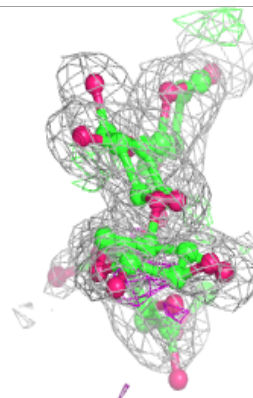
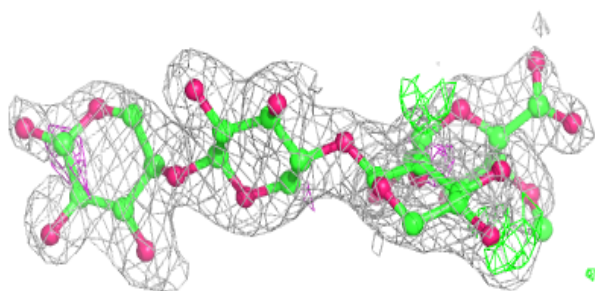
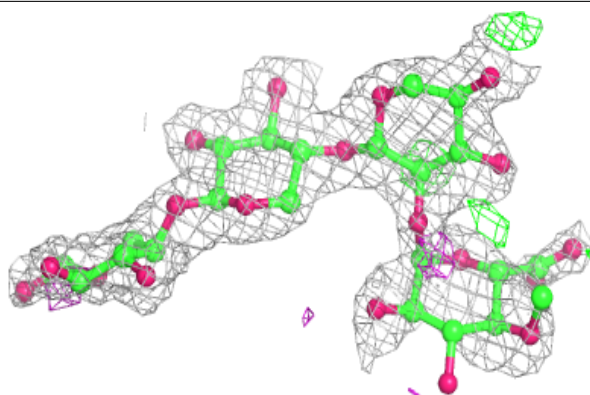
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



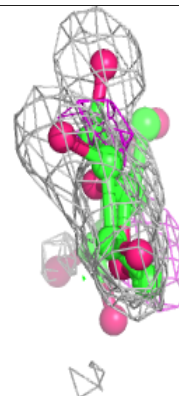
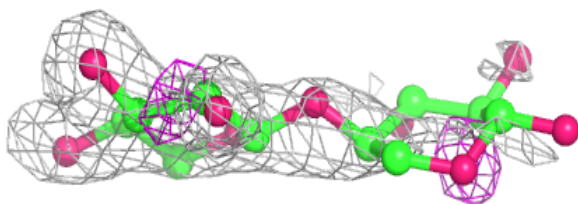
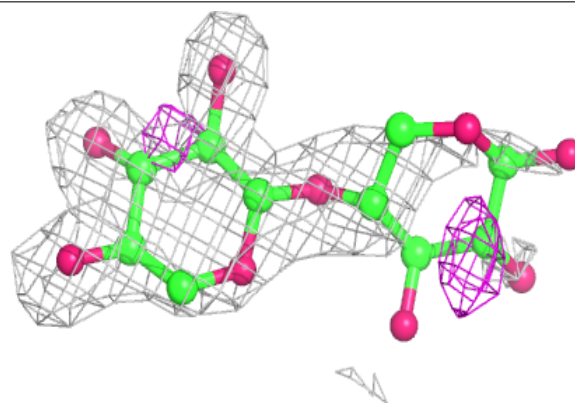


**Electron density around Chain L:**

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

**Electron density around Chain Q:**

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



## 6.4 Ligands ⓘ

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
7	NA	D	304	1/1	0.82	0.29	45,45,45,45	0
7	NA	C	307	1/1	0.91	0.19	43,43,43,43	0
6	CL	D	303	1/1	0.92	0.26	43,43,43,43	0
7	NA	I	313	1/1	0.92	0.32	43,43,43,43	0
7	NA	F	303	1/1	0.93	0.16	44,44,44,44	0
7	NA	D	306	1/1	0.94	0.19	41,41,41,41	0
7	NA	A	406	1/1	0.94	0.10	38,38,38,38	0
7	NA	D	305	1/1	0.94	0.22	42,42,42,42	0
7	NA	E	306	1/1	0.94	0.14	44,44,44,44	0
7	NA	I	311	1/1	0.96	0.14	50,50,50,50	0
7	NA	I	314	1/1	0.96	0.13	39,39,39,39	0
7	NA	I	312	1/1	0.96	0.19	37,37,37,37	0
6	CL	C	305	1/1	0.97	0.15	45,45,45,45	0
6	CL	E	303	1/1	0.97	0.09	41,41,41,41	0
6	CL	I	310	1/1	0.97	0.20	43,43,43,43	0
7	NA	B	303	1/1	0.97	0.12	40,40,40,40	0
6	CL	C	301	1/1	0.97	0.06	33,33,33,33	0
6	CL	F	301	1/1	0.97	0.19	41,41,41,41	0
6	CL	D	302	1/1	0.97	0.08	40,40,40,40	0
6	CL	I	304	1/1	0.97	0.16	45,45,45,45	0
6	CL	I	308	1/1	0.98	0.15	42,42,42,42	0
6	CL	H	301	1/1	0.98	0.09	40,40,40,40	0
6	CL	I	303	1/1	0.98	0.14	42,42,42,42	0
6	CL	C	306	1/1	0.98	0.07	37,37,37,37	0
6	CL	H	302	1/1	0.98	0.07	37,37,37,37	0
6	CL	G	302	1/1	0.98	0.06	39,39,39,39	0
7	NA	D	307	1/1	0.98	0.05	42,42,42,42	0
6	CL	E	301	1/1	0.98	0.11	35,35,35,35	0
6	CL	I	307	1/1	0.98	0.08	42,42,42,42	0
6	CL	E	304	1/1	0.98	0.07	41,41,41,41	0
6	CL	I	309	1/1	0.98	0.13	43,43,43,43	0
6	CL	H	304	1/1	0.99	0.03	35,35,35,35	0
6	CL	H	303	1/1	0.99	0.13	41,41,41,41	0
6	CL	D	308	1/1	0.99	0.07	36,36,36,36	0
6	CL	B	302	1/1	0.99	0.06	33,33,33,33	0
6	CL	C	304	1/1	0.99	0.05	31,31,31,31	0
6	CL	A	401	1/1	0.99	0.07	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	G	304	1/1	0.99	0.13	39,39,39,39	0
6	CL	D	301	1/1	0.99	0.04	38,38,38,38	0
6	CL	A	404	1/1	0.99	0.06	30,30,30,30	0
6	CL	C	302	1/1	0.99	0.05	38,38,38,38	0
6	CL	E	305	1/1	0.99	0.06	32,32,32,32	0
6	CL	A	402	1/1	0.99	0.11	37,37,37,37	0
6	CL	G	301	1/1	0.99	0.12	37,37,37,37	0
6	CL	A	403	1/1	0.99	0.10	40,40,40,40	0
6	CL	D	309	1/1	0.99	0.04	32,32,32,32	0
6	CL	C	303	1/1	0.99	0.04	34,34,34,34	0
6	CL	E	302	1/1	0.99	0.03	32,32,32,32	0
6	CL	I	301	1/1	0.99	0.14	42,42,42,42	0
6	CL	I	306	1/1	0.99	0.15	40,40,40,40	0
6	CL	F	302	1/1	0.99	0.10	40,40,40,40	0
6	CL	B	301	1/1	0.99	0.06	36,36,36,36	0
6	CL	I	305	1/1	1.00	0.04	27,27,27,27	0
6	CL	I	302	1/1	1.00	0.06	33,33,33,33	0
6	CL	A	405	1/1	1.00	0.05	29,29,29,29	0
6	CL	G	303	1/1	1.00	0.04	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.