



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 10:49 AM BST

PDB ID : 3VPL  
Title : Crystal structure of a 2-fluoroxylotriosyl complex of the Vibrio sp. AX-4 Beta-1,3-xylanase  
Authors : Watanabe, N.; Sakaguchi, K.  
Deposited on : 2012-03-05  
Resolution : 1.20 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 : 2.13.1  
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

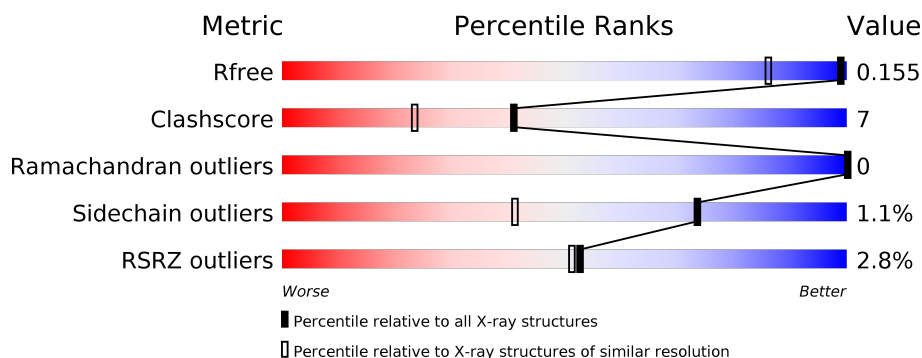
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	333	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
3	C	3	<div> <div>33%</div> <div>67%</div> </div>

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
2	BXF	B	1	X	-	-	-
4	DNX	A	1004	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3278 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 Beta-1,3-xylanase XYL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2700	1726	447	523	4	2	30	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	HIS	-	expression tag	UNP D5MP61
A	329	HIS	-	expression tag	UNP D5MP61
A	330	HIS	-	expression tag	UNP D5MP61
A	331	HIS	-	expression tag	UNP D5MP61
A	332	HIS	-	expression tag	UNP D5MP61
A	333	HIS	-	expression tag	UNP D5MP61

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-3)-2-deoxy-2-fluoro-beta-D-xylopyranose.



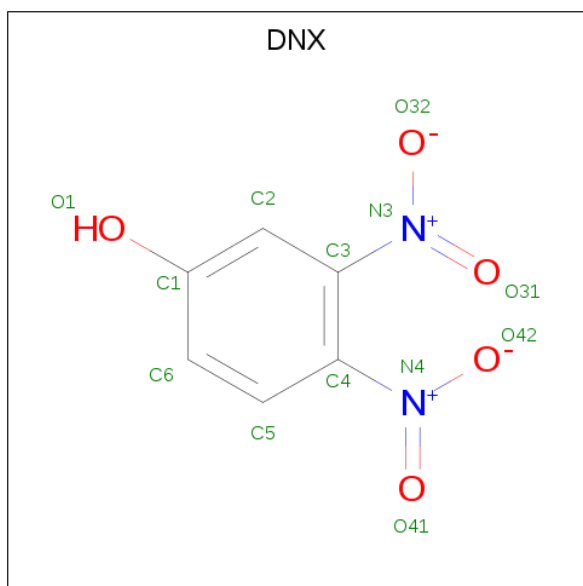
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	F	O			
2	B	3	27	15	1	11	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-3)-2-deoxy-2-fluoro-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	F	O	0	0	0
			27	15	1	11			

- Molecule 4 is 3,4-dinitrophenol (three-letter code: DNX) (formula:  $C_6H_4N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	6	2	5		

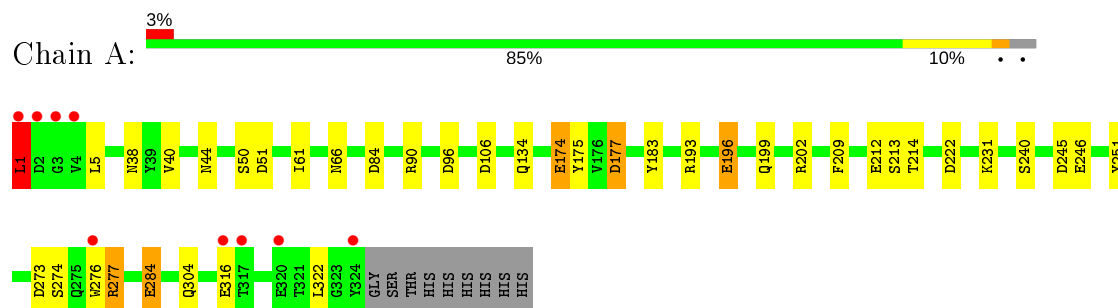
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	511	Total	O	0	0
			511	511		

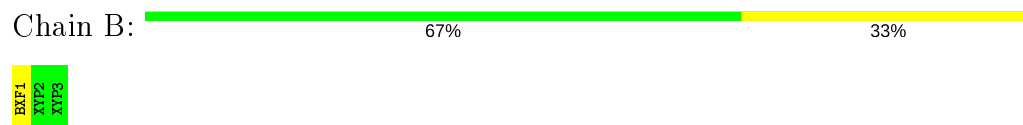
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-1,3-xylanase XYL4



- Molecule 2: beta-D-xylopyranose-(1-3)-beta-D-xylopyranose-(1-3)-2-deoxy-2-fluoro-beta-D-xylopyranose



- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-3)-2-deoxy-2-fluoro-beta-D-xylopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.34Å 75.44Å 81.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 1.20 28.65 – 1.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.61-1.20) 96.9 (28.65-1.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.64 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.141 , 0.156 0.140 , 0.155	Depositor DCC
$R_{free}$ test set	4931 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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, DNX, BXF

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	1.41	12/2866 (0.4%)	1.30	21/3918 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLU	CD-OE2	8.86	1.35	1.25
1	A	276	TRP	CD2-CE2	7.96	1.50	1.41
1	A	212	GLU	CD-OE1	7.51	1.33	1.25
1	A	90	ARG	CD-NE	7.00	1.58	1.46
1	A	251	TYR	CE1-CZ	-6.89	1.29	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	CB-CG-OD1	15.44	132.19	118.30
1	A	273	ASP	CB-CG-OD2	-11.61	107.86	118.30
1	A	202	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	A	51	ASP	CB-CG-OD1	8.17	125.65	118.30
1	A	245	ASP	CB-CG-OD1	7.93	125.44	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	1[A]	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2700	0	2606	34	0
2	B	27	0	6	0	0
3	C	27	0	6	5	0
4	A	13	0	3	2	2
5	A	511	0	0	19	2
All	All	3278	0	2621	38	2

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 7.

The worst 5 of 38 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1[A]:LEU:HD11	5:A:1557:HOH:O	1.17	1.28
1:A:199[B]:GLN:OE1	5:A:1322:HOH:O	1.91	0.89
1:A:40[B]:VAL:CG2	1:A:61:ILE:HD12	2.03	0.88
1:A:1[A]:LEU:CD1	5:A:1164:HOH:O	2.22	0.87
1:A:134[A]:GLN:HG2	5:A:1289:HOH:O	1.76	0.85

All (2) 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)
4:A:1004:DNX:O42	5:A:1604:HOH:O[4_445]	1.75	0.45
4:A:1004:DNX:O1	5:A:1451:HOH:O[4_445]	1.80	0.40

## 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	354/333 (106%)	346 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	297/272 (109%)	294 (99%)	3 (1%)	76	47

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	209	PHE
1	A	214	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	303	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 ⓘ

6 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	BXF	B	1	1,2	9,9,10	1.12	1 (11%)	7,12,14	1.56	2 (28%)
2	XYP	B	2	2	9,9,10	0.90	0	10,12,14	0.89	0
2	XYP	B	3	2	9,9,10	0.88	0	10,12,14	0.90	0
3	BXF	C	1	3,4	9,9,10	2.88	5 (55%)	7,12,14	4.94	5 (71%)
3	XYP	C	2	3	9,9,10	2.26	2 (22%)	10,12,14	2.97	6 (60%)
3	XYP	C	3	3	9,9,10	0.63	0	10,12,14	2.08	5 (50%)

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	BXF	B	1	1,2	1/1/3/4	-	0/1/1/1
2	XYP	B	2	2	-	-	0/1/1/1
2	XYP	B	3	2	-	-	0/1/1/1
3	BXF	C	1	3,4	-	-	0/1/1/1
3	XYP	C	2	3	-	-	0/1/1/1
3	XYP	C	3	3	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	BXF	C1-C2	-5.69	1.44	1.52
3	C	2	XYP	O5-C5	5.49	1.53	1.42
3	C	1	BXF	O5-C5	-4.30	1.34	1.42
2	B	1	BXF	C4-C3	-2.85	1.48	1.52
3	C	2	XYP	O5-C1	2.71	1.48	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	BXF	O4-C4-C3	8.64	127.45	110.14
3	C	1	BXF	O4-C4-C5	-8.23	92.32	109.15
3	C	2	XYP	C5-O5-C1	-6.73	101.18	111.52
3	C	2	XYP	O3-C3-C4	-3.89	102.54	109.99
3	C	1	BXF	C5-O5-C1	3.85	117.45	111.52

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	BXF	C1

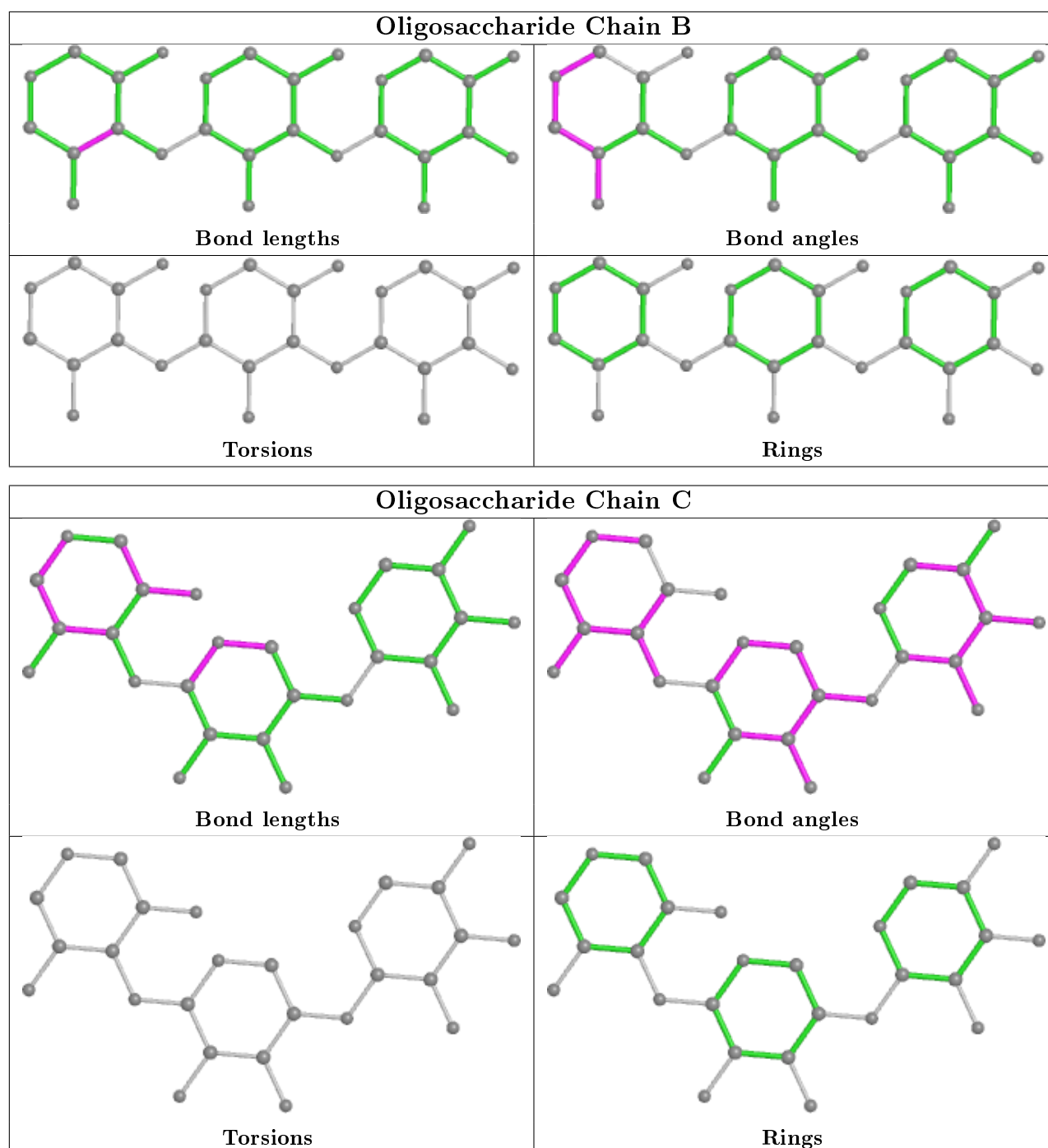
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	BXF	3	0
3	C	2	XYP	2	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](#)

1 ligand is 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	$\# Z  > 2$
4	DNX	A	1004	3	11,13,13	3.17	6 (54%)	11,18,18	4.04	7 (63%)

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
4	DNX	A	1004	3	-	1/4/8/8	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1004	DNX	O31-N3	-6.30	1.12	1.22
4	A	1004	DNX	C4-C3	4.11	1.46	1.40
4	A	1004	DNX	C5-C4	-4.09	1.31	1.39
4	A	1004	DNX	O41-N4	-3.66	1.16	1.22
4	A	1004	DNX	C3-N3	-3.41	1.39	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	DNX	C5-C6-C1	9.61	130.42	119.88
4	A	1004	DNX	C3-C2-C1	-5.36	114.51	118.46
4	A	1004	DNX	C2-C3-C4	4.99	124.15	118.68
4	A	1004	DNX	C5-C4-N4	3.44	120.15	116.47
4	A	1004	DNX	C6-C1-C2	-2.47	117.46	120.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	DNX	C5-C4-N4-O41

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DNX	2	2

## 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	324/333 (97%)	0.01	9 (2%) 53 51	5, 9, 16, 46	1 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	LEU	6.4
1	A	2	ASP	5.6
1	A	4	VAL	4.8
1	A	276	TRP	3.5
1	A	324	TYR	3.3

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	XYP	C	2	9/10	0.82	0.22	9,10,12,15	9
3	BXF	C	1	9/10	0.84	0.22	7,8,10,10	9
3	XYP	C	3	9/10	0.90	0.15	10,12,13,15	9
2	BXF	B	1	9/10	0.99	0.08	5,5,6,6	0
2	XYP	B	2	9/10	0.99	0.06	5,5,6,6	0
2	XYP	B	3	9/10	0.99	0.05	5,6,8,8	0

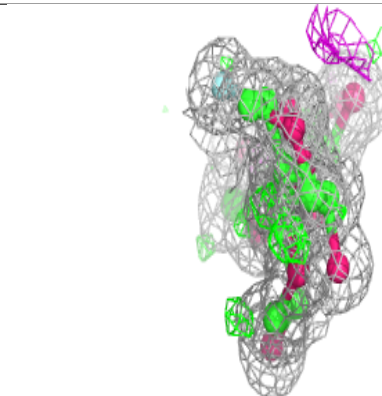
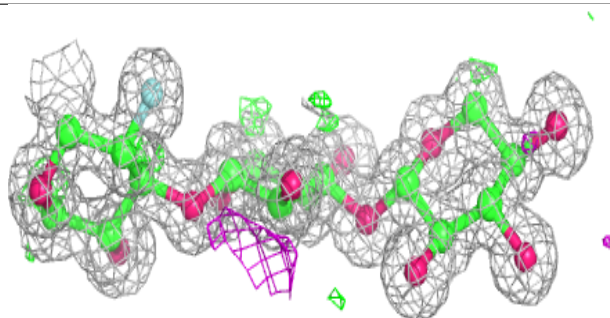
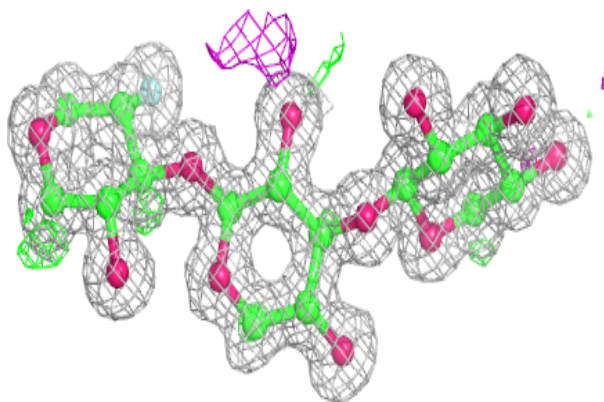
The following is a graphical depiction of the model fit to experimental electron density for oligosac-



charide. Each fit is shown from different orientation to approximate a three-dimensional view.

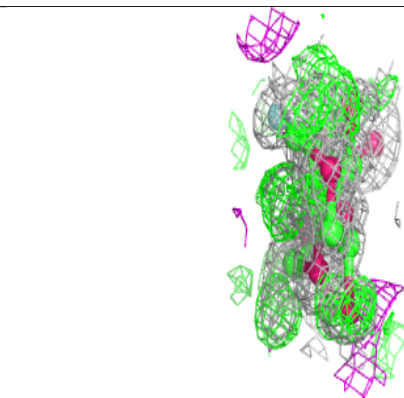
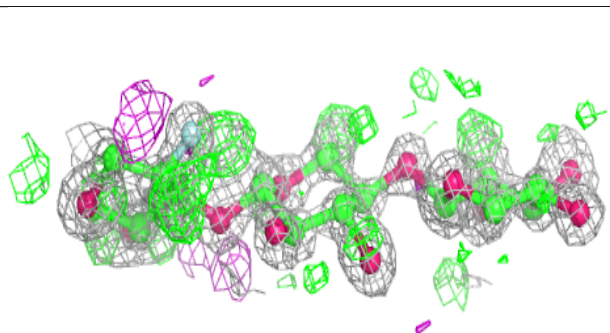
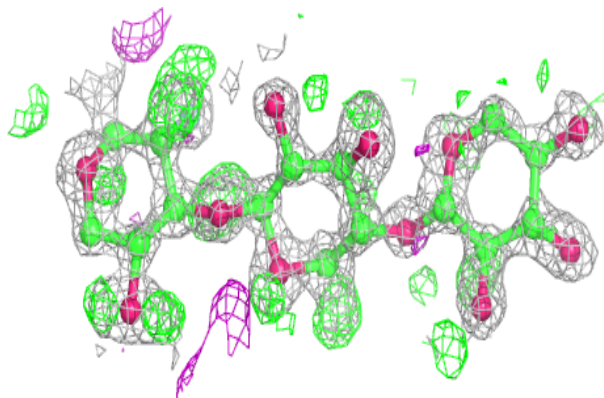
**Electron density around Chain B:**

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



**Electron density around Chain C:**

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



## 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( $\text{\AA}^2$ )	Q<0.9
4	DNX	A	1004	13/13	0.85	0.22	7,10,14,18	13

## 6.5 Other polymers

There are no such residues in this entry.