



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 07:49 AM BST

PDB ID : 5UAS  
Title : Structure of a new family of Polysaccharide lyase PL25-Ulvanlyase bound to  
-[GlcA(1-4)Rha3S]-  
Authors : Ulaganathan, T.S.; Cygler, M.  
Deposited on : 2016-12-20  
Resolution : 1.60 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

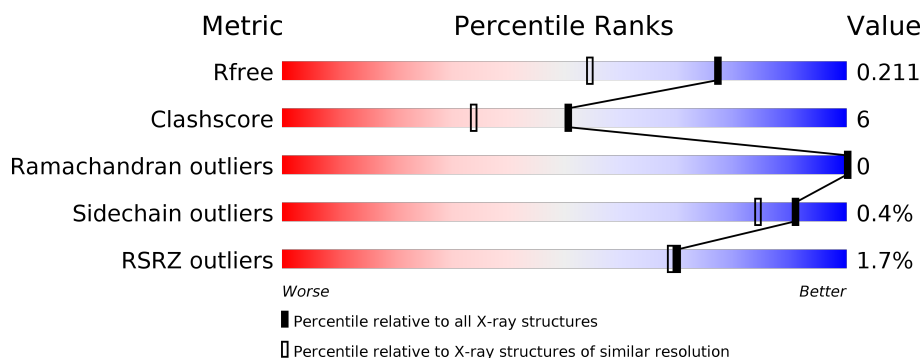
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	473	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
1	B	473	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
2	D	4	<div> <div>25%</div> <div>75%</div> </div>

## 2 Entry composition [i](#)

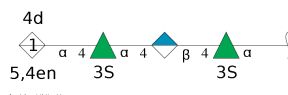
There are 7 unique types of molecules in this entry. The entry contains 8306 atoms, of which 92 are hydrogens and 0 are deuteriums.

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 UlvanLyase-PL25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	1	0
			3472	2176	624	662	10			
1	B	440	Total	C	N	O	S	0	3	0
			3484	2187	625	660	12			

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	O	S	0	0	0
			83	24	31	26	2			
2	D	4	Total	C	H	O	S	0	0	0
			83	24	31	26	2			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

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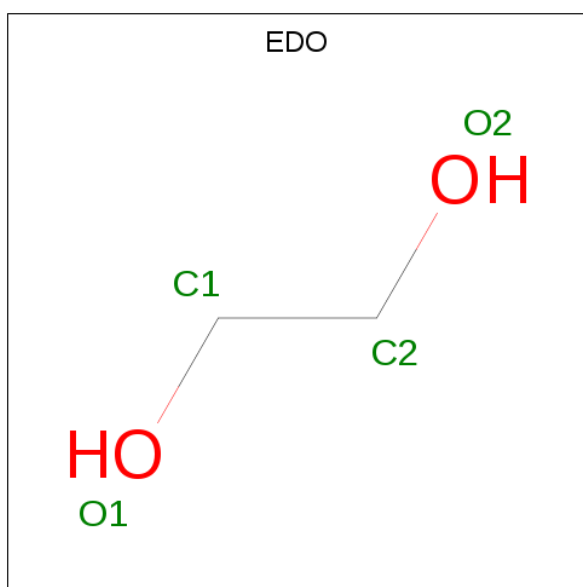
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

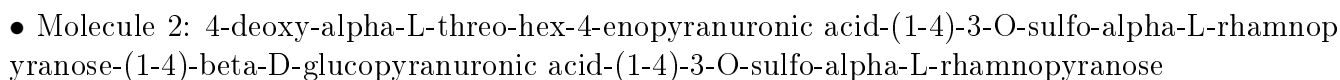
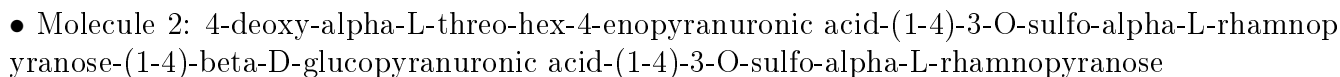


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	594	Total 594	O 594	0	0
7	B	534	Total 534	O 534	0	0

- Molecule 1: UlvanLyase-PL25





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.62Å 71.81Å 109.27Å 90.00° 122.44° 90.00°	Depositor
Resolution (Å)	47.80 – 1.60 47.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (47.80-1.60) 96.1 (47.81-1.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.182 , 0.212 0.182 , 0.211	Depositor DCC
$R_{free}$ test set	7184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4609e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GCD, CL, K, 83Y, EDO, BDP

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	0.46	0/3569	0.63	0/4837
1	B	0.46	0/3587	0.62	0/4859
All	All	0.46	0/7156	0.62	0/9696

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

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	3472	0	3273	41	1
1	B	3484	0	3302	36	0
2	C	52	31	11	0	0
2	D	52	31	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	12	18	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	12	12	1	0
7	A	594	0	0	22	7
7	B	534	0	0	17	7
All	All	8214	92	6627	78	8

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 6.

The worst 5 of 78 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:396:ASN:HB2	7:B:1100:HOH:O	1.72	0.89
1:A:396:ASN:HB2	7:A:1041:HOH:O	1.72	0.87
1:B:293:LYS:NZ	7:B:703:HOH:O	2.08	0.86
1:B:151:LYS:HE3	7:B:934:HOH:O	1.79	0.81
1:A:405:GLN:NE2	7:A:704:HOH:O	2.15	0.76

The worst 5 of 8 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)
7:A:932:HOH:O	7:B:1037:HOH:O[1_565]	2.00	0.20
7:A:714:HOH:O	7:B:1053:HOH:O[1_565]	2.01	0.19
7:A:839:HOH:O	7:B:1086:HOH:O[1_565]	2.01	0.19
7:A:1161:HOH:O	7:B:1080:HOH:O[4_555]	2.06	0.14
7:A:1070:HOH:O	7:B:1099:HOH:O[4_556]	2.07	0.13

## 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	439/473 (93%)	422 (96%)	17 (4%)	0	100	100
1	B	441/473 (93%)	425 (96%)	16 (4%)	0	100	100
All	All	880/946 (93%)	847 (96%)	33 (4%)	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	360/391 (92%)	358 (99%)	2 (1%)	86	77
1	B	362/391 (93%)	361 (100%)	1 (0%)	92	87
All	All	722/782 (92%)	719 (100%)	3 (0%)	91	84

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

Mol	Chain	Res	Type
1	A	146	GLN
1	A	370	GLU
1	B	146	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	HIS

### 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 ⓘ

8 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	83Y	C	1	2	15,15,15	0.68	0	17,23,23	0.60	0
2	BDP	C	2	2	9,12,13	1.80	2 (22%)	12,17,19	1.89	4 (33%)
2	83Y	C	3	2	14,14,15	0.88	1 (7%)	16,21,23	1.27	2 (12%)
2	GCD	C	4	2	7,11,12	2.34	1 (14%)	8,15,17	1.50	1 (12%)
2	83Y	D	1	2	15,15,15	0.65	0	17,23,23	1.07	1 (5%)
2	BDP	D	2	2	9,12,13	1.44	2 (22%)	12,17,19	2.27	6 (50%)
2	83Y	D	3	2	14,14,15	0.86	0	16,21,23	1.03	0
2	GCD	D	4	2	7,11,12	2.32	1 (14%)	8,15,17	1.27	1 (12%)

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	83Y	C	1	2	-	0/5/25/25	0/1/1/1
2	BDP	C	2	2	-	0/0/21/24	0/1/1/1
2	83Y	C	3	2	-	0/5/22/25	0/1/1/1
2	GCD	C	4	2	-	0/0/17/20	0/1/1/1
2	83Y	D	1	2	-	0/5/25/25	0/1/1/1
2	BDP	D	2	2	-	0/0/21/24	0/1/1/1
2	83Y	D	3	2	-	0/5/22/25	0/1/1/1
2	GCD	D	4	2	-	0/0/17/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GCD	O5-C5	5.91	1.45	1.37
2	D	4	GCD	O5-C5	5.74	1.45	1.37
2	C	2	BDP	O5-C5	-3.87	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	BDP	C4-C3	3.10	1.60	1.52
2	D	2	BDP	C4-C5	2.66	1.59	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BDP	O4-C4-C3	4.30	120.29	110.35
2	D	2	BDP	C1-O5-C5	4.07	119.35	112.17
2	D	1	83Y	C4-C3-C2	-3.82	105.35	110.85
2	C	4	GCD	O5-C5-C4	-3.53	121.83	124.81
2	D	2	BDP	O5-C1-C2	3.35	115.94	110.77

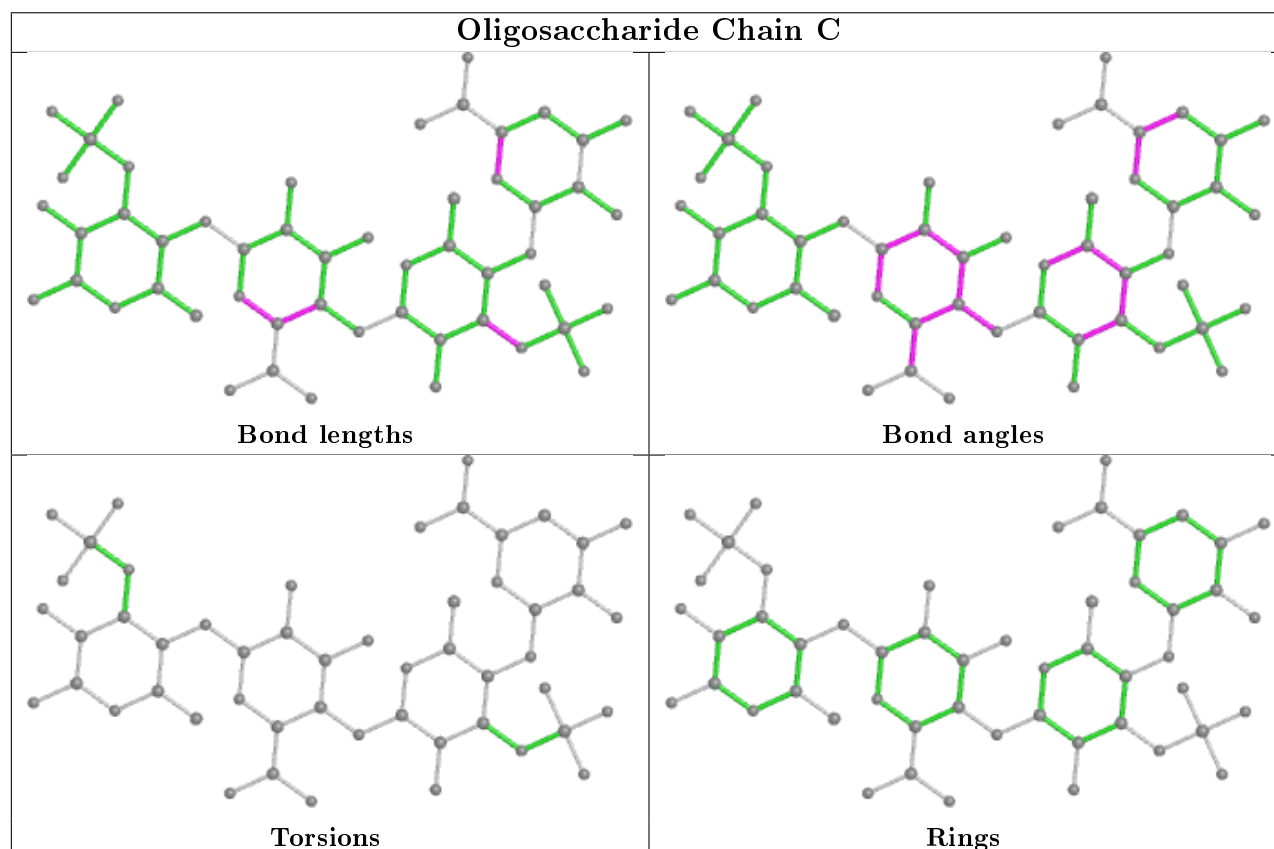
There are no chirality outliers.

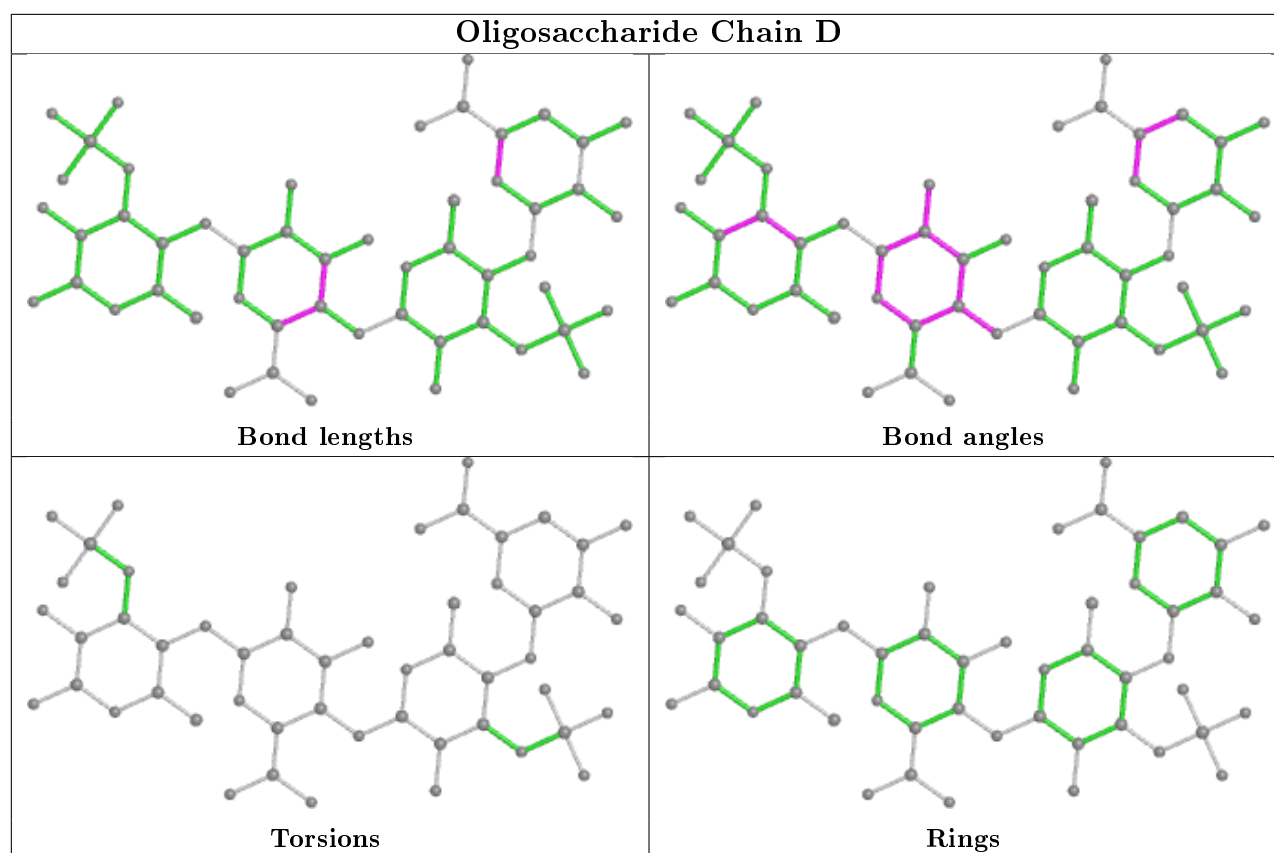
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	EDO	A	608	-	3,3,3	0.42	0	2,2,2	0.34	0
6	EDO	B	608	-	3,3,3	0.45	0	2,2,2	0.22	0
6	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.30	0
6	EDO	A	610	-	3,3,3	0.55	0	2,2,2	0.20	0
6	EDO	B	609	-	3,3,3	0.58	0	2,2,2	0.06	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
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	B	608	-	-	1/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
6	EDO	B	609	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	608	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	EDO	1	0
6	B	608	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	440/473 (93%)	-0.39	6 (1%) 75 75	11, 18, 37, 62	0
1	B	440/473 (93%)	-0.27	9 (2%) 65 64	12, 20, 41, 72	0
All	All	880/946 (93%)	-0.33	15 (1%) 70 69	11, 19, 39, 72	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	VAL	9.1
1	B	272	GLY	5.5
1	B	274	ASN	5.0
1	A	273	VAL	4.0
1	A	275	GLY	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
2	83Y	C	1	15/15	0.82	0.14	20,40,56,60	0
2	83Y	D	1	15/15	0.85	0.14	21,49,67,70	0
2	GCD	C	4	11/12	0.94	0.09	16,24,30,36	0
2	GCD	D	4	11/12	0.95	0.06	18,23,30,36	0
2	BDP	D	2	12/13	0.95	0.07	14,20,26,28	0

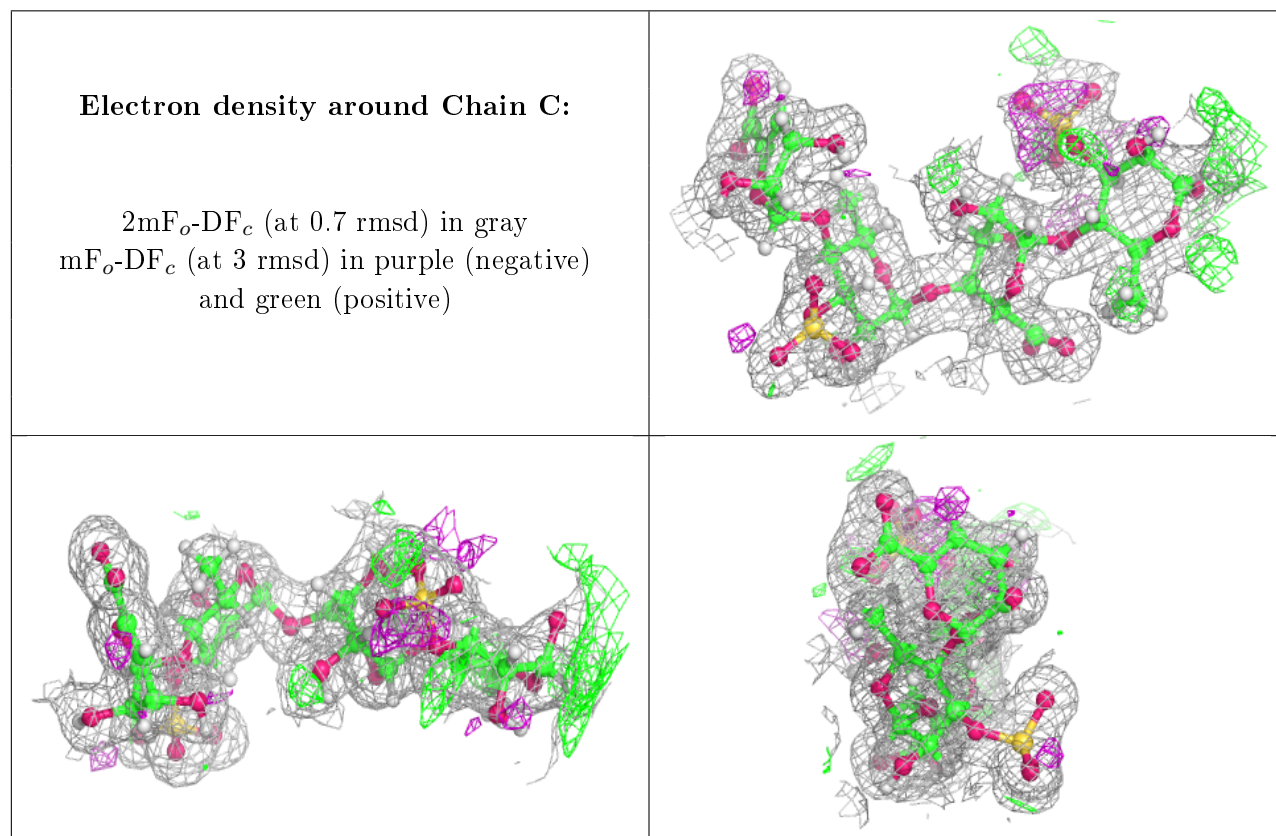
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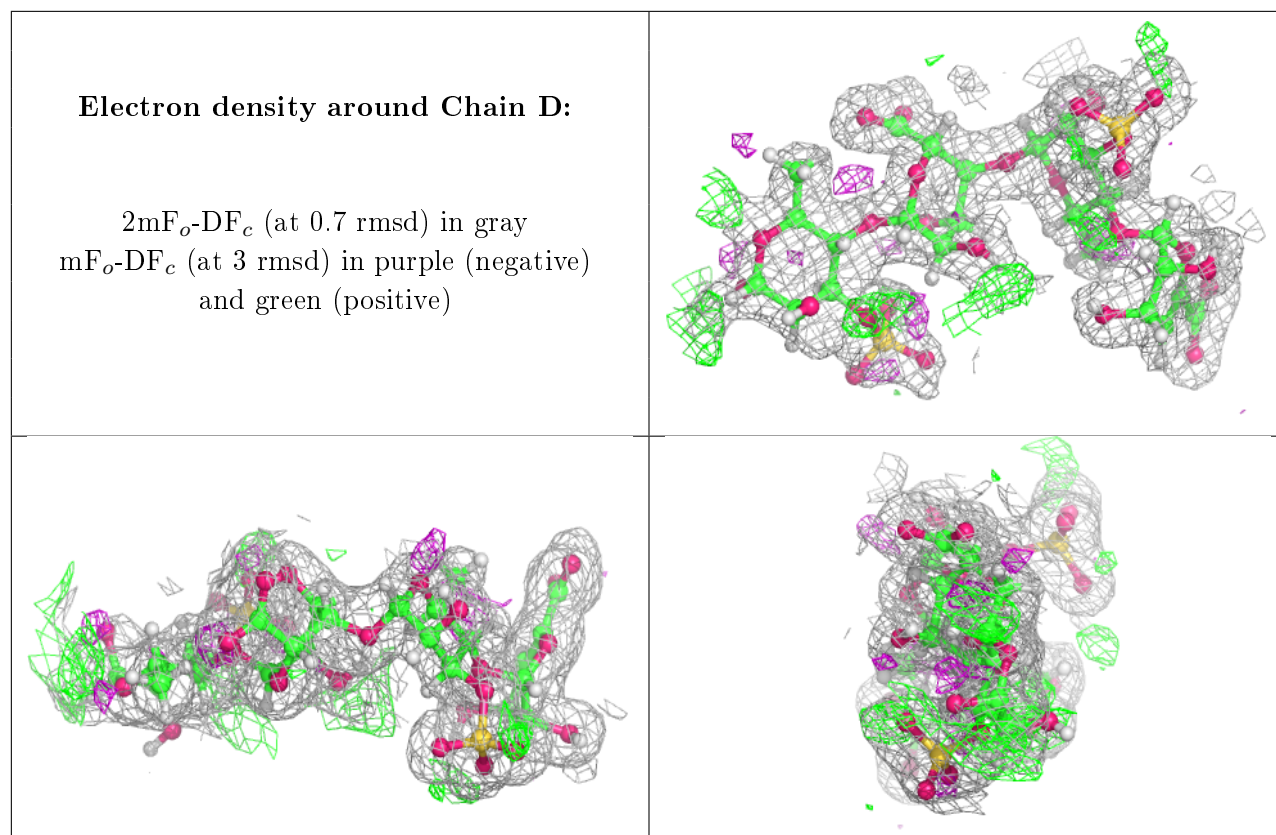


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BDP	C	2	12/13	0.96	0.06	14,18,23,25	0
2	83Y	D	3	14/15	0.97	0.07	16,18,22,22	0
2	83Y	C	3	14/15	0.98	0.06	13,16,18,19	0

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.





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	B	608	4/4	0.82	0.20	42,50,59,60	0
6	EDO	B	609	4/4	0.90	0.11	19,32,38,38	0
6	EDO	A	608	4/4	0.90	0.09	40,48,55,55	0
6	EDO	A	610	4/4	0.92	0.10	19,27,32,32	0
6	EDO	A	609	4/4	0.93	0.12	39,47,49,49	0
3	ZN	A	601	1/1	0.99	0.05	21,21,21,21	0
4	K	B	602	1/1	0.99	0.05	16,16,16,16	0
3	ZN	B	601	1/1	0.99	0.04	20,20,20,20	0
5	CL	B	603	1/1	0.99	0.06	31,31,31,31	0
5	CL	A	603	1/1	0.99	0.07	29,29,29,29	0
4	K	A	602	1/1	1.00	0.05	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.