

Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 04:56 AM EDT

PDB ID : 3PFZ

Title: Crystal structure of Cel7A from Talaromyces emersonii in complex with cel-

lotetraose

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Deposited on : 2010-10-29

Resolution : 1.10 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

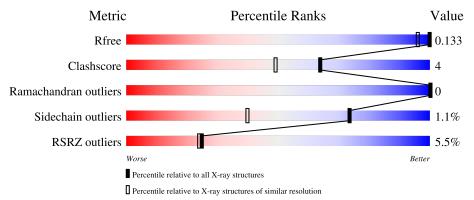
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 >=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 <=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	437	5%	94%	6%			
2	В	4		75%	25%			
3	С	4	25%	50%	25%			
4	D	2	50 ^c	%	50%			



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7470 atoms, of which 3134 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 Cellobiohydrolase 1 catalytic domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	436	Total 6301	C 2040	H 2996	N 541	O 697	S 27	0	7	0

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(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
9	D	4	Total	С	Н	N	О	0	0	0
	Б	4	93	28	43	2	20	U	0	U

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	С	4	Total 83		H 38	 0	0	0

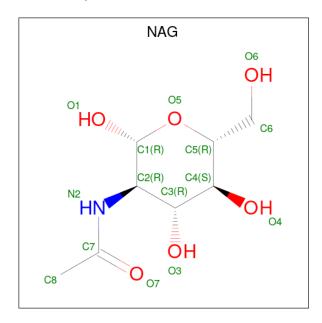
• Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.





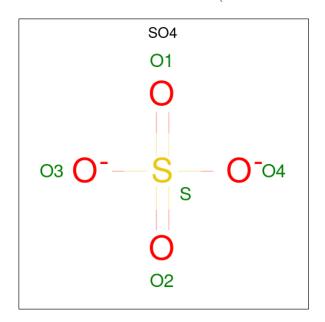
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total 90	C 24	H 44	O 22	0	2	0

 \bullet Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
E	Λ	1	Total	С	Н	N	О	0	0
) 3	O A	1	27	8	13	1	5	U	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

$\bullet\,$ Molecule 7 is water.

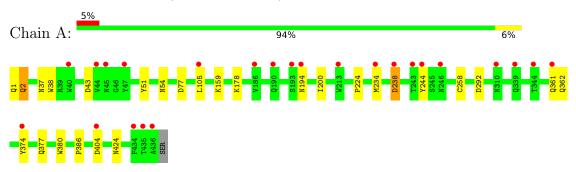
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	866	Total O 866 866	0	2



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: Cellobiohydrolase 1 catalytic domain



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

Chain B: 75% 25%

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

Chain C: 25% 50% 25%

BGC1 BGC2 BGC3 BGC4

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

Chain D: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 41 21 2	Depositor	
Cell constants	74.72Å 74.72Å 169.92Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	28.78 - 1.10	Depositor	
Resolution (A)	28.78 - 1.10	EDS	
% Data completeness	95.4 (28.78-1.10)	Depositor	
(in resolution range)	95.4 (28.78-1.10)	EDS	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.24 (at 1.10Å)	Xtriage	
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor	
R, R_{free}	0.126 , 0.143	Depositor	
It, It free	0.115 , 0.133	DCC	
R_{free} test set	2000 reflections (1.06%)	wwPDB-VP	
Wilson B-factor (Å ²)	6.9	Xtriage	
Anisotropy	0.427	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 40.4	EDS	
L-test for twinning ²	$ < L > = 0.49, < L^2 > = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.98	EDS	
Total number of atoms	7470	wwPDB-VP	
Average B, all atoms (Å ²)	10.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: BMA, NAG, PCA, BGC, MAN, SO4

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	Boı	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	1/3400 (0.0%)	0.71	4/4649 (0.1%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	234	MET	CB-CG	6.83	1.73	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	105	LEU	CA-CB-CG	-5.89	101.75	115.30
1	A	238	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	292	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	238	ASP	CB-CG-OD2	-5.13	113.69	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3305	2996	2997	26	0
2	В	50	43	43	0	0
3	С	45	38	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	46	44	42	4	0
5	A	14	13	13	0	0
6	A	10	0	0	0	0
7	A	866	0	0	17	1
All	All	4336	3134	3134	28	1

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (28) 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:77:ASP:OD1	7:A:657:HOH:O	1.86	0.94
1:A:386:PRO:HD3	7:A:494:HOH:O	1.86	0.75
1:A:200:ILE:HD11	1:A:244:TYR:CD1	2.25	0.72
1:A:178:LYS:HE2	7:A:1022:HOH:O	1.88	0.71
1:A:361:GLN:HG2	7:A:906:HOH:O	1.91	0.69
1:A:244:TYR:CE2	7:A:674:HOH:O	2.44	0.69
1:A:404:ASP:OD2	7:A:1196:HOH:O	2.11	0.67
1:A:374[B]:TYR:O	7:A:528:HOH:O	2.17	0.60
1:A:361:GLN:CG	7:A:906:HOH:O	2.49	0.59
1:A:178:LYS:CE	7:A:1022:HOH:O	2.48	0.57
1:A:404:ASP:HB3	7:A:688:HOH:O	2.06	0.56
1:A:2:GLN:HE22	1:A:159:LYS:HD2	1.71	0.54
1:A:361:GLN:HG2	7:A:604:HOH:O	2.08	0.53
7:A:588:HOH:O	4:D:2[A]:BGC:H4	2.07	0.53
1:A:424[B]:ASN:ND2	7:A:1207:HOH:O	2.42	0.52
1:A:200:ILE:CD1	1:A:244:TYR:CD1	2.91	0.52
1:A:362:GLN:NE2	7:A:1249:HOH:O	2.32	0.51
1:A:380:TRP:CZ2	4:D:2[B]:BGC:H5	2.47	0.50
1:A:194:ASN:O	1:A:374[B]:TYR:CE1	2.65	0.48
1:A:2:GLN:NE2	1:A:159:LYS:HD2	2.28	0.48
7:A:1134:HOH:O	4:D:2[A]:BGC:H6C1	2.14	0.46
1:A:224:PRO:HD2	1:A:258:CYS:O	2.17	0.43
1:A:380:TRP:CE2	4:D:2[B]:BGC:H5	2.52	0.43
1:A:238:ASP:HB3	7:A:1063:HOH:O	2.19	0.42
1:A:200:ILE:HD12	1:A:244:TYR:HB3	2.01	0.42
1:A:38:TRP:CZ3	3:C:2:BGC:H6C1	2.56	0.41
1:A:374[B]:TYR:C	7:A:528:HOH:O	2.57	0.40
1:A:51:TYR:CZ	1:A:54:ASN:HA	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			Clash overlap (Å)	
7:A:1171:HOH:O	7:A:1310:HOH:O[7_465]	1.88	0.32	

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		
1	A	441/437 (101%)	434 (98%)	7 (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 Pero		entiles
1	A	366/361 (101%)	362 (99%)	4 (1%)	73	40

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	37	ASN
1	A	43	ASP
1	A	377	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	132	ASN
1	A	190	GLN
1	A	361	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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		
	MIOI	туре	Chain	rtes	Lilik	Counts	Counts RMSZ $\# Z > 2$			RMSZ	# Z > 2
ſ	1	PCA	A	1	1	7,8,9	1.57	3 (42%)	9,10,12	1.25	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	1	PCA	CD-N	2.64	1.41	1.34
1	A	1	PCA	CA-N	-2.08	1.44	1.46
1	A	1	PCA	CG-CD	2.02	1.56	1.50

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	1	PCA	CB-CA-N	2.14	109.43	103.30
1	A	1	PCA	O-C-CA	-2.02	119.48	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

12 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).

Mal	Trino	Chain	Dag	Link	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	0.59	0	17,19,21	1.15	1 (5%)
2	NAG	В	2	2	14,14,15	0.50	0	17,19,21	0.71	0
2	BMA	В	3	2	11,11,12	0.55	0	15,15,17	0.71	0
2	MAN	В	4	2	11,11,12	0.54	0	15,15,17	0.57	0
3	BGC	С	1	3	12,12,12	0.56	0	17,17,17	0.84	0
3	BGC	С	2	3	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
3	BGC	С	3	3	11,11,12	1.12	2 (18%)	15,15,17	1.24	2 (13%)
3	BGC	С	4	3	11,11,12	0.88	1 (9%)	15,15,17	0.76	0
4	BGC	D	1[A]	4	12,12,12	0.56	0	17,17,17	1.26	2 (11%)
4	BGC	D	1[B]	4	12,12,12	0.60	0	17,17,17	1.24	1 (5%)
4	BGC	D	2[A]	4	11,11,12	0.68	0	15,15,17	2.69	7 (46%)
4	BGC	D	2[B]	4	11,11,12	0.83	0	15,15,17	1.78	4 (26%)

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	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
2	BMA	В	3	2	-	0/2/19/22	0/1/1/1
2	MAN	В	4	2	-	0/2/19/22	0/1/1/1
3	BGC	С	1	3	-	0/2/22/22	0/1/1/1
3	BGC	С	2	3	-	0/2/19/22	0/1/1/1
3	BGC	С	3	3	-	0/2/19/22	0/1/1/1
3	BGC	С	4	3	-	0/2/19/22	0/1/1/1
4	BGC	D	1[A]	4	-	0/2/22/22	0/1/1/1
4	BGC	D	1[B]	4	-	0/2/22/22	0/1/1/1
4	BGC	D	2[A]	4	_	0/2/19/22	0/1/1/1
4	BGC	D	2[B]	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
3	С	3	BGC	O5-C1	-2.22	1.40	1.43
3	С	3	BGC	O5-C5	-2.19	1.39	1.43
3	С	4	BGC	O5-C1	-2.08	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
4	D	2[A]	BGC	O4-C4-C3	-5.54	97.53	110.35
4	D	2[A]	BGC	C3-C4-C5	-4.92	101.46	110.24
4	D	2[A]	BGC	O4-C4-C5	3.98	119.18	109.30
4	D	2[A]	BGC	C1-C2-C3	-3.64	105.19	109.67
4	D	2[B]	BGC	C1-C2-C3	-3.49	105.38	109.67
2	В	1	NAG	O5-C1-C2	-3.42	105.89	111.29
4	D	2[B]	BGC	C3-C4-C5	-3.29	104.38	110.24
4	D	2[A]	BGC	O3-C3-C2	-2.98	104.29	109.99
4	D	2[B]	BGC	O3-C3-C2	-2.91	104.42	109.99
3	С	3	BGC	O3-C3-C2	-2.40	105.39	109.99
3	С	3	BGC	O5-C1-C2	-2.40	107.07	110.77
4	D	2[A]	BGC	O2-C2-C3	2.32	114.78	110.14
4	D	1[A]	BGC	C1-C2-C3	-2.31	105.51	110.31
4	D	1[B]	BGC	O2-C2-C1	-2.30	103.83	109.16
4	D	2[A]	BGC	C2-C3-C4	2.21	114.71	110.89
3	С	2	BGC	O5-C5-C6	2.17	110.61	107.20
4	D	1[A]	BGC	C4-C3-C2	2.09	114.47	110.82
4	D	2[B]	BGC	O5-C1-C2	-2.02	107.66	110.77
3	С	2	BGC	O4-C4-C5	2.01	114.30	109.30



There are no chirality outliers.

There are no torsion outliers.

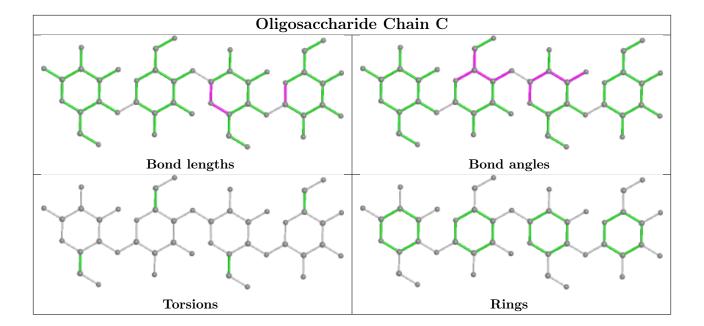
There are no ring outliers.

3 monomers are involved in 5 short contacts:

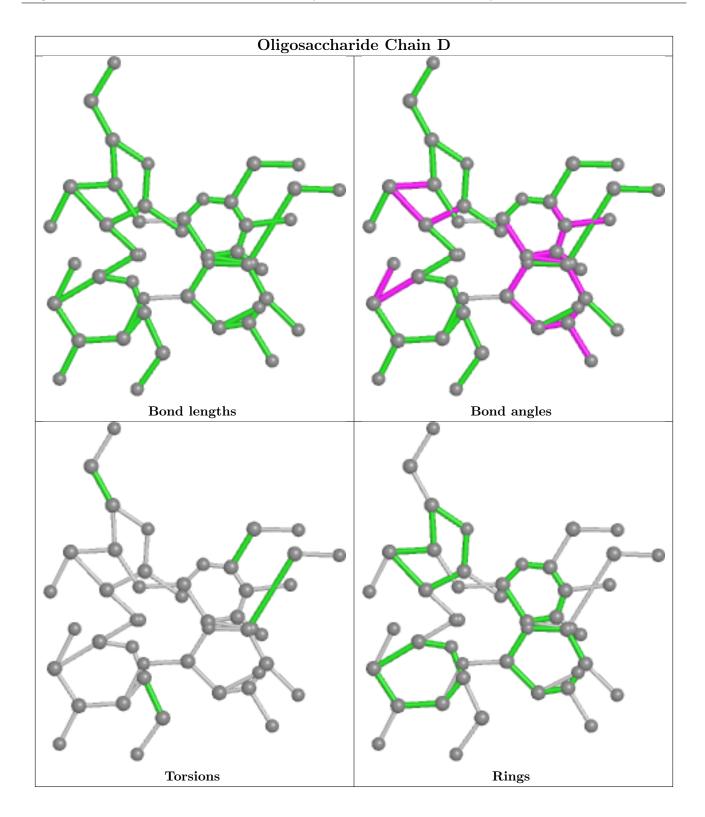
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2[A]	BGC	2	0
4	D	2[B]	BGC	2	0
3	С	2	BGC	1	0

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









5.6 Ligand geometry (i)

3 ligands 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	Bo	nd leng	$ ag{ths}$	В	ond ang	eles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	441	-	4,4,4	0.17	0	6,6,6	0.32	0
6	SO4	A	444	-	4,4,4	0.38	0	6,6,6	0.29	0
5	NAG	A	440	1	14,14,15	0.67	0	17,19,21	0.78	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
5	NAG	A	440	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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	435/437 (99%)	0.99	24 (5%) 25 24	4, 7, 16, 31	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	6.5
1	A	435	THR	5.6
1	A	47	TYR	4.8
1	A	194	ASN	3.8
1	A	246	ASN	3.6
1	A	436	ALA	3.5
1	A	190	GLN	3.2
1	A	45	ASN	2.9
1	A	44	VAL	2.9
1	A	193	SER	2.9
1	A	186	VAL	2.7
1	A	238	ASP	2.6
1	A	234	MET	2.5
1	A	243	THR	2.5
1	A	434	PHE	2.4
1	A	339	GLN	2.4
1	A	310	ASN	2.4
1	A	404	ASP	2.3
1	A	40	TRP	2.2
1	A	105	LEU	2.2
1	A	361	GLN	2.1
1	A	374[A]	TYR	2.1
1	A	344[A]	THR	2.0
1	A	213	TRP	2.0



6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	PCA	A	1	8/9	0.98	0.10	5,6,7,7	0

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^{th} 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.

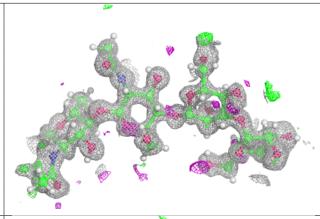
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	В	3	11/12	0.80	0.23	16,25,37,37	0
2	MAN	В	4	11/12	0.84	0.20	16,23,29,33	0
2	NAG	В	2	14/15	0.92	0.15	9,14,21,21	0
2	NAG	В	1	14/15	0.94	0.12	8,12,37,37	0
3	BGC	С	2	11/12	0.94	0.12	7,9,11,13	0
4	BGC	D	1[A]	12/12	0.94	0.15	6,8,10,12	23
4	BGC	D	1[B]	12/12	0.94	0.15	3,6,7,8	23
4	BGC	D	2[A]	11/12	0.94	0.14	8,14,19,19	22
4	BGC	D	2[B]	11/12	0.94	0.14	3,4,8,10	22
3	BGC	С	4	11/12	0.95	0.16	6,10,13,16	0
3	BGC	С	3	11/12	0.96	0.15	6,8,10,11	0
3	BGC	С	1	12/12	0.96	0.11	6,9,16,20	1

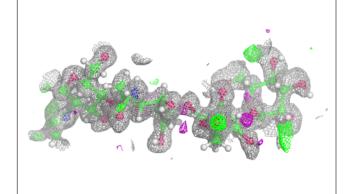
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

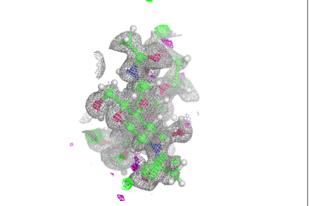


Electron density around Chain B:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

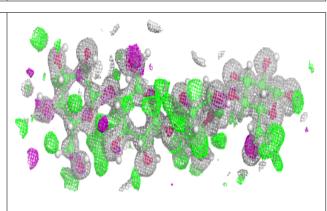


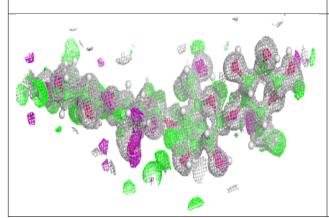


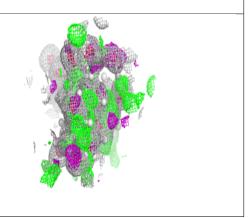


Electron density around Chain C:

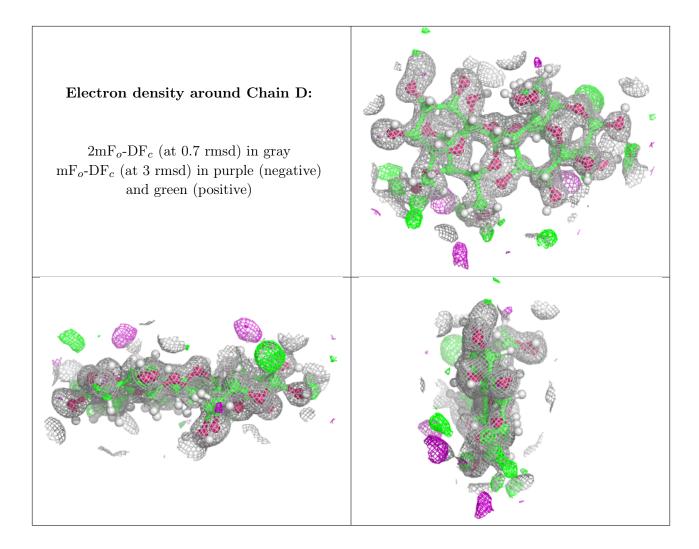
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
6	SO4	A	441	5/5	0.75	0.26	6,13,17,17	5
5	NAG	A	440	14/15	0.86	0.12	15,22,33,33	0
6	SO4	A	444	5/5	0.90	0.19	7,11,13,16	5

6.5 Other polymers (i)

There are no such residues in this entry.

