

# Full wwPDB X-ray Structure Validation Report (i)

#### Jul 18, 2022 – 04:30 pm BST

PDB ID	:	7P43
Title	:	Structure of CgGBE in complex with maltotriose
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Deposited on	:	2021-07-09
Resolution	:	1.93  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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.93 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
$R_{free}$	130704	4310 (1.96-1.92)		
Clashscore	141614	1023 (1.94-1.94)		
Ramachandran outliers	138981	1007 (1.94-1.94)		
Sidechain outliers	138945	1007 (1.94-1.94)		
RSRZ outliers	127900	4250 (1.96-1.92)		

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	А	706	<sup>2%</sup> 91%	7% •
1	В	706	83%	15% •
2	С	3	100%	
2	D	3	100%	

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	GLC	D	1	-	-	-	Х



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11641 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 1,4-alpha-glucan-branching enzyme.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	687	Total 5551	C 3552	N 954	O 1025	S 20	0	0	0
1	В	690	Total 5330	C 3376	N 940	O 996	S 18	0	0	0

• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	С	3	Total 34	C 18	O 16	0	0	0
2	D	3	Total 34	C 18	O 16	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	552	Total O 552 552	0	0
3	В	140	Total         O           140         140	0	0





# 3 Residue-property plots (i)

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



• Molecule 1: 1,4-alpha-glucan-branching enzyme



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e

Chain C:

100%

#### GLC1 GLC2 GLC3 GLC3

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos e

Chain D: 100%

GLC1 GLC2 GLC3 GLC3



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	88.72Å 210.70Å 90.52Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	47.05 - 1.93	Depositor
Resolution (A)	47.05 - 1.93	EDS
% Data completeness	99.5 (47.05-1.93)	Depositor
(in resolution range)	99.5(47.05-1.93)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.11 (at 1.92 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D	0.192 , $0.217$	Depositor
$\Lambda, \Lambda_{free}$	0.191 , $0.216$	DCC
$R_{free}$ test set	6404 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.1	Xtriage
Anisotropy	0.928	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: GLC

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.57	0/5711	0.69	0/7760	
1	В	0.35	0/5476	0.58	0/7453	
All	All	0.48	0/11187	0.64	0/15213	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5551	0	5262	31	0
1	В	5330	0	4809	70	0
2	С	34	0	29	0	0
2	D	34	0	29	0	0
3	А	552	0	0	6	0
3	В	140	0	0	2	0
All	All	11641	0	10129	101	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 5.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:459:ASP:OD2	1:B:697:ARG:NH2	2.27	0.67	
1:A:133:LYS:NZ	1:A:296:GLU:OE2	2.29	0.66	
1:B:383:TYR:HB2	1:B:384:LEU:HD12	1.77	0.66	
1:A:466:HIS:HD2	3:A:1257:HOH:O	1.78	0.65	
1:B:428:CYS:HB2	1:B:478:GLU:HB3	1.78	0.64	
1:B:361:THR:HG23	1:B:422:SER:HB3	1.80	0.62	
1:A:704:ARG:NH1	3:A:806:HOH:O	2.33	0.62	
1:B:216:LYS:NZ	1:B:270:GLU:OE1	2.33	0.62	
1:A:483:TYR:CE2	1:A:486:SER:HB2	2.36	0.61	
1:B:615:HIS:HB3	1:B:618:ASP:O	2.01	0.60	
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.66	0.60	
1:B:63:THR:O	1:B:78:ARG:HD3	2.02	0.59	
1:B:547:GLY:HA2	1:B:550:PHE:CE1	2.38	0.59	
1:B:633:ASN:ND2	1:B:694:ILE:O	2.34	0.59	
1:B:639:SER:HB3	1:B:695:PRO:HA	1.83	0.59	
1:B:487:HIS:HB3	1:B:545:PHE:CD2	2.38	0.58	
1:B:320:HIS:HD2	1:B:323:TRP:H	1.51	0.58	
1:A:145:TYR:O	1:A:146:ARG:HD3	2.04	0.57	
1:A:410:LEU:HB2	1:A:414:ALA:HB2	1.87	0.57	
1:B:471:LEU:HD23	1:B:537:LEU:HD23	1.86	0.57	
1:B:121:ASN:ND2	3:B:808:HOH:O	2.39	0.55	
1:A:443:ALA:HB2	1:A:480:VAL:CG1	2.36	0.55	
1:B:428:CYS:SG	1:B:441:ARG:HB3	2.48	0.54	
1:B:464:MET:HB3	1:B:621:ILE:HD11	1.89	0.54	
1:B:619:LYS:O	1:B:634:PHE:N	2.37	0.54	
1:A:663:GLU:HG2	3:A:883:HOH:O	2.07	0.54	
1:A:644:ARG:HG2	1:A:689:PHE:CD2	2.43	0.54	
1:B:385:SER:N	1:B:389:SER:OG	2.41	0.54	
1:B:661:ARG:NH2	1:B:672:GLU:OE1	2.41	0.53	
1:B:463:ASP:O	1:B:467:ILE:HD12	2.09	0.53	
1:B:319:GLU:OE1	1:B:320:HIS:N	2.43	0.52	
1:B:695:PRO:HD2	1:B:698:THR:HG21	1.92	0.52	
1:B:410:LEU:HB2	1:B:414:ALA:HB2	1.92	0.52	
1:A:495:LYS:HB3	1:A:499:PHE:HB3	1.92	0.51	
1:B:383:TYR:CB	1:B:384:LEU:HD12	2.40	0.51	
1:B:583:ARG:HG2	1:B:583:ARG:NH1	2.26	0.50	
1:B:384:LEU:HD11	1:B:425:PRO:HG2	1.92	0.50	
1:B:682:GLU:HA	1:B:686:ARG:O	2.12	0.50	
1:A:265:PRO:HB3	1:A:350:TYR:OH	2.12	0.50	
1:B:191:LEU:HD22	3:B:847:HOH:O	2.12	0.50	
1:B:512:VAL:HG12	1:B:581:LEU:O	2.11	0.50	



	le as pagem	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:197:LYS:HD2	1:A:595:GLN:OE1	2.12	0.50
1:A:96:TRP:HZ3	1:A:133:LYS:HG3	1.76	0.49
1:A:443:ALA:HB2	1:A:480:VAL:HG13	1.95	0.48
1:B:443:ALA:HB2	1:B:480:VAL:CG1	2.43	0.48
1:B:121:ASN:HB3	1:B:123:ASP:H	1.76	0.48
1:B:206:SER:HB3	1:B:222:VAL:HG21	1.96	0.48
1:B:464:MET:HE1	1:B:619:LYS:HB3	1.96	0.47
1:B:443:ALA:HB1	1:B:446:LEU:HG	1.95	0.47
1:B:320:HIS:CD2	1:B:323:TRP:H	2.30	0.47
1:B:168:THR:HG21	1:B:296:GLU:HG2	1.96	0.47
1:B:293:LYS:NZ	1:B:319:GLU:OE2	2.28	0.46
1:A:66:LEU:HG	1:A:77:TYR:CD1	2.50	0.46
1:B:379:ASP:O	1:B:382:GLU:HG3	2.15	0.46
1:B:487:HIS:HB3	1:B:545:PHE:HD2	1.80	0.46
1:B:611:VAL:HA	1:B:623:PHE:HB3	1.97	0.45
1:B:320:HIS:HB2	1:B:327:LEU:HD21	1.98	0.45
1:B:522:ARG:HG3	1:B:697:ARG:NH1	2.32	0.45
1:B:573:GLN:HB3	1:B:576:LEU:HG	1.99	0.44
1:B:187:PRO:HG2	1:B:281:LEU:HD23	1.99	0.44
1:A:206:SER:HB3	1:A:222:VAL:HG21	1.99	0.43
1:B:559:PRO:HG2	1:B:567:TYR:CE1	2.52	0.43
1:B:197:LYS:HE3	1:B:232:ASP:OD2	2.18	0.43
1:A:466:HIS:CD2	3:A:1257:HOH:O	2.63	0.43
1:B:347:ILE:O	1:B:351:GLN:HA	2.18	0.43
1:A:406:VAL:HG12	1:A:414:ALA:HB1	2.01	0.43
1:A:510:MET:HB3	1:A:510:MET:HE3	1.92	0.43
1:B:560:ARG:HD2	1:B:560:ARG:HA	1.84	0.43
1:B:440:TYR:HB3	1:B:481:VAL:HG23	2.01	0.43
1:A:356:ARG:HD2	1:A:442:LEU:HD11	2.01	0.43
1:B:547:GLY:HA2	1:B:550:PHE:HE1	1.82	0.42
1:B:531:ARG:HH21	1:B:591:ASP:HB2	1.84	0.42
1:B:619:LYS:HB2	1:B:635:HIS:N	2.35	0.42
1:B:464:MET:CE	1:B:619:LYS:HB3	2.49	0.42
1:A:591:ASP:O	1:A:595:GLN:HG2	2.20	0.42
1:B:400:MET:HB3	1:B:431:ARG:CD	2.49	0.42
1:A:475:ARG:HD2	3:A:809:HOH:O	2.20	0.42
1:B:522:ARG:HG2	1:B:526:LEU:HD12	2.01	0.42
1:B:159:LYS:O	1:B:163:GLN:HG2	2.20	0.42
1:A:615:HIS:HE1	1:A:617:VAL:HB	1.85	0.42
1:B:22:PRO:HG2	1:B:23:PHE:CE1	2.55	0.41
1:A:96:TRP:CZ3	1:A:133:LYS:HG3	2.54	0.41



Atom-1	Atom-2	Interatomic $distance (\hat{\lambda})$	Clash
		distance (A)	overlap (A)
1:B:591:ASP:O	1:B:595:GLN:HG2	2.21	0.41
1:A:17:ASP:OD2	1:A:475:ARG:NH2	2.52	0.41
1:A:317:ARG:NH2	3:A:819:HOH:O	2.44	0.41
1:B:527:HIS:O	1:B:531:ARG:HD3	2.19	0.41
1:A:239:ILE:HB	1:A:284:LEU:HD11	2.03	0.41
1:B:156:GLN:HG3	1:B:157:PRO:HD2	2.03	0.41
1:B:197:LYS:NZ	1:B:599:SER:OG	2.45	0.41
1:B:554:GLU:HB3	1:B:555:TRP:H	1.69	0.41
1:B:300:ASN:OD1	1:B:326:ARG:NH1	2.54	0.41
1:B:620:VAL:HA	1:B:632:PHE:O	2.21	0.41
1:A:168:THR:HG21	1:A:296:GLU:HG2	2.03	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.92	0.41
1:B:487:HIS:H	1:B:487:HIS:CD2	2.38	0.41
1:A:239:ILE:HB	1:A:284:LEU:CD1	2.51	0.41
1:B:618:ASP:HB3	1:B:640:PHE:CZ	2.56	0.41
1:B:163:GLN:HE21	1:B:163:GLN:HA	1.87	0.40
1:B:295:SER:O	1:B:297:ASP:N	2.51	0.40
1:B:550:PHE:CZ	1:B:552:HIS:HD2	2.38	0.40
1:A:6:ILE:HD11	1:A:21:GLU:HG2	2.03	0.40

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	Perce	ntiles
1	А	683/706~(97%)	666~(98%)	17 (2%)	0	100	100
1	В	682/706~(97%)	654 (96%)	28 (4%)	0	100	100
All	All	1365/1412~(97%)	1320 (97%)	45 (3%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	582/607~(96%)	575~(99%)	7 (1%)	71 64		
1	В	518/607~(85%)	510 (98%)	8 (2%)	65 56		
All	All	1100/1214 (91%)	1085~(99%)	15 (1%)	67 58		

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	73	LYS
1	А	191	LEU
1	А	248	PHE
1	А	285	ASP
1	А	452	LYS
1	А	499	PHE
1	А	565	ASP
1	В	207	SER
1	В	248	PHE
1	В	285	ASP
1	В	332	SER
1	В	382	GLU
1	В	459	ASP
1	В	464	MET
1	В	500	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	59	ASN
1	А	458	GLN
1	В	163	GLN
1	В	228	HIS
1	В	242	HIS
1	В	320	HIS
1	В	487	HIS



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Mol	Chain	$\mathbf{Res}$	Type
1	В	596	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

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).

Mal	Turne	Chain	Dog	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
	туре	Unann	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	С	1	2	12,12,12	1.41	1 (8%)	17,17,17	0.63	0
2	GLC	С	2	2	11,11,12	2.05	2 (18%)	15,15,17	1.35	2 (13%)
2	GLC	С	3	2	11,11,12	1.81	3 (27%)	15,15,17	1.11	1 (6%)
2	GLC	D	1	2	12,12,12	1.50	1 (8%)	17,17,17	0.73	0
2	GLC	D	2	2	11,11,12	1.94	3 (27%)	$15,\!15,\!17$	1.12	0
2	GLC	D	3	2	11,11,12	1.99	3 (27%)	15,15,17	0.93	1 (6%)

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	GLC	С	1	2	-	2/2/22/22	0/1/1/1
2	GLC	С	2	2	-	2/2/19/22	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	С	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1

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All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
2	С	2	GLC	O5-C1	5.32	1.52	1.43
2	D	3	GLC	O5-C1	4.99	1.51	1.43
2	D	2	GLC	O5-C1	4.99	1.51	1.43
2	С	3	GLC	O5-C1	4.07	1.50	1.43
2	D	1	GLC	O5-C1	3.99	1.52	1.42
2	С	1	GLC	O5-C1	3.72	1.52	1.42
2	С	3	GLC	O3-C3	2.80	1.49	1.43
2	D	3	GLC	O5-C5	2.58	1.48	1.43
2	С	2	GLC	O5-C5	2.43	1.48	1.43
2	D	2	GLC	C2-C3	-2.32	1.49	1.52
2	С	3	GLC	O5-C5	2.29	1.48	1.43
2	D	3	GLC	O3-C3	2.19	1.48	1.43
2	D	2	GLC	O5-C5	2.10	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	3	GLC	C1-C2-C3	3.17	113.57	109.67
2	С	2	GLC	C3-C4-C5	-2.59	105.61	110.24
2	С	2	GLC	O4-C4-C3	2.39	115.89	110.35
2	D	3	GLC	C1-C2-C3	2.16	112.32	109.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GLC	O5-C5-C6-O6
2	С	2	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	С	1	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
2	С	1	GLC	C4-C5-C6-O6
2	С	3	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	С	2	GLC	C4-C5-C6-O6
2	С	3	GLC	C4-C5-C6-O6

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)

There are no ligands in this entry.

# 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	< <b>RSRZ</b> >	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	687/706~(97%)	0.33	12 (1%) 70 75	27, 38, 64, 153	0
1	В	690/706~(97%)	1.13	143 (20%) 1 1	39, 70, 118, 184	0
All	All	1377/1412~(97%)	0.73	155 (11%) 5 8	27, 50, 109, 184	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	492	VAL	6.6
1	В	677	PHE	5.5
1	В	665	GLY	5.4
1	В	653	TYR	5.3
1	В	555	TRP	4.9
1	А	493	GLY	4.8
1	В	533	ILE	4.8
1	В	574	PHE	4.8
1	В	632	PHE	4.7
1	В	23	PHE	4.7
1	В	651	GLY	4.7
1	В	48	GLY	4.6
1	В	462	TRP	4.6
1	В	643	TYR	4.5
1	А	490	ALA	4.5
1	В	611	VAL	4.5
1	В	657	LEU	4.5
1	В	380	TYR	4.5
1	В	567	TYR	4.5
1	В	645	ILE	4.5
1	В	561	VAL	4.4
1	В	686	ARG	4.4
1	В	513	LEU	4.4
1	В	17	ASP	4.3



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Mol	Chain	Res	Type	RSRZ			
1	В	699	ALA	4.3			
1	А	5	LYS	4.2			
1	В	700	ILE	4.2			
1	В	685	ASN	4.2			
1	В	684	ASN	4.2			
1	В	586	HIS	4.1			
1	В	584	TYR	4.1			
1	В	621	ILE	4.1			
1	В	210	PRO	4.0			
1	В	692	VAL	4.0			
1	В	652	THR	4.0			
1	В	701	VAL	4.0			
1	В	165	TYR	3.9			
1	А	460	ASP	3.9			
1	В	664	PHE	3.9			
1	В	27	LEU	3.9			
1	В	610	TYR	3.9			
1	В	641	THR	3.8			
1	В	20	LEU	3.8			
1	В	576	LEU	3.8			
1	В	631	VAL	3.8			
1	В	560	ARG	3.8			
1	В	682	GLU	3.8			
1	В	681	LEU	3.8			
1	В	671	ASP	3.7			
1	В	698	THR	3.7			
1	В	676	PHE	3.7			
1	В	570	ALA	3.6			
1	В	374	GLY	3.6			
1	В	630	PHE	3.6			
1	В	673	ALA	3.6			
1	В	453	LEU	3.6			
1	В	497	LEU	3.6			
1	В	666	GLY	3.6			
1	А	4	THR	3.5			
1	A	3	LEU	3.5			
1	В	500	TRP	3.5			
1	В	679	THR	3.5			
1	В	581	LEU	3.4			
1	В	490	ALA	3.4			
1	В	465	GLY	3.4			
1	В	689	PHE	3.4			



7P43
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Mol	Chain	Res	Type	RSRZ
1	В	18	PRO	3.4
1	А	1	MET	3.4
1	В	609	ALA	3.3
1	В	690	ILE	3.3
1	В	467	ILE	3.3
1	В	456	THR	3.3
1	В	687	ARG	3.3
1	В	14	VAL	3.2
1	В	7	PRO	3.2
1	В	21	GLU	3.2
1	В	16	ILE	3.2
1	В	646	GLY	3.1
1	В	642	ASP	3.1
1	В	655	ILE	3.1
1	В	13	ALA	3.1
1	В	670	ILE	3.1
1	В	694	ILE	3.1
1	В	527	HIS	3.1
1	В	616	GLU	3.0
1	В	590	PHE	3.0
1	В	640	PHE	3.0
1	В	457	LYS	2.9
1	В	450	TRP	2.9
1	В	660	ASP	2.9
1	В	24	ALA	2.9
1	В	163	GLN	2.9
1	В	466	HIS	2.8
1	В	22	PRO	2.8
1	В	512	VAL	2.8
1	В	504	ALA	2.8
1	В	577	VAL	2.8
1	В	566	SER	2.8
1	А	491	LEU	2.8
1	В	613	LEU	2.8
1	В	476	HIS	2.7
1	В	15	SER	2.7
1	В	693	TYR	2.7
1	В	10	VAL	2.6
1	В	683	TRP	2.6
1	В	647	VAL	2.6
1	В	503	ASP	2.6
1	В	461	ASP	2.5



7P43	
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Mol	Chain	Res	Type	RSRZ
1	В	426	THR	2.5
1	В	662	ALA	2.5
1	В	471	LEU	2.5
1	В	105	HIS	2.5
1	В	47	ASP	2.5
1	В	323	TRP	2.5
1	В	688	ASN	2.5
1	В	137	VAL	2.5
1	В	470	THR	2.5
1	В	620	VAL	2.4
1	В	387	ASP	2.4
1	В	537	LEU	2.4
1	B	704	ARG	2.4
1	В	25	ASP	2.4
1	B	451	ILE	2.4
1	В	562	GLY	2.4
1	В	375	ALA	2.3
1	В	248	PHE	2.3
1	В	703	THR	2.3
1	В	199	TYR	2.3
1	В	510	MET	2.3
1	В	384	LEU	2.3
1	В	145	TYR	2.3
1	В	659	THR	2.2
1	В	552	HIS	2.2
1	В	523	GLY	2.2
1	В	658	ASN	2.2
1	В	618	ASP	2.2
1	В	515	GLU	2.2
1	В	579	ASP	2.2
1	В	603	TRP	2.1
1	В	32	TYR	2.1
1	В	587	LEU	2.1
1	В	635	HIS	2.1
1	В	468	VAL	2.1
1	В	538	GLY	2.1
1	A	161	THR	2.1
1	В	695	PRO	2.1
1	В	8	GLU	2.1
1	В	575	ASN	2.1
1	B	551	GLY	2.1
1	В	617	VAL	2.1



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Mol	Chain	Res	Type	RSRZ
1	В	458	GLN	2.1
1	А	594	MET	2.0
1	А	400	MET	2.0
1	В	534	THR	2.0
1	В	526	LEU	2.0

### 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,  $95^{th}$  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	$B-factors(Å^2)$	Q<0.9
2	GLC	D	1	12/12	0.59	0.44	100,114,119,119	0
2	GLC	D	3	11/12	0.62	0.34	86,93,96,99	0
2	GLC	С	1	12/12	0.70	0.26	78,112,121,150	0
2	GLC	С	3	11/12	0.74	0.27	69,71,76,77	0
2	GLC	С	2	11/12	0.79	0.30	65,74,79,84	0
2	GLC	D	2	11/12	0.87	0.33	89,94,98,99	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)

There are no ligands in this entry.

# 6.5 Other polymers (i)

There are no such residues in this entry.

