

Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 12:22 am GMT

PDB ID : 4CCE

Title : STRUCTURE OF MOUSE GALACTOCEREBROSIDASE WITH GALAC-

TOSE: ENZYME- PRODUCT COMPLEX

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Deposited on : 2013-10-21

Resolution : 2.06 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 : 2.36

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)

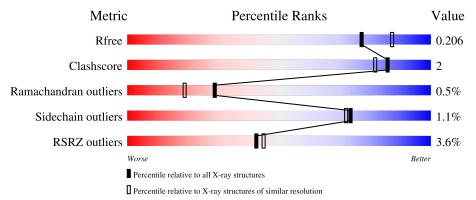
Validation Pipeline (wwPDB-VP) : 2.36

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 2.06 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	654	91%	7% •
2	В	2	100%	
2	С	2	50% 50%	
2	D	2	100%	



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5436 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 GALACTOCEREBROSIDASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	٨	640	Total	С	N	О	S	0	0	0
1	A	040	5119	3315	850	939	15	0	0	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	-	expression tag	UNP P54818
A	16	HIS	-	expression tag	UNP P54818
A	17	HIS	-	expression tag	UNP P54818
A	18	HIS	-	expression tag	UNP P54818
A	19	HIS	-	expression tag	UNP P54818
A	20	HIS	-	expression tag	UNP P54818
A	21	ILE	-	expression tag	UNP P54818
A	22	GLU	-	expression tag	UNP P54818
A	23	GLY	-	expression tag	UNP P54818
A	24	ARG	-	expression tag	UNP P54818

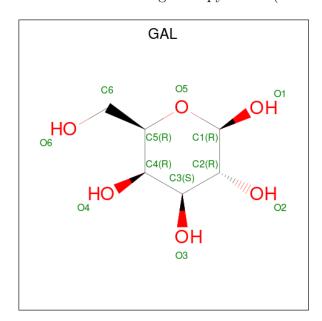
• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0
2	С	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0

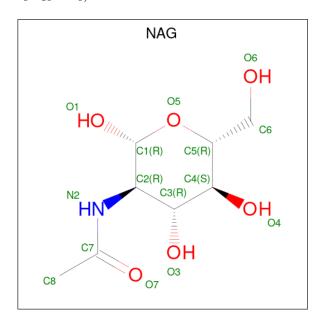


• Molecule 3 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 0	C O 6	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0



• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

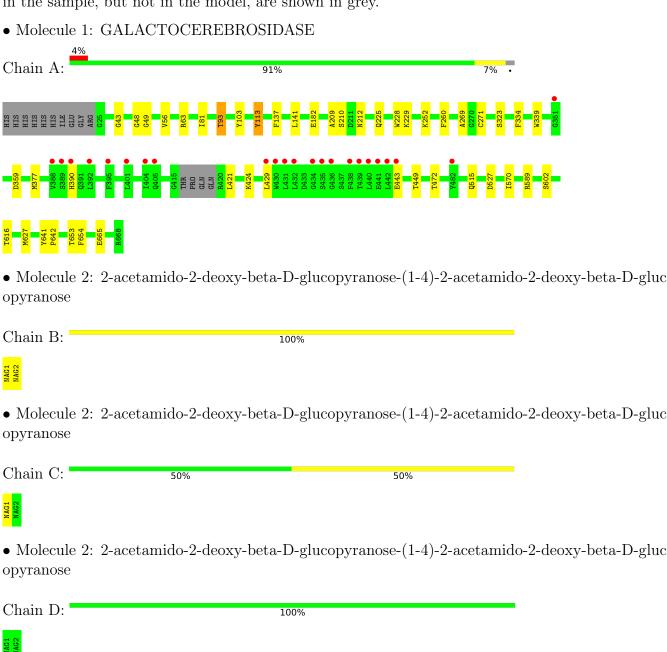
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	206	Total O 206 206	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	248.75Å 248.75Å 77.63Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.25 - 2.06	Depositor
Resolution (A)	47.01 - 2.06	EDS
% Data completeness	99.9 (44.25-2.06)	Depositor
(in resolution range)	99.9 (47.01-2.06)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.33 (at 2.07Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.172 , 0.206	Depositor
R, R_{free}	0.172 , 0.206	DCC
R_{free} test set	2857 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 52.0	EDS
L-test for twinning ²	$ < L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.09% 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: GAL, CA, NAG

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
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.39	0/5282	0.53	0/7202

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	A	5119	0	4868	22	0
2	В	28	0	25	0	0
2	С	28	0	25	0	0
2	D	28	0	25	0	0
3	A	12	0	12	1	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
6	A	206	0	0	1	0
All	All	5436	0	4968	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (22) 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:339:TRP:CE2	1:A:359:ASP:HB3	2.39	0.57
1:A:43:GLY:HA3	1:A:81:ILE:HB	1.87	0.56
1:A:269:ALA:HB2	1:A:323:SER:HB2	1.89	0.55
1:A:616:THR:HB	1:A:627:MET:HB2	1.88	0.55
1:A:63:ARG:NH2	6:A:2014:HOH:O	2.40	0.54
1:A:390:HIS:HD2	1:A:443:GLU:HG2	1.74	0.52
1:A:421:LEU:HB3	1:A:424:LYS:HD3	1.92	0.51
1:A:641:TYR:CD1	1:A:642:PRO:HA	2.46	0.50
1:A:48:GLY:N	1:A:49:GLY:HA2	2.26	0.49
1:A:137:PHE:HB3	1:A:141:LEU:HD12	1.95	0.48
1:A:225:GLN:HG2	1:A:229:LYS:HE3	1.96	0.47
1:A:228:TRP:CE2	1:A:252:LYS:HE2	2.50	0.47
1:A:56:VAL:HG11	1:A:113:TYR:HB3	1.97	0.46
1:A:334:PHE:CD2	1:A:449:THR:HG21	2.53	0.45
1:A:589:ARG:HD3	1:A:602:SER:HB3	1.98	0.44
1:A:641:TYR:CG	1:A:642:PRO:HA	2.53	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.85	0.43
1:A:472:THR:O	1:A:665:GLU:HA	2.19	0.42
1:A:182:GLU:OE1	3:A:1001:GAL:O1	2.38	0.41
1:A:209:ALA:HA	1:A:210:SER:HA	1.84	0.41
1:A:653:THR:OG1	1:A:654:PHE:N	2.52	0.41
1:A:93:THR:HA	1:A:570:ILE:HG23	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed Outliers		Percentiles		
1	A	636/654 (97%)	607 (95%)	26 (4%)	3 (0%)	29 19		

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	93	THR
1	A	260	PHE
1	A	212	ASN

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	533/555 (96%)	527 (99%)	6 (1%)	73 72	

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	113	TYR
1	A	271	CYS
1	A	377	MET
1	A	515	GLN
1	A	527	ASP

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

Mol	Chain	Res	Type	
1	A	390	HIS	

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).

Mol	Trino	Chain	Dag	Link	Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	1.12	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	В	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.57	0
2	NAG	С	1	2,1	14,14,15	0.66	1 (7%)	17,19,21	0.59	0
2	NAG	С	2	2	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	0.41	0
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.35	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
2	NAG	В	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	В	2	2	-	1/6/23/26	0/1/1/1
2	NAG	С	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	В	1	NAG	O5-C1	-4.01	1.37	1.43
2	В	2	NAG	O5-C1	-2.25	1.40	1.43
2	С	1	NAG	O5-C1	-2.15	1.40	1.43

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	В	1	NAG	C4-C3-C2	2.53	114.73	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

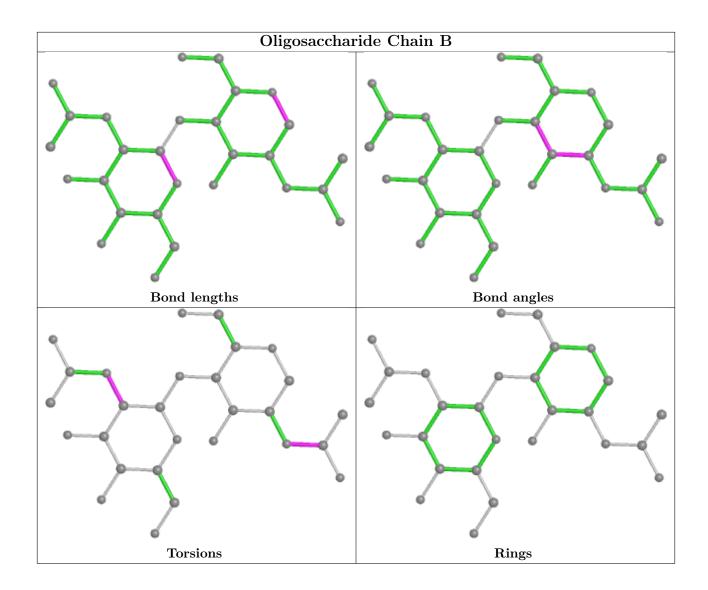
Mol	Chain	Res	Type	Atoms
2	С	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	В	1	NAG	C8-C7-N2-C2
2	В	1	NAG	O7-C7-N2-C2
2	С	1	NAG	C4-C5-C6-O6
2	С	1	NAG	O5-C5-C6-O6
2	В	2	NAG	C1-C2-N2-C7
2	С	1	NAG	C3-C2-N2-C7

There are no ring outliers.

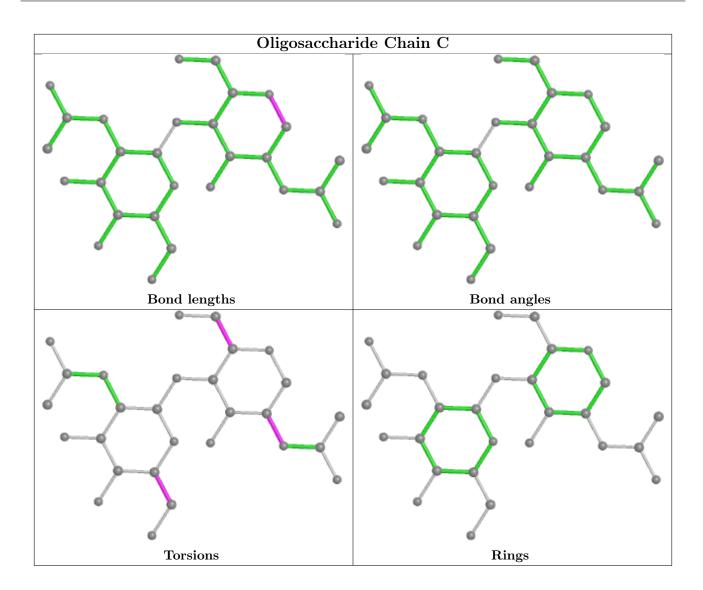
No monomer is involved in short contacts.

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

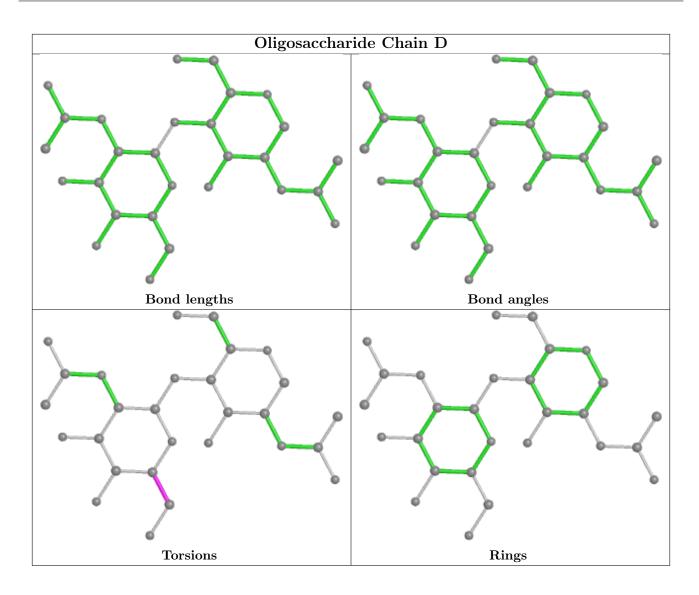












5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Dag	Link	Bond lengths			Bond angles		
MIOI	Туре	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	A	1001	-	12,12,12	1.04	0	17,17,17	0.95	0
4	NAG	A	1387	1	14,14,15	0.35	0	17,19,21	0.38	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
3	GAL	A	1001	-	-	0/2/22/22	0/1/1/1
4	NAG	A	1387	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1387	NAG	O5-C5-C6-O6
4	A	1387	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GAL	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^{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	l Chain Analysed		<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	640/654 (97%)	-0.23	23 (3%)	42	45	22, 42, 77, 111	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	LEU	6.0
1	A	431	LEU	5.9
1	A	404	ILE	5.3
1	A	392	LEU	4.2
1	A	430	TRP	3.7
1	A	438	PHE	3.6
1	A	436	GLY	3.6
1	A	405	GLN	3.4
1	A	434	GLY	3.4
1	A	390	HIS	3.1
1	A	440	LEU	3.1
1	A	429	LEU	2.9
1	A	401	LEU	2.9
1	A	441	GLU	2.7
1	A	482	TYR	2.7
1	A	435	SER	2.4
1	A	395	PHE	2.3
1	A	351	GLY	2.3
1	A	443	GLU	2.2
1	A	389	SER	2.1
1	A	439	THR	2.1
1	A	442	LEU	2.0
1	A	388	VAL	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	NAG	В	2	14/15	0.70	0.34	105,109,112,113	0
2	NAG	С	2	14/15	0.81	0.39	93,105,111,111	0
2	NAG	D	2	14/15	0.81	0.25	76,86,90,92	0
2	NAG	В	1	14/15	0.88	0.16	55,72,79,94	0
2	NAG	С	1	14/15	0.92	0.23	64,80,83,93	0
2	NAG	D	1	14/15	0.93	0.16	48,60,71,77	0

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

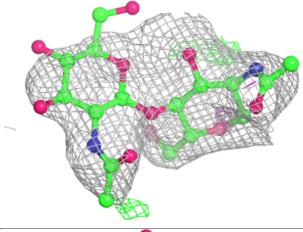


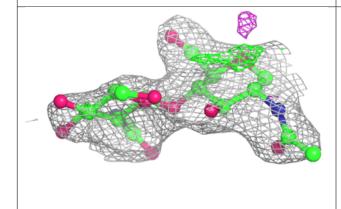
Electron density around Chain B: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

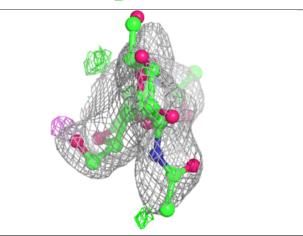


Electron density around Chain C:

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

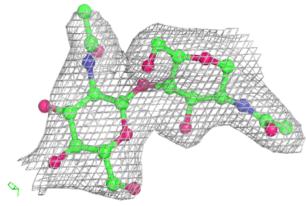


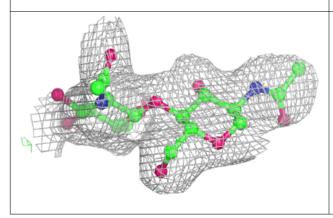


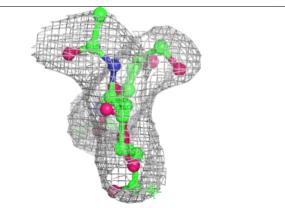


Electron density around Chain D:

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









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
4	NAG	A	1387	14/15	0.78	0.33	74,86,90,92	0
3	GAL	A	1001	12/12	0.95	0.09	28,43,52,55	0
5	CA	A	4001	1/1	0.98	0.11	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.

