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4-Formylphenyl 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranoside

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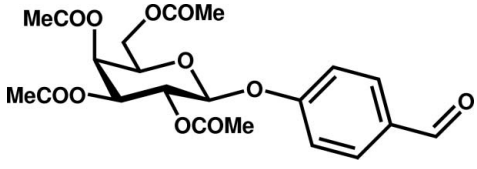
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.086; data-to-parameter ratio = 9.4.

The galactose ring in the title compound, $C_{21}H_{24}O_{11}$, has a chair conformation with the substituted benzene ring occupying an equatorial position. The crystal packing features C—H···O interactions that lead to the formation of supramolecular layers in the *ab* plane.

Related literature

For the synthesis, see: Benassi *et al.* (2007); Patil *et al.* (2008). For the biological activity of related structures, see: Zheng *et al.* (2010). For the structure of the isomeric allopyranoside and glucopyranoside derivatives, see: Ye *et al.* (2009); Heidelberg *et al.* (2011). For conformational analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{21}H_{24}O_{11}$
M_r = 452.40
Monoclinic, $P2_1$
a = 11.8358 (4) Å
b = 5.6664 (2) Å
c = 17.5079 (6) Å
β = 109.616 (4)°
V = 1106.05 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.05 mm

Data collection

Agilent Supernova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.596, T_{max} = 1.000
10396 measured reflections
2768 independent reflections
2535 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.05
2768 reflections
293 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O9^{i}	1.00	2.39	3.199 (3)	137
C5—H5···O9^{i}	1.00	2.45	3.268 (3)	139
C10—H10b···O3^{ii}	0.98	2.46	3.307 (3)	145
C12—H12b···O5^{iii}	0.98	2.57	3.548 (3)	172
C14—H14c···O11^{iv}	0.98	2.50	3.415 (4)	155

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $-x+2, y+\frac{1}{2}, -z+1$; (iv) $x+1, y, z$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2236).

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