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

Thorsten Heidelberg,‡ Rusnah Syahila Duali Hussen, Nasrul Zamani Mohd Rodzi, Seik Weng Ng and Edward R. T. Tiekink*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: edward.tiekink@gmail.com

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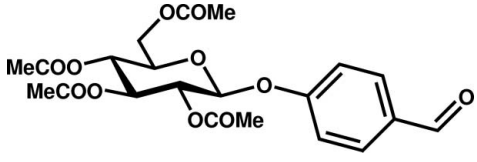
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 14.0.

The pyranoside 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 is dominated by C—H···O interactions that lead to the formation of supramolecular layers in the *ab* plane.

Related literature

For synthesis, see: Bao *et al.* (2004); Hongu *et al.* (1999); Patil & Ravindranathan Kartha (2008). For the natural anti-oxidant glucosylated resveratrol, see: La Torre *et al.* (2004). For the biological activity of related structures, see: Wen *et al.* (2008); Yan *et al.* (2009). For the structure of the isomeric allopyranoside and galactose derivatives, see: Ye *et al.* (2009); Hussen *et al.* (2011). For conformational analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{21}H_{24}O_{11}$
M_r = 452.40
Triclinic, $P\overline{1}$
a = 5.7868 (2) Å
b = 8.9166 (3) Å
c = 11.4716 (3) Å
α = 102.473 (3)°
β = 93.481 (2)°
γ = 102.780 (3)°
V = 559.96 (3) Å^3
Z = 1
Cu $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.20 mm

Data collection

Agilent Supernova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
T_{min} = 0.919, T_{max} = 1.000
7392 measured reflections
4097 independent reflections
4087 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.07
4097 reflections
293 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 1855 Friedel pairs
Flack parameter: -0.02(12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O5^{i}	1.00	2.51	3.356 (2)	143
C3—H3···O5^{i}	1.00	2.35	3.207 (2)	143
C6—H6*A*···O9^{ii}	0.99	2.40	3.324 (2)	155
C8—H8*C*···O11^{iii}	0.98	2.54	3.475 (3)	160

Symmetry codes: (i) $x+1, y, z$; (ii) $x, y+1, z$; (iii) $x-1, y, z$.

Data collection: *CrysAlis PRO* (Agilent Technologies, 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: EZ2235).

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‡ Additional correspondence author, e-mail: heidelberg@um.edu.my.