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1,5-Di-*O*-acetyl-2,3,4-tri-*O*-benzyl-α-D-mannopyranoside

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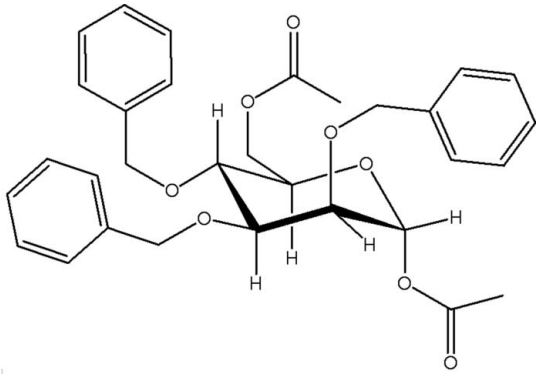
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.053; wR factor = 0.089; data-to-parameter ratio = 8.2.

In the title compound, $C_{31}H_{34}O_8$, the three benzene rings are nearly perpendicular to each other. The six-membered mannopyranoside ring displays a typical chair conformation. Intermolecular C—H···O hydrogen bonding helps to stabilize the crystal structure.

Related literature

For synthesis, see: Tennant-Eyles *et al.* (2000).



Experimental

Crystal data

$C_{31}H_{34}O_8$
M_r = 534.58
Trigonal, $R\overline{3}$
a = 24.001 (3) Å
c = 13.441 (3) Å
V = 6705.5 (19) Å^3
Z = 9
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.50 × 0.45 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: none
16963 measured reflections
2627 independent reflections
1277 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.089
S = 1.03
2627 reflections
319 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23A···O1^{i}	0.97	2.53	3.496 (9)	175

Symmetry code: (i) $-y+2, x-y+1, z$.

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2242).

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supplementary materials

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1,5-Di-*O*-acetyl-2,3,4-tri-*O*-benzyl-*α*-D-mannopyranoside

Z.-J. Liu, D. Han, L.-N. Wang, X.-B. Meng and Z.-J. Li

Comment

The title compound, 1,6-di-*O*-acetyl-2,3,4-tri-*O*-benzyl-α-*D*-mannopyranoside, (I), is obtained from methyl-2,3,4,6-tetra-*O*-benzyl-α-*D*-mannopyranoside with acetic anhydride, acetic acid and concentrated sulfuric acid in ice bath yields 90% as a white solid.

The title compound is a derivative of mannopyranoside, and the six-membered ring has a chair conformation. All five hydroxyl groups are substituted by three benzyloxy groups and two acetoxy groups respectively. The dihedral angles of three benzene rings are 94.4 (2)° (A/B), 103.9 (2)° (A/C), and 110.8 (2)° (B/C). The weak C–H···O hydrogen bonding helps to stabilize the crystal structure (Table 1).

Experimental

The title compound was synthesized according to the procedure of Tennant-Eyles *et al.* (2000). The compound was crystallized from hexane/ethyl acetate solution (4:1, *v*/*v*) to yield colorless block-like crystals after a week at room temperature.

Refinement

All H-atoms were refined using a riding model with C—H = 0.93 Å and U_{iso}=1.2U_{eq}(C) for aromatic, 0.98 Å and U_{iso} = 1.2U_{eq} (C) for CH, 0.97 Å and U_{iso} = 1.2U_{eq}(C) for CH_2, 0.96 Å and U_{iso} = 1.5U_{eq}(C) for CH_3. In the absence of significant anomalous dispersion effects, Freidel pairs were merged.

Figures

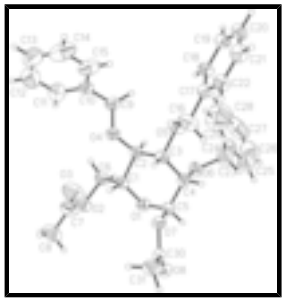


Fig. 1. A view of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

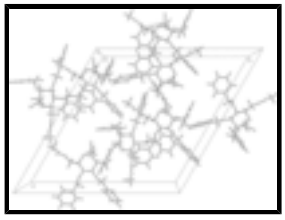


Fig. 2. The molecular packing of (I) viewed along the *c* axis. Dashed lines indicate hydrogen bonding interactions.

1,5-Di-*O*-acetyl-2,3,4-tri-*O*-benzyl-α-*D*-mannopyranoside

Crystal data

$C_{31}H_{34}O_8$	$Z = 9$
$M_r = 534.58$	$F_{000} = 2556$
Trigonal, $R3$	$D_x = 1.191$ Mg m^{-3}
Hall symbol: R 3	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 24.001$ (3) Å	Cell parameters from 16963 reflections
$b = 24.001$ (3) Å	$\theta = 2.4$–25.0°
$c = 13.441$ (3) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 90^\circ$	$T = 298$ (2) K
$\beta = 90^\circ$	Block, colorless
$\gamma = 120^\circ$	0.50 × 0.45 × 0.25 mm
$V = 6705.5$ (19) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2627 independent reflections
Radiation source: fine-focus sealed tube	1277 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.056$
Detector resolution: 10.00 pixels mm^{-1}	$\theta_{max} = 25.0^\circ$
$T = 298$(2) K	$\theta_{min} = 2.4^\circ$
Ω scans	$h = -28 \rightarrow 28$
Absorption correction: none	$k = -28 \rightarrow 26$
16963 measured reflections	$l = -13 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0156P)^2 + 0.731P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2627 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
319 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00248 (10)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8308 (2)	0.89609 (18)	0.0017 (3)	0.0589 (11)
O2	0.7086 (2)	0.8907 (2)	0.0209 (3)	0.0832 (14)
O3	0.6777 (4)	0.9119 (4)	0.1583 (6)	0.169 (3)
O4	0.71440 (19)	0.72464 (19)	0.0247 (3)	0.0593 (11)
O5	0.8332 (2)	0.7232 (2)	0.0228 (3)	0.0640 (12)
O6	0.9087 (2)	0.8540 (2)	0.0925 (3)	0.0690 (13)
O7	0.86749 (18)	0.88162 (18)	−0.1512 (3)	0.0562 (11)
O8	0.9173 (2)	0.9883 (2)	−0.1794 (4)	0.0791 (14)
C1	0.7701 (3)	0.8374 (3)	0.0044 (4)	0.0516 (16)
H1A	0.7513	0.8282	−0.0624	0.062*
C2	0.7752 (3)	0.7796 (3)	0.0409 (4)	0.0506 (16)
H2A	0.7851	0.7841	0.1122	0.061*
C3	0.8278 (3)	0.7760 (3)	−0.0153 (4)	0.0547 (17)
H3A	0.8152	0.7675	−0.0855	0.066*
C4	0.8894 (3)	0.8393 (3)	−0.0087 (4)	0.0570 (17)
H4A	0.9232	0.8373	−0.0470	0.068*
C5	0.8803 (3)	0.8924 (3)	−0.0467 (5)	0.0568 (17)
H5A	0.9205	0.9332	−0.0374	0.068*
C6	0.7279 (3)	0.8491 (3)	0.0724 (5)	0.0680 (19)
H6A	0.6902	0.8086	0.0900	0.082*
H6B	0.7510	0.8697	0.1330	0.082*
C7	0.6824 (4)	0.9177 (5)	0.0706 (7)	0.105 (3)
C8	0.6651 (5)	0.9575 (4)	0.0146 (7)	0.128 (3)
H8A	0.6391	0.9685	0.0550	0.192*
H8B	0.6412	0.9345	−0.0433	0.192*
H8C	0.7033	0.9960	−0.0055	0.192*
C9	0.6919 (3)	0.6800 (3)	0.1058 (5)	0.077 (2)
H9A	0.6883	0.7004	0.1658	0.092*
H9B	0.7212	0.6640	0.1183	0.092*
C10	0.6280 (2)	0.6269 (3)	0.0754 (4)	0.0682 (19)
C11	0.5738 (3)	0.6333 (3)	0.0843 (4)	0.125 (3)
H11A	0.5774	0.6706	0.1116	0.150*
C12	0.5143 (2)	0.5841 (4)	0.0526 (5)	0.160 (4)

H12A	0.4780	0.5884	0.0586	0.192*
C13	0.5090 (3)	0.5284 (3)	0.0118 (4)	0.132 (4)
H13A	0.4691	0.4955	−0.0094	0.158*
C14	0.5631 (4)	0.5220 (3)	0.0028 (4)	0.144 (4)
H14A	0.5596	0.4847	−0.0244	0.173*
C15	0.6227 (3)	0.5712 (3)	0.0346 (4)	0.105 (3)
H15A	0.6589	0.5669	0.0286	0.126*
C16	0.8486 (4)	0.6916 (4)	−0.0499 (5)	0.094 (2)
H16A	0.8883	0.7223	−0.0824	0.113*
H16B	0.8149	0.6741	−0.0998	0.113*
C17	0.8561 (2)	0.63855 (18)	−0.0072 (3)	0.0570 (17)
C18	0.8460 (2)	0.6219 (2)	0.0929 (3)	0.0638 (17)
H18A	0.8323	0.6431	0.1357	0.077*
C19	0.8564 (2)	0.5736 (2)	0.1290 (3)	0.0689 (18)
H19A	0.8497	0.5624	0.1960	0.083*
C20	0.8769 (2)	0.54193 (18)	0.0651 (4)	0.076 (2)
H20A	0.8839	0.5096	0.0893	0.091*
C21	0.8870 (2)	0.5586 (2)	−0.0350 (4)	0.081 (2)
H21A	0.9007	0.5374	−0.0778	0.097*
C22	0.8766 (2)	0.6069 (2)	−0.0712 (2)	0.0679 (19)
H22A	0.8834	0.6180	−0.1381	0.082*
C23	0.9567 (4)	0.8403 (5)	0.1229 (6)	0.111 (3)
H23A	0.9962	0.8663	0.0861	0.133*
H23B	0.9429	0.7953	0.1120	0.133*
C24	0.9667 (4)	0.8558 (4)	0.2296 (4)	0.097 (3)
C25	1.0186 (3)	0.9125 (4)	0.2651 (6)	0.131 (3)
H25A	1.0479	0.9426	0.2207	0.157*
C26	1.0267 (3)	0.9240 (3)	0.3668 (7)	0.176 (5)
H26A	1.0615	0.9619	0.3905	0.212*
C27	0.9830 (5)	0.8790 (5)	0.4332 (4)	0.169 (5)
H27A	0.9885	0.8867	0.5013	0.203*
C28	0.9311 (4)	0.8223 (4)	0.3978 (5)	0.165 (5)
H28A	0.9019	0.7922	0.4422	0.198*
C29	0.9230 (3)	0.8108 (3)	0.2960 (6)	0.140 (4)
H29A	0.8883	0.7729	0.2723	0.169*
C30	0.8914 (3)	0.9350 (4)	−0.2107 (5)	0.0642 (19)
C31	0.8804 (4)	0.9152 (4)	−0.3171 (5)	0.089 (2)
H31A	0.9109	0.9500	−0.3578	0.134*
H31B	0.8375	0.9044	−0.3358	0.134*
H31C	0.8856	0.8784	−0.3264	0.134*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.066 (3)	0.048 (3)	0.062 (3)	0.027 (3)	0.005 (2)	0.001 (2)
O2	0.113 (4)	0.092 (4)	0.078 (3)	0.076 (3)	0.025 (3)	0.018 (3)
O3	0.139 (7)	0.125 (7)	0.106 (5)	0.086 (6)	0.054 (5)	0.036 (5)
O4	0.062 (3)	0.053 (3)	0.049 (3)	0.019 (2)	−0.004 (2)	0.011 (2)

O5	0.097 (3)	0.066 (3)	0.048 (3)	0.055 (3)	0.009 (2)	0.000 (2)
O6	0.065 (3)	0.084 (3)	0.063 (3)	0.041 (3)	−0.014 (2)	0.000 (2)
O7	0.059 (3)	0.051 (3)	0.051 (2)	0.021 (2)	0.002 (2)	0.007 (2)
O8	0.068 (3)	0.057 (3)	0.100 (4)	0.022 (3)	−0.002 (3)	0.012 (3)
C1	0.060 (4)	0.054 (4)	0.043 (3)	0.030 (4)	0.001 (3)	0.004 (3)
C2	0.058 (4)	0.048 (4)	0.044 (4)	0.025 (4)	−0.003 (3)	0.002 (3)
C3	0.065 (5)	0.051 (4)	0.052 (4)	0.031 (4)	−0.005 (3)	−0.005 (3)
C4	0.059 (4)	0.059 (5)	0.049 (4)	0.027 (4)	0.001 (3)	0.002 (3)
C5	0.055 (4)	0.051 (4)	0.060 (5)	0.024 (3)	−0.006 (4)	−0.001 (3)
C6	0.083 (5)	0.074 (5)	0.061 (4)	0.049 (4)	0.017 (4)	0.017 (4)
C7	0.143 (8)	0.133 (8)	0.082 (7)	0.101 (7)	0.046 (6)	0.037 (6)
C8	0.141 (7)	0.129 (6)	0.112 (7)	0.116 (6)	0.023 (6)	0.028 (6)
C9	0.068 (4)	0.067 (4)	0.079 (5)	0.021 (4)	−0.002 (4)	0.019 (4)
C10	0.091 (5)	0.084 (5)	0.077 (4)	0.026 (4)	0.004 (4)	0.021 (4)
C11	0.092 (6)	0.114 (6)	0.160 (8)	0.044 (5)	−0.012 (5)	0.013 (6)
C12	0.131 (6)	0.131 (7)	0.170 (7)	0.069 (5)	−0.021 (5)	0.033 (6)
C13	0.119 (7)	0.115 (7)	0.080 (6)	−0.003 (5)	−0.027 (5)	0.022 (5)
C14	0.141 (9)	0.102 (7)	0.102 (6)	0.026 (6)	0.024 (7)	−0.002 (5)
C15	0.120 (6)	0.076 (5)	0.097 (6)	0.031 (5)	0.028 (5)	0.011 (5)
C16	0.094 (7)	0.080 (5)	0.062 (5)	0.056 (5)	0.010 (4)	0.011 (4)
C17	0.065 (4)	0.054 (4)	0.055 (4)	0.032 (4)	0.010 (3)	−0.005 (3)
C18	0.086 (5)	0.063 (4)	0.061 (5)	0.051 (4)	0.004 (4)	−0.001 (4)
C19	0.078 (5)	0.066 (5)	0.070 (4)	0.041 (4)	−0.002 (4)	−0.005 (4)
C20	0.084 (5)	0.071 (5)	0.088 (6)	0.051 (4)	−0.004 (4)	−0.006 (5)
C21	0.091 (6)	0.096 (6)	0.063 (5)	0.053 (5)	0.007 (4)	−0.014 (4)
C22	0.082 (5)	0.075 (5)	0.062 (4)	0.050 (4)	0.012 (4)	−0.003 (4)
C23	0.080 (6)	0.132 (7)	0.084 (5)	0.064 (5)	−0.015 (5)	0.007 (5)
C24	0.092 (6)	0.133 (7)	0.085 (6)	0.041 (5)	−0.030 (5)	0.008 (6)
C25	0.106 (8)	0.131 (9)	0.162 (11)	0.063 (8)	−0.026 (7)	−0.002 (8)
C26	0.135 (9)	0.153 (9)	0.160 (9)	0.073 (7)	−0.036 (8)	−0.032 (8)
C27	0.151 (15)	0.162 (13)	0.105 (8)	0.061 (12)	−0.044 (10)	−0.058 (10)
C28	0.189 (9)	0.157 (8)	0.101 (8)	0.072 (7)	−0.027 (7)	0.021 (6)
C29	0.199 (11)	0.153 (10)	0.066 (6)	0.084 (9)	−0.044 (7)	−0.007 (6)
C30	0.047 (4)	0.066 (5)	0.078 (5)	0.028 (4)	0.008 (4)	0.015 (4)
C31	0.110 (6)	0.104 (6)	0.057 (5)	0.055 (5)	0.019 (4)	0.023 (4)

Geometric parameters (Å, °)

O1—C5	1.396 (7)	C12—H12A	0.9300
O1—C1	1.434 (7)	C13—C14	1.3900
O2—C7	1.291 (9)	C13—H13A	0.9300
O2—C6	1.469 (7)	C14—C15	1.3900
O3—C7	1.186 (9)	C14—H14A	0.9300
O4—C2	1.411 (6)	C15—H15A	0.9300
O4—C9	1.431 (7)	C16—C17	1.487 (7)
O5—C16	1.395 (7)	C16—H16A	0.9700
O5—C3	1.433 (7)	C16—H16B	0.9700
O6—C23	1.409 (8)	C17—C18	1.3900
O6—C4	1.423 (6)	C17—C22	1.3900

O7—C30	1.369 (7)	C18—C19	1.3900
O7—C5	1.433 (6)	C18—H18A	0.9300
O8—C30	1.186 (7)	C19—C20	1.3900
C1—C6	1.490 (8)	C19—H19A	0.9300
C1—C2	1.534 (7)	C20—C21	1.3900
C1—H1A	0.9800	C20—H20A	0.9300
C2—C3	1.509 (8)	C21—C22	1.3900
C2—H2A	0.9800	C21—H21A	0.9300
C3—C4	1.501 (8)	C22—H22A	0.9300
C3—H3A	0.9800	C23—C24	1.472 (9)
C4—C5	1.488 (8)	C23—H23A	0.9700
C4—H4A	0.9800	C23—H23B	0.9700
C5—H5A	0.9800	C24—C25	1.3900
C6—H6A	0.9700	C24—C29	1.3900
C6—H6B	0.9700	C25—C26	1.3900
C7—C8	1.430 (11)	C25—H25A	0.9300
C8—H8A	0.9600	C26—C27	1.3900
C8—H8B	0.9600	C26—H26A	0.9300
C8—H8C	0.9600	C27—C28	1.3900
C9—C10	1.479 (7)	C27—H27A	0.9300
C9—H9A	0.9700	C28—C29	1.3900
C9—H9B	0.9700	C28—H28A	0.9300
C10—C11	1.3900	C29—H29A	0.9300
C10—C15	1.3900	C30—C31	1.490 (9)
C11—C12	1.3900	C31—H31A	0.9600
C11—H11A	0.9300	C31—H31B	0.9600
C12—C13	1.3900	C31—H31C	0.9600
C5—O1—C1	115.4 (4)	C12—C13—C14	120.0
C7—O2—C6	119.7 (6)	C12—C13—H13A	120.0
C2—O4—C9	114.1 (5)	C14—C13—H13A	120.0
C16—O5—C3	113.4 (4)	C15—C14—C13	120.0
C23—O6—C4	114.9 (5)	C15—C14—H14A	120.0
C30—O7—C5	116.9 (5)	C13—C14—H14A	120.0
O1—C1—C6	106.5 (5)	C14—C15—C10	120.0
O1—C1—C2	113.3 (5)	C14—C15—H15A	120.0
C6—C1—C2	110.1 (5)	C10—C15—H15A	120.0
O1—C1—H1A	109.0	O5—C16—C17	111.9 (5)
C6—C1—H1A	109.0	O5—C16—H16A	109.2
C2—C1—H1A	109.0	C17—C16—H16A	109.2
O4—C2—C3	111.9 (5)	O5—C16—H16B	109.2
O4—C2—C1	106.4 (5)	C17—C16—H16B	109.2
C3—C2—C1	109.8 (5)	H16A—C16—H16B	107.9
O4—C2—H2A	109.6	C18—C17—C22	120.0
C3—C2—H2A	109.6	C18—C17—C16	122.7 (4)
C1—C2—H2A	109.6	C22—C17—C16	117.2 (4)
O5—C3—C4	113.1 (5)	C19—C18—C17	120.0
O5—C3—C2	108.6 (5)	C19—C18—H18A	120.0
C4—C3—C2	110.1 (5)	C17—C18—H18A	120.0
O5—C3—H3A	108.3	C18—C19—C20	120.0

C4—C3—H3A	108.3	C18—C19—H19A	120.0
C2—C3—H3A	108.3	C20—C19—H19A	120.0
O6—C4—C5	106.5 (5)	C21—C20—C19	120.0
O6—C4—C3	109.9 (5)	C21—C20—H20A	120.0
C5—C4—C3	110.6 (5)	C19—C20—H20A	120.0
O6—C4—H4A	109.9	C20—C21—C22	120.0
C5—C4—H4A	109.9	C20—C21—H21A	120.0
C3—C4—H4A	109.9	C22—C21—H21A	120.0
O1—C5—O7	110.8 (5)	C21—C22—C17	120.0
O1—C5—C4	112.9 (5)	C21—C22—H22A	120.0
O7—C5—C4	107.0 (5)	C17—C22—H22A	120.0
O1—C5—H5A	108.7	O6—C23—C24	105.8 (6)
O7—C5—H5A	108.7	O6—C23—H23A	110.6
C4—C5—H5A	108.7	C24—C23—H23A	110.6
O2—C6—C1	108.3 (5)	O6—C23—H23B	110.6
O2—C6—H6A	110.0	C24—C23—H23B	110.6
C1—C6—H6A	110.0	H23A—C23—H23B	108.7
O2—C6—H6B	110.0	C25—C24—C29	120.0
C1—C6—H6B	110.0	C25—C24—C23	122.3 (7)
H6A—C6—H6B	108.4	C29—C24—C23	117.7 (7)
O3—C7—O2	119.9 (8)	C26—C25—C24	120.0
O3—C7—C8	123.9 (9)	C26—C25—H25A	120.0
O2—C7—C8	116.0 (8)	C24—C25—H25A	120.0
C7—C8—H8A	109.5	C25—C26—C27	120.0
C7—C8—H8B	109.5	C25—C26—H26A	120.0
H8A—C8—H8B	109.5	C27—C26—H26A	120.0
C7—C8—H8C	109.5	C28—C27—C26	120.0
H8A—C8—H8C	109.5	C28—C27—H27A	120.0
H8B—C8—H8C	109.5	C26—C27—H27A	120.0
O4—C9—C10	106.0 (5)	C27—C28—C29	120.0
O4—C9—H9A	110.5	C27—C28—H28A	120.0
C10—C9—H9A	110.5	C29—C28—H28A	120.0
O4—C9—H9B	110.5	C28—C29—C24	120.0
C10—C9—H9B	110.5	C28—C29—H29A	120.0
H9A—C9—H9B	108.7	C24—C29—H29A	120.0
C11—C10—C15	120.0	O8—C30—O7	123.5 (7)
C11—C10—C9	120.3 (6)	O8—C30—C31	126.8 (7)
C15—C10—C9	119.7 (6)	O7—C30—C31	109.8 (6)
C10—C11—C12	120.0	C30—C31—H31A	109.5
C10—C11—H11A	120.0	C30—C31—H31B	109.5
C12—C11—H11A	120.0	H31A—C31—H31B	109.5
C13—C12—C11	120.0	C30—C31—H31C	109.5
C13—C12—H12A	120.0	H31A—C31—H31C	109.5
C11—C12—H12A	120.0	H31B—C31—H31C	109.5
C5—O1—C1—C6	171.0 (5)	O4—C9—C10—C11	−80.9 (6)
C5—O1—C1—C2	49.9 (6)	O4—C9—C10—C15	97.0 (5)
C9—O4—C2—C3	103.7 (6)	C15—C10—C11—C12	0.0
C9—O4—C2—C1	−136.4 (5)	C9—C10—C11—C12	177.9 (5)
O1—C1—C2—O4	−171.0 (5)	C10—C11—C12—C13	0.0

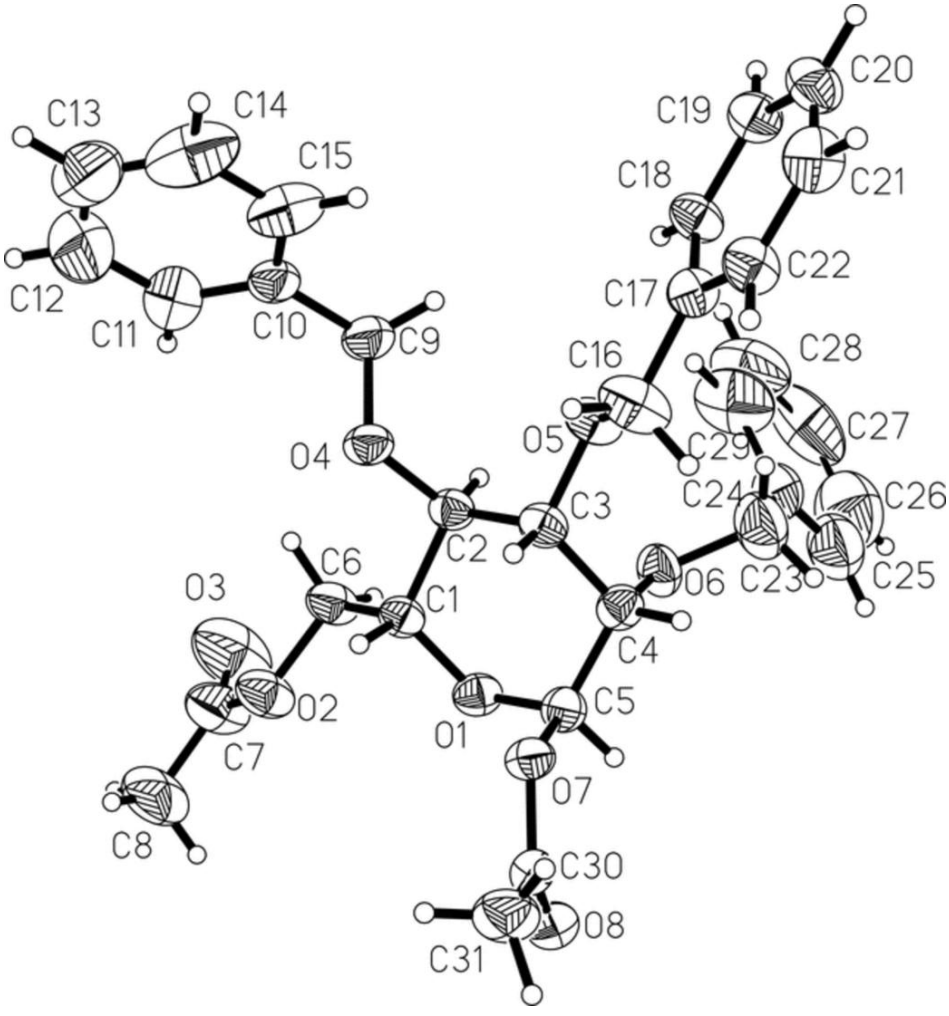
C6—C1—C2—O4	69.9 (6)	C11—C12—C13—C14	0.0
O1—C1—C2—C3	−49.7 (6)	C12—C13—C14—C15	0.0
C6—C1—C2—C3	−168.7 (5)	C13—C14—C15—C10	0.0
C16—O5—C3—C4	−92.8 (7)	C11—C10—C15—C14	0.0
C16—O5—C3—C2	144.7 (6)	C9—C10—C15—C14	−177.9 (5)
O4—C2—C3—O5	−64.3 (6)	C3—O5—C16—C17	178.0 (5)
C1—C2—C3—O5	177.8 (5)	O5—C16—C17—C18	2.6 (8)
O4—C2—C3—C4	171.3 (5)	O5—C16—C17—C22	−174.8 (4)
C1—C2—C3—C4	53.4 (6)	C22—C17—C18—C19	0.0
C23—O6—C4—C5	−140.2 (6)	C16—C17—C18—C19	−177.4 (5)
C23—O6—C4—C3	99.9 (7)	C17—C18—C19—C20	0.0
O5—C3—C4—O6	−61.1 (7)	C18—C19—C20—C21	0.0
C2—C3—C4—O6	60.6 (6)	C19—C20—C21—C22	0.0
O5—C3—C4—C5	−178.4 (5)	C20—C21—C22—C17	0.0
C2—C3—C4—C5	−56.7 (7)	C18—C17—C22—C21	0.0
C1—O1—C5—O7	67.4 (6)	C16—C17—C22—C21	177.5 (5)
C1—O1—C5—C4	−52.6 (7)	C4—O6—C23—C24	−177.2 (6)
C30—O7—C5—O1	91.6 (6)	O6—C23—C24—C25	−101.6 (7)
C30—O7—C5—C4	−144.9 (5)	O6—C23—C24—C29	80.1 (7)
O6—C4—C5—O1	−63.7 (6)	C29—C24—C25—C26	0.0
C3—C4—C5—O1	55.7 (7)	C23—C24—C25—C26	−178.3 (6)
O6—C4—C5—O7	174.1 (4)	C24—C25—C26—C27	0.0
C3—C4—C5—O7	−66.5 (6)	C25—C26—C27—C28	0.0
C7—O2—C6—C1	−166.6 (7)	C26—C27—C28—C29	0.0
O1—C1—C6—O2	73.5 (6)	C27—C28—C29—C24	0.0
C2—C1—C6—O2	−163.3 (5)	C25—C24—C29—C28	0.0
C6—O2—C7—O3	4.6 (14)	C23—C24—C29—C28	178.4 (6)
C6—O2—C7—C8	−180.0 (7)	C5—O7—C30—O8	−5.9 (9)
C2—O4—C9—C10	179.4 (5)	C5—O7—C30—C31	173.5 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23A···O1^{i}	0.97	2.53	3.496 (9)	175

Symmetry codes: (i) −*y*+2, *x*−*y*+1, *z*.

Fig. 1


C20
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O3
C4
O2
C5
O1
C7
O7
C8
C30
O8
C31

Fig. 2