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2,2′-(Propane-1,3-diyldioxy)dibenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.110
Data-to-parameter ratio = 10.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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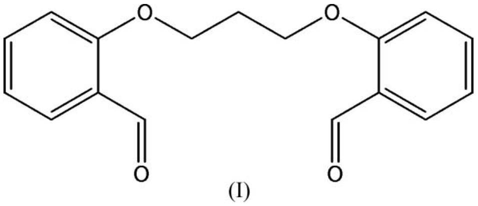
Molecules of the title compound, $C_{17}H_{16}O_4$, form a chain along the *c* axis *via* π–π stacking interactions involving neighboring aromatic rings. The chains are linked through intermolecular C—H···O hydrogen bonds, resulting in a zigzag packing arrangement.

Comment

Much attention has been paid to the synthesis, coordination chemistry and catalytic application of salicylaldehyde, its Schiff bases and metal complexes (Hata *et al.*, 2004; Scherhag & Spicer, 2000; Mukherjee *et al.*, 2001; Li *et al.*, 2000), leading to the characterization of many derivatives. Meanwhile, interactions, such as C—H···π, π–π and weak hydrogen-bonding interactions (C—H···*X*: *X* = O, N, Cl, Br), are known to play crucial roles in molecular self-assembly and crystal symmetry in biology, chemistry and materials science (Leininger *et al.*, 2000; Müller-Dethlefs & Hobza, 2000; Conn & Rebek, 1997; Hunter *et al.*, 1991; Desiraju, 2005).



(I)

In the title molecule, (I), four intramolecular C—H···O hydrogen bonds are observed (Table 1). The planes of the aromatic rings form a dihedral angle of 99.88 (5)°, with the aldehyde groups oriented in opposite directions (Fig. 1). Interestingly, the C1–C6 benzene ring is offset-stacked along

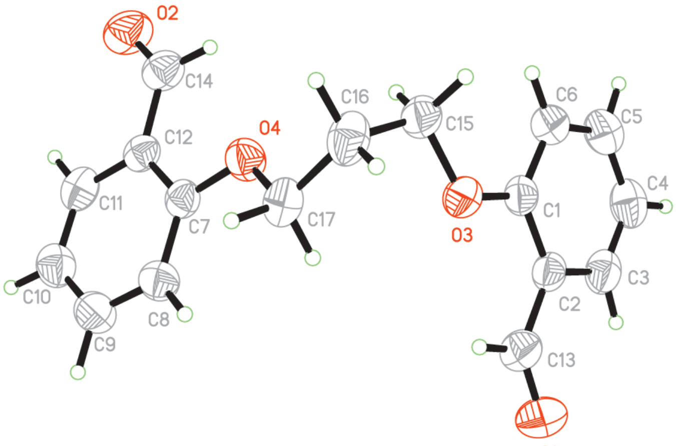


Figure 1
View of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

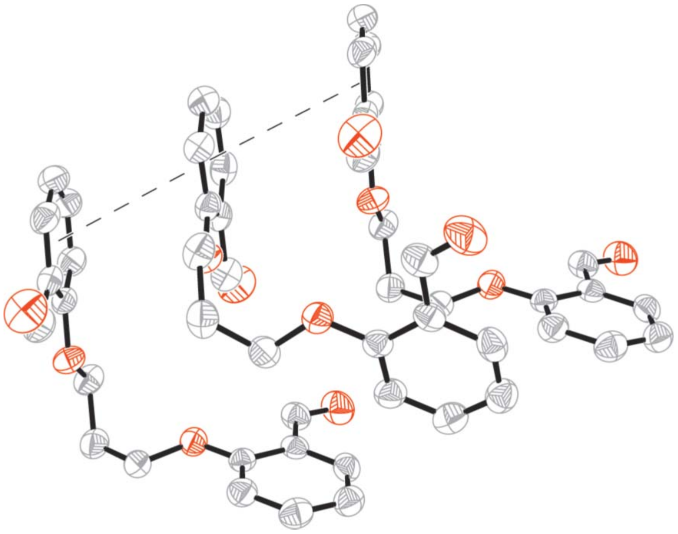


Figure 2
The one-dimensional chain structure of (I) formed by π–π interactions along the *c* axis (dashed lines represent the π–π interactions). H atoms have been omitted.

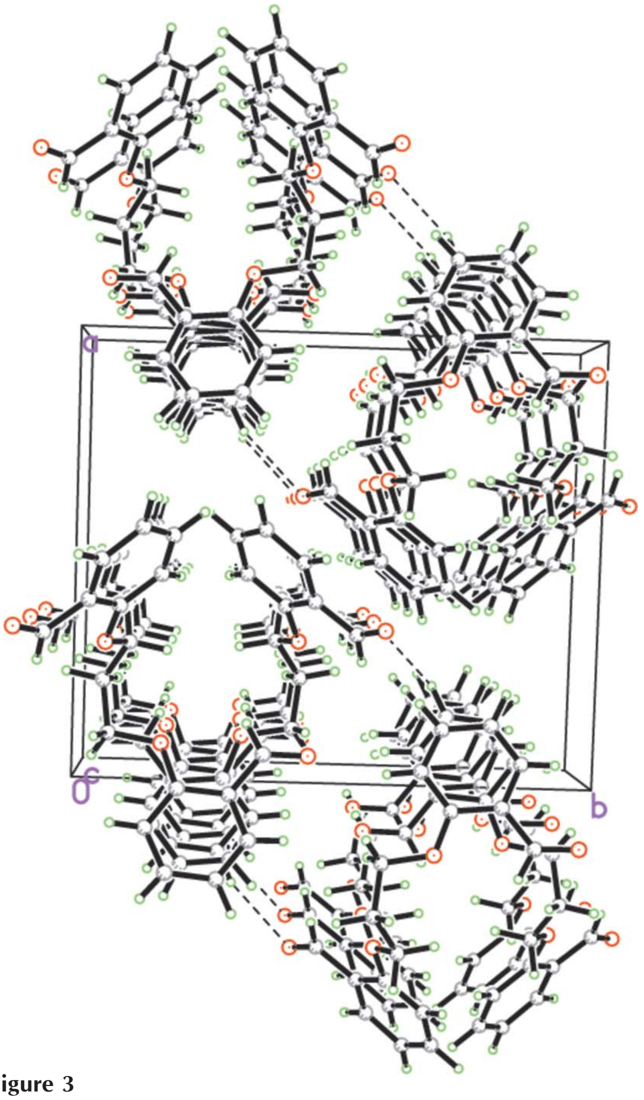


Figure 3
A packing diagram of (I), viewed down the *c* axis. Dashed lines denote C—H···O hydrogen bonds.

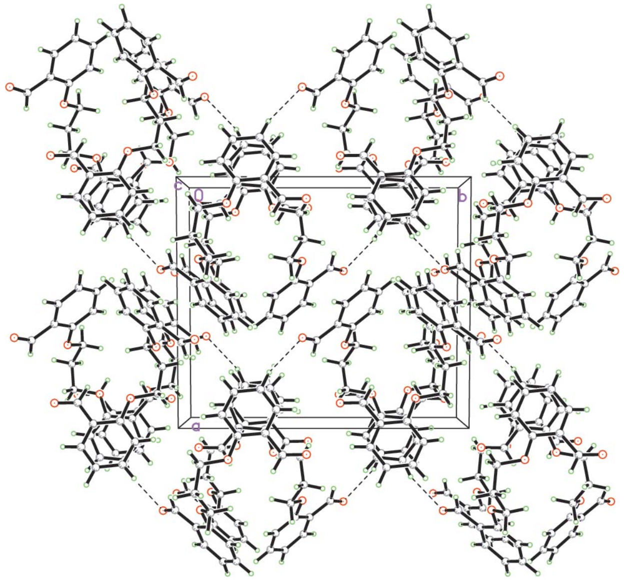


Figure 4
The zigzag packing arrangement of (I) parallel to the *ab* plane. C—H···O hydrogen bonds are shown as dashed lines.

the *c* axis with respect to the corresponding rings of neighboring molecules at $(x, \frac{1}{2} - y, -\frac{1}{2} + z)$ and $(x, \frac{1}{2} - y, \frac{1}{2} + z)$ (Fig. 2). The dihedral angle formed by adjacent rings is 3.53 (7)°. The centroid–centroid distance between two neighbouring ring centers is 3.915 (3) Å and the perpendicular distances of the center of a benzene ring to two neighboring rings are 3.532 (4) and 3.539 (4) Å. These values indicate the presence of reasonable π–π aromatic interactions (Hunter & Sanders, 1990), which greatly contribute to the stabilization of the one-dimensional chain structure. There is a weak C—H···O hydrogen bond between adjacent chains (Table 1), resulting in a two-dimensional zigzag packing arrangement parallel to the *ab* plane.

Experimental

The title compound was prepared according to the literature method Atkins *et al.* (1994). A mixture of salicylaldehyde (60 mmol), 1,3-dibromopropane (30 mmol) and anhydrous K_2CO_3 (60 mmol) was stirred under N_2 in anhydrous dimethylformamide (60 ml) for 20 h, then cooled to room temperature in an ice-water bath to ensure precipitation. After filtration, the precipitate was recrystallized from 95% ethanol to give the title compound (70% yield). A small amount of the precipitate was dissolved in 95% ethanol to make a clear solution and kept at room temperature for a week to give light-yellow pillar-shaped crystals suitable for X-ray diffraction analysis.

Crystal data

$C_{17}H_{16}O_4$
$M_r = 284.30$
Monoclinic, $P2_1/c$
$a = 12.8275$ (12) Å
$b = 14.8431$ (13) Å
$c = 7.8272$ (7) Å
$\beta = 95.334$ (2)°
$V = 1483.8$ (2) Å^3
$Z = 4$

$D_x = 1.273$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1628 reflections
$\theta = 3.0$–19.1°
$\mu = 0.09$ mm^{-1}
$T = 295$ (2) K
Pillar, light yellow
0.21 × 0.18 × 0.13 mm

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Data collection

Bruker SMART APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.981$, $T_{\max} = 0.988$
10969 measured reflections
2758 independent reflections
1562 reflections with I > 2šI)
$R_{\rm int} = 0.030$
$\theta_{\max} = 25.5°$
$h = -15 \rightarrow 15$
$k = -17 \rightarrow 17$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.110$
$S = 1.01$
2758 reflections
255 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.1205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.11$ e Å^{-3}
$\Delta\rho_{\min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0093 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1	0.93 (2)	2.51 (2)	2.871 (3)	103 (1)
C11—H11···O2	0.95 (2)	2.50 (2)	2.828 (3)	100 (1)
C13—H13···O3	0.98 (2)	2.36 (2)	2.737 (3)	102 (2)
C14—H14···O4	0.98 (2)	2.43 (2)	2.786 (3)	101 (1)
C4—H4···O2$^{\rm i}$	1.04 (2)	2.48 (2)	3.454 (3)	156 (2)

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

The H atoms were located in a difference Fourier map and refined isotropically [C—H = 0.93–(2)–1.04–(2)–Å].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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