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3,5-Di-*tert*-butyl-2-hydroxybenzaldehyde

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The title compound, $C_{15}H_{22}O_2$, crystallizes in the monoclinic space group $P2_1/c$, with two molecules in the asymmetric unit related by a non-crystallographic inversion centre. The O—H···O hydrogen bonding is exclusively intramolecular.

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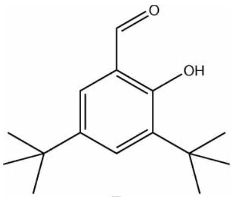
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.053
wR factor = 0.146
Data-to-parameter ratio = 16.2

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

Comment

During the course of research into metal complexes with extended chelating ligands, the structure of the title compound, (I), was determined (Fig. 1).



(I)

The asymmetric unit contains two crystallographically independent molecules, one of which includes a disordered *tert*-butyl group, with relative occupancies of 69.6 (3) and 30.4 (3)% for the two components. Small (10 Å^3) voids are found close to the disordered moieties.

A local pseudo-inversion centre is located between the two crystallographically independent molecules, and is broken by the disorder of the *tert*-butyl group involving atom C23. It is, in fact, the major component of the disorder that breaks the symmetry, and not the minor (Fig. 2).

The only strong hydrogen bonds are intramolecular, between H2 and O1, and between H4 and O3, and the molecules pack in layers parallel to the (101) plane in the crystal structure (Fig. 3).

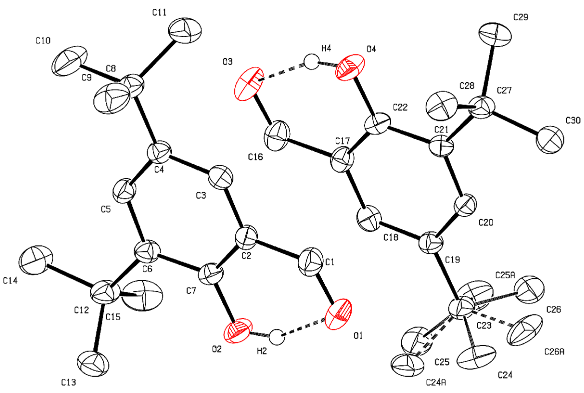


Figure 1
The asymmetric unit of the title compound, with the atom-numbering scheme. Both disorder components are included. Dashed bonds represent hydrogen bonds. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

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Experimental

The title compound, recovered unchanged from a reaction mixture in which it was one of the intended reagents, was recrystallized from hot methanol, giving large good-quality single crystals.

Crystal data

$C_{15}H_{22}O_2$
$M_r = 234.33$
Monoclinic, $P2_1/c$
$a = 11.627$ (1) Å
$b = 10.1214$ (7) Å
$c = 25.461$ (2) Å
$\beta = 111.326$ (3)°
$V = 2791.1$ (4) Å^3
$Z = 8$
$D_x = 1.115$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 56 reflections
$\theta = 4.0$–18.3°
$\mu = 0.07$ mm^{-1}
$T = 150$ K
Block, colourless
0.30 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
28855 measured reflections
5782 independent reflections
4178 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.063$
$\theta_{\rm max} = 26.5°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.146$
$S = 1.04$
5782 reflections
358 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 1.0702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.36$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O3—C16	1.227 (2)	O1—C1	1.226 (2)
O4—C22	1.3560 (18)	O2—C7	1.3584 (18)
O3—C16—C17	125.00 (16)	O1—C1—C2	125.03 (16)
O4—C22—C21	119.60 (14)	O2—C7—C6	119.89 (14)
O4—C22—C17	120.03 (14)	O2—C7—C2	120.05 (14)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.88 (2)	1.80 (2)	2.6122 (18)	151.5 (19)
O4—H4···O3	0.88 (3)	1.79 (2)	2.6075 (18)	153.7 (19)

Atoms H2 and H4 were refined freely with individual isotropic displacement parameters. All remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H atoms, and C—H = 0.95 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for all other H atoms. The *tert*-butyl group containing atom C23 was rotationally disordered over two positions. The final occupancies of the two sites were 69.6 (3) and 30.4 (3)% for the major and minor components, respectively.

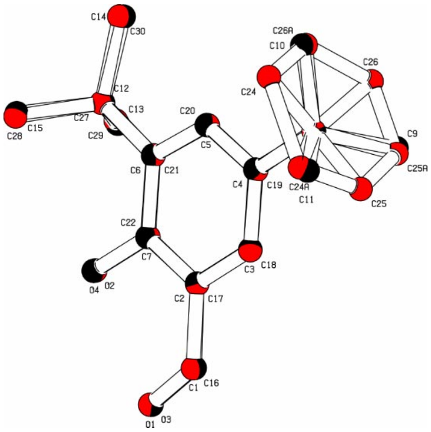

Figure 2
Plot of the fit between the two molecules related by a pseudo-inversion centre (one molecule has been inverted). It is the major component that breaks the symmetry, and not the minor.

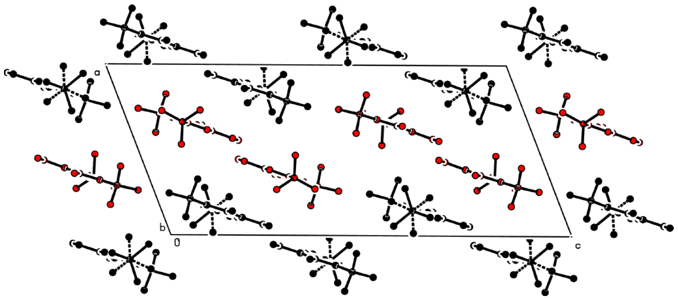

Figure 3
Projection of the structure down the *b* axis, demonstrating the packing of the two crystallographically independent molecules in layers parallel to the (101) plane.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVAL*14 (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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