organic compounds

2,6-Di-*tert*-butyl-4-(morpholinomethyl)-phenol monohydrate

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In the title compound, $C_{19}H_{31}NO_2 \cdot H_2O$, the morpholine ring adopts a chair conformation, while the phenolic hydroxyl group is sterically hindered by the adjacent *tert*-butyl groups. The crystal structure is stabilized by a number of O—H⋯O, O—H⋯N and C—H⋯O hydrogen-bonding interactions, involving both the organic and the solvent molecules.

Related literature

For related literature, see: Shu *et al.* (2005); Zeng & Chen (2006); Zeng *et al.* (2006); Yamazaki & Seguchi (1997); Steiner (1996); Rieker (1968).
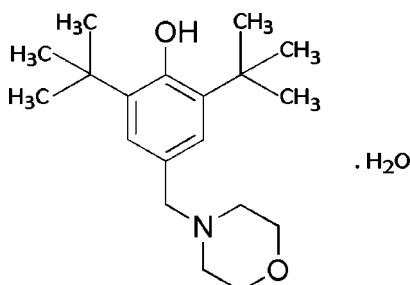
Experimental

Crystal data

$C_{19}H_{31}NO_2 \cdot H_2O$
$M_r = 323.46$
Monoclinic, $P2_1/n$
$a = 10.1461 (14)$ Å
$b = 9.7118 (12)$ Å
$c = 19.966 (2)$ Å
$\beta = 95.166 (8)°$
$V = 1959.4 (4)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 294 (2)$ K
$0.32 \times 0.30 \times 0.26$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.97$, $T_{max} = 0.98$
9174 measured reflections
3412 independent reflections
2098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.151$
$S = 1.03$
3412 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H3B⋯O2^i	0.86 (3)	2.13 (3)	2.884 (2)	146 (3)
O3—H3A⋯N1^{ii}	0.83 (3)	2.10 (3)	2.915 (2)	170 (3)
O1—H1⋯O3	0.85 (3)	1.91 (3)	2.734 (2)	162 (3)
C12—H12B⋯O3	0.96	2.47	3.410 (3)	167

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$.

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2147).

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supporting information

2,6-Di-*tert*-butyl-4-(morpholinomethyl)phenol monohydrate

Tao Zeng and Wan-Zhong Ren

S1. Comment

Hindered phenol antioxidants are widely used in polymers and lubricants. They can protect polymers by increasing both their process and long-term stability against oxidative degradation (Yamazaki & Seguchi, 1997). In our research, derivates of 2,6-di-*tert*-butyl-4-(alkylamino)methylphenol have been studied (Shu *et al.*, 2005; Zeng *et al.*, 2006; Zeng & Chen, 2006). In a former paper, we have reported the transformation of 2,6-di-*tert*-butyl-4-(alkylamino)methyl-phenols to *N*,*N*-bis(3,5-di-*tert*-butyl- 4-hydroxylbenzyl)-*N*-alkylamines (Zeng *et al.*, 2006), and proposed a mechanism by which 2,6-di-*tert*-butyl-4-(alkylamino)methyl-phenols could trnsform to 2,6-di-*tert*-butyl-4-methylenecyclohexa-2,5-dienone and then react with another molecule of 2,6-di-*tert*-butyl-4-(alkylamino)methyl-phenols to yield the *N*,*N*-bis(3,5-di-*tert*-butyl-4-hydroxylbenzyl)-*N*-alkylamines. To confirm this mechanism, a number of experiments have been carried out, *viz.*, the reaction of 2,6-di-*tert*-butyl-4-(alkylamino)methyl-phenol with different amines, and the products were analysed carefully. For example, when 2,6-di-*tert*-butyl-4-(butylamino)methyl-phenol reacts with morpholine the title compound (I) was obtained, but the same result was obtained when different 2,6-di-*tert*-butyl-4-(alkylamino)methyl-phenols such as 2,6-di-*tert*-butyl-4-(propylamino)methylphenol or 2,6-di-*tert*-butyl-4-(iso-propylamino)methylphenol were used instead. This behaviour proves the mechanism proposed.

In the title compound, $C_{19}H_{33}NO_3$, the morpholine ring adopts a chair conformation, while the phenolic hydroxyl is hindered by the adjacent *tert*-butyl groups. The crystal structure is stabilized by a number of O—H⋯O, O—H⋯N and C—H⋯O hydrogen-bonding interactions, where both the organic and the solvato molecules take part (Table 1).

S2. Experimental

The 2,6-di-*tert*-butyl-4-(butylamino)methylphenol was prepared by the indirect reductive amination of 3,5-di-*tert*-butyl-4-hydroxybenzaldehyde with butlyamine and sodium borhydride, and then separated by silica gel flash column chromatography in 61.5% yield. 2,6-Di-*tert*-butyl-4-(butylamino)methylphenol (2.91 g, 0.01 mol) and morpholine (1.3 g, 0.015 mol) was dissolved in THF (30 ml) and heated to reflux for 6 h. Then the THF and the extra morpholine was evaporated under reduced pressure.The residue was washed with methanol(10 ml) and the title product (2.89 g) was obtained in 89.5% yield. Suitable crystals were obtained by slow evaporation of a mixture of ethyl acetate and THF.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) and 0.96 Å (methyl) with $U_{iso}(H) = 1.2$(aromatic) or 1.5(methyl)$U_{eq}(C)$. H atoms attached to O were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.85 (3) Å) with $U_{iso}(H) = 1.5U_{eq}(O)$.
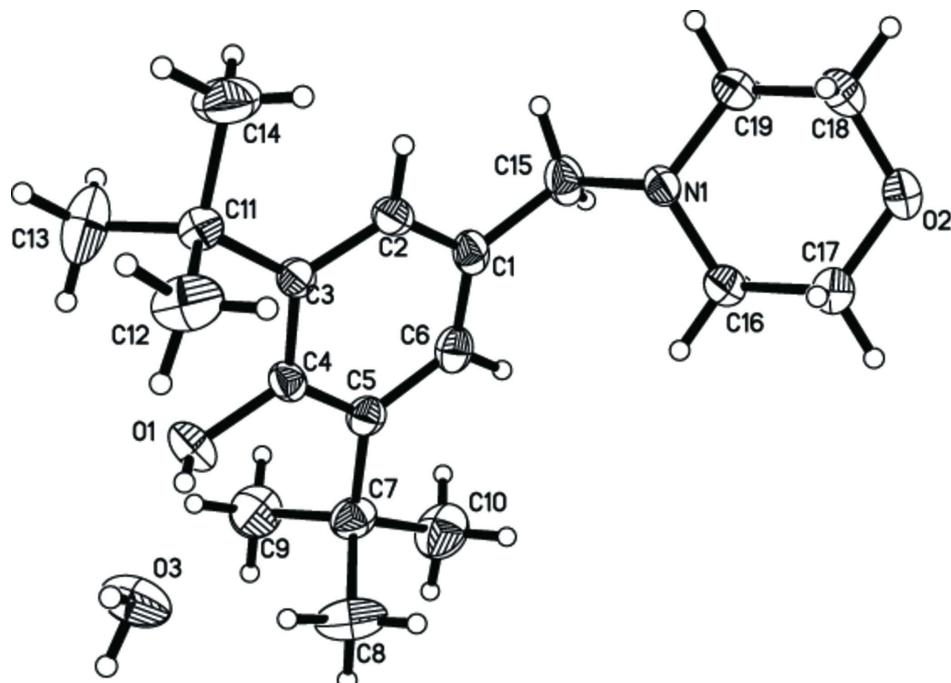
Figure 1

Molecular diagram of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.
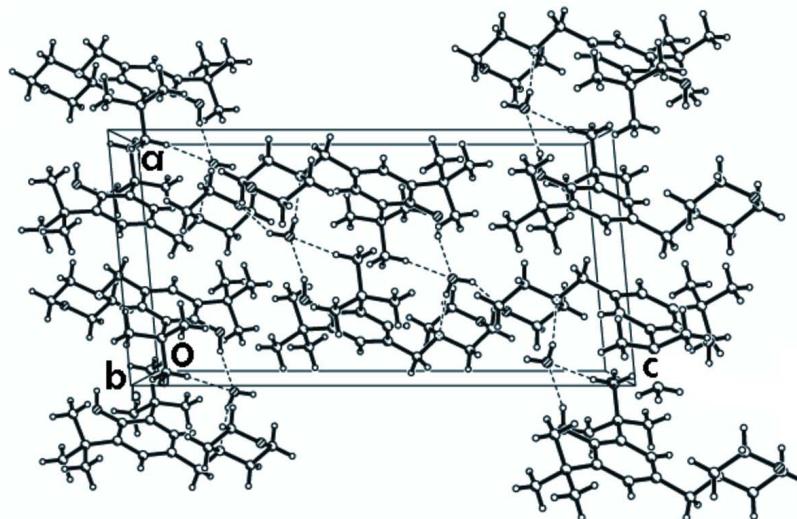
Figure 2

Packing diagram of (I) viewed down the unique crystallographic *b* axis, showing H-bonding interactions in dashed lines.

2,6-Di-*tert*-butyl-4-(morpholinomethyl)phenol monohydrate

Crystal data

$C_{19}H_{31}NO_2 \cdot H_2O$	Monoclinic, $P2_1/n$
$M_r = 323.46$	Hall symbol: -P 2yn

$a = 10.1461\ (14)$ Å
$b = 9.7118\ (12)$ Å
$c = 19.966\ (2)$ Å
$\beta = 95.166\ (8)°$
$V = 1959.4\ (4)$ Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.097$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2606 reflections
$\theta = 2.2–24.6°$
$\mu = 0.07$ mm^{-1}
$T = 294$ K
Block, colourless
$0.32 \times 0.30 \times 0.26$ mm

Data collection

Bruker SMART CCD area-detector
   diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
   (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.97$, $T_{max} = 0.98$

9174 measured reflections
3412 independent reflections
2098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow12$
$k = -11\rightarrow11$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.151$
$S = 1.04$
3412 reflections
224 parameters
0 restraints
Primary atom site location: structure-invariant
   direct methods
Secondary atom site location: difference Fourier
   map

Hydrogen site location: inferred from
   neighbouring sites
H atoms treated by a mixture of independent
   and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2 + 0.2168P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97*,
   $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.059 (5)

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	0.67458 (16)	0.44480 (17)	0.64823 (7)	0.0583 (5)
H1	0.591 (3)	0.445 (3)	0.6451 (13)	0.087*
O2	0.77839 (18)	0.91614 (16)	0.27118 (7)	0.0722 (5)
N1	0.83158 (15)	0.70489 (15)	0.36930 (8)	0.0416 (4)
C1	0.85010 (18)	0.5892 (2)	0.48162 (10)	0.0439 (5)
C2	0.78398 (19)	0.4645 (2)	0.47924 (9)	0.0434 (5)
H2	0.7801	0.4139	0.4396	0.052*

C3	0.72305 (17)	0.41118 (19)	0.53319 (9)	0.0387 (5)
C4	0.72865 (18)	0.4931 (2)	0.59152 (9)	0.0404 (5)
C5	0.79608 (19)	0.6196 (2)	0.59699 (9)	0.0423 (5)
C6	0.85611 (19)	0.6634 (2)	0.54058 (10)	0.0470 (5)
H6	0.9022	0.7464	0.5429	0.056*
C7	0.8063 (2)	0.7062 (2)	0.66190 (11)	0.0547 (6)
C8	0.6688 (3)	0.7499 (3)	0.67925 (14)	0.0918 (10)
H8A	0.6181	0.6697	0.6883	0.138*
H8B	0.6249	0.7994	0.6420	0.138*
H8C	0.6770	0.8081	0.7183	0.138*
C9	0.8780 (3)	0.6257 (3)	0.72030 (11)	0.0782 (8)
H9A	0.8814	0.6803	0.7605	0.117*
H9B	0.9664	0.6047	0.7100	0.117*
H9C	0.8311	0.5417	0.7270	0.117*
C10	0.8867 (3)	0.8386 (3)	0.65505 (14)	0.0845 (9)
H10A	0.8905	0.8893	0.6964	0.127*
H10B	0.8452	0.8939	0.6193	0.127*
H10C	0.9749	0.8153	0.6451	0.127*
C11	0.6553 (2)	0.2692 (2)	0.52747 (10)	0.0473 (5)
C12	0.5064 (2)	0.2830 (3)	0.52936 (14)	0.0780 (8)
H12A	0.4723	0.3461	0.4950	0.117*
H12B	0.4874	0.3171	0.5726	0.117*
H12C	0.4655	0.1946	0.5216	0.117*
C13	0.7121 (3)	0.1735 (3)	0.58367 (15)	0.0959 (10)
H13A	0.6686	0.0858	0.5794	0.144*
H13B	0.6983	0.2132	0.6265	0.144*
H13C	0.8053	0.1614	0.5804	0.144*
C14	0.6772 (3)	0.1980 (3)	0.46143 (15)	0.0934 (10)
H14A	0.7703	0.1846	0.4586	0.140*
H14B	0.6419	0.2542	0.4245	0.140*
H14C	0.6333	0.1104	0.4595	0.140*
C15	0.9192 (2)	0.6354 (2)	0.42175 (10)	0.0561 (6)
H15A	0.9903	0.6978	0.4371	0.067*
H15B	0.9587	0.5558	0.4021	0.067*
C16	0.8039 (2)	0.8458 (2)	0.38799 (10)	0.0503 (5)
H16A	0.8864	0.8958	0.3967	0.060*
H16B	0.7591	0.8459	0.4289	0.060*
C17	0.7184 (3)	0.9162 (2)	0.33275 (11)	0.0682 (7)
H17A	0.6336	0.8696	0.3264	0.082*
H17B	0.7025	1.0105	0.3459	0.082*
C18	0.8050 (3)	0.7790 (2)	0.25213 (11)	0.0656 (7)
H18A	0.8471	0.7798	0.2104	0.079*
H18B	0.7224	0.7288	0.2444	0.079*
C19	0.8934 (2)	0.7072 (2)	0.30551 (10)	0.0558 (6)
H19A	0.9098	0.6136	0.2914	0.067*
H19B	0.9778	0.7547	0.3118	0.067*
O3	0.41145 (17)	0.4475 (2)	0.66808 (10)	0.0767 (6)
H3A	0.346 (3)	0.403 (3)	0.6527 (16)	0.115*

H3B	0.399 (3)	0.471 (3)	0.7087 (16)	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0548 (9)	0.0818 (11)	0.0398 (8)	−0.0044 (8)	0.0121 (7)	0.0068 (7)
O2	0.1162 (14)	0.0551 (10)	0.0476 (10)	0.0132 (9)	0.0196 (9)	0.0160 (8)
N1	0.0445 (9)	0.0453 (10)	0.0363 (9)	0.0052 (7)	0.0108 (7)	0.0080 (7)
C1	0.0354 (11)	0.0524 (12)	0.0441 (12)	0.0105 (9)	0.0040 (9)	0.0157 (10)
C2	0.0432 (11)	0.0515 (12)	0.0356 (11)	0.0133 (9)	0.0045 (9)	0.0030 (9)
C3	0.0363 (10)	0.0429 (11)	0.0370 (11)	0.0086 (8)	0.0040 (8)	0.0052 (9)
C4	0.0377 (10)	0.0491 (12)	0.0347 (11)	0.0070 (9)	0.0054 (8)	0.0077 (9)
C5	0.0406 (11)	0.0436 (11)	0.0420 (11)	0.0091 (9)	−0.0003 (9)	0.0033 (9)
C6	0.0422 (12)	0.0452 (12)	0.0522 (13)	0.0024 (9)	−0.0030 (9)	0.0102 (10)
C7	0.0603 (14)	0.0503 (13)	0.0521 (13)	0.0063 (10)	−0.0022 (11)	−0.0082 (10)
C8	0.083 (2)	0.092 (2)	0.102 (2)	0.0162 (16)	0.0144 (17)	−0.0440 (18)
C9	0.102 (2)	0.0789 (18)	0.0495 (14)	0.0049 (15)	−0.0180 (14)	−0.0085 (13)
C10	0.103 (2)	0.0620 (16)	0.0854 (19)	−0.0092 (15)	−0.0098 (16)	−0.0134 (14)
C11	0.0504 (13)	0.0439 (12)	0.0481 (12)	0.0047 (9)	0.0067 (10)	−0.0006 (9)
C12	0.0541 (15)	0.0781 (17)	0.102 (2)	−0.0066 (13)	0.0081 (14)	−0.0257 (15)
C13	0.109 (2)	0.0592 (16)	0.113 (2)	−0.0132 (15)	−0.0220 (19)	0.0291 (16)
C14	0.118 (3)	0.0663 (17)	0.103 (2)	−0.0170 (16)	0.0472 (19)	−0.0360 (16)
C15	0.0447 (12)	0.0689 (15)	0.0561 (13)	0.0127 (10)	0.0117 (10)	0.0226 (11)
C16	0.0641 (14)	0.0479 (12)	0.0399 (11)	0.0012 (10)	0.0097 (10)	−0.0008 (10)
C17	0.097 (2)	0.0583 (14)	0.0510 (14)	0.0245 (13)	0.0166 (13)	0.0106 (11)
C18	0.0961 (18)	0.0651 (16)	0.0373 (12)	0.0021 (13)	0.0152 (12)	0.0048 (11)
C19	0.0669 (15)	0.0560 (13)	0.0477 (13)	0.0063 (11)	0.0230 (11)	0.0037 (10)
O3	0.0590 (11)	0.1028 (15)	0.0710 (12)	−0.0152 (9)	0.0209 (9)	−0.0255 (10)

Geometric parameters (Å, º)

O1—C4	1.384 (2)	C10—H10B	0.9600
O1—H1	0.85 (3)	C10—H10C	0.9600
O2—C18	1.418 (3)	C11—C12	1.520 (3)
O2—C17	1.420 (3)	C11—C14	1.523 (3)
N1—C16	1.452 (2)	C11—C13	1.529 (3)
N1—C19	1.470 (2)	C12—H12A	0.9600
N1—C15	1.475 (2)	C12—H12B	0.9600
C1—C6	1.377 (3)	C12—H12C	0.9600
C1—C2	1.383 (3)	C13—H13A	0.9600
C1—C15	1.508 (3)	C13—H13B	0.9600
C2—C3	1.389 (3)	C13—H13C	0.9600
C2—H2	0.9300	C14—H14A	0.9600
C3—C4	1.407 (3)	C14—H14B	0.9600
C3—C11	1.540 (3)	C14—H14C	0.9600
C4—C5	1.406 (3)	C15—H15A	0.9700
C5—C6	1.394 (3)	C15—H15B	0.9700
C5—C7	1.541 (3)	C16—C17	1.505 (3)

C6—H6	0.9300	C16—H16A	0.9700
C7—C8	1.527 (3)	C16—H16B	0.9700
C7—C9	1.532 (3)	C17—H17A	0.9700
C7—C10	1.535 (3)	C17—H17B	0.9700
C8—H8A	0.9600	C18—C19	1.501 (3)
C8—H8B	0.9600	C18—H18A	0.9700
C8—H8C	0.9600	C18—H18B	0.9700
C9—H9A	0.9600	C19—H19A	0.9700
C9—H9B	0.9600	C19—H19B	0.9700
C9—H9C	0.9600	O3—H3A	0.83 (3)
C10—H10A	0.9600	O3—H3B	0.86 (3)
C4—O1—H1	114.2 (18)	C14—C11—C3	111.80 (18)
C18—O2—C17	109.84 (16)	C13—C11—C3	110.69 (17)
C16—N1—C19	108.42 (15)	C11—C12—H12A	109.5
C16—N1—C15	111.52 (16)	C11—C12—H12B	109.5
C19—N1—C15	110.19 (15)	H12A—C12—H12B	109.5
C6—C1—C2	118.17 (18)	C11—C12—H12C	109.5
C6—C1—C15	122.24 (19)	H12A—C12—H12C	109.5
C2—C1—C15	119.50 (19)	H12B—C12—H12C	109.5
C1—C2—C3	123.23 (18)	C11—C13—H13A	109.5
C1—C2—H2	118.4	C11—C13—H13B	109.5
C3—C2—H2	118.4	H13A—C13—H13B	109.5
C2—C3—C4	116.30 (18)	C11—C13—H13C	109.5
C2—C3—C11	120.20 (17)	H13A—C13—H13C	109.5
C4—C3—C11	123.50 (17)	H13B—C13—H13C	109.5
O1—C4—C5	117.30 (17)	C11—C14—H14A	109.5
O1—C4—C3	119.73 (17)	C11—C14—H14B	109.5
C5—C4—C3	122.79 (17)	H14A—C14—H14B	109.5
C6—C5—C4	116.67 (18)	C11—C14—H14C	109.5
C6—C5—C7	120.78 (18)	H14A—C14—H14C	109.5
C4—C5—C7	122.54 (18)	H14B—C14—H14C	109.5
C1—C6—C5	122.79 (19)	N1—C15—C1	113.94 (16)
C1—C6—H6	118.6	N1—C15—H15A	108.8
C5—C6—H6	118.6	C1—C15—H15A	108.8
C8—C7—C9	110.5 (2)	N1—C15—H15B	108.8
C8—C7—C10	106.9 (2)	C1—C15—H15B	108.8
C9—C7—C10	106.0 (2)	H15A—C15—H15B	107.7
C8—C7—C5	110.41 (18)	N1—C16—C17	110.61 (17)
C9—C7—C5	110.66 (17)	N1—C16—H16A	109.5
C10—C7—C5	112.2 (2)	C17—C16—H16A	109.5
C7—C8—H8A	109.5	N1—C16—H16B	109.5
C7—C8—H8B	109.5	C17—C16—H16B	109.5
H8A—C8—H8B	109.5	H16A—C16—H16B	108.1
C7—C8—H8C	109.5	O2—C17—C16	111.77 (19)
H8A—C8—H8C	109.5	O2—C17—H17A	109.3
H8B—C8—H8C	109.5	C16—C17—H17A	109.3
C7—C9—H9A	109.5	O2—C17—H17B	109.3

C7—C9—H9B	109.5	C16—C17—H17B	109.3
H9A—C9—H9B	109.5	H17A—C17—H17B	107.9
C7—C9—H9C	109.5	O2—C18—C19	111.22 (19)
H9A—C9—H9C	109.5	O2—C18—H18A	109.4
H9B—C9—H9C	109.5	C19—C18—H18A	109.4
C7—C10—H10A	109.5	O2—C18—H18B	109.4
C7—C10—H10B	109.5	C19—C18—H18B	109.4
H10A—C10—H10B	109.5	H18A—C18—H18B	108.0
C7—C10—H10C	109.5	N1—C19—C18	110.34 (18)
H10A—C10—H10C	109.5	N1—C19—H19A	109.6
H10B—C10—H10C	109.5	C18—C19—H19A	109.6
C12—C11—C14	106.5 (2)	N1—C19—H19B	109.6
C12—C11—C13	110.2 (2)	C18—C19—H19B	109.6
C14—C11—C13	106.5 (2)	H19A—C19—H19B	108.1
C12—C11—C3	110.90 (17)	H3A—O3—H3B	108 (3)
C6—C1—C2—C3	0.3 (3)	C6—C5—C7—C10	0.1 (3)
C15—C1—C2—C3	176.91 (17)	C4—C5—C7—C10	179.16 (19)
C1—C2—C3—C4	1.6 (3)	C2—C3—C11—C12	−113.3 (2)
C1—C2—C3—C11	−177.92 (17)	C4—C3—C11—C12	67.3 (2)
C2—C3—C4—O1	−177.58 (16)	C2—C3—C11—C14	5.5 (3)
C11—C3—C4—O1	1.9 (3)	C4—C3—C11—C14	−174.0 (2)
C2—C3—C4—C5	−2.5 (3)	C2—C3—C11—C13	124.1 (2)
C11—C3—C4—C5	177.00 (17)	C4—C3—C11—C13	−55.4 (3)
O1—C4—C5—C6	176.67 (16)	C16—N1—C15—C1	77.3 (2)
C3—C4—C5—C6	1.4 (3)	C19—N1—C15—C1	−162.21 (18)
O1—C4—C5—C7	−2.4 (3)	C6—C1—C15—N1	−99.6 (2)
C3—C4—C5—C7	−177.63 (17)	C2—C1—C15—N1	84.0 (2)
C2—C1—C6—C5	−1.5 (3)	C19—N1—C16—C17	56.5 (2)
C15—C1—C6—C5	−177.96 (17)	C15—N1—C16—C17	177.96 (17)
C4—C5—C6—C1	0.6 (3)	C18—O2—C17—C16	57.6 (3)
C7—C5—C6—C1	179.70 (17)	N1—C16—C17—O2	−57.9 (3)
C6—C5—C7—C8	119.3 (2)	C17—O2—C18—C19	−58.2 (3)
C4—C5—C7—C8	−61.6 (3)	C16—N1—C19—C18	−57.2 (2)
C6—C5—C7—C9	−118.0 (2)	C15—N1—C19—C18	−179.50 (18)
C4—C5—C7—C9	61.0 (3)	O2—C18—C19—N1	59.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*B*···O2[i]	0.86 (3)	2.13 (3)	2.884 (2)	146 (3)
O3—H3*A*···N1[ii]	0.83 (3)	2.10 (3)	2.915 (2)	170 (3)
O1—H1···O3	0.85 (3)	1.91 (3)	2.734 (2)	162 (3)
C12—H12*B*···O3	0.96	2.47	3.410 (3)	167

Symmetry codes: (i) $x-1/2$, $-y+3/2$, $z+1/2$; (ii) $-x+1$, $-y+1$, $-z+1$.