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

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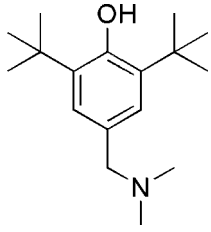
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 10.5.

The title compound, $C_{17}H_{29}NO$, is an important hindered phenol derivative. The asymmetric unit contains two molecules. Molecules interact through O—H···N hydrogen bonds to form a tetramer arranged around a twofold rotation axis.

Related literature

For related literature, see: Ciba-Geigy AG (1978); Eggensperger *et al.* (1974, 1976); Yamazaki & Seguchi (1997). For the synthesis, see: Coffield (1965); Coffield & Mich (1965); Rieker *et al.* (1968).



Experimental

Crystal data

$C_{17}H_{29}NO$
M_r = 263.41
Monoclinic, $C2$
a = 28.731 (9) Å
b = 8.912 (3) Å
c = 16.112 (5) Å
β = 122.965 (5)°
V = 3461.4 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.989
6903 measured reflections
3752 independent reflections
2317 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 0.99
3752 reflections
359 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.85	2.20	2.836 (3)	132
O2—H2···N1^{i}	0.86	2.26	2.933 (3)	135

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

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); 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: DN2296).

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S1. Comment

Hindered phenol antioxidants are widely used in polymers and lubricants. It could protect polymers by increasing both their process stability and long-term stability against oxidative degradation (Yamazaki & Seguchi, 1997). Moreover, ester of 3,5-di-*tert*-butyl-4-hydroxyphenol acetic acid is one important kind of antioxidant derivative. An important route to prepare these compounds is to react an α-halo ester compound with the title compound in the presence of a strong base (Eggensperger *et al.*, 1974, 1976; Eggensperger *et al.*, 1976; Ciba-Geigy AG, 1978). The title compound is ususlly called a Mannich base. The title compound was prepared from 4-bromomethyl-2,6-di-*tert*-butyl-phenol and *N*,*N*-dimethyl-amine.It can also be easily obtained by a Mannich reaction from 2,6-di-*tert*-butylphenol,formaldehyde and dimethyl-amine (Coffield, 1965; Coffield & Mich, 1965).

The asymmetric unit of the title compound contains two molecules which are linked by a weak O—H···N hydrogen bond (Fig. 1). Each pseudo dimer interacts with a symmetry related one to build up like a crown arranged around axis parallele to the *b* axis through O—H··· hydrogen bonds (Table 1, Fig. 2).

S2. Experimental

The 4-bromomethyl-2,6-di-*tert*-butyl-phenol was synthesized according to the method described by Rieker(Rieker *et al.*,1968). Dimethylamine (2.7 g, 0.06 mol) and 4-bromomethyl-2,6-di-*tert*-butyl-phenol (9.0 g, 0.03 mol) were added, with stirring to THF(60 ml)at 273 K. The reaction mixture was stirred at 273 K for a further 2 h. The solvent THF was evaporated under reduced pressure and the residual was washed with water (30 ml). The product (7.39 g) was obtained in a yield of 93.6%. Suitable crystals were obtained by slow evaporation of a mixture of ethyl acetate and ethanol.

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 (methyle) with U_{iso}(H) = 1.2(aromatic) or 1.5(methyle)U_{eq}(C). H atoms of hydroxyle group were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.85 (1) Å) with U_{iso}(H) = 1.5U_{eq}(O). In the final stage of refinement, they were treated as riding on their parent O atoms.

In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined and then the Friedel pairs were merged and any references to the Flack parameter were removed.

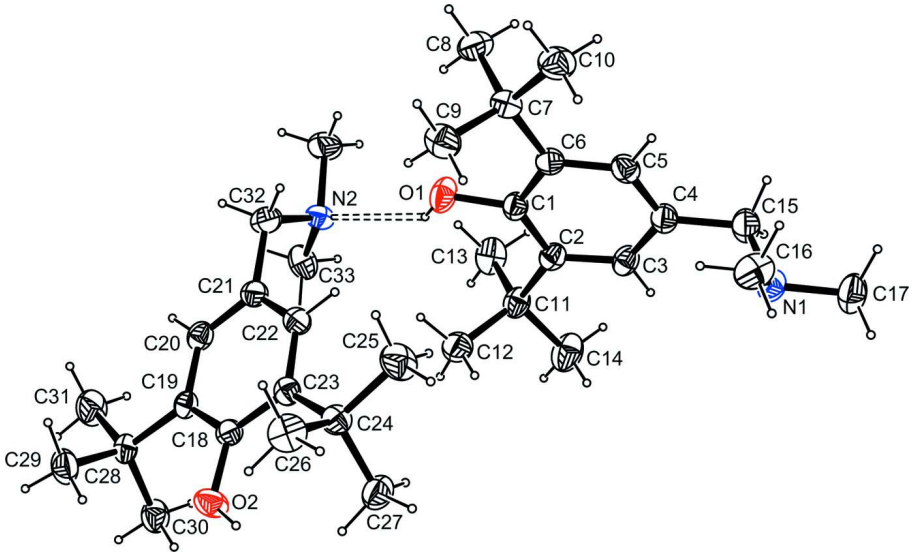

Figure 1

View of the two crystallygraphically independent molecules with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bond is shown as dashed line. H atoms are represented as small spheres of arbitrary radii.

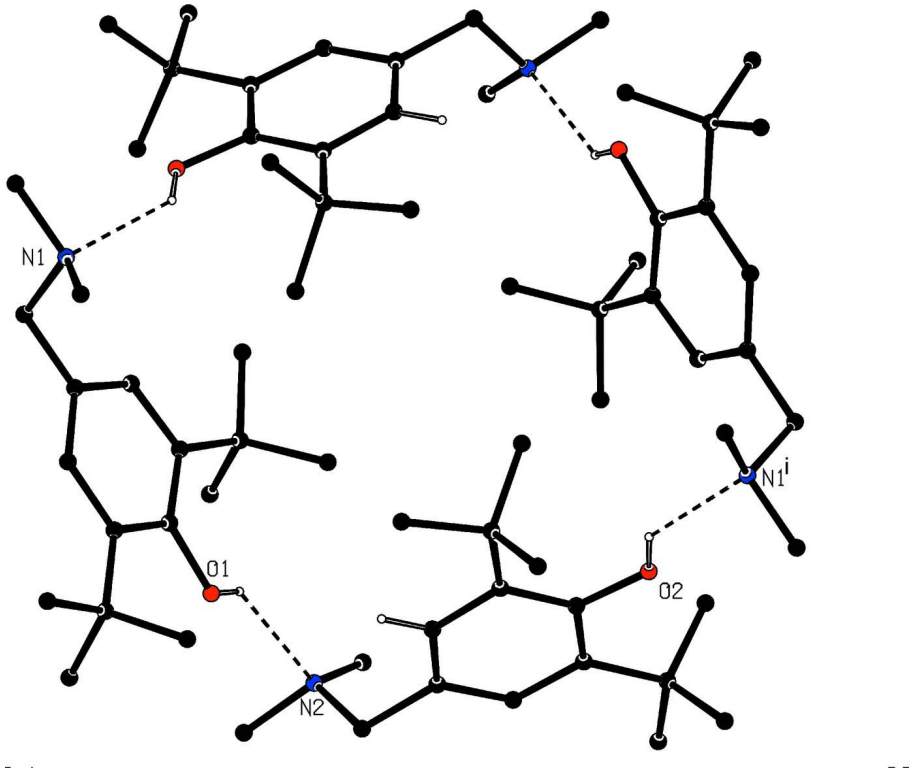

Figure 2

View of the crown formed by the assembly of four molecules through O—H···N hydrogen bonds. Dashed lines indicate the hydrogen bonds.H atoms not involved in hydrogen bonding have been omitted for clarity.

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

Crystal data

$C_{17}H_{29}NO$
$M_r = 263.41$
Monoclinic, $C2$
Hall symbol: C 2y
$a = 28.731$ (9) Å
$b = 8.912$ (3) Å
$c = 16.112$ (5) Å
$\beta = 122.965$ (5)°
$V = 3461.4$ (19) Å^3
$Z = 8$
$F(000) = 1168$
$D_x = 1.011$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2365 reflections
$\theta = 2.4$–$21.0°$
$\mu = 0.06$ mm^{-1}
$T = 294$ K
Block, colourless
0.24 × 0.22 × 0.20 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)
$T_{min} = 0.978$, $T_{max} = 0.989$
6903 measured reflections
3752 independent reflections
2317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 26.4°$, $\theta_{min} = 1.5°$
$h = -35 \rightarrow 29$
$k = -11 \rightarrow 11$
$l = 0 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.112$
$S = 0.99$
3752 reflections
359 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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	0.96396 (9)	−0.0075 (3)	0.26691 (14)	0.0632 (7)
H1	0.9775	−0.0898	0.2629	0.076*
O2	1.20963 (9)	0.0785 (3)	0.24701 (16)	0.0604 (6)
H2	1.1990	0.1526	0.2069	0.073*

N1	0.76397 (10)	0.2845 (3)	−0.13626 (17)	0.0531 (7)
N2	1.05111 (10)	−0.2181 (3)	0.37179 (17)	0.0466 (6)
C1	0.91498 (12)	0.0341 (3)	0.1819 (2)	0.0442 (7)
C2	0.89225 (12)	−0.0421 (3)	0.0907 (2)	0.0442 (7)
C3	0.84136 (12)	0.0109 (4)	0.0118 (2)	0.0478 (8)
H3	0.8253	−0.0377	−0.0488	0.057*
C4	0.81353 (12)	0.1321 (4)	0.0193 (2)	0.0486 (8)
C5	0.83809 (12)	0.2039 (4)	0.1103 (2)	0.0488 (8)
H5	0.8198	0.2850	0.1163	0.059*
C6	0.88894 (12)	0.1598 (3)	0.1930 (2)	0.0445 (8)
C7	0.91528 (13)	0.2442 (4)	0.2931 (2)	0.0503 (8)
C8	0.91655 (15)	0.1407 (4)	0.3709 (2)	0.0657 (10)
H8A	0.9389	0.0542	0.3808	0.099*
H8B	0.8795	0.1093	0.3481	0.099*
H8C	0.9320	0.1940	0.4322	0.099*
C9	0.97393 (13)	0.3002 (4)	0.3292 (3)	0.0663 (10)
H9A	0.9881	0.3577	0.3887	0.099*
H9B	0.9726	0.3621	0.2792	0.099*
H9C	0.9978	0.2158	0.3424	0.099*
C10	0.88150 (15)	0.3852 (4)	0.2835 (3)	0.0685 (10)
H10A	0.8984	0.4338	0.3467	0.103*
H10B	0.8443	0.3565	0.2614	0.103*
H10C	0.8808	0.4530	0.2365	0.103*
C11	0.92034 (13)	−0.1804 (4)	0.0773 (2)	0.0517 (8)
C12	0.97975 (13)	−0.1438 (4)	0.1057 (2)	0.0610 (9)
H12A	0.9948	−0.2285	0.0913	0.091*
H12B	1.0025	−0.1214	0.1751	0.091*
H12C	0.9789	−0.0585	0.0684	0.091*
C13	0.91972 (15)	−0.3122 (4)	0.1393 (3)	0.0674 (10)
H13A	0.8821	−0.3347	0.1180	0.101*
H13B	0.9403	−0.2846	0.2080	0.101*
H13C	0.9364	−0.3990	0.1305	0.101*
C14	0.88828 (15)	−0.2344 (5)	−0.0307 (2)	0.0774 (11)
H14A	0.8867	−0.1550	−0.0724	0.116*
H14B	0.8513	−0.2623	−0.0507	0.116*
H14C	0.9068	−0.3195	−0.0364	0.116*
C15	0.75856 (13)	0.1836 (4)	−0.0695 (2)	0.0594 (9)
H15A	0.7373	0.0961	−0.1066	0.071*
H15B	0.7379	0.2349	−0.0463	0.071*
C16	0.78926 (17)	0.4270 (4)	−0.0877 (3)	0.0712 (11)
H16A	0.7927	0.4902	−0.1323	0.107*
H16B	0.8253	0.4087	−0.0296	0.107*
H16C	0.7663	0.4757	−0.0694	0.107*
C17	0.70858 (14)	0.3107 (5)	−0.2253 (3)	0.0816 (12)
H17A	0.6856	0.3598	−0.2071	0.122*
H17B	0.6922	0.2164	−0.2563	0.122*
H17C	0.7118	0.3730	−0.2706	0.122*
C18	1.17964 (12)	0.0384 (3)	0.2871 (2)	0.0412 (7)

C19	1.20150 (11)	−0.0867 (3)	0.3518 (2)	0.0404 (7)
C20	1.17375 (11)	−0.1308 (4)	0.3964 (2)	0.0458 (7)
H20	1.1880	−0.2108	0.4406	0.055*
C21	1.12606 (12)	−0.0621 (4)	0.3786 (2)	0.0446 (7)
C22	1.10584 (12)	0.0591 (4)	0.3143 (2)	0.0441 (7)
H22	1.0739	0.1067	0.3023	0.053*
C23	1.13113 (12)	0.1136 (3)	0.2665 (2)	0.0412 (7)
C24	1.10825 (12)	0.2547 (3)	0.2001 (2)	0.0483 (8)
C25	1.05452 (14)	0.3120 (4)	0.1893 (3)	0.0717 (10)
H25A	1.0268	0.2348	0.1605	0.108*
H25B	1.0414	0.3991	0.1475	0.108*
H25C	1.0620	0.3379	0.2533	0.108*
C26	1.15096 (15)	0.3832 (4)	0.2467 (3)	0.0664 (10)
H26A	1.1587	0.4053	0.3114	0.100*
H26B	1.1362	0.4709	0.2058	0.100*
H26C	1.1846	0.3534	0.2520	0.100*
C27	1.09303 (14)	0.2209 (4)	0.0937 (2)	0.0634 (10)
H27A	1.1259	0.1938	0.0956	0.095*
H27B	1.0768	0.3085	0.0532	0.095*
H27C	1.0670	0.1395	0.0664	0.095*
C28	1.25469 (11)	−0.1685 (3)	0.3744 (2)	0.0468 (8)
C29	1.30491 (13)	−0.0619 (5)	0.4262 (2)	0.0657 (10)
H29A	1.3382	−0.1173	0.4467	0.099*
H29B	1.3076	−0.0179	0.4830	0.099*
H29C	1.3003	0.0159	0.3811	0.099*
C30	1.24665 (13)	−0.2338 (4)	0.2788 (2)	0.0596 (9)
H30A	1.2413	−0.1533	0.2348	0.089*
H30B	1.2147	−0.2981	0.2473	0.089*
H30C	1.2789	−0.2904	0.2947	0.089*
C31	1.26844 (15)	−0.3037 (5)	0.4444 (3)	0.0738 (11)
H31A	1.3006	−0.3546	0.4547	0.111*
H31B	1.2376	−0.3717	0.4152	0.111*
H31C	1.2757	−0.2688	0.5067	0.111*
C32	1.09783 (13)	−0.1136 (4)	0.4303 (2)	0.0552 (9)
H32A	1.1252	−0.1622	0.4919	0.066*
H32B	1.0843	−0.0261	0.4466	0.066*
C33	1.06835 (14)	−0.3538 (4)	0.3442 (3)	0.0620 (9)
H33A	1.0960	−0.4056	0.4029	0.093*
H33B	1.0835	−0.3266	0.3059	0.093*
H33C	1.0368	−0.4181	0.3057	0.093*
C34	1.02793 (14)	−0.2575 (5)	0.4305 (3)	0.0706 (11)
H34A	0.9968	−0.3233	0.3929	0.106*
H34B	1.0161	−0.1680	0.4470	0.106*
H34C	1.0557	−0.3072	0.4902	0.106*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0632 (14)	0.0591 (14)	0.0435 (12)	0.0226 (12)	0.0135 (11)	−0.0036 (11)
O2	0.0607 (14)	0.0630 (14)	0.0759 (15)	0.0133 (12)	0.0490 (12)	0.0255 (13)
N1	0.0567 (16)	0.0494 (16)	0.0451 (14)	0.0094 (14)	0.0225 (13)	0.0080 (13)
N2	0.0505 (15)	0.0470 (15)	0.0540 (14)	0.0018 (13)	0.0359 (13)	0.0041 (13)
C1	0.0402 (17)	0.0464 (19)	0.0407 (16)	0.0025 (15)	0.0185 (14)	0.0058 (15)
C2	0.0463 (18)	0.0427 (18)	0.0411 (17)	−0.0050 (15)	0.0222 (15)	0.0025 (15)
C3	0.0455 (18)	0.0478 (19)	0.0395 (16)	−0.0097 (15)	0.0162 (15)	0.0009 (14)
C4	0.0409 (17)	0.054 (2)	0.0487 (18)	−0.0009 (16)	0.0227 (15)	0.0098 (16)
C5	0.0469 (18)	0.0479 (18)	0.058 (2)	0.0057 (15)	0.0327 (17)	0.0112 (16)
C6	0.0457 (18)	0.0461 (19)	0.0457 (17)	−0.0019 (15)	0.0276 (16)	0.0043 (15)
C7	0.0529 (19)	0.050 (2)	0.0565 (19)	−0.0006 (16)	0.0356 (16)	−0.0011 (16)
C8	0.080 (3)	0.071 (2)	0.055 (2)	0.004 (2)	0.0430 (19)	0.0030 (19)
C9	0.063 (2)	0.065 (2)	0.076 (2)	−0.0129 (19)	0.0405 (19)	−0.015 (2)
C10	0.080 (2)	0.063 (2)	0.072 (2)	0.010 (2)	0.048 (2)	−0.003 (2)
C11	0.0546 (19)	0.0449 (18)	0.0439 (17)	0.0024 (16)	0.0193 (15)	−0.0038 (15)
C12	0.065 (2)	0.062 (2)	0.0564 (19)	0.0093 (19)	0.0335 (17)	−0.0006 (18)
C13	0.071 (2)	0.044 (2)	0.072 (2)	−0.0013 (18)	0.029 (2)	0.0050 (18)
C14	0.084 (3)	0.065 (2)	0.056 (2)	0.006 (2)	0.0209 (19)	−0.014 (2)
C15	0.0464 (19)	0.065 (2)	0.058 (2)	0.0038 (17)	0.0227 (16)	0.0119 (18)
C16	0.101 (3)	0.049 (2)	0.070 (2)	0.006 (2)	0.050 (2)	0.0000 (18)
C17	0.070 (2)	0.093 (3)	0.060 (2)	0.028 (2)	0.021 (2)	0.019 (2)
C18	0.0420 (17)	0.0431 (17)	0.0387 (15)	−0.0036 (14)	0.0220 (14)	−0.0010 (14)
C19	0.0360 (16)	0.0428 (18)	0.0347 (15)	−0.0041 (13)	0.0144 (13)	−0.0039 (13)
C20	0.0453 (18)	0.0444 (17)	0.0399 (16)	−0.0064 (15)	0.0182 (14)	0.0009 (14)
C21	0.0435 (18)	0.0500 (19)	0.0414 (16)	−0.0099 (16)	0.0238 (14)	−0.0088 (15)
C22	0.0419 (17)	0.0453 (18)	0.0465 (16)	−0.0054 (15)	0.0248 (15)	−0.0100 (15)
C23	0.0392 (16)	0.0386 (17)	0.0423 (16)	−0.0044 (14)	0.0199 (14)	−0.0079 (13)
C24	0.0528 (18)	0.0432 (18)	0.0509 (17)	0.0055 (16)	0.0296 (15)	−0.0011 (15)
C25	0.075 (2)	0.059 (2)	0.089 (3)	0.023 (2)	0.050 (2)	0.012 (2)
C26	0.080 (2)	0.0441 (19)	0.076 (2)	−0.0067 (19)	0.043 (2)	−0.0042 (19)
C27	0.067 (2)	0.067 (2)	0.0489 (19)	0.016 (2)	0.0262 (17)	0.0066 (18)
C28	0.0370 (16)	0.0526 (19)	0.0404 (17)	0.0061 (15)	0.0144 (14)	0.0058 (15)
C29	0.0404 (18)	0.081 (3)	0.062 (2)	−0.0071 (18)	0.0188 (16)	−0.013 (2)
C30	0.0496 (18)	0.061 (2)	0.059 (2)	0.0088 (18)	0.0236 (17)	−0.0061 (18)
C31	0.063 (2)	0.074 (3)	0.076 (2)	0.021 (2)	0.032 (2)	0.028 (2)
C32	0.062 (2)	0.061 (2)	0.0483 (18)	−0.0064 (18)	0.0341 (17)	−0.0044 (17)
C33	0.052 (2)	0.049 (2)	0.081 (2)	0.0040 (17)	0.0329 (18)	0.0002 (19)
C34	0.073 (2)	0.086 (3)	0.072 (2)	0.003 (2)	0.052 (2)	0.020 (2)

Geometric parameters (Å, º)

O1—C1	1.377 (3)	C16—H16B	0.9600
O1—H1	0.8495	C16—H16C	0.9600
O2—C18	1.376 (3)	C17—H17A	0.9600
O2—H2	0.8557	C17—H17B	0.9600

N1—C16	1.461 (4)	C17—H17C	0.9600
N1—C17	1.470 (4)	C18—C23	1.413 (4)
N1—C15	1.474 (4)	C18—C19	1.419 (4)
N2—C33	1.465 (4)	C19—C20	1.389 (4)
N2—C34	1.466 (4)	C19—C28	1.547 (4)
N2—C32	1.477 (4)	C20—C21	1.381 (4)
C1—C6	1.411 (4)	C20—H20	0.9300
C1—C2	1.415 (4)	C21—C22	1.387 (4)
C2—C3	1.398 (4)	C21—C32	1.515 (4)
C2—C11	1.552 (5)	C22—C23	1.403 (4)
C3—C4	1.387 (4)	C22—H22	0.9300
C3—H3	0.9300	C23—C24	1.547 (4)
C4—C5	1.390 (4)	C24—C26	1.542 (4)
C4—C15	1.514 (4)	C24—C25	1.543 (4)
C5—C6	1.395 (4)	C24—C27	1.551 (4)
C5—H5	0.9300	C25—H25A	0.9600
C6—C7	1.552 (4)	C25—H25B	0.9600
C7—C9	1.536 (4)	C25—H25C	0.9600
C7—C8	1.541 (4)	C26—H26A	0.9600
C7—C10	1.543 (5)	C26—H26B	0.9600
C8—H8A	0.9600	C26—H26C	0.9600
C8—H8B	0.9600	C27—H27A	0.9600
C8—H8C	0.9600	C27—H27B	0.9600
C9—H9A	0.9600	C27—H27C	0.9600
C9—H9B	0.9600	C28—C29	1.540 (4)
C9—H9C	0.9600	C28—C30	1.543 (4)
C10—H10A	0.9600	C28—C31	1.547 (5)
C10—H10B	0.9600	C29—H29A	0.9600
C10—H10C	0.9600	C29—H29B	0.9600
C11—C14	1.537 (4)	C29—H29C	0.9600
C11—C12	1.542 (4)	C30—H30A	0.9600
C11—C13	1.549 (5)	C30—H30B	0.9600
C12—H12A	0.9600	C30—H30C	0.9600
C12—H12B	0.9600	C31—H31A	0.9600
C12—H12C	0.9600	C31—H31B	0.9600
C13—H13A	0.9600	C31—H31C	0.9600
C13—H13B	0.9600	C32—H32A	0.9700
C13—H13C	0.9600	C32—H32B	0.9700
C14—H14A	0.9600	C33—H33A	0.9600
C14—H14B	0.9600	C33—H33B	0.9600
C14—H14C	0.9600	C33—H33C	0.9600
C15—H15A	0.9700	C34—H34A	0.9600
C15—H15B	0.9700	C34—H34B	0.9600
C16—H16A	0.9600	C34—H34C	0.9600

C1—O1—H1	114.8	H17A—C17—H17B	109.5
C18—O2—H2	119.8	N1—C17—H17C	109.5
C16—N1—C17	110.1 (3)	H17A—C17—H17C	109.5

C16—N1—C15	111.0 (2)	H17B—C17—H17C	109.5
C17—N1—C15	108.7 (3)	O2—C18—C23	123.8 (2)
C33—N2—C34	110.2 (3)	O2—C18—C19	114.1 (2)
C33—N2—C32	112.0 (2)	C23—C18—C19	122.1 (3)
C34—N2—C32	108.3 (2)	C20—C19—C18	117.0 (3)
O1—C1—C6	114.4 (2)	C20—C19—C28	121.1 (3)
O1—C1—C2	123.2 (3)	C18—C19—C28	121.9 (3)
C6—C1—C2	122.4 (3)	C21—C20—C19	123.4 (3)
C3—C2—C1	116.4 (3)	C21—C20—H20	118.3
C3—C2—C11	120.5 (3)	C19—C20—H20	118.3
C1—C2—C11	123.1 (3)	C20—C21—C22	117.8 (3)
C4—C3—C2	123.5 (3)	C20—C21—C32	121.2 (3)
C4—C3—H3	118.3	C22—C21—C32	121.0 (3)
C2—C3—H3	118.3	C21—C22—C23	123.3 (3)
C3—C4—C5	117.6 (3)	C21—C22—H22	118.4
C3—C4—C15	120.6 (3)	C23—C22—H22	118.4
C5—C4—C15	121.8 (3)	C22—C23—C18	116.5 (3)
C4—C5—C6	123.0 (3)	C22—C23—C24	120.6 (3)
C4—C5—H5	118.5	C18—C23—C24	122.8 (3)
C6—C5—H5	118.5	C26—C24—C25	106.9 (3)
C5—C6—C1	117.0 (3)	C26—C24—C23	109.9 (2)
C5—C6—C7	121.4 (3)	C25—C24—C23	111.7 (3)
C1—C6—C7	121.6 (3)	C26—C24—C27	110.7 (3)
C9—C7—C8	110.5 (3)	C25—C24—C27	106.1 (3)
C9—C7—C10	105.9 (3)	C23—C24—C27	111.3 (3)
C8—C7—C10	107.7 (3)	C24—C25—H25A	109.5
C9—C7—C6	111.4 (2)	C24—C25—H25B	109.5
C8—C7—C6	109.7 (2)	H25A—C25—H25B	109.5
C10—C7—C6	111.5 (3)	C24—C25—H25C	109.5
C7—C8—H8A	109.5	H25A—C25—H25C	109.5
C7—C8—H8B	109.5	H25B—C25—H25C	109.5
H8A—C8—H8B	109.5	C24—C26—H26A	109.5
C7—C8—H8C	109.5	C24—C26—H26B	109.5
H8A—C8—H8C	109.5	H26A—C26—H26B	109.5
H8B—C8—H8C	109.5	C24—C26—H26C	109.5
C7—C9—H9A	109.5	H26A—C26—H26C	109.5
C7—C9—H9B	109.5	H26B—C26—H26C	109.5
H9A—C9—H9B	109.5	C24—C27—H27A	109.5
C7—C9—H9C	109.5	C24—C27—H27B	109.5
H9A—C9—H9C	109.5	H27A—C27—H27B	109.5
H9B—C9—H9C	109.5	C24—C27—H27C	109.5
C7—C10—H10A	109.5	H27A—C27—H27C	109.5
C7—C10—H10B	109.5	H27B—C27—H27C	109.5
H10A—C10—H10B	109.5	C29—C28—C30	111.1 (3)
C7—C10—H10C	109.5	C29—C28—C19	110.6 (3)
H10A—C10—H10C	109.5	C30—C28—C19	110.5 (2)
H10B—C10—H10C	109.5	C29—C28—C31	107.1 (2)
C14—C11—C12	106.7 (3)	C30—C28—C31	105.9 (3)

C14—C11—C13	106.5 (3)	C19—C28—C31	111.5 (3)
C12—C11—C13	111.6 (3)	C28—C29—H29A	109.5
C14—C11—C2	111.7 (3)	C28—C29—H29B	109.5
C12—C11—C2	111.5 (3)	H29A—C29—H29B	109.5
C13—C11—C2	108.8 (2)	C28—C29—H29C	109.5
C11—C12—H12A	109.5	H29A—C29—H29C	109.5
C11—C12—H12B	109.5	H29B—C29—H29C	109.5
H12A—C12—H12B	109.5	C28—C30—H30A	109.5
C11—C12—H12C	109.5	C28—C30—H30B	109.5
H12A—C12—H12C	109.5	H30A—C30—H30B	109.5
H12B—C12—H12C	109.5	C28—C30—H30C	109.5
C11—C13—H13A	109.5	H30A—C30—H30C	109.5
C11—C13—H13B	109.5	H30B—C30—H30C	109.5
H13A—C13—H13B	109.5	C28—C31—H31A	109.5
C11—C13—H13C	109.5	C28—C31—H31B	109.5
H13A—C13—H13C	109.5	H31A—C31—H31B	109.5
H13B—C13—H13C	109.5	C28—C31—H31C	109.5
C11—C14—H14A	109.5	H31A—C31—H31C	109.5
C11—C14—H14B	109.5	H31B—C31—H31C	109.5
H14A—C14—H14B	109.5	N2—C32—C21	114.4 (2)
C11—C14—H14C	109.5	N2—C32—H32A	108.7
H14A—C14—H14C	109.5	C21—C32—H32A	108.7
H14B—C14—H14C	109.5	N2—C32—H32B	108.7
N1—C15—C4	113.8 (3)	C21—C32—H32B	108.7
N1—C15—H15A	108.8	H32A—C32—H32B	107.6
C4—C15—H15A	108.8	N2—C33—H33A	109.5
N1—C15—H15B	108.8	N2—C33—H33B	109.5
C4—C15—H15B	108.8	H33A—C33—H33B	109.5
H15A—C15—H15B	107.7	N2—C33—H33C	109.5
N1—C16—H16A	109.5	H33A—C33—H33C	109.5
N1—C16—H16B	109.5	H33B—C33—H33C	109.5
H16A—C16—H16B	109.5	N2—C34—H34A	109.5
N1—C16—H16C	109.5	N2—C34—H34B	109.5
H16A—C16—H16C	109.5	H34A—C34—H34B	109.5
H16B—C16—H16C	109.5	N2—C34—H34C	109.5
N1—C17—H17A	109.5	H34A—C34—H34C	109.5
N1—C17—H17B	109.5	H34B—C34—H34C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.85	2.20	2.836 (3)	132
O2—H2···N1^{i}	0.86	2.26	2.933 (3)	135

Symmetry code: (i) −*x*+2, *y*, −*z*.