organic compounds

2-Ethoxy-6-{(*E*)-[(4-methylphenyl)imino]-methyl}phenol

Muhammad Ashraf Shaheen,[a] **M. Nawaz Tahir,**[b]* **Rana Muhammad Irfan,**[a] **Shahid Iqbal**[a] **and Saeed Ahmad**[c]

[a]Department of Chemistry, University of Sargodha, Sargodha, Pakistan, [b]Department of Physics, University of Sargodha, Sargodha, Pakistan, and [c]Department of Chemistry, University of Engineering and Technology, Lahore 54890, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

The asymmetric unit of the title compound, $C_{16}H_{17}NO_2$, contains two molecules in which the dihedral angles between the 3-ethoxy-2-hydroxybenzaldehyde and toluidine moieties are 16.87 (8) and 19.93 (6)°. $S(6)$ rings are present in both molecules due to intramolecular O—H···N hydrogen bonds. In the crystal, one of the molecules is dimerized with an inversion-generated partner, due to two C—H···O interactions. This generates an $R_2^2(8)$ loop.

Related literature

For related crystal structures, see: Albayrak *et al.* (2010); Özek *et al.* (2010).

Experimental

Crystal data

$C_{16}H_{17}NO_2$	V = 5574.9 (4) Å^3
M_r = 255.31	Z = 16
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 29.5126 (11) Å	μ = 0.08 mm^{-1}
b = 6.8703 (3) Å	T = 296 K
c = 28.2167 (13) Å	0.30 × 0.25 × 0.22 mm
β = 102.986 (3)°	

Data collection

Bruker Kappa APEXII CCD diffractometer	20559 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	5040 independent reflections
	2075 reflections with $I > 2\sigma(I)$
T_{min} = 0.975, T_{max} = 0.985	R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064	346 parameters
$wR(F^2)$ = 0.181	H-atom parameters constrained
S = 0.98	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
5040 reflections	$\Delta\rho_{min}$ = −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···N1	0.82	1.86	2.584 (4)	147
O3—H3···N2	0.82	1.86	2.585 (3)	147
C24—H24A···O4^i	0.96	2.59	3.470 (4)	153

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

References

Albayrak, Ç., Koşar, B., Demir, S., Odabaşoğlu, M. & Büyükgüngör, O. (2010). *J. Mol. Struct.* **963**, 211–218.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Özek, A., Koşar, B., Albayrak, Ç. & Büyükgüngör, O. (2010). *Acta Cryst.* E**66**, o684.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

2-Ethoxy-6-{(*E*)-[(4-methylphenyl)imino]methyl}phenol

Muhammad Ashraf Shaheen, M. Nawaz Tahir, Rana Muhammad Irfan, Shahid Iqbal and Saeed Ahmad

Comment

The title compound (I), (Fig. 1) has been synthesized as a derivative for the complexation and other studies.

The crystal structures of 2-ethoxy-6-((phenylimino)methyl)phenol (Albayrak *et al.*, 2010) and (*E*)-2-ethoxy-6-[(4-ethoxyphenyl)iminomethyl]phenol (Özek *et al.*, 2010) have been published which are related to the title compound (I).

In (I), two molecules in the asymmetric unit are present, which differ slightly from each other geometrically. In one molecule, the group A (C1—C9/O1/O2) of 3-ethoxy-2-hydroxybenzaldehyde and group B (N1/C10—C16) of toluidine moieties are planar with r. m. s. deviation of 0.0270 Å and 0.0105 Å, respectively. The dihedral angle between A/B is 19.93 (6)°. In second molecule, the similar groups C (C18—C25/O3/O4) and D (N2/C26—C32) are also planar with r. m. s. deviation of 0.0184 Å and 0.0193 Å, respectively and the dihedral angle between C/D is 16.87 (8)°. In both molecules S(6) ring motif is present due to classical H–bonding of O—H···N type (Table 1, Fig. 2). The second molecule which is more planar is dimerized with itself from ethoxy groups with $R_2^2(8)$ ring motif due to C—H···O type of H–bonding (Table 1, Fig. 2).

Experimental

Equal molar ratio of 4-toluidine and 3-ethoxy-2-hydroxybenzaldehyde was refluxed in methanol for 2 h and orange prisms of (I) were obtained after 72 h by the slow evaporation at room temperature.

Refinement

The H-atoms were positioned geometrically at C—H = 0.93—0.97 and O—H = 0.82 Å, respectively and included in the refinement as riding with $U_{iso}(H) = xU_{eq}(C, O)$, where $x = 1.5$ for metyl H-atoms and $x = 1.2$ for all other H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).
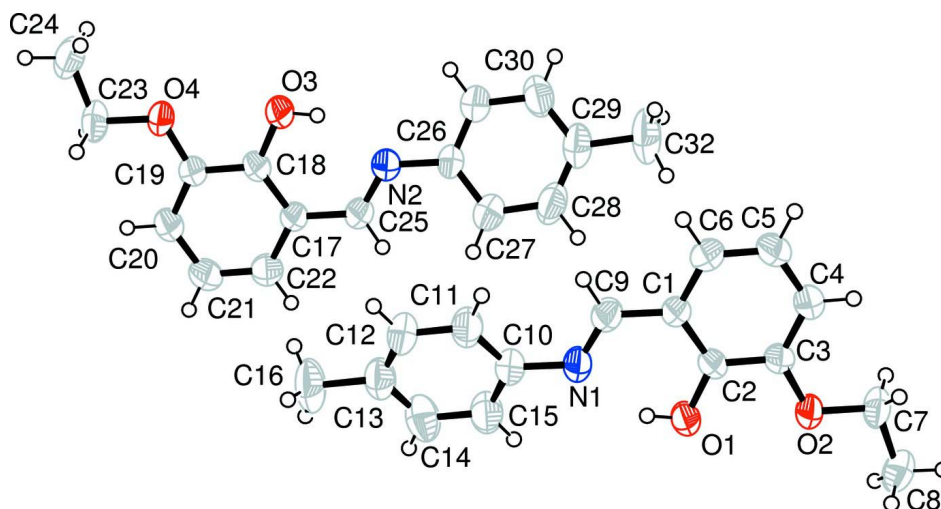
Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level.
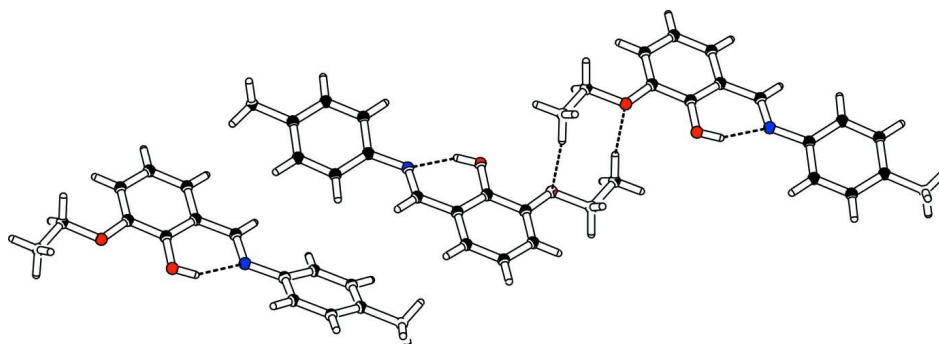
Figure 2

The partial packing, which shows that molecules form S(6) ring motif and one molecule is also dimerized with itself.

2-Ethoxy-6-{(*E*)-[(4-methylphenyl)imino]methyl}phenol

Crystal data

$C_{16}H_{17}NO_2$	$F(000) = 2176$
$M_r = 255.31$	$D_x = 1.217$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 2075 reflections
$a = 29.5126$ (11) Å	$\theta = 1.8–25.3°$
$b = 6.8703$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 28.2167$ (13) Å	$T = 296$ K
$\beta = 102.986$ (3)°	Prism, orange
$V = 5574.9$ (4) Å^3	$0.30 \times 0.25 \times 0.22$ mm
$Z = 16$	

Data collection

Bruker Kappa APEXII CCD diffractometer	ω scans
	Absorption correction: multi-scan
Radiation source: fine-focus sealed tube	(*SADABS*; Bruker, 2005)
Graphite monochromator	$T_{min} = 0.975$, $T_{max} = 0.985$
Detector resolution: 8.10 pixels mm^{-1}	20559 measured reflections

5040 independent reflections
2075 reflections with $I > 2\sigma(I)$
$R_{int} = 0.083$
$\theta_{max} = 25.3°$, $\theta_{min} = 1.8°$

$h = -35\rightarrow35$
$k = -8\rightarrow8$
$l = -33\rightarrow33$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.181$	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2]$
$S = 0.98$	where $P = (F_o^2 + 2F_c^2)/3$
5040 reflections	$(\Delta/\sigma)_{max} = 0.001$
346 parameters	$\Delta\rho_{max} = 0.25$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0022 (8)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.10580 (7)	0.6814 (3)	0.19524 (10)	0.0684 (10)
O2	0.01761 (7)	0.6161 (3)	0.18973 (9)	0.0585 (10)
N1	0.18746 (9)	0.5514 (5)	0.19299 (10)	0.0550 (11)
C1	0.12297 (10)	0.3411 (5)	0.19135 (12)	0.0461 (12)
C2	0.09199 (11)	0.4939 (5)	0.19246 (12)	0.0473 (14)
C3	0.04488 (11)	0.4545 (5)	0.18944 (12)	0.0468 (12)
C4	0.02948 (11)	0.2647 (5)	0.18598 (12)	0.0574 (16)
C5	0.06006 (12)	0.1118 (5)	0.18585 (13)	0.0629 (17)
C6	0.10630 (11)	0.1513 (5)	0.18828 (12)	0.0580 (16)
C7	−0.03139 (10)	0.5835 (6)	0.18454 (13)	0.0620 (16)
C8	−0.05326 (11)	0.7791 (6)	0.18882 (13)	0.0721 (16)
C9	0.17137 (11)	0.3781 (5)	0.19224 (12)	0.0527 (16)
C10	0.23446 (11)	0.5901 (6)	0.19178 (12)	0.0533 (14)
C11	0.27089 (11)	0.4584 (6)	0.20317 (13)	0.0670 (16)
C12	0.31500 (12)	0.5126 (7)	0.19954 (15)	0.0753 (18)
C13	0.32467 (12)	0.6948 (7)	0.18545 (13)	0.0665 (19)
C14	0.28869 (14)	0.8279 (7)	0.17494 (14)	0.0794 (17)
C15	0.24410 (12)	0.7749 (6)	0.17846 (14)	0.0710 (16)
C16	0.37347 (8)	0.7535 (4)	0.18219 (13)	0.097 (2)
O3	0.39693 (6)	0.0489 (3)	0.05775 (9)	0.0672 (10)
O4	0.48472 (7)	0.1144 (3)	0.06181 (8)	0.0594 (10)

N2	0.31507 (8)	0.1776 (4)	0.05970 (10)	0.0540 (11)
C17	0.37945 (10)	0.3890 (5)	0.06123 (12)	0.0470 (12)
C18	0.41055 (10)	0.2363 (5)	0.05998 (12)	0.0479 (12)
C19	0.45777 (11)	0.2768 (5)	0.06204 (12)	0.0493 (14)
C20	0.47255 (11)	0.4658 (6)	0.06428 (13)	0.0578 (16)
C21	0.44186 (12)	0.6194 (5)	0.06494 (13)	0.0636 (17)
C22	0.39611 (11)	0.5794 (5)	0.06345 (12)	0.0598 (16)
C23	0.53338 (10)	0.1477 (6)	0.06427 (14)	0.0652 (16)
C24	0.55535 (11)	−0.0499 (6)	0.06255 (14)	0.0765 (16)
C25	0.33127 (10)	0.3496 (5)	0.06107 (12)	0.0519 (16)
C26	0.26797 (10)	0.1379 (6)	0.06073 (12)	0.0520 (16)
C27	0.23819 (12)	0.2710 (6)	0.07524 (13)	0.0686 (16)
C28	0.19325 (13)	0.2127 (7)	0.07633 (14)	0.0766 (19)
C29	0.17740 (12)	0.0278 (7)	0.06428 (14)	0.0694 (18)
C30	0.20727 (12)	−0.1006 (6)	0.05007 (14)	0.0743 (17)
C31	0.25229 (11)	−0.0466 (6)	0.04814 (14)	0.0666 (16)
C32	0.12886 (12)	−0.0360 (7)	0.06682 (16)	0.101 (2)
H1	0.13371	0.68676	0.19605	0.1027*
H4	−0.00187	0.23879	0.18369	0.0689*
H5	0.04949	−0.01611	0.18414	0.0755*
H6	0.12678	0.04878	0.18786	0.0694*
H7A	−0.03675	0.49650	0.20979	0.0740*
H7B	−0.04466	0.52550	0.15315	0.0740*
H8A	−0.04101	0.83189	0.22062	0.1082*
H8B	−0.08634	0.76427	0.18387	0.1082*
H8C	−0.04637	0.86579	0.16469	0.1082*
H9	0.19133	0.27337	0.19226	0.0633*
H11	0.26559	0.33328	0.21328	0.0803*
H12	0.33892	0.42183	0.20695	0.0901*
H14	0.29434	0.95355	0.16546	0.0954*
H15	0.22034	0.86659	0.17166	0.0848*
H16A	0.39353	0.75171	0.21409	0.1453*
H16B	0.37283	0.88227	0.16884	0.1453*
H16C	0.38490	0.66367	0.16157	0.1453*
H3	0.36940	0.04294	0.05871	0.1006*
H20	0.50366	0.49238	0.06538	0.0696*
H21	0.45232	0.74747	0.06637	0.0763*
H22	0.37562	0.68183	0.06394	0.0715*
H23A	0.54759	0.21451	0.09421	0.0781*
H23B	0.53738	0.22683	0.03703	0.0781*
H24A	0.54192	−0.11186	0.03213	0.1145*
H24B	0.54986	−0.12861	0.08882	0.1145*
H24C	0.58822	−0.03496	0.06560	0.1145*
H25	0.31139	0.45384	0.06200	0.0619*
H27	0.24816	0.39701	0.08407	0.0823*
H28	0.17328	0.30243	0.08558	0.0922*
H30	0.19725	−0.22678	0.04151	0.0891*
H31	0.27184	−0.13652	0.03824	0.0798*
H32A	0.11408	0.06568	0.08117	0.1515*

H32B	0.13071	−0.15157	0.08630	0.1515*
H32C	0.11102	−0.06260	0.03461	0.1515*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0416 (14)	0.0433 (17)	0.122 (2)	−0.0037 (11)	0.0222 (14)	−0.0038 (15)
O2	0.0341 (14)	0.0511 (17)	0.0919 (19)	0.0002 (11)	0.0178 (11)	−0.0033 (14)
N1	0.0366 (17)	0.054 (2)	0.075 (2)	0.0002 (15)	0.0137 (13)	0.0008 (18)
C1	0.040 (2)	0.040 (2)	0.059 (2)	0.0006 (17)	0.0126 (15)	−0.0014 (18)
C2	0.041 (2)	0.038 (2)	0.063 (3)	−0.0057 (16)	0.0121 (15)	−0.0018 (18)
C3	0.043 (2)	0.038 (2)	0.060 (2)	−0.0002 (18)	0.0128 (15)	−0.0001 (19)
C4	0.044 (2)	0.052 (3)	0.077 (3)	−0.0044 (19)	0.0155 (17)	−0.004 (2)
C5	0.057 (3)	0.042 (3)	0.090 (3)	−0.0063 (19)	0.017 (2)	−0.001 (2)
C6	0.052 (2)	0.047 (3)	0.076 (3)	0.0087 (18)	0.0163 (17)	−0.001 (2)
C7	0.035 (2)	0.076 (3)	0.077 (3)	0.0011 (18)	0.0166 (17)	0.006 (2)
C8	0.045 (2)	0.085 (3)	0.088 (3)	0.016 (2)	0.0186 (18)	0.003 (2)
C9	0.043 (2)	0.050 (3)	0.065 (3)	0.0067 (18)	0.0122 (16)	0.004 (2)
C10	0.041 (2)	0.061 (3)	0.059 (2)	−0.0005 (19)	0.0138 (16)	0.001 (2)
C11	0.046 (2)	0.066 (3)	0.090 (3)	0.000 (2)	0.0172 (19)	0.007 (2)
C12	0.042 (2)	0.088 (4)	0.097 (3)	0.003 (2)	0.018 (2)	−0.007 (3)
C13	0.049 (3)	0.093 (4)	0.060 (3)	−0.010 (2)	0.0175 (19)	−0.008 (3)
C14	0.063 (3)	0.087 (3)	0.089 (3)	−0.017 (3)	0.019 (2)	0.019 (3)
C15	0.051 (2)	0.070 (3)	0.092 (3)	−0.001 (2)	0.0161 (19)	0.014 (3)
C16	0.052 (2)	0.150 (5)	0.095 (3)	−0.025 (3)	0.031 (2)	−0.005 (3)
O3	0.0427 (14)	0.0433 (17)	0.119 (2)	−0.0046 (12)	0.0256 (12)	0.0009 (15)
O4	0.0348 (14)	0.0553 (18)	0.0910 (19)	−0.0002 (11)	0.0202 (12)	−0.0012 (14)
N2	0.0412 (18)	0.048 (2)	0.073 (2)	−0.0004 (14)	0.0135 (13)	−0.0014 (17)
C17	0.038 (2)	0.039 (2)	0.064 (2)	0.0015 (16)	0.0112 (15)	0.0012 (19)
C18	0.042 (2)	0.042 (2)	0.061 (2)	−0.0069 (17)	0.0141 (16)	0.0009 (19)
C19	0.040 (2)	0.044 (3)	0.065 (2)	−0.0029 (18)	0.0142 (16)	−0.003 (2)
C20	0.045 (2)	0.051 (3)	0.077 (3)	−0.0080 (19)	0.0131 (17)	0.000 (2)
C21	0.060 (3)	0.044 (3)	0.087 (3)	−0.008 (2)	0.017 (2)	0.000 (2)
C22	0.053 (2)	0.047 (3)	0.079 (3)	0.0012 (19)	0.0142 (18)	0.003 (2)
C23	0.035 (2)	0.083 (3)	0.080 (3)	−0.0020 (19)	0.0182 (17)	0.007 (2)
C24	0.046 (2)	0.095 (3)	0.090 (3)	0.015 (2)	0.0184 (19)	−0.005 (3)
C25	0.041 (2)	0.047 (3)	0.067 (3)	0.0054 (17)	0.0106 (16)	0.001 (2)
C26	0.034 (2)	0.059 (3)	0.063 (3)	0.0003 (18)	0.0109 (16)	−0.004 (2)
C27	0.053 (2)	0.075 (3)	0.083 (3)	0.002 (2)	0.0261 (19)	−0.011 (2)
C28	0.048 (3)	0.101 (4)	0.087 (3)	0.006 (2)	0.028 (2)	−0.014 (3)
C29	0.043 (2)	0.103 (4)	0.065 (3)	−0.007 (2)	0.0181 (18)	0.000 (3)
C30	0.051 (3)	0.086 (3)	0.088 (3)	−0.017 (2)	0.020 (2)	−0.009 (3)
C31	0.049 (2)	0.067 (3)	0.088 (3)	−0.003 (2)	0.0244 (19)	−0.005 (2)
C32	0.052 (3)	0.158 (5)	0.101 (4)	−0.023 (3)	0.035 (2)	−0.003 (3)

Geometric parameters (Å, º)

O1—C2	1.348 (4)	C12—H12	0.9300
O2—C3	1.372 (4)	C14—H14	0.9300
O2—C7	1.438 (4)	C15—H15	0.9300

O1—H1	0.8200	C16—H16C	0.9600
O3—C18	1.346 (4)	C16—H16A	0.9600
O4—C19	1.371 (4)	C16—H16B	0.9600
O4—C23	1.440 (4)	C17—C22	1.394 (5)
O3—H3	0.8200	C17—C25	1.447 (4)
N1—C9	1.280 (5)	C17—C18	1.400 (5)
N1—C10	1.420 (4)	C18—C19	1.409 (5)
N2—C25	1.272 (4)	C19—C20	1.367 (5)
N2—C26	1.423 (4)	C20—C21	1.394 (5)
C1—C6	1.390 (5)	C21—C22	1.369 (5)
C1—C2	1.397 (5)	C23—C24	1.510 (6)
C1—C9	1.446 (5)	C26—C31	1.369 (6)
C2—C3	1.400 (5)	C26—C27	1.392 (5)
C3—C4	1.377 (5)	C27—C28	1.392 (5)
C4—C5	1.386 (5)	C28—C29	1.370 (7)
C5—C6	1.378 (5)	C29—C32	1.515 (5)
C7—C8	1.507 (6)	C29—C30	1.369 (6)
C10—C15	1.372 (6)	C30—C31	1.392 (5)
C10—C11	1.387 (5)	C20—H20	0.9300
C11—C12	1.380 (5)	C21—H21	0.9300
C12—C13	1.363 (7)	C22—H22	0.9300
C13—C14	1.382 (6)	C23—H23A	0.9700
C13—C16	1.518 (5)	C23—H23B	0.9700
C14—C15	1.390 (6)	C24—H24A	0.9600
C4—H4	0.9300	C24—H24B	0.9600
C5—H5	0.9300	C24—H24C	0.9600
C6—H6	0.9300	C25—H25	0.9300
C7—H7A	0.9700	C27—H27	0.9300
C7—H7B	0.9700	C28—H28	0.9300
C8—H8C	0.9600	C30—H30	0.9300
C8—H8A	0.9600	C31—H31	0.9300
C8—H8B	0.9600	C32—H32A	0.9600
C9—H9	0.9300	C32—H32B	0.9600
C11—H11	0.9300	C32—H32C	0.9600
C3—O2—C7	116.8 (3)	H16A—C16—H16B	109.00
C2—O1—H1	109.00	C13—C16—H16A	109.00
C19—O4—C23	116.3 (3)	C13—C16—H16B	109.00
C18—O3—H3	110.00	C18—C17—C22	118.6 (3)
C9—N1—C10	122.3 (3)	C18—C17—C25	120.6 (3)
C25—N2—C26	122.7 (3)	C22—C17—C25	120.8 (3)
C2—C1—C6	118.8 (3)	O3—C18—C19	118.2 (3)
C2—C1—C9	121.1 (3)	C17—C18—C19	119.9 (3)
C6—C1—C9	120.1 (3)	O3—C18—C17	121.8 (3)
O1—C2—C3	118.1 (3)	O4—C19—C20	126.4 (3)
O1—C2—C1	121.9 (3)	C18—C19—C20	119.5 (3)
C1—C2—C3	120.0 (3)	O4—C19—C18	114.1 (3)
C2—C3—C4	119.7 (3)	C19—C20—C21	121.2 (3)
O2—C3—C4	125.6 (3)	C20—C21—C22	119.1 (3)

O2—C3—C2	114.8 (3)	C17—C22—C21	121.7 (3)
C3—C4—C5	120.9 (3)	O4—C23—C24	106.6 (3)
C4—C5—C6	119.3 (3)	N2—C25—C17	122.4 (3)
C1—C6—C5	121.4 (3)	N2—C26—C31	116.6 (3)
O2—C7—C8	107.0 (3)	C27—C26—C31	119.1 (3)
N1—C9—C1	121.7 (3)	N2—C26—C27	124.3 (3)
C11—C10—C15	118.0 (3)	C26—C27—C28	119.0 (4)
N1—C10—C15	116.3 (3)	C27—C28—C29	122.4 (4)
N1—C10—C11	125.7 (4)	C28—C29—C30	117.6 (4)
C10—C11—C12	120.1 (4)	C28—C29—C32	122.0 (4)
C11—C12—C13	122.2 (4)	C30—C29—C32	120.4 (4)
C12—C13—C14	118.0 (4)	C29—C30—C31	121.5 (4)
C14—C13—C16	120.3 (4)	C26—C31—C30	120.4 (3)
C12—C13—C16	121.7 (3)	C19—C20—H20	119.00
C13—C14—C15	120.4 (4)	C21—C20—H20	119.00
C10—C15—C14	121.3 (4)	C20—C21—H21	120.00
C5—C4—H4	120.00	C22—C21—H21	120.00
C3—C4—H4	120.00	C17—C22—H22	119.00
C6—C5—H5	120.00	C21—C22—H22	119.00
C4—C5—H5	120.00	O4—C23—H23A	110.00
C5—C6—H6	119.00	O4—C23—H23B	110.00
C1—C6—H6	119.00	C24—C23—H23A	110.00
O2—C7—H7B	110.00	C24—C23—H23B	110.00
H7A—C7—H7B	109.00	H23A—C23—H23B	109.00
C8—C7—H7A	110.00	C23—C24—H24A	109.00
C8—C7—H7B	110.00	C23—C24—H24B	109.00
O2—C7—H7A	110.00	C23—C24—H24C	109.00
H8A—C8—H8B	109.00	H24A—C24—H24B	109.00
H8A—C8—H8C	109.00	H24A—C24—H24C	109.00
H8B—C8—H8C	109.00	H24B—C24—H24C	109.00
C7—C8—H8A	109.00	N2—C25—H25	119.00
C7—C8—H8B	109.00	C17—C25—H25	119.00
C7—C8—H8C	109.00	C26—C27—H27	120.00
N1—C9—H9	119.00	C28—C27—H27	120.00
C1—C9—H9	119.00	C27—C28—H28	119.00
C12—C11—H11	120.00	C29—C28—H28	119.00
C10—C11—H11	120.00	C29—C30—H30	119.00
C13—C12—H12	119.00	C31—C30—H30	119.00
C11—C12—H12	119.00	C26—C31—H31	120.00
C13—C14—H14	120.00	C30—C31—H31	120.00
C15—C14—H14	120.00	C29—C32—H32A	109.00
C10—C15—H15	119.00	C29—C32—H32B	109.00
C14—C15—H15	119.00	C29—C32—H32C	109.00
C13—C16—H16C	109.00	H32A—C32—H32B	109.00
H16A—C16—H16C	109.00	H32A—C32—H32C	109.00
H16B—C16—H16C	109.00	H32B—C32—H32C	109.00
C7—O2—C3—C2	177.4 (3)	C10—C11—C12—C13	0.8 (6)
C7—O2—C3—C4	−1.9 (5)	C11—C12—C13—C14	0.5 (6)

C3—O2—C7—C8	176.8 (3)	C11—C12—C13—C16	179.2 (4)
C19—O4—C23—C24	−179.0 (3)	C16—C13—C14—C15	−179.3 (3)
C23—O4—C19—C20	0.1 (5)	C12—C13—C14—C15	−0.5 (6)
C23—O4—C19—C18	−179.5 (3)	C13—C14—C15—C10	−0.8 (6)
C9—N1—C10—C15	161.4 (3)	C22—C17—C18—O3	−179.9 (3)
C10—N1—C9—C1	−177.3 (3)	C22—C17—C18—C19	1.4 (5)
C9—N1—C10—C11	−19.1 (5)	C25—C17—C18—O3	1.2 (5)
C25—N2—C26—C31	165.7 (3)	C25—C17—C18—C19	−177.6 (3)
C25—N2—C26—C27	−16.7 (5)	C18—C17—C22—C21	−0.7 (5)
C26—N2—C25—C17	178.4 (3)	C25—C17—C22—C21	178.2 (3)
C9—C1—C2—O1	−1.2 (5)	C18—C17—C25—N2	−0.2 (5)
C9—C1—C2—C3	177.2 (3)	C22—C17—C25—N2	−179.1 (3)
C6—C1—C2—C3	−1.4 (5)	O3—C18—C19—O4	−0.4 (4)
C6—C1—C2—O1	−179.8 (3)	O3—C18—C19—C20	179.9 (3)
C2—C1—C9—N1	−1.6 (5)	C17—C18—C19—O4	178.4 (3)
C2—C1—C6—C5	0.7 (5)	C17—C18—C19—C20	−1.3 (5)
C9—C1—C6—C5	−178.0 (3)	O4—C19—C20—C21	−179.1 (3)
C6—C1—C9—N1	177.0 (3)	C18—C19—C20—C21	0.5 (5)
C1—C2—C3—O2	−178.5 (3)	C19—C20—C21—C22	0.2 (5)
O1—C2—C3—O2	−0.1 (4)	C20—C21—C22—C17	−0.1 (5)
O1—C2—C3—C4	179.3 (3)	N2—C26—C27—C28	−177.7 (3)
C1—C2—C3—C4	0.8 (5)	C31—C26—C27—C28	−0.3 (5)
O2—C3—C4—C5	179.8 (3)	N2—C26—C31—C30	177.3 (3)
C2—C3—C4—C5	0.5 (5)	C27—C26—C31—C30	−0.3 (6)
C3—C4—C5—C6	−1.3 (5)	C26—C27—C28—C29	1.0 (6)
C4—C5—C6—C1	0.7 (5)	C27—C28—C29—C30	−1.0 (6)
N1—C10—C15—C14	−178.5 (3)	C27—C28—C29—C32	178.4 (4)
C15—C10—C11—C12	−2.0 (5)	C28—C29—C30—C31	0.4 (6)
N1—C10—C11—C12	178.6 (3)	C32—C29—C30—C31	−179.0 (4)
C11—C10—C15—C14	2.0 (6)	C29—C30—C31—C26	0.3 (6)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯N1	0.82	1.86	2.584 (4)	147
O3—H3⋯N2	0.82	1.86	2.585 (3)	147
C24—H24A⋯O4[i]	0.96	2.59	3.470 (4)	153

Symmetry code: (i) −x+1, −y, −z.