Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-Hydroxy-2-{[(2-phenylethyl)-iminiumyl]methyl}phenolate

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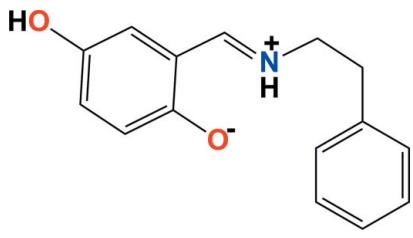
Received 2 June 2012; accepted 4 June 2012

Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.107; data-to-parameter ratio = 17.0.

The title Schiff base compound, $C_{15}H_{15}NO_2$, crystallized as the iminium–phenolate zwitterion. The H atom is localized on the imine N atom, forming a strong intramolecular hydrogen bond with the phenolate O atom, and giving rise to an S(6) ring motif. The molecule has an E conformation about the C=N bond. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains propagating along [010]. There are also C—H···O interactions present.

Related literature

For general background to the characteristics of Schiff bases, see: Krause *et al.* (1995); Hadjoudis *et al.* (2004). For related structures, see: Dominiak *et al.* (2006); Santos-Contreras *et al.* (2009); Ng (2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Monoclinic, $P2_1/c$
a = 9.5010 (19) Å
b = 12.936 (3) Å
c = 12.551 (4) Å
β = 124.81 (2)°
V = 1266.5 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 170 K
0.50 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: for a sphere (Dwiggins, 1975)
T_{min} = 0.861, T_{max} = 0.862
15718 measured reflections
2773 independent reflections
2367 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.107
S = 1.02
2773 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 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
N8—H8···O1	0.86	1.90	2.5884 (15)	137
O4—H4···O1^{i}	0.82	1.87	2.6902 (15)	176
C6—H6···O4^{ii}	0.95	2.59	3.2818 (18)	130

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO/SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

The authors gratefully acknowledge financial support from FRABA-Universidad de Colima 764/11, CINVESTAV-IPN and SIP-IPN

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2447).

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supplementary materials

Acta Cryst. (2012). E**68**, o2075 [doi:10.1107/S1600536812025408]

(*E*)-4-Hydroxy-2-{[(2-phenylethyl)iminiumyl]methyl}phenolate

David Ortegon-Reyna, Cesar Garcias-Morales, Efren V. García-Báez, Armando Ariza-Castolo and Francisco J. Martínez-Martínez

Comment

Schiff base compounds are highly versatile compounds widely applied in different study fields. They have been used as selective prodrugs for histamine (Krause *et al.*, 1995). and as materials of interest because of their thermochromic and photochromic properties (Hadjoudis *et al.*, 2004). When an OH functionality is also present in the same molecule, tautomeric N—H or O—H equilibrium can be performed, thus these compounds can exist as O—H···N (imines), O···H—N (enamines) and also as N^+—H···O^- zwitterionic forms (Dominiak *et al.*, 2006, Ng, 2008, Santos-Contreras *et al.*, 2009) Herein we demonstrate that the title compound exist as the N^+—H···O^- zwitterionic form, with the H atom closing a six membered ring.

The title compound, Fig. 1, exists as a zwitterion with the hydrogen atom being localized on the imine N atom N8. The C1═O1 and N8═C7 bond lengths [1.3206 (14) and 1.2985 (16) Å, respectively] reveal significant double-bond character. The phenolate ring shows a certain distortion in the C—C bond lengths, but nevertheless an alternating long-short pattern is observed, in agreement with delocalized bonding. The C2—C7 bond distance of 1.4407 (16) Å is in the range for a single bond character. The intramolecular N8-H8···O1 hydrogen bond gives rise to the formation of an S(6) ring motif (Table 1; Bernstein *et al.*, 1995).

In the crystal, an O-H···O hydrogen bond links the molecules to form C(7) chains (Bernstein *et al.*, 1995) that propagate along the b axis direction (Table 1 and Fig. 2). There are also C-H···O interactions present (Table 1).

The title structure closely resembles that of *N*,-bis(2,5-dihydroxybezyl idene)-1,2-diaminobenzene (Dominiak *et al.*, 2006) and 4-chloro-2-[tris(hydroxymethyl)methyliminiomethyl]phenolate (Ng, 2008).

Experimental

The title compound was prepared by condensation of 5-hydroxysalicylaldehyde (0.5 g, 3.62 mmol) with phenethylamine (0.438 g, 0.454 ml, 3.62 mmol) in toluene, at 298 K with stirring for 5 min. Orange crystals, suitable for X-ray analysis, were obtained by slow evaporation from a saturated dimethylsulfoxide solution [Yield of 0.78 g (90%); *M*.p. 396–397 K]. Spectroscopic data for the title compound are available in the archived CIF.

Refinement

The amino and OH H atoms were located in a difference Fourier map. In the final cycles of refinement they and the C-bound H atoms were included in calculated positions and treated as riding atoms: O-H = 0.82 Å, N-H = 0.86 Å, C-H = 0.95 and 0.99 Å for CH and CH_2 H atoms, respectively, with U_{iso}(H) = k × Ueq(O,N,C) where k = 1.5 for the OH H atom and = 1.2 for other H atoms.

Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

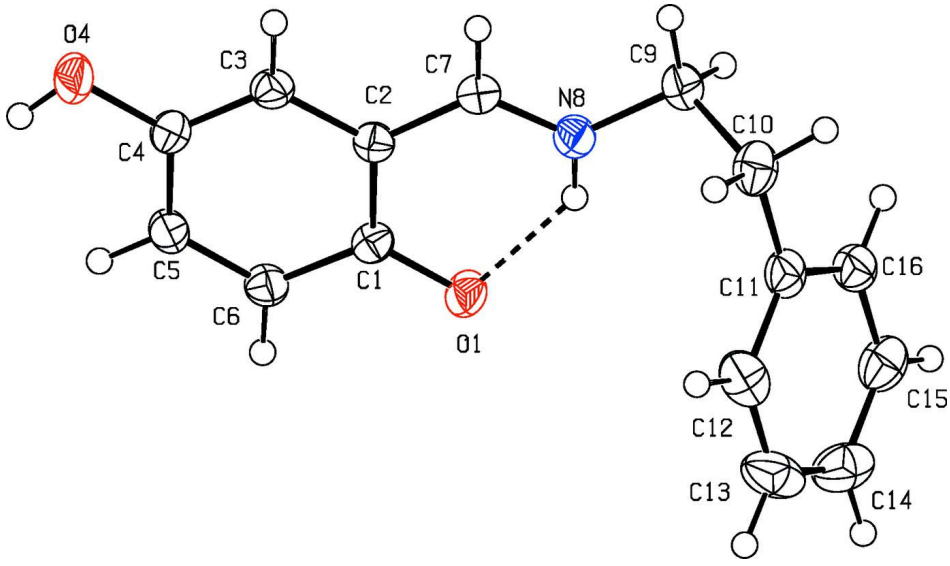

Figure 1

The molecular structure of the title compound with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular N-H···O bond is shown as a dashed line.

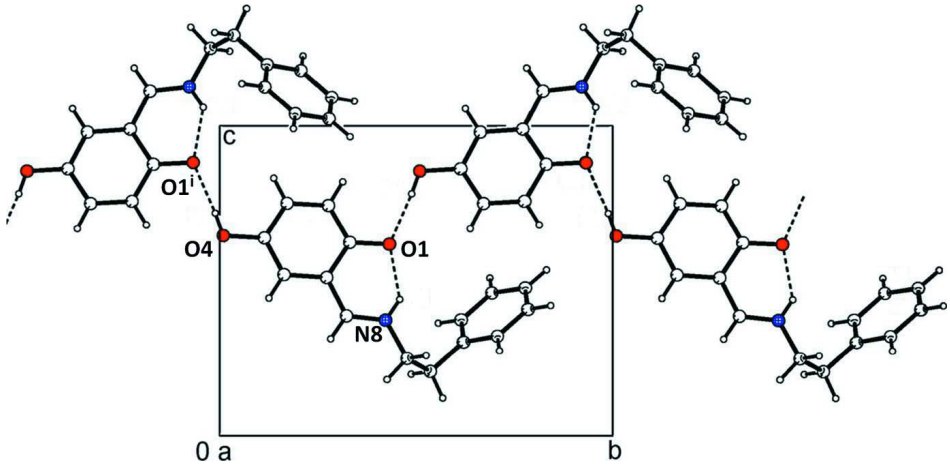

Figure 2

A partial view along the a axis of the crystal packing of the title compound. The N-H···O and O-H..O hydrogen bonds are shown as dashed lines [symmetry code: (i) -*x*+2, *y*-1/2, -*z*+3/2].

(*E*)-4-Hydroxy-2-{[(2-phenylethyl)iminiumyl]methyl}phenolate

Crystal data

$C_{15}H_{15}NO_2$
$M_r = 241.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.5010$ (19) Å
$b = 12.936$ (3) Å
$c = 12.551$ (4) Å
$\beta = 124.81$ (2)°
$V = 1266.5$ (6) Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.265$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14042 reflections
$\theta = 2.9$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 170$ K
Prism, orange
0.50 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
Absorption correction: for a sphere (Dwiggins, 1975)
$T_{min} = 0.861$, $T_{max} = 0.862$
15718 measured reflections
2773 independent reflections
2367 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$, $\theta_{min} = 4.1°$
$h = -10 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.107$
$S = 1.02$
2773 reflections
163 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.3688P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Experimental. Spectroscopic data for the title compound: FT—IR by ATR (cm^{-1}): 1643 (C═N as intense band), 1496 (Asymmetrical C=C—O···H stretch), 3311 (free phenolic O—H intense broad band), 3059 (intramolecular hydrogen bonding N—H···O, as a weak broad band). LC/MS/TOF on HPLC-methanol solution, m/z (%) calculated: 242.1181 (100); found 242.1175 (100) $[M+H]^+$, molecular formula $C_{15}H_{15}NO_2$. ^{1}H NMR ($CDCl_3$, 300.1MHz): δ 6.83 (m, H5 and H6), 6.67 (s, H3), 8.12 (s, H7), 3.84 (t, H9), 3.00 (t, H10), 7.19–7.32 (m, H12—H16). ^{13}C NMR ($CDCl_3$, 75.4MHz): δ 147.5 (C1), 118.4 (C2), 116.6 (C3), 144.0 (C4), 119.9 (C5), 117.6 (C6), 164.5 (C7), 61.1 (C9), 37.3 (C10), 139.3 (C11), 128.9 (C13, C15), 128.5 (C12, C16), 126.4 (C14).

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.88467 (11)	0.43206 (6)	0.61806 (8)	0.0320 (3)
O4	0.99566 (15)	0.00918 (7)	0.64559 (9)	0.0460 (3)
N8	0.75925 (13)	0.42202 (8)	0.37321 (9)	0.0284 (3)
C1	0.90916 (14)	0.33115 (8)	0.62390 (11)	0.0245 (3)
C2	0.85954 (14)	0.27185 (8)	0.51050 (10)	0.0241 (3)
C3	0.88858 (15)	0.16354 (9)	0.51983 (11)	0.0272 (3)
C4	0.96636 (16)	0.11344 (9)	0.63837 (11)	0.0290 (3)
C5	1.01496 (15)	0.17148 (9)	0.75028 (11)	0.0288 (3)
C6	0.98611 (15)	0.27637 (9)	0.74326 (11)	0.0276 (3)
C7	0.78312 (14)	0.32274 (9)	0.38709 (11)	0.0256 (3)
C9	0.68816 (16)	0.47659 (9)	0.24949 (12)	0.0325 (4)
C10	0.52322 (16)	0.53653 (10)	0.20739 (13)	0.0364 (4)
C11	0.55332 (15)	0.62068 (9)	0.30222 (11)	0.0314 (3)
C12	0.48187 (17)	0.61459 (12)	0.37397 (13)	0.0408 (4)
C13	0.51032 (18)	0.69276 (14)	0.46060 (14)	0.0495 (5)
C14	0.60966 (18)	0.77808 (13)	0.47683 (14)	0.0470 (5)
C15	0.68349 (17)	0.78487 (10)	0.40787 (13)	0.0399 (4)
C16	0.65511 (16)	0.70707 (10)	0.32130 (12)	0.0332 (4)
H3	0.85445	0.12504	0.44421	0.0326*
H4	1.03190	−0.01141	0.71879	0.0689*
H5	1.06841	0.13740	0.83162	0.0345*
H6	1.01819	0.31299	0.81963	0.0332*
H7	0.74885	0.28207	0.31297	0.0307*
H8	0.78653	0.45796	0.44009	0.0341*
H9A	0.66198	0.42590	0.18137	0.0389*
H9B	0.77472	0.52552	0.25890	0.0389*
H10A	0.47519	0.56802	0.12123	0.0437*
H10B	0.43734	0.48727	0.19847	0.0437*
H12	0.41353	0.55663	0.36330	0.0490*
H13	0.46162	0.68769	0.50873	0.0594*
H14	0.62724	0.83176	0.53491	0.0565*
H15	0.75308	0.84257	0.42000	0.0479*
H16	0.70530	0.71235	0.27424	0.0398*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0424 (5)	0.0208 (4)	0.0295 (4)	0.0003 (3)	0.0185 (4)	−0.0023 (3)
O4	0.0827 (8)	0.0218 (4)	0.0385 (5)	0.0085 (5)	0.0376 (5)	0.0045 (4)
N8	0.0316 (5)	0.0272 (5)	0.0248 (5)	0.0016 (4)	0.0151 (4)	0.0004 (4)
C1	0.0234 (5)	0.0229 (5)	0.0270 (6)	−0.0020 (4)	0.0142 (5)	−0.0025 (4)
C2	0.0230 (5)	0.0248 (6)	0.0249 (6)	−0.0016 (4)	0.0140 (5)	−0.0007 (4)
C3	0.0324 (6)	0.0245 (6)	0.0272 (6)	−0.0024 (4)	0.0185 (5)	−0.0041 (4)
C4	0.0374 (6)	0.0209 (5)	0.0327 (6)	0.0000 (5)	0.0223 (5)	−0.0001 (4)
C5	0.0340 (6)	0.0269 (6)	0.0260 (6)	−0.0001 (5)	0.0175 (5)	0.0025 (4)
C6	0.0309 (6)	0.0266 (6)	0.0242 (6)	−0.0024 (5)	0.0150 (5)	−0.0034 (4)
C7	0.0250 (5)	0.0266 (6)	0.0262 (6)	−0.0006 (4)	0.0152 (5)	−0.0022 (4)

C9	0.0375 (7)	0.0311 (6)	0.0282 (6)	0.0038 (5)	0.0184 (5)	0.0049 (5)
C10	0.0318 (6)	0.0347 (7)	0.0327 (7)	0.0034 (5)	0.0125 (5)	0.0044 (5)
C11	0.0253 (6)	0.0348 (6)	0.0299 (6)	0.0077 (5)	0.0132 (5)	0.0087 (5)
C12	0.0288 (6)	0.0540 (8)	0.0385 (7)	0.0031 (6)	0.0185 (6)	0.0116 (6)
C13	0.0347 (7)	0.0833 (12)	0.0348 (7)	0.0142 (7)	0.0224 (6)	0.0074 (7)
C14	0.0340 (7)	0.0616 (10)	0.0349 (8)	0.0144 (7)	0.0134 (6)	−0.0054 (6)
C15	0.0324 (7)	0.0371 (7)	0.0403 (7)	0.0061 (5)	0.0149 (6)	0.0020 (5)
C16	0.0312 (6)	0.0356 (7)	0.0342 (7)	0.0058 (5)	0.0195 (5)	0.0065 (5)

Geometric parameters (Å, º)

O1—C1	1.3206 (14)	C12—C13	1.394 (2)
O4—C4	1.3696 (16)	C13—C14	1.390 (3)
O4—H4	0.8200	C14—C15	1.394 (3)
N8—C7	1.2985 (16)	C15—C16	1.3898 (19)
N8—C9	1.4725 (16)	C3—H3	0.9500
N8—H8	0.8600	C5—H5	0.9500
C1—C6	1.4250 (17)	C6—H6	0.9500
C1—C2	1.4389 (16)	C7—H7	0.9500
C2—C7	1.4407 (16)	C9—H9A	0.9900
C2—C3	1.4199 (16)	C9—H9B	0.9900
C3—C4	1.3872 (17)	C10—H10A	0.9900
C4—C5	1.4175 (17)	C10—H10B	0.9900
C5—C6	1.3771 (17)	C12—H12	0.9500
C9—C10	1.546 (2)	C13—H13	0.9500
C10—C11	1.5148 (19)	C14—H14	0.9500
C11—C16	1.406 (2)	C15—H15	0.9500
C11—C12	1.406 (2)	C16—H16	0.9500
C4—O4—H4	109.00	C4—C3—H3	120.00
C7—N8—C9	123.74 (10)	C4—C5—H5	119.00
C9—N8—H8	118.00	C6—C5—H5	119.00
C7—N8—H8	118.00	C1—C6—H6	119.00
O1—C1—C2	121.62 (10)	C5—C6—H6	119.00
O1—C1—C6	121.22 (10)	N8—C7—H7	119.00
C2—C1—C6	117.17 (10)	C2—C7—H7	119.00
C1—C2—C7	119.95 (10)	N8—C9—H9A	109.00
C1—C2—C3	120.40 (10)	N8—C9—H9B	109.00
C3—C2—C7	119.64 (10)	C10—C9—H9A	109.00
C2—C3—C4	120.59 (11)	C10—C9—H9B	109.00
O4—C4—C3	119.65 (11)	H9A—C9—H9B	108.00
C3—C4—C5	119.21 (11)	C9—C10—H10A	109.00
O4—C4—C5	121.14 (10)	C9—C10—H10B	109.00
C4—C5—C6	121.21 (11)	C11—C10—H10A	109.00
C1—C6—C5	121.41 (11)	C11—C10—H10B	109.00
N8—C7—C2	122.58 (11)	H10A—C10—H10B	108.00
N8—C9—C10	111.47 (13)	C11—C12—H12	120.00
C9—C10—C11	113.07 (12)	C13—C12—H12	120.00
C10—C11—C12	121.30 (13)	C12—C13—H13	120.00
C10—C11—C16	120.53 (14)	C14—C13—H13	120.00

C12—C11—C16	118.18 (12)	C13—C14—H14	120.00
C11—C12—C13	120.64 (15)	C15—C14—H14	120.00
C12—C13—C14	120.24 (17)	C14—C15—H15	120.00
C13—C14—C15	119.97 (15)	C16—C15—H15	120.00
C14—C15—C16	119.87 (15)	C11—C16—H16	119.00
C11—C16—C15	121.08 (15)	C15—C16—H16	119.00
C2—C3—H3	120.00		

C9—N8—C7—C2	177.35 (15)	O4—C4—C5—C6	179.78 (16)
C7—N8—C9—C10	121.46 (15)	C3—C4—C5—C6	0.1 (3)
C6—C1—C2—C3	−0.5 (2)	C4—C5—C6—C1	−1.1 (2)
C6—C1—C2—C7	−179.18 (14)	N8—C9—C10—C11	62.54 (15)
O1—C1—C6—C5	−178.71 (15)	C9—C10—C11—C12	−113.64 (16)
C2—C1—C6—C5	1.3 (2)	C9—C10—C11—C16	65.94 (16)
O1—C1—C2—C7	0.8 (2)	C10—C11—C12—C13	−179.82 (14)
O1—C1—C2—C3	179.54 (14)	C16—C11—C12—C13	0.6 (2)
C7—C2—C3—C4	178.19 (15)	C10—C11—C16—C15	179.90 (13)
C1—C2—C3—C4	−0.5 (2)	C12—C11—C16—C15	−0.5 (2)
C3—C2—C7—N8	−177.33 (15)	C11—C12—C13—C14	0.2 (2)
C1—C2—C7—N8	1.4 (2)	C12—C13—C14—C15	−1.0 (2)
C2—C3—C4—C5	0.7 (2)	C13—C14—C15—C16	1.1 (2)
C2—C3—C4—O4	−178.96 (15)	C14—C15—C16—C11	−0.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···O1	0.86	1.90	2.5884 (15)	137
O4—H4···O1^{i}	0.82	1.87	2.6902 (15)	176
C6—H6···O4^{ii}	0.95	2.59	3.2818 (18)	130

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