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(*E*)-2-({2-[(*E*)-(Hydroxyimino)methyl]-phenoxy}methyl)-3-phenylacrylonitrile

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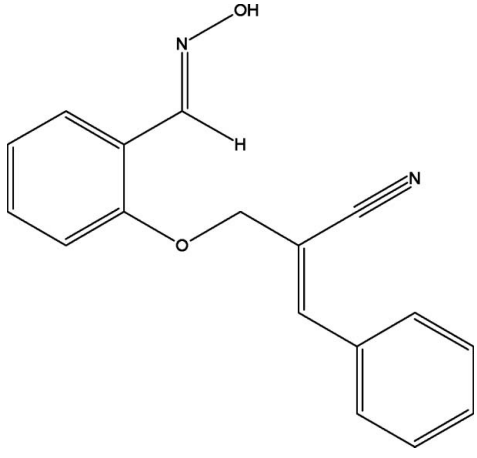
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.131; data-to-parameter ratio = 23.5.

In the title compound, $C_{17}H_{14}N_2O_2$, the hydroxyethanimine group adopts an antiperiplanar conformation. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming zigzag chains running along the c axis.

Related literature

For the structures of other acrylate derivatives, see: Zhang *et al.* (2009); Wang *et al.* (2011); SakthiMurugesan *et al.* (2011); Govindan *et al.* (2011). For the use of oxime ligands in coordination chemistry, see: Chaudhuri (2003). For the biological activity of caffeic acids, see: Hwang *et al.* (2001); Altug *et al.* (2008); Ates *et al.* (2006); Atik *et al.* (2006); Padinchare *et al.* (2001).



Experimental

Crystal data

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1/c$
a = 15.8867 (5) Å
b = 6.2381 (2) Å
c = 15.1874 (4) Å
β = 107.199 (2)°
V = 1437.81 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.2 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur-S diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.980, T_{max} = 0.990
19516 measured reflections
4490 independent reflections
2774 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.131
S = 0.99
4490 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2^{i}	0.82	2.10	2.9187 (17)	178

Symmetry code: (i) $x, -y-\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5765).

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supplementary materials

Acta Cryst. (2012). E**68**, o596 [doi:10.1107/S1600536812003923]

(*E*)-2-({2-[(*E*)-(Hydroxyimino)methyl]phenoxy}methyl)-3-phenylacrylonitrile

Suresh Govindan, Sabari Vijayakumar, Srinivasan Jayakumar, Bakthadoss Mannickam and Aravindhan Sanmargam

Comment

Recently, 2-cyanoacrylates have been extensively used as agrochemicals because of their unique mechanism of action and good environmental profiles (Zhang *et al.*, 2009). Oximes are a classical type of chelating ligands which are widely used in coordination and analytical chemistry (Chaudhuri, 2003). Some naturally occurring caffeic acids and their esters attract much attention in biology and medicine (Hwang *et al.*, 2001; Altug *et al.*, 2008). These compounds show antiviral, antibacterial, vasoactive, antiatherogenic, antiproliferative, antioxidant and antiinflammatory properties (Atik *et al.*, 2006; Padinchare *et al.*, 2001; Ates *et al.*, 2006). Against this background, and in order to obtain detailed information on molecular conformations in the solid state, an X-ray study of the title compound was carried out and the results are presented here. X-Ray analysis confirms the molecular structure and atom connectivity as illustrated in Fig. 1. The oxime group has the C=N bond in an E configuration. The hydroxy ethanimine group is essentially coplanar with the ring to which it is attached. The crystal packing is stabilized by an O—H···N hydrogen bond(Fig. 2).

Experimental

To a stirred solution of (*E*)-2-((2-formylphenoxy)methyl)-3-phenylacrylonitrile (4 mmol) in 10 ml of EtOH/H2O mixture (1:1) was added NH2OH.HCl (6 mmol) in the presence of 50% NaOH at room temperature. Then the reaction mixture was allowed to stir at room temperature for 1.5 h. After completion of the reaction, solvent was removed and the crude mass was diluted with water (15 ml) and extracted with ethyl acetate (3 *τ*imes 15 ml). The combined organic layer was washed with brine (2 *τ*imes 10 ml) and dried over anhydrous Na2SO4 and then evaporated under reduced pressure to obtain (*E*)-2-((2-((*E*)-(Hydroxyimino)methyl)phenoxy)methyl)-3-phenylacrylonitrile as a colourless solid.

Refinement

H atoms were positioned at calculated positions and refined using a riding model with O-H=0.82Å, $C_{aromatic}$-H = 0.93Å and $C_{methylene}$-H= 0.97Å and U(H) set to 1.2U_{eq}(C) or 1.5U_{eq}(O).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 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); software used to prepare material for publication: *PLATON* (Spek, 2009).

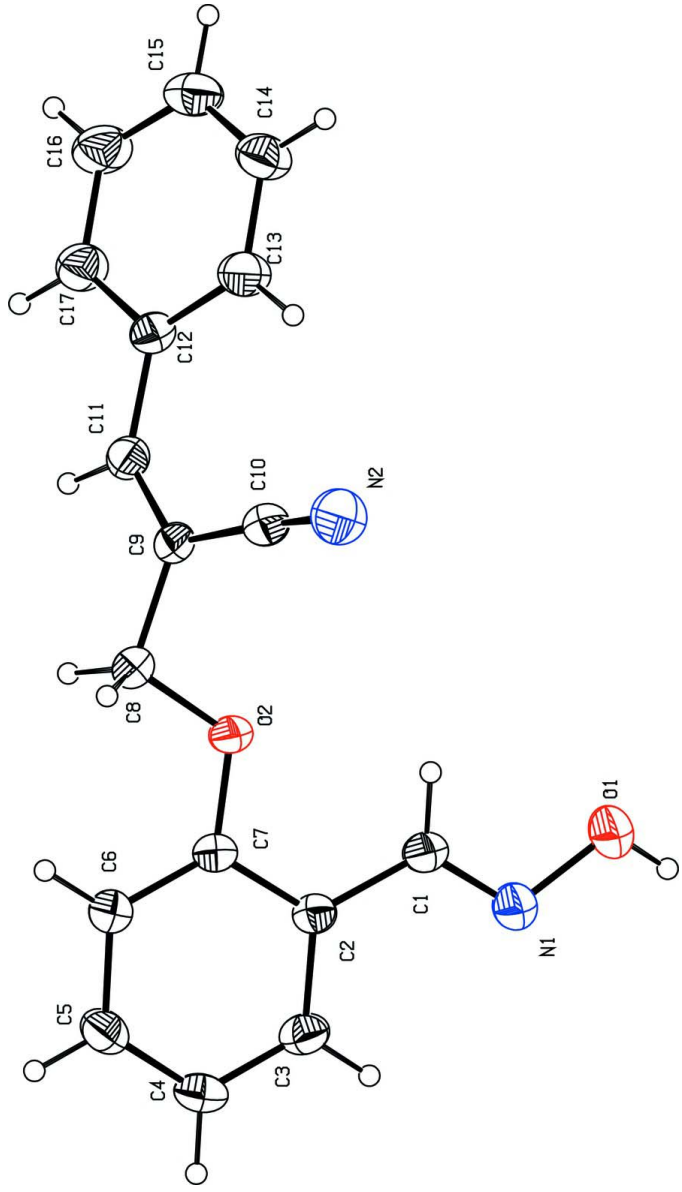

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms.

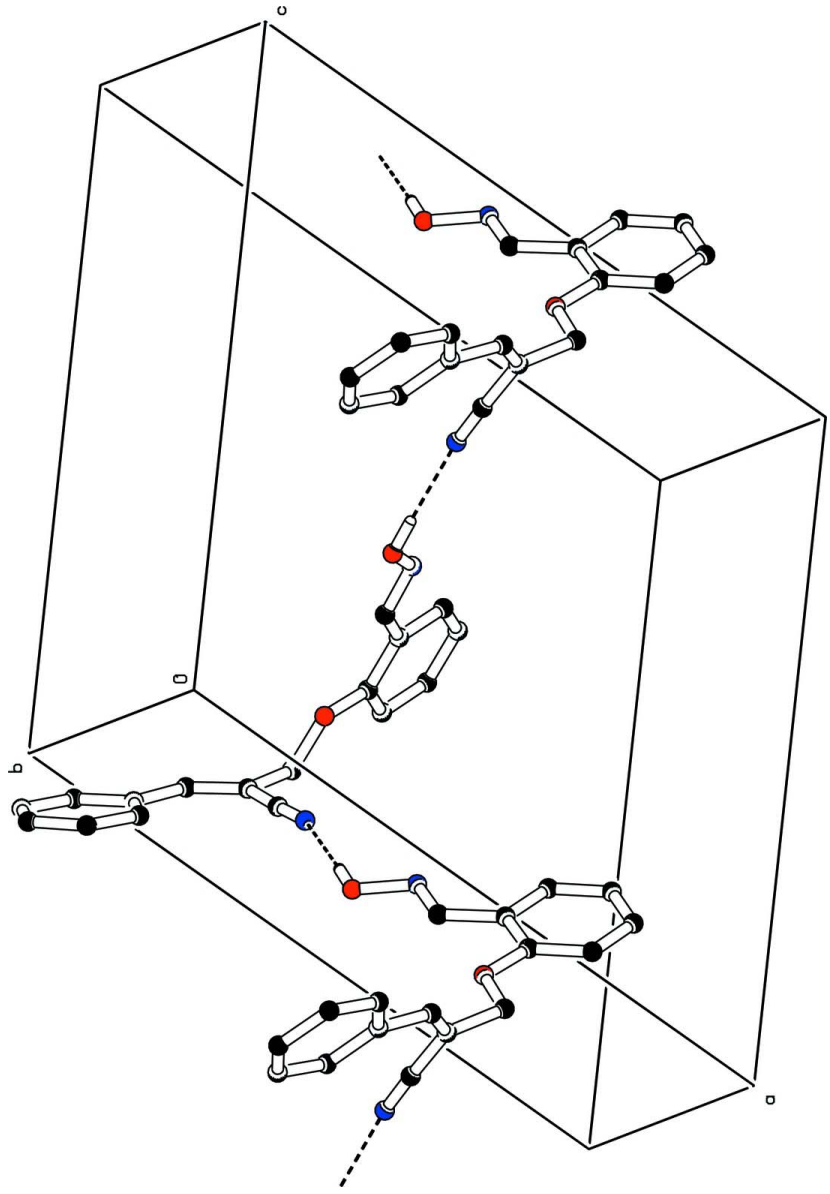

Figure 2

A view of the crystal packing. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

(*E*)-2-({2-[(*E*)-(Hydroxyimino)methyl]phenoxy}methyl)-3- phenylacrylonitrile

Crystal data

$C_{17}H_{14}N_2O_2$
$M_r = 278.30$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.8867$ (5) Å
$b = 6.2381$ (2) Å
$c = 15.1874$ (4) Å
$\beta = 107.199$ (2)°
$V = 1437.81$ (7) Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8725 reflections
$\theta = 2.8$–29.1°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Monoclinic, colourless
0.2 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur-S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9948 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.980, T_{max} = 0.990
19516 measured reflections
4490 independent reflections
2774 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 31.4°, θ_{min} = 2.7°
h = −20→23
k = −9→9
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.131
S = 0.99
4490 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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}
C1	0.30906 (9)	0.0194 (2)	0.29768 (9)	0.0471 (3)
H1	0.2662	0.0231	0.2407	0.057*
C2	0.37843 (8)	0.1812 (2)	0.31995 (8)	0.0405 (3)
C3	0.44575 (9)	0.1763 (2)	0.40269 (9)	0.0500 (3)
H3	0.4456	0.0697	0.4455	0.060*
C4	0.51256 (9)	0.3247 (2)	0.42297 (9)	0.0525 (3)
H4	0.5574	0.3176	0.4784	0.063*
C5	0.51234 (9)	0.4837 (2)	0.36050 (10)	0.0542 (4)
H5	0.5574	0.5849	0.3740	0.065*
C6	0.44610 (9)	0.4954 (2)	0.27781 (9)	0.0488 (3)
H6	0.4464	0.6041	0.2360	0.059*
C7	0.37943 (8)	0.3449 (2)	0.25758 (8)	0.0399 (3)
C8	0.30879 (9)	0.5024 (2)	0.11052 (9)	0.0474 (3)
H8A	0.3612	0.4952	0.0904	0.057*
H8B	0.3058	0.6435	0.1363	0.057*
C9	0.22813 (8)	0.4609 (2)	0.03129 (8)	0.0411 (3)

C10	0.22894 (9)	0.2607 (2)	−0.01427 (9)	0.0486 (3)
C11	0.16197 (9)	0.6014 (2)	0.00727 (8)	0.0444 (3)
H11	0.1718	0.7251	0.0431	0.053*
C12	0.07740 (9)	0.5990 (2)	−0.06398 (8)	0.0435 (3)
C13	0.04331 (10)	0.4260 (2)	−0.12169 (10)	0.0577 (4)
H13	0.0768	0.3021	−0.1177	0.069*
C14	−0.03912 (10)	0.4363 (3)	−0.18424 (10)	0.0629 (4)
H14	−0.0607	0.3196	−0.2223	0.075*
C15	−0.08983 (10)	0.6164 (3)	−0.19123 (11)	0.0633 (4)
H15	−0.1460	0.6212	−0.2330	0.076*
C16	−0.05728 (11)	0.7892 (3)	−0.13634 (12)	0.0694 (5)
H16	−0.0911	0.9128	−0.1414	0.083*
C17	0.02527 (10)	0.7807 (2)	−0.07360 (10)	0.0577 (4)
H17	0.0466	0.8996	−0.0368	0.069*
N1	0.30657 (8)	−0.12586 (19)	0.35497 (8)	0.0527 (3)
N2	0.23413 (9)	0.0992 (2)	−0.04726 (10)	0.0728 (4)
O1	0.23639 (8)	−0.26430 (19)	0.31926 (8)	0.0716 (3)
H1A	0.2369	−0.3587	0.3570	0.107*
O2	0.31108 (6)	0.34087 (15)	0.17729 (6)	0.0487 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0432 (7)	0.0502 (8)	0.0433 (7)	0.0001 (6)	0.0055 (6)	0.0077 (6)
C2	0.0369 (6)	0.0437 (7)	0.0396 (6)	0.0029 (5)	0.0093 (5)	0.0023 (5)
C3	0.0488 (8)	0.0581 (8)	0.0397 (7)	0.0044 (7)	0.0079 (6)	0.0084 (6)
C4	0.0455 (8)	0.0654 (9)	0.0387 (7)	0.0008 (7)	0.0004 (6)	−0.0043 (6)
C5	0.0488 (8)	0.0567 (9)	0.0514 (8)	−0.0101 (7)	0.0061 (6)	−0.0076 (7)
C6	0.0479 (8)	0.0474 (8)	0.0470 (7)	−0.0046 (6)	0.0075 (6)	0.0040 (6)
C7	0.0359 (6)	0.0441 (7)	0.0372 (6)	0.0032 (5)	0.0070 (5)	0.0013 (5)
C8	0.0481 (8)	0.0434 (7)	0.0456 (7)	−0.0020 (6)	0.0060 (6)	0.0092 (6)
C9	0.0460 (7)	0.0386 (6)	0.0367 (6)	−0.0009 (5)	0.0090 (5)	0.0048 (5)
C10	0.0443 (8)	0.0476 (8)	0.0497 (7)	0.0045 (6)	0.0076 (6)	0.0034 (6)
C11	0.0524 (8)	0.0397 (7)	0.0387 (6)	0.0005 (6)	0.0096 (6)	−0.0009 (5)
C12	0.0453 (7)	0.0462 (7)	0.0377 (6)	0.0033 (6)	0.0104 (5)	0.0028 (5)
C13	0.0551 (9)	0.0542 (9)	0.0547 (8)	0.0079 (7)	0.0023 (7)	−0.0070 (7)
C14	0.0565 (10)	0.0695 (10)	0.0541 (9)	−0.0032 (8)	0.0030 (7)	−0.0095 (7)
C15	0.0449 (8)	0.0833 (12)	0.0551 (9)	0.0031 (8)	0.0048 (7)	0.0054 (8)
C16	0.0536 (10)	0.0700 (11)	0.0773 (11)	0.0192 (8)	0.0080 (8)	0.0012 (9)
C17	0.0551 (9)	0.0527 (9)	0.0602 (9)	0.0091 (7)	0.0093 (7)	−0.0048 (7)
N1	0.0521 (7)	0.0517 (7)	0.0522 (7)	−0.0081 (5)	0.0119 (5)	0.0032 (5)
N2	0.0731 (10)	0.0553 (8)	0.0837 (10)	0.0116 (7)	0.0136 (8)	−0.0131 (7)
O1	0.0701 (8)	0.0631 (7)	0.0727 (7)	−0.0239 (6)	0.0074 (6)	0.0106 (6)
O2	0.0427 (5)	0.0525 (5)	0.0421 (5)	−0.0062 (4)	−0.0009 (4)	0.0133 (4)

Geometric parameters (Å, º)

C1—N1	1.2649 (16)	C9—C11	1.3339 (18)
C1—C2	1.4583 (18)	C9—C10	1.4296 (19)
C1—H1	0.9300	C10—N2	1.1392 (17)

C2—C3	1.3889 (18)	C11—C12	1.4548 (18)
C2—C7	1.3962 (17)	C11—H11	0.9300
C3—C4	1.373 (2)	C12—C17	1.3857 (19)
C3—H3	0.9300	C12—C13	1.3951 (19)
C4—C5	1.372 (2)	C13—C14	1.373 (2)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.3814 (19)	C14—C15	1.368 (2)
C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.3804 (18)	C15—C16	1.367 (2)
C6—H6	0.9300	C15—H15	0.9300
C7—O2	1.3725 (14)	C16—C17	1.375 (2)
C8—O2	1.4225 (14)	C16—H16	0.9300
C8—C9	1.4983 (18)	C17—H17	0.9300
C8—H8A	0.9700	N1—O1	1.3876 (15)
C8—H8B	0.9700	O1—H1A	0.8200

N1—C1—C2	120.76 (12)	C11—C9—C8	121.58 (12)
N1—C1—H1	119.6	C10—C9—C8	114.31 (11)
C2—C1—H1	119.6	N2—C10—C9	176.18 (16)
C3—C2—C7	118.02 (12)	C9—C11—C12	132.56 (12)
C3—C2—C1	121.43 (12)	C9—C11—H11	113.7
C7—C2—C1	120.55 (11)	C12—C11—H11	113.7
C4—C3—C2	121.70 (13)	C17—C12—C13	117.24 (13)
C4—C3—H3	119.2	C17—C12—C11	117.49 (12)
C2—C3—H3	119.2	C13—C12—C11	125.23 (12)
C5—C4—C3	119.26 (12)	C14—C13—C12	120.79 (14)
C5—C4—H4	120.4	C14—C13—H13	119.6
C3—C4—H4	120.4	C12—C13—H13	119.6
C4—C5—C6	120.82 (13)	C15—C14—C13	120.76 (15)
C4—C5—H5	119.6	C15—C14—H14	119.6
C6—C5—H5	119.6	C13—C14—H14	119.6
C7—C6—C5	119.64 (12)	C16—C15—C14	119.48 (14)
C7—C6—H6	120.2	C16—C15—H15	120.3
C5—C6—H6	120.2	C14—C15—H15	120.3
O2—C7—C6	124.30 (11)	C15—C16—C17	120.22 (15)
O2—C7—C2	115.14 (11)	C15—C16—H16	119.9
C6—C7—C2	120.56 (11)	C17—C16—H16	119.9
O2—C8—C9	106.60 (10)	C16—C17—C12	121.48 (15)
O2—C8—H8A	110.4	C16—C17—H17	119.3
C9—C8—H8A	110.4	C12—C17—H17	119.3
O2—C8—H8B	110.4	C1—N1—O1	111.22 (11)
C9—C8—H8B	110.4	N1—O1—H1A	109.5
H8A—C8—H8B	108.6	C7—O2—C8	117.86 (9)
C11—C9—C10	124.11 (12)		

N1—C1—C2—C3	2.7 (2)	C8—C9—C11—C12	−178.61 (12)
N1—C1—C2—C7	−178.10 (13)	C9—C11—C12—C17	−176.32 (13)
C7—C2—C3—C4	−1.05 (19)	C9—C11—C12—C13	5.7 (2)
C1—C2—C3—C4	178.19 (12)	C17—C12—C13—C14	−0.9 (2)

C2—C3—C4—C5	0.8 (2)	C11—C12—C13—C14	177.09 (14)
C3—C4—C5—C6	−0.2 (2)	C12—C13—C14—C15	−0.2 (2)
C4—C5—C6—C7	−0.2 (2)	C13—C14—C15—C16	1.1 (3)
C5—C6—C7—O2	−179.43 (12)	C14—C15—C16—C17	−1.0 (3)
C5—C6—C7—C2	0.0 (2)	C15—C16—C17—C12	−0.1 (3)
C3—C2—C7—O2	−179.90 (11)	C13—C12—C17—C16	1.1 (2)
C1—C2—C7—O2	0.86 (16)	C11—C12—C17—C16	−177.09 (14)
C3—C2—C7—C6	0.63 (18)	C2—C1—N1—O1	−178.97 (12)
C1—C2—C7—C6	−178.62 (12)	C6—C7—O2—C8	0.00 (18)
O2—C8—C9—C11	116.39 (13)	C2—C7—O2—C8	−179.45 (11)
O2—C8—C9—C10	−63.22 (14)	C9—C8—O2—C7	−179.66 (10)
C10—C9—C11—C12	1.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N2^{i}	0.82	2.10	2.9187 (17)	178

Symmetry code: (i) *x*, −*y*−1/2, *z*+1/2.