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(*E*)-2,4-Dimethyl-*N*′-(2-methylbenzylidene)benzohydrazide

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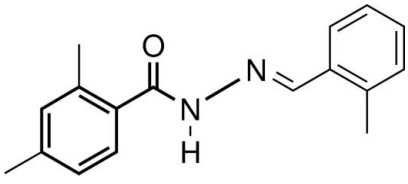
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.080; data-to-parameter ratio = 13.6.

In the title benzoylhydrazide derivative, $C_{17}H_{18}N_2O$, the dihedral angle between the benzene rings is 88.45 (8)° and the azomethine double bond adopts an *E* conformation. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds, forming a chain along the *b* axis.

Related literature

For the applications and biological activity of Schiff bases, see: Musharraf *et al.* (2012); Khan *et al.* (2012). For the crystal structures of related compounds, see: Taha *et al.* (2012*a*,*b*); Naz *et al.* (2012).



Experimental

Crystal data

$C_{17}H_{18}N_2O$
M_r = 266.33
Orthorhombic, $Pca2_1$
a = 26.1151 (10) Å
b = 4.9484 (2) Å
c = 11.3933 (4) Å
V = 1472.33 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 273 K
0.56 × 0.55 × 0.23 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.959, T_{max} = 0.983
8023 measured reflections
2577 independent reflections
2483 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.04
2577 reflections
189 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.833 (15)	2.000 (15)	2.8150 (14)	166.1 (14)
C8—H8A···O1^{i}	0.93	2.52	3.2696 (19)	138

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5246).

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supplementary materials

Acta Cryst. (2013). E**69**, o400 [doi:10.1107/S1600536813004388]

(*E*)-2,4-Dimethyl-*N*′-(2-methylbenzylidene)benzohydrazide

Muhammad Taha, Nor Hadiani Ismail, Faridahanim Mohd Jaafar, Khalid M. Khan and Sammer Yousuf

Comment

Benzohydrazides represents an important class of organic compounds with a wide range of biological applications (Musharraf *et al.*, 2012; Khan *et al.*, 2012). The title compound was obtained in continuation of our work to synthesize and study the biological activities of benzohydrazide derivatives. Previously, we have published crystal structures of many benzohydrazides derivatives with different substitution pattern on two phenyl rings (Taha *et al.*, 2012*a*,*b*; Naz *et al.*, 2012). In the title compound two methyl substituted phenyl rings (C1–C6 and C9–C14) are each planner with dihedral angle of 88.45 (8)° between them. The bond lengths and angles were found to be similar as in structurally related benzohydrazide derivatives (Taha *et al.*, 2012*a*,*b*; Naz *et al.*, 2012). The crystal structure stabilize by intermolecular N1—H1A···O1^{i} and C8—H8A···O1^{i} interactions to form a chain along the *b* axis (symmetry code as in Table 1).

Experimental

The title compound was synthesized by using (0.328 g) 2 mmol of 2,4-dimethylbenzohydrazide and (0.240 g) 2 mmol 2-methylbenzaldehyde as starting material under same conditions and solvents as described in our previous publications (Taha *et al.*, 2012*a*,*b*; Naz *et al.*, 2012). The compound was recrystallized by dissolving in methanol to obtain colorless needles (0.474 g, 89% yield). All chemicals were purchased by sigma Aldrich Germany.

Refinement

H atoms on methyl and phenyl groups were positioned geometrically with C—H = 0.96 and 0.93 Å, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = 1.5U_{eq}(C_{methyl}) or 1.2U_{eq}(C_{phenyl}). A rotating group model was applied to the methyl groups. The H atoms on the nitrogen was located in a difference Fourier map and refined isotropically [N—H = 0.832 (15) Å]. The Hooft y parameter was -0.3 (5).

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

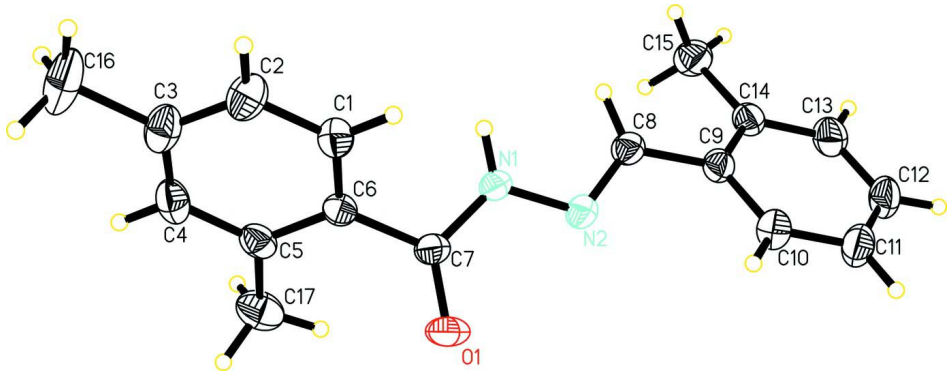

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at 30% probability level.

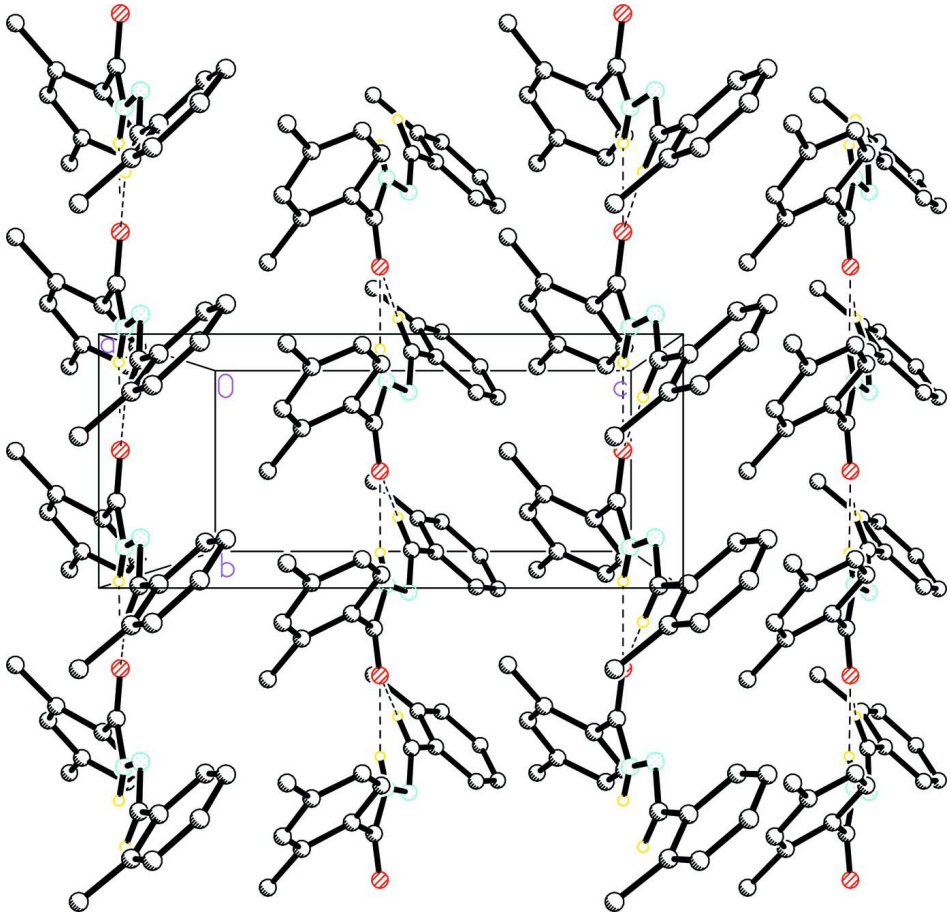

Figure 2

A crystal packing diagram of the title compound. Only hydrogen atoms involved in the hydrogen bonds (dashed lines) are shown.

(*E*)-2,4-Dimethyl-*N*′-(2-methylbenzylidene)benzohydrazide

Crystal data

$C_{17}H_{18}N_2O$
$M_r = 266.33$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 26.1151$ (10) Å
$b = 4.9484$ (2) Å
$c = 11.3933$ (4) Å
$V = 1472.33$ (10) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.202$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4590 reflections
$\theta = 2.4$–$27.4°$
$\mu = 0.08$ mm^{-1}
$T = 273$ K
Block, colorles
0.56 × 0.55 × 0.23 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.959$, $T_{max} = 0.983$
8023 measured reflections
2577 independent reflections
2483 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.4°$
$h = -25 \rightarrow 31$
$k = -5 \rightarrow 5$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.080$
$S = 1.04$
2577 reflections
189 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.1205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.016 (2)

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	0.40241 (5)	0.5493 (2)	0.43046 (18)	0.0938 (6)
N1	0.38352 (4)	0.1086 (2)	0.44326 (11)	0.0438 (3)
H1A	0.3925 (5)	−0.050 (3)	0.4301 (13)	0.039 (4)*

N2	0.33498 (4)	0.1558 (2)	0.48752 (10)	0.0448 (3)
C1	0.49419 (6)	0.0399 (3)	0.44104 (14)	0.0500 (3)
H1B	0.4797	−0.0346	0.5082	0.060*
C2	0.54235 (6)	−0.0412 (3)	0.40641 (15)	0.0600 (4)
H2B	0.5601	−0.1679	0.4510	0.072*
C3	0.56461 (6)	0.0633 (4)	0.30653 (15)	0.0605 (4)
C4	0.53740 (6)	0.2556 (4)	0.24413 (14)	0.0588 (4)
H4A	0.5524	0.3297	0.1775	0.071*
C5	0.48869 (6)	0.3437 (3)	0.27612 (13)	0.0488 (4)
C6	0.46699 (5)	0.2308 (3)	0.37737 (12)	0.0426 (3)
C7	0.41514 (5)	0.3145 (3)	0.41905 (14)	0.0480 (3)
C8	0.30625 (5)	−0.0517 (3)	0.49163 (13)	0.0459 (3)
H8A	0.3181	−0.2157	0.4624	0.055*
C9	0.25464 (5)	−0.0345 (3)	0.54203 (13)	0.0458 (3)
C10	0.24424 (6)	0.1476 (3)	0.63203 (14)	0.0553 (4)
H10A	0.2703	0.2579	0.6602	0.066*
C11	0.19599 (7)	0.1674 (4)	0.68005 (15)	0.0656 (5)
H11A	0.1893	0.2922	0.7392	0.079*
C12	0.15778 (7)	0.0008 (4)	0.63967 (17)	0.0665 (5)
H12A	0.1252	0.0108	0.6722	0.080*
C13	0.16772 (6)	−0.1808 (3)	0.55115 (18)	0.0628 (4)
H13A	0.1414	−0.2922	0.5248	0.075*
C14	0.21564 (5)	−0.2029 (3)	0.50006 (14)	0.0500 (3)
C15	0.22448 (7)	−0.3941 (3)	0.39994 (17)	0.0652 (4)
H15A	0.1940	−0.4979	0.3862	0.098*
H15B	0.2522	−0.5136	0.4189	0.098*
H15C	0.2329	−0.2933	0.3306	0.098*
C16	0.61613 (7)	−0.0348 (6)	0.2648 (2)	0.0969 (8)
H16A	0.6383	−0.0606	0.3311	0.145*
H16B	0.6308	0.0969	0.2129	0.145*
H16C	0.6120	−0.2030	0.2239	0.145*
C17	0.46107 (8)	0.5471 (4)	0.20175 (18)	0.0736 (5)
H17A	0.4250	0.5091	0.2028	0.110*
H17B	0.4735	0.5370	0.1226	0.110*
H17C	0.4670	0.7251	0.2323	0.110*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0731 (8)	0.0328 (5)	0.1753 (17)	0.0011 (5)	0.0407 (10)	−0.0067 (8)
N1	0.0394 (6)	0.0335 (5)	0.0587 (7)	0.0032 (4)	0.0055 (5)	−0.0042 (5)
N2	0.0388 (6)	0.0451 (6)	0.0505 (6)	0.0038 (5)	0.0034 (5)	−0.0020 (5)
C1	0.0471 (8)	0.0556 (8)	0.0472 (8)	−0.0015 (6)	0.0033 (7)	0.0003 (7)
C2	0.0467 (8)	0.0745 (10)	0.0586 (10)	0.0108 (7)	−0.0058 (8)	−0.0036 (8)
C3	0.0421 (8)	0.0810 (11)	0.0583 (9)	−0.0034 (7)	0.0019 (8)	−0.0175 (8)
C4	0.0589 (10)	0.0728 (10)	0.0448 (8)	−0.0218 (8)	0.0111 (7)	−0.0100 (7)
C5	0.0555 (9)	0.0431 (7)	0.0477 (8)	−0.0127 (6)	−0.0011 (7)	−0.0043 (6)
C6	0.0429 (7)	0.0367 (6)	0.0482 (8)	−0.0057 (5)	0.0015 (6)	−0.0066 (5)
C7	0.0460 (8)	0.0349 (6)	0.0630 (9)	−0.0006 (5)	0.0038 (7)	−0.0038 (6)
C8	0.0415 (7)	0.0427 (6)	0.0534 (8)	0.0024 (6)	0.0011 (6)	−0.0018 (6)

C9	0.0414 (7)	0.0469 (7)	0.0492 (7)	0.0032 (6)	0.0032 (6)	0.0059 (6)
C10	0.0508 (9)	0.0632 (9)	0.0520 (8)	−0.0002 (7)	0.0027 (7)	−0.0012 (7)
C11	0.0663 (11)	0.0764 (11)	0.0541 (9)	0.0055 (9)	0.0177 (8)	−0.0022 (8)
C12	0.0499 (9)	0.0789 (11)	0.0707 (11)	0.0030 (8)	0.0207 (9)	0.0056 (9)
C13	0.0458 (8)	0.0650 (9)	0.0774 (11)	−0.0079 (7)	0.0060 (9)	0.0036 (9)
C14	0.0454 (8)	0.0459 (7)	0.0586 (8)	−0.0005 (6)	0.0026 (7)	0.0066 (6)
C15	0.0578 (9)	0.0578 (9)	0.0800 (12)	−0.0053 (7)	0.0007 (9)	−0.0111 (9)
C16	0.0501 (11)	0.150 (2)	0.0910 (16)	0.0072 (12)	0.0129 (10)	−0.0378 (15)
C17	0.0953 (15)	0.0592 (10)	0.0664 (11)	−0.0078 (9)	−0.0073 (11)	0.0132 (8)

Geometric parameters (Å, º)

O1—C7	1.2156 (17)	C9—C14	1.400 (2)
N1—C7	1.3401 (17)	C10—C11	1.377 (2)
N1—N2	1.3842 (16)	C10—H10A	0.9300
N1—H1A	0.832 (15)	C11—C12	1.374 (3)
N2—C8	1.2723 (18)	C11—H11A	0.9300
C1—C2	1.378 (2)	C12—C13	1.376 (3)
C1—C6	1.387 (2)	C12—H12A	0.9300
C1—H1B	0.9300	C13—C14	1.384 (2)
C2—C3	1.378 (3)	C13—H13A	0.9300
C2—H2B	0.9300	C14—C15	1.500 (2)
C3—C4	1.384 (3)	C15—H15A	0.9600
C3—C16	1.507 (2)	C15—H15B	0.9600
C4—C5	1.393 (2)	C15—H15C	0.9600
C4—H4A	0.9300	C16—H16A	0.9600
C5—C6	1.401 (2)	C16—H16B	0.9600
C5—C17	1.500 (2)	C16—H16C	0.9600
C6—C7	1.4933 (19)	C17—H17A	0.9600
C8—C9	1.4675 (19)	C17—H17B	0.9600
C8—H8A	0.9300	C17—H17C	0.9600
C9—C10	1.392 (2)		

C7—N1—N2	120.73 (11)	C11—C10—H10A	119.4
C7—N1—H1A	120.4 (10)	C9—C10—H10A	119.4
N2—N1—H1A	118.9 (10)	C12—C11—C10	119.26 (16)
C8—N2—N1	114.66 (11)	C12—C11—H11A	120.4
C2—C1—C6	121.07 (15)	C10—C11—H11A	120.4
C2—C1—H1B	119.5	C11—C12—C13	120.04 (15)
C6—C1—H1B	119.5	C11—C12—H12A	120.0
C1—C2—C3	120.80 (16)	C13—C12—H12A	120.0
C1—C2—H2B	119.6	C12—C13—C14	122.03 (16)
C3—C2—H2B	119.6	C12—C13—H13A	119.0
C2—C3—C4	117.73 (14)	C14—C13—H13A	119.0
C2—C3—C16	121.07 (18)	C13—C14—C9	117.84 (15)
C4—C3—C16	121.17 (18)	C13—C14—C15	120.58 (15)
C3—C4—C5	123.35 (14)	C9—C14—C15	121.54 (14)
C3—C4—H4A	118.3	C14—C15—H15A	109.5
C5—C4—H4A	118.3	C14—C15—H15B	109.5
C4—C5—C6	117.36 (14)	H15A—C15—H15B	109.5

C4—C5—C17	120.09 (15)	C14—C15—H15C	109.5
C6—C5—C17	122.54 (15)	H15A—C15—H15C	109.5
C1—C6—C5	119.67 (13)	H15B—C15—H15C	109.5
C1—C6—C7	119.13 (13)	C3—C16—H16A	109.5
C5—C6—C7	121.19 (13)	C3—C16—H16B	109.5
O1—C7—N1	122.42 (14)	H16A—C16—H16B	109.5
O1—C7—C6	123.16 (13)	C3—C16—H16C	109.5
N1—C7—C6	114.42 (11)	H16A—C16—H16C	109.5
N2—C8—C9	120.62 (12)	H16B—C16—H16C	109.5
N2—C8—H8A	119.7	C5—C17—H17A	109.5
C9—C8—H8A	119.7	C5—C17—H17B	109.5
C10—C9—C14	119.67 (14)	H17A—C17—H17B	109.5
C10—C9—C8	120.32 (13)	C5—C17—H17C	109.5
C14—C9—C8	120.01 (13)	H17A—C17—H17C	109.5
C11—C10—C9	121.14 (15)	H17B—C17—H17C	109.5

C7—N1—N2—C8	170.77 (14)	C5—C6—C7—O1	−49.4 (2)
C6—C1—C2—C3	−0.8 (2)	C1—C6—C7—N1	−49.99 (18)
C1—C2—C3—C4	1.3 (2)	C5—C6—C7—N1	130.66 (14)
C1—C2—C3—C16	−176.88 (17)	N1—N2—C8—C9	176.93 (12)
C2—C3—C4—C5	−1.2 (2)	N2—C8—C9—C10	−30.9 (2)
C16—C3—C4—C5	177.01 (16)	N2—C8—C9—C14	149.45 (15)
C3—C4—C5—C6	0.5 (2)	C14—C9—C10—C11	−0.6 (2)
C3—C4—C5—C17	−178.19 (16)	C8—C9—C10—C11	179.71 (15)
C2—C1—C6—C5	0.0 (2)	C9—C10—C11—C12	1.2 (3)
C2—C1—C6—C7	−179.36 (14)	C10—C11—C12—C13	−0.9 (3)
C4—C5—C6—C1	0.16 (19)	C11—C12—C13—C14	0.0 (3)
C17—C5—C6—C1	178.77 (14)	C12—C13—C14—C9	0.6 (2)
C4—C5—C6—C7	179.50 (12)	C12—C13—C14—C15	−177.14 (17)
C17—C5—C6—C7	−1.9 (2)	C10—C9—C14—C13	−0.2 (2)
N2—N1—C7—O1	−2.7 (3)	C8—C9—C14—C13	179.43 (14)
N2—N1—C7—C6	177.21 (12)	C10—C9—C14—C15	177.45 (15)
C1—C6—C7—O1	129.9 (2)	C8—C9—C14—C15	−2.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.833 (15)	2.000 (15)	2.8150 (14)	166.1 (14)
C8—H8*A*···O1^{i}	0.93	2.52	3.2696 (19)	138

Symmetry code: (i) *x*, *y*−1, *z*.