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(*E*)-*N*′-(4-Methoxybenzylidene)-2-*m*-tolylacetohydrazide

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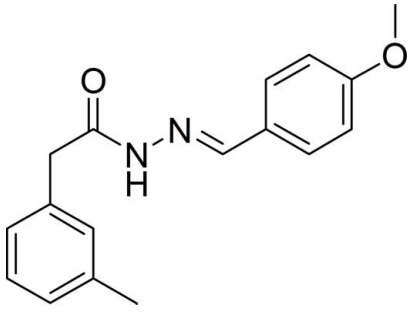
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.158; data-to-parameter ratio = 14.7.

In the title molecule, $C_{17}H_{18}N_2O_2$, the benzene rings form a dihedral angle of 83.0 (7)°. In the crystal, N—H···O hydrogen bonds, in an $R_2^2(8)$ graph-set motif, link molecules into centrocymmetric dimers, and weak C—H···π interactions further link these dimers into columns in [100].

Related literature

For the biological activity of Schiff bases, see: Desai *et al.* (2001); El-Masry *et al.* (2000); Hodnett & Dunn (1970); Pandey *et al.* (1999); Singh & Dash (1988). For Schiff bases employed as ligands for complexation of metal ions, see: Aydogan *et al.* (2001). For Schiff bases with applications in dyes and pigments, see: Taggi *et al.* (2002). For related structures, see: Akkurt *et al.* (2011); Lv *et al.* (2009*a*,*b*); Yu & Lv (2010). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{17}H_{18}N_2O_2$
M_r = 282.33
Triclinic, $P\overline{1}$
a = 6.4961 (8) Å
b = 9.8047 (10) Å
c = 12.7464 (13) Å
α = 112.130 (9)°
β = 95.507 (10)°
γ = 96.601 (9)°
V = 738.45 (14) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 173 K
0.34 × 0.14 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.735, T_{max} = 1.000
4418 measured reflections
2840 independent reflections
2032 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.158
S = 1.04
2840 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg is the centroid of the C3–C8 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.04	2.902 (2)	178
C15—H15···*Cg*^{ii}	0.93	2.63	3.557 (2)	173

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x+2, -y, -z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); 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*.

ASP thanks UOM for research facilities. JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5364).

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supporting information

Acta Cryst. (2012). E**68**, o3435 [doi:10.1107/S1600536812047113]

(*E*)-*N*′-(4-Methoxybenzylidene)-2-*m*-tolylacetohydrazide

A. S. Praveen, Jerry P. Jasinski, Amanda C. Keeley, H. S. Yathirajan and B. Narayana

S1. Comment

Schiff bases are known to have biological activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh *et al.*, 1988), antitumor (Hodnett *et al.*, 1970; Desai *et al.*, 2001), and as herbicides. Schiff bases have also been employed as ligands for complexation of metal ions (Aydogan *et al.*, 2001). On the industrial scale, they have wide range of applications such as dyes and pigments (Taggi *et al.*, 2002). The crystal structures of some Schiff base hydrazines, viz., N′-(2-methoxybenzylidene) acetohydrazide (Yu & Lv, 2010), 2-[6-(4-chlorophenyl)imidazo[2,1-b][1,3] thiazol-2-yl]-N′-[(E)-4-methoxybenzylidene]acetohydrazide (Akkurt *et al.*, 2011), N′-(3-methoxybenzyl-idene)acetohydrazide and N′-(3,4-dimethoxybenzylidene)acetohydrazide (Lv *et al.*, 2009*a*,*b*). In view of the importance of hydrazides, the crystal structure of title compound (I) is reported.

In the title molecule, $C_{17}H_{18}N_2O_2$, two benzene rings form a dihedral angle of 83.0 (7)° (Fig. 1). Bond lengths are in normal ranges (Allen, 1987). In the crystal, N—H···O hydrogen bonds (Table 1), in an $R^2_2(8)$ graph set motif, link molecules into centrocymmetric dimers, and weak C–H···π interactions (Table 1) link further these dimers into columns in [100] (Fig. 2).

S2. Experimental

To a stirred solution of 2-m-tolylacetohydrazide (1 g, 6.09 mmol) in ethanol (10 mL), 4-methoxybenzaldehyde (0.79 g, 6.09 mmol) was added (Fig. 3) and strirred at room temperature for 30 minutes. Precipitated solid was filtered and dried. The single crystal was grown from ethyl acetate by slow evaporation method and yield of the compound was 94% (m.p.: 403-405 K).

S3. Refinement

All H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93Å (CH), 0.97Å (CH_2), 0.96Å (CH_3) or 0.86Å (NH). Isotropic displacement parameters for these atoms were set to 1.19-1.21 (CH, CH_2), 1.49 (CH_3) or 1.21 (NH) times U_{eq} of the parent atom.

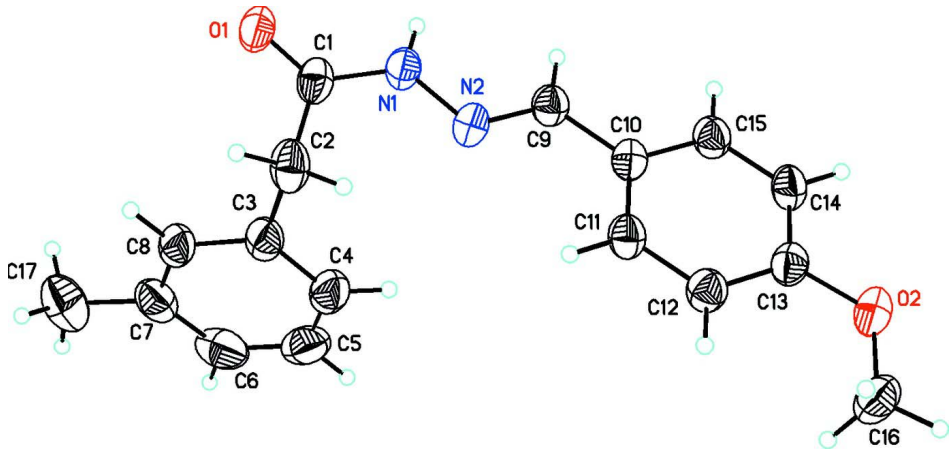

Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

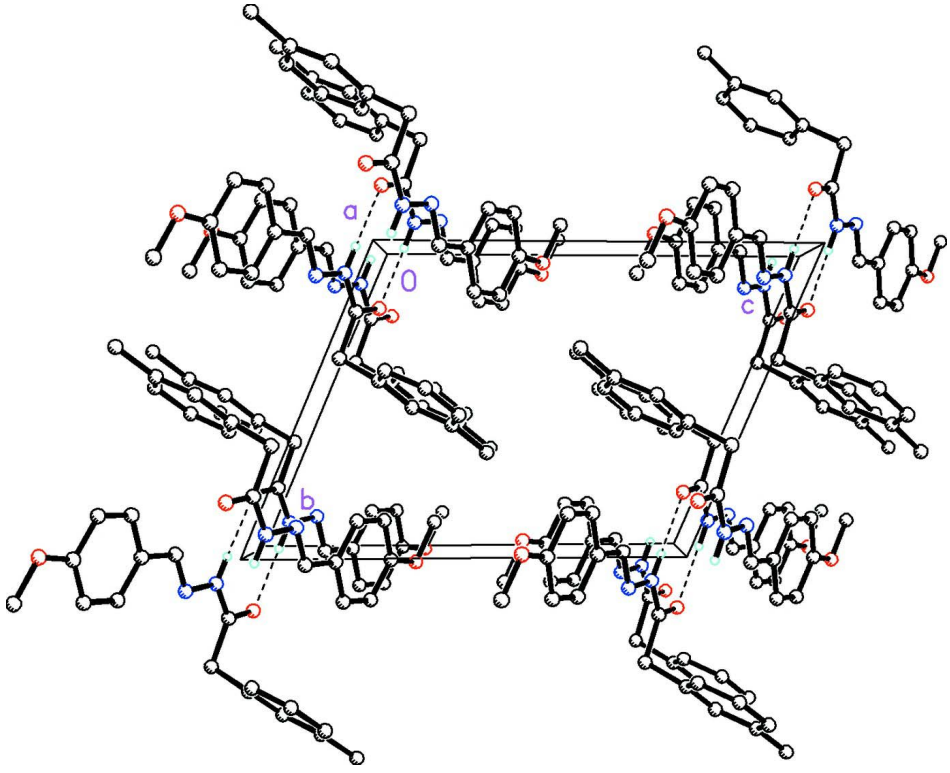

Figure 2

Packing diagram of the title compound viewed along the *a* axis. Dashed lines indicate N—H···O hydrogen bonds. The remaining H atoms have been removed for clarity.

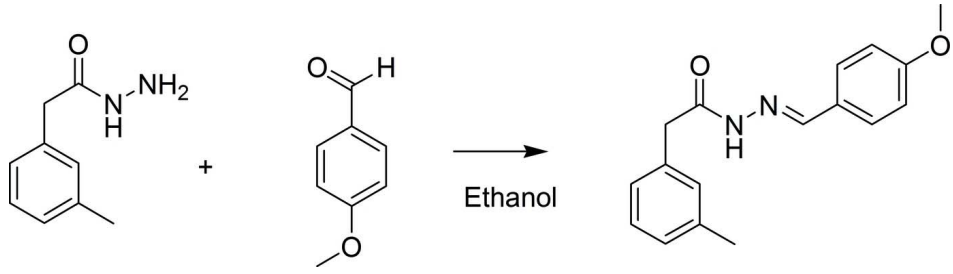

Figure 3

Synthesis of the title compound.

(*E*)-*N*′-(4-Methoxybenzylidene)-2-*m*-tolylacetohydrazide

Crystal data

$C_{17}H_{18}N_2O_2$
M_r = 282.33
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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c = 12.7464 (13) Å
α = 112.130 (9)°
β = 95.507 (10)°
γ = 96.601 (9)°
V = 738.45 (14) Å^3
Z = 2
$F(000)$ = 300
D_x = 1.270 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1237 reflections
θ = 3.8–72.4°
μ = 0.68 mm^{-1}
T = 173 K
Chunk, colorless
0.34 × 0.14 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.735, T_{max} = 1.000
4418 measured reflections
2840 independent reflections
2032 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 72.6°, θ_{min} = 3.8°
h = −8→7
k = −12→8
l = −11→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.158
S = 1.04
2840 reflections
193 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
$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 0.071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0097 (12)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4694 (2)	0.19694 (16)	0.05426 (13)	0.0429 (4)
O2	1.6491 (2)	−0.04156 (17)	−0.38486 (13)	0.0482 (4)
N1	0.7161 (2)	0.09164 (19)	−0.04553 (14)	0.0363 (4)
H1	0.6645	0.0052	−0.0486	0.044*
N2	0.8879 (2)	0.10557 (19)	−0.09800 (14)	0.0365 (4)
C1	0.6266 (3)	0.2111 (2)	0.01087 (17)	0.0376 (5)
C2	0.7332 (4)	0.3634 (2)	0.02237 (19)	0.0447 (5)
H2A	0.8138	0.3528	−0.0397	0.054*
H2B	0.6288	0.4255	0.0188	0.054*
C3	0.8763 (3)	0.4349 (2)	0.13628 (19)	0.0397 (5)
C4	1.0802 (4)	0.4059 (2)	0.1471 (2)	0.0488 (6)
H4	1.1354	0.3504	0.0826	0.059*
C5	1.2004 (4)	0.4600 (3)	0.2543 (3)	0.0584 (7)
H5	1.3365	0.4402	0.2617	0.070*
C6	1.1199 (4)	0.5432 (3)	0.3507 (3)	0.0596 (7)
H6	1.2023	0.5784	0.4222	0.071*
C7	0.9182 (4)	0.5748 (2)	0.3419 (2)	0.0487 (6)
C8	0.7994 (3)	0.5198 (2)	0.2336 (2)	0.0419 (5)
H8	0.6640	0.5408	0.2262	0.050*
C9	0.9579 (3)	−0.0161 (2)	−0.14981 (17)	0.0353 (5)
H9	0.8927	−0.1052	−0.1490	0.042*
C10	1.1381 (3)	−0.0163 (2)	−0.20977 (16)	0.0336 (4)
C11	1.2404 (3)	0.1120 (2)	−0.21651 (17)	0.0365 (5)
H11	1.1929	0.2020	−0.1818	0.044*
C12	1.4114 (3)	0.1087 (2)	−0.27377 (18)	0.0376 (5)
H12	1.4781	0.1958	−0.2771	0.045*
C13	1.4832 (3)	−0.0259 (2)	−0.32644 (17)	0.0362 (5)
C14	1.3827 (3)	−0.1543 (2)	−0.31983 (18)	0.0403 (5)
H14	1.4310	−0.2441	−0.3541	0.048*
C15	1.2124 (3)	−0.1503 (2)	−0.26320 (17)	0.0379 (5)
H15	1.1458	−0.2377	−0.2603	0.045*
C16	1.7630 (3)	0.0894 (3)	−0.3878 (2)	0.0523 (6)
H16A	1.6733	0.1318	−0.4272	0.078*
H16B	1.8807	0.0643	−0.4272	0.078*
H16C	1.8118	0.1605	−0.3109	0.078*

C17	0.8251 (5)	0.6648 (3)	0.4450 (2)	0.0709 (8)
H17A	0.7722	0.7457	0.4325	0.106*
H17B	0.9312	0.7039	0.5114	0.106*
H17C	0.7128	0.6020	0.4568	0.106*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0382 (8)	0.0476 (9)	0.0442 (8)	0.0160 (7)	0.0149 (7)	0.0148 (7)
O2	0.0452 (9)	0.0510 (10)	0.0483 (9)	0.0128 (7)	0.0216 (7)	0.0144 (7)
N1	0.0370 (9)	0.0360 (9)	0.0391 (9)	0.0108 (7)	0.0137 (7)	0.0150 (7)
N2	0.0349 (9)	0.0411 (10)	0.0373 (9)	0.0126 (7)	0.0123 (7)	0.0163 (8)
C1	0.0375 (11)	0.0448 (12)	0.0347 (10)	0.0177 (9)	0.0081 (9)	0.0164 (9)
C2	0.0544 (13)	0.0416 (12)	0.0501 (13)	0.0228 (10)	0.0188 (10)	0.0245 (10)
C3	0.0438 (12)	0.0301 (10)	0.0523 (13)	0.0117 (9)	0.0164 (10)	0.0204 (9)
C4	0.0453 (13)	0.0380 (12)	0.0692 (16)	0.0117 (10)	0.0231 (12)	0.0232 (11)
C5	0.0348 (12)	0.0457 (14)	0.096 (2)	0.0049 (10)	0.0052 (13)	0.0307 (14)
C6	0.0587 (16)	0.0412 (13)	0.0705 (18)	−0.0021 (11)	−0.0082 (13)	0.0199 (12)
C7	0.0599 (14)	0.0317 (11)	0.0513 (14)	0.0062 (10)	0.0098 (11)	0.0127 (10)
C8	0.0418 (12)	0.0312 (10)	0.0584 (14)	0.0134 (9)	0.0173 (10)	0.0194 (10)
C9	0.0378 (11)	0.0337 (10)	0.0366 (10)	0.0095 (8)	0.0089 (8)	0.0144 (8)
C10	0.0347 (10)	0.0361 (10)	0.0310 (10)	0.0106 (8)	0.0071 (8)	0.0126 (8)
C11	0.0397 (11)	0.0330 (10)	0.0391 (11)	0.0134 (8)	0.0097 (9)	0.0135 (9)
C12	0.0389 (11)	0.0360 (11)	0.0403 (11)	0.0089 (8)	0.0086 (9)	0.0160 (9)
C13	0.0348 (10)	0.0428 (11)	0.0310 (10)	0.0098 (8)	0.0075 (8)	0.0130 (9)
C14	0.0429 (12)	0.0357 (11)	0.0405 (11)	0.0149 (9)	0.0126 (9)	0.0091 (9)
C15	0.0426 (11)	0.0320 (10)	0.0400 (11)	0.0095 (8)	0.0103 (9)	0.0132 (9)
C16	0.0429 (13)	0.0643 (16)	0.0530 (14)	0.0051 (11)	0.0186 (11)	0.0249 (12)
C17	0.096 (2)	0.0541 (16)	0.0542 (16)	0.0169 (15)	0.0162 (15)	0.0096 (13)

Geometric parameters (Å, º)

O1—C1	1.225 (2)	C7—C17	1.508 (3)
O2—C13	1.358 (2)	C8—H8	0.9300
O2—C16	1.422 (3)	C9—C10	1.457 (3)
N1—C1	1.352 (2)	C9—H9	0.9300
N1—N2	1.374 (2)	C10—C11	1.390 (3)
N1—H1	0.8600	C10—C15	1.399 (3)
N2—C9	1.286 (2)	C11—C12	1.383 (3)
C1—C2	1.520 (3)	C11—H11	0.9300
C2—C3	1.513 (3)	C12—C13	1.394 (3)
C2—H2A	0.9700	C12—H12	0.9300
C2—H2B	0.9700	C13—C14	1.386 (3)
C3—C8	1.385 (3)	C14—C15	1.374 (3)
C3—C4	1.391 (3)	C14—H14	0.9300
C4—C5	1.383 (4)	C15—H15	0.9300
C4—H4	0.9300	C16—H16A	0.9600
C5—C6	1.383 (4)	C16—H16B	0.9600

C5—H5	0.9300	C16—H16C	0.9600
C6—C7	1.384 (3)	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C7—C8	1.389 (3)	C17—H17C	0.9600

C13—O2—C16	117.66 (17)	N2—C9—H9	119.5
C1—N1—N2	121.37 (17)	C10—C9—H9	119.5
C1—N1—H1	119.3	C11—C10—C15	118.04 (18)
N2—N1—H1	119.3	C11—C10—C9	122.64 (18)
C9—N2—N1	115.66 (17)	C15—C10—C9	119.32 (18)
O1—C1—N1	121.0 (2)	C12—C11—C10	121.44 (18)
O1—C1—C2	121.47 (18)	C12—C11—H11	119.3
N1—C1—C2	117.52 (18)	C10—C11—H11	119.3
C3—C2—C1	108.30 (17)	C11—C12—C13	119.67 (19)
C3—C2—H2A	110.0	C11—C12—H12	120.2
C1—C2—H2A	110.0	C13—C12—H12	120.2
C3—C2—H2B	110.0	O2—C13—C14	116.24 (18)
C1—C2—H2B	110.0	O2—C13—C12	124.44 (19)
H2A—C2—H2B	108.4	C14—C13—C12	119.32 (19)
C8—C3—C4	118.9 (2)	C15—C14—C13	120.69 (19)
C8—C3—C2	119.98 (19)	C15—C14—H14	119.7
C4—C3—C2	120.8 (2)	C13—C14—H14	119.7
C5—C4—C3	119.6 (2)	C14—C15—C10	120.84 (19)
C5—C4—H4	120.2	C14—C15—H15	119.6
C3—C4—H4	120.2	C10—C15—H15	119.6
C4—C5—C6	120.6 (2)	O2—C16—H16A	109.5
C4—C5—H5	119.7	O2—C16—H16B	109.5
C6—C5—H5	119.7	H16A—C16—H16B	109.5
C5—C6—C7	120.8 (3)	O2—C16—H16C	109.5
C5—C6—H6	119.6	H16A—C16—H16C	109.5
C7—C6—H6	119.6	H16B—C16—H16C	109.5
C6—C7—C8	117.9 (2)	C7—C17—H17A	109.5
C6—C7—C17	122.3 (3)	C7—C17—H17B	109.5
C8—C7—C17	119.8 (2)	H17A—C17—H17B	109.5
C3—C8—C7	122.1 (2)	C7—C17—H17C	109.5
C3—C8—H8	119.0	H17A—C17—H17C	109.5
C7—C8—H8	119.0	H17B—C17—H17C	109.5
N2—C9—C10	120.92 (18)		

C1—N1—N2—C9	−179.39 (18)	C17—C7—C8—C3	−179.1 (2)
N2—N1—C1—O1	177.62 (17)	N1—N2—C9—C10	179.35 (16)
N2—N1—C1—C2	−4.8 (3)	N2—C9—C10—C11	−1.4 (3)
O1—C1—C2—C3	83.1 (2)	N2—C9—C10—C15	178.72 (18)
N1—C1—C2—C3	−94.5 (2)	C15—C10—C11—C12	−0.2 (3)
C1—C2—C3—C8	−88.4 (2)	C9—C10—C11—C12	179.85 (18)
C1—C2—C3—C4	85.9 (2)	C10—C11—C12—C13	0.2 (3)
C8—C3—C4—C5	1.0 (3)	C16—O2—C13—C14	−176.56 (19)
C2—C3—C4—C5	−173.3 (2)	C16—O2—C13—C12	3.1 (3)

C3—C4—C5—C6	−0.3 (3)	C11—C12—C13—O2	179.91 (18)
C4—C5—C6—C7	−0.3 (4)	C11—C12—C13—C14	−0.5 (3)
C5—C6—C7—C8	0.3 (4)	O2—C13—C14—C15	−179.62 (18)
C5—C6—C7—C17	179.8 (2)	C12—C13—C14—C15	0.7 (3)
C4—C3—C8—C7	−1.2 (3)	C13—C14—C15—C10	−0.7 (3)
C2—C3—C8—C7	173.23 (19)	C11—C10—C15—C14	0.5 (3)
C6—C7—C8—C3	0.5 (3)	C9—C10—C15—C14	−179.58 (18)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C3–C8 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.04	2.902 (2)	178
C15—H15···*Cg*^{ii}	0.93	2.63	3.557 (2)	173

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