Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-1-{6-[1-(2,6-Dimethylphenylimino)-ethyl]pyridin-2-yl}ethanone

Qing Su[a] and Qing Zhao[b]*

[a]School of Chemistry, Jilin University, Changchun 130012, People's Republic of China, and [b]Department of Neurology, China-Japan Union Hospital, Jilin University, Changchun 130033, People's Republic of China
Correspondence e-mail: qingzhao888@hotmail.com

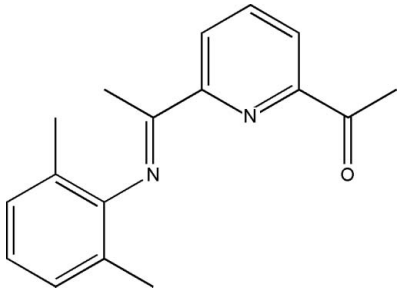
Received 16 December 2011; accepted 31 December 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.143; data-to-parameter ratio = 18.2.

In the title compound, $C_{17}H_{18}N_2O$, the dijedral angle between the mean planes of the pyridine and benzene rings is 78.0 (1)°. In the crystal, pairs of C—H···O interactions with graph-set motif $R_2^2(10)$ form inversion dimers. Adjacent dimers are further connected into a three-dimensional network by C—H···O connections. There is also an interaction between the carbonyl groups in adjacent molecules with an O···C distance of 3.176 (2) Å.

Related literature

For the synthesis of mono- and bis(imino)pyridine ligands and catalytic applications of their metal complexes, see: Schmidt *et al.* (2002); Bianchini *et al.* (2003); Britovsek *et al.* (1999); Mecking *et al.* (2001); Gibson *et al.* (2007). For graph-set analysis of hydrogen-bonded networks, see: Bernstein *et al.* (1995). For carbonyl–carbonyl interactions, see: Allen *et al.* (1998).



Experimental

Crystal data

$C_{17}H_{18}N_2O$
M_r = 266.33
Triclinic, $P\overline{1}$
a = 6.2988 (13) Å
b = 7.9684 (16) Å
c = 16.009 (3) Å
α = 99.57 (3)°
β = 96.40 (3)°
γ = 108.31 (3)°
V = 740.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.48 × 0.39 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.965, T_{max} = 0.984
7308 measured reflections
3359 independent reflections
2372 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.06
3359 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.64	3.459 (2)	147
C9—H9C···O1^{ii}	0.96	2.59	3.366 (2)	138

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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*.

We thank Jilin Province Science and Technology Division for financial support (grant Nos. 200505174; 20100751). We are also grateful for support by the Frontiers of Science and Interdisciplinary Innovation Project of Jilin University (grant No. 450060445023).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2044).

References

Allen, F. H., Baalham, C. A., Lommerse, J. P. M. & Raithby, P. R. (1998). *Acta Cryst.* B**54**, 320–329.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bianchini, C., Mantovani, G., Meli, A., Migliacci, F., Zanobini, F., Laschi, F. & Sommazzi, A. (2003). *Eur. J. Inorg. Chem.* pp. 1620–1631.
Britovsek, G. J. P., Gibson, V. C. & Wass, D. F. (1999). *Angew. Chem. Int. Ed.* **38**, 428–447.
Gibson, V. C., Redshaw, C. & Solan, G. A. (2007). *Chem. Rev.* **107**, 1745–1776.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Mecking, S. (2001). *Angew. Chem. Int. Ed.* **40**, 534–540.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Schmidt, R., Welch, M. B., Palackal, S. J. & Alt, H. G. (2002). *J. Mol. Catal. A Chem.* **179**, 155–173.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o360 [doi:10.1107/S1600536811056327]

(*E*)-1-{6-[1-(2,6-Dimethylphenylimino)ethyl]pyridin-2-yl}ethanone

Qing Su and Qing Zhao

S1. Comment

Bis(imino)pyridine iron and cobalt complexes have been well-known as catalyst precursors for olefin oligomerization and polymerization. Considerable efforts have been focused on improving catalyst performance with a view to enhancing catalytic activity and control of the microstructure of the resulting polymer. (Britovsek, *et al.*, 1999; Mecking, *et al.*, 2001; Gibson, *et al.*, 2007;) The nature of the bis(imino)pyridine ligands was found to be a crucial factor affecting the catalyst performance and it has also been shown that similar complexes of mono(imino)pyridine ligands can function as active catalysts (Bianchini *et al.*, 2003).

In the title molecule, Fig. 1, the angle between the mean planes of the pyridine and benzene rings is 78.04 (6)°. In the crystal, there exist intermolecular C2—H2···O1 interactions with the graph-set motif $R_2^2(10)$ (Bernstein *et al.*, 1995) which form a dimer (Fig.2 and Table 1). The adjacent dimers are connected into a 3-dimensional network by intermolecular C9—H9C···O1 interactions (Fig.2 and Table 1), and significant interactions between centrosymmetrically-related pairs of carbonyl groups (Allen, *et al.*, 1998) in adjacent molecules with an O1···C6^{iii} distance of 3.176 (2) Å and a C6=O1···C6^{iii} angle of 93.48 (9)° [(iii) -x, -1-y, 1-z].

S2. Experimental

Compound (I) was prepared as described in the litererature (Schmidt *et al.*, 2002; Bianchini *et al.*, 2003) with 2,6-di-acetylpyridine and 2,6-dimethylaniline as starting material. Crystals suitable for X-ray analysis were obtained by recrystallization from a petroleum ether solution at room temperature.

S3. Refinement

The C-bound H atoms were positioned geometrically with C—H = 0.93 Å (aromatic carbon), and 0.96 (methyl) Å, and allowed to ride on their parent atoms in the riding model approximation with U_{iso}(H) = 1.2 (1.5 for methyl) U_{eq}(C).

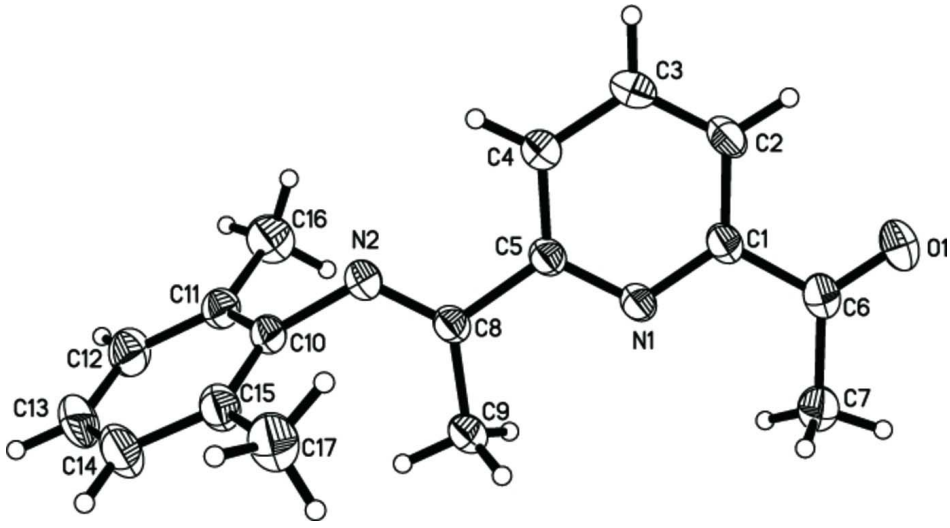


Figure 1

View of the molecule of (I) showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

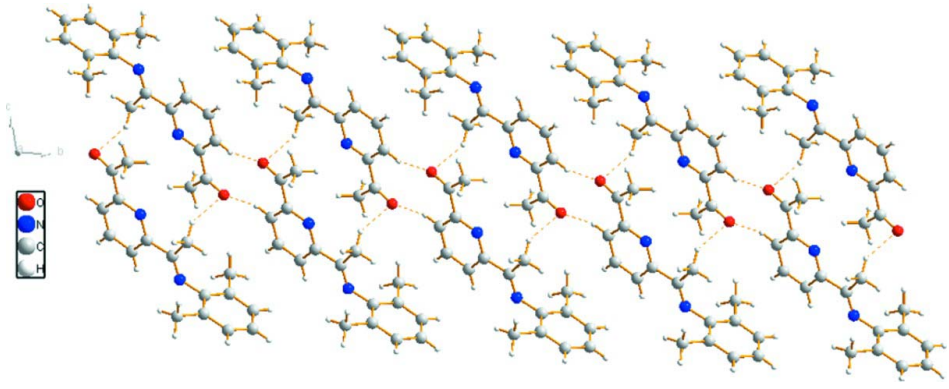


Figure 2

The molecular packing of (I). Hydrogen bonds are indicated by dashed lines.

(*E*)-1-{6-[1-(2,6-Dimethylphenylimino)ethyl]pyridin-2-yl}ethanone

Crystal data

$C_{17}H_{18}N_2O$
$M_r = 266.33$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.2988\ (13)$ Å
$b = 7.9684\ (16)$ Å
$c = 16.009\ (3)$ Å
$\alpha = 99.57\ (3)°$
$\beta = 96.40\ (3)°$
$\gamma = 108.31\ (3)°$
$V = 740.6\ (3)$ Å^3
$Z = 2$
$F(000) = 284$
$D_x = 1.194$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5656 reflections
$\theta = 3.3–27.5°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, yellow
0.48 × 0.39 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.965, T_{max} = 0.984
7308 measured reflections
3359 independent reflections
2372 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −8→8
k = −10→10
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.06
3359 reflections
185 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
$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 0.0412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	−0.1379 (2)	−0.37717 (16)	0.54963 (7)	0.0681 (3)
N1	−0.01368 (18)	−0.15963 (14)	0.37828 (7)	0.0422 (3)
N2	−0.0626 (2)	0.02226 (15)	0.19274 (7)	0.0471 (3)
C1	−0.1418 (2)	−0.27314 (17)	0.42051 (9)	0.0434 (3)
C2	−0.3694 (2)	−0.37081 (19)	0.39062 (10)	0.0531 (4)
H2	−0.4536	−0.4474	0.4220	0.064*
C3	−0.4679 (3)	−0.3518 (2)	0.31350 (11)	0.0607 (4)
H3	−0.6201	−0.4171	0.2914	0.073*
C4	−0.3396 (2)	−0.23533 (19)	0.26906 (10)	0.0524 (4)
H4	−0.4038	−0.2206	0.2168	0.063*
C5	−0.1126 (2)	−0.14023 (16)	0.30375 (8)	0.0410 (3)
C6	−0.0265 (3)	−0.28860 (19)	0.50480 (9)	0.0494 (3)
C7	0.2229 (3)	−0.1950 (2)	0.53064 (10)	0.0616 (4)
H7A	0.2725	−0.2148	0.5859	0.092*
H7B	0.2578	−0.0676	0.5338	0.092*
H7C	0.2994	−0.2421	0.4889	0.092*

C8	0.0334 (2)	−0.00400 (16)	0.26111 (8)	0.0410 (3)
C9	0.2751 (2)	0.0919 (2)	0.30375 (10)	0.0543 (4)
H9A	0.3439	0.1871	0.2753	0.081*
H9B	0.3561	0.0078	0.3003	0.081*
H9C	0.2806	0.1426	0.3630	0.081*
C10	0.0553 (2)	0.15611 (17)	0.14995 (8)	0.0445 (3)
C11	0.0037 (2)	0.31576 (18)	0.15929 (9)	0.0496 (3)
C12	0.1034 (3)	0.4428 (2)	0.11335 (11)	0.0632 (4)
H12	0.0720	0.5502	0.1193	0.076*
C13	0.2480 (3)	0.4132 (2)	0.05903 (12)	0.0746 (5)
H13	0.3128	0.4997	0.0283	0.090*
C14	0.2970 (3)	0.2554 (3)	0.05017 (12)	0.0724 (5)
H14	0.3953	0.2366	0.0133	0.087*
C15	0.2030 (3)	0.1238 (2)	0.09492 (9)	0.0545 (4)
C16	−0.1539 (3)	0.3483 (2)	0.21889 (13)	0.0713 (5)
H16A	−0.0827	0.3648	0.2773	0.107*
H16B	−0.2920	0.2460	0.2060	0.107*
H16C	−0.1879	0.4547	0.2114	0.107*
C17	0.2582 (4)	−0.0483 (2)	0.08336 (12)	0.0711 (5)
H17A	0.2760	−0.0826	0.0249	0.107*
H17B	0.1370	−0.1427	0.0966	0.107*
H17C	0.3968	−0.0294	0.1212	0.107*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0754 (8)	0.0750 (7)	0.0612 (6)	0.0197 (6)	0.0261 (6)	0.0361 (6)
N1	0.0402 (6)	0.0407 (6)	0.0481 (6)	0.0116 (5)	0.0132 (5)	0.0164 (5)
N2	0.0446 (6)	0.0447 (6)	0.0520 (6)	0.0100 (5)	0.0094 (5)	0.0201 (5)
C1	0.0459 (7)	0.0389 (6)	0.0500 (7)	0.0144 (6)	0.0172 (6)	0.0162 (5)
C2	0.0467 (8)	0.0496 (8)	0.0653 (9)	0.0088 (6)	0.0208 (7)	0.0255 (7)
C3	0.0391 (8)	0.0600 (9)	0.0748 (10)	0.0014 (6)	0.0079 (7)	0.0239 (8)
C4	0.0440 (8)	0.0520 (8)	0.0586 (8)	0.0087 (6)	0.0061 (6)	0.0217 (7)
C5	0.0396 (7)	0.0381 (6)	0.0473 (7)	0.0121 (5)	0.0119 (5)	0.0140 (5)
C6	0.0586 (9)	0.0457 (7)	0.0500 (7)	0.0195 (6)	0.0178 (6)	0.0174 (6)
C7	0.0593 (10)	0.0645 (9)	0.0594 (9)	0.0157 (8)	0.0052 (7)	0.0225 (7)
C8	0.0399 (7)	0.0380 (6)	0.0467 (7)	0.0116 (5)	0.0121 (5)	0.0133 (5)
C9	0.0433 (8)	0.0586 (8)	0.0565 (8)	0.0048 (6)	0.0096 (6)	0.0236 (7)
C10	0.0421 (7)	0.0430 (7)	0.0462 (7)	0.0081 (6)	0.0054 (6)	0.0177 (6)
C11	0.0490 (8)	0.0449 (7)	0.0533 (8)	0.0125 (6)	0.0049 (6)	0.0155 (6)
C12	0.0712 (11)	0.0462 (8)	0.0739 (10)	0.0168 (7)	0.0091 (8)	0.0255 (7)
C13	0.0807 (13)	0.0666 (11)	0.0852 (12)	0.0158 (9)	0.0293 (10)	0.0481 (9)
C14	0.0790 (12)	0.0786 (11)	0.0771 (11)	0.0297 (10)	0.0398 (10)	0.0411 (9)
C15	0.0587 (9)	0.0548 (8)	0.0557 (8)	0.0198 (7)	0.0171 (7)	0.0221 (7)
C16	0.0746 (12)	0.0665 (10)	0.0844 (12)	0.0338 (9)	0.0261 (9)	0.0204 (9)
C17	0.0866 (13)	0.0702 (11)	0.0733 (11)	0.0400 (10)	0.0308 (9)	0.0236 (9)

Geometric parameters (Å, º)

O1—C6	1.2147 (17)	C9—H9B	0.9600
N1—C5	1.3386 (18)	C9—H9C	0.9600
N1—C1	1.3388 (16)	C10—C11	1.3977 (19)
N2—C8	1.2712 (17)	C10—C15	1.4022 (19)
N2—C10	1.4202 (16)	C11—C12	1.382 (2)
C1—C2	1.383 (2)	C11—C16	1.501 (2)
C1—C6	1.502 (2)	C12—C13	1.373 (3)
C2—C3	1.372 (2)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.375 (3)
C3—C4	1.377 (2)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.384 (2)
C4—C5	1.389 (2)	C14—H14	0.9300
C4—H4	0.9300	C15—C17	1.506 (2)
C5—C8	1.4997 (17)	C16—H16A	0.9600
C6—C7	1.487 (2)	C16—H16B	0.9600
C7—H7A	0.9600	C16—H16C	0.9600
C7—H7B	0.9600	C17—H17A	0.9600
C7—H7C	0.9600	C17—H17B	0.9600
C8—C9	1.494 (2)	C17—H17C	0.9600
C9—H9A	0.9600		

C5—N1—C1	117.90 (12)	H9A—C9—H9C	109.5
C8—N2—C10	121.37 (12)	H9B—C9—H9C	109.5
N1—C1—C2	123.17 (13)	C11—C10—C15	121.17 (12)
N1—C1—C6	116.46 (12)	C11—C10—N2	117.17 (12)
C2—C1—C6	120.37 (12)	C15—C10—N2	121.46 (12)
C3—C2—C1	118.35 (13)	C12—C11—C10	118.41 (14)
C3—C2—H2	120.8	C12—C11—C16	121.22 (14)
C1—C2—H2	120.8	C10—C11—C16	120.37 (13)
C2—C3—C4	119.49 (14)	C13—C12—C11	121.19 (15)
C2—C3—H3	120.3	C13—C12—H12	119.4
C4—C3—H3	120.3	C11—C12—H12	119.4
C3—C4—C5	118.80 (14)	C12—C13—C14	119.88 (14)
C3—C4—H4	120.6	C12—C13—H13	120.1
C5—C4—H4	120.6	C14—C13—H13	120.1
N1—C5—C4	122.27 (12)	C13—C14—C15	121.44 (15)
N1—C5—C8	116.15 (12)	C13—C14—H14	119.3
C4—C5—C8	121.54 (12)	C15—C14—H14	119.3
O1—C6—C7	121.86 (14)	C14—C15—C10	117.91 (14)
O1—C6—C1	119.54 (14)	C14—C15—C17	120.26 (14)
C7—C6—C1	118.60 (12)	C10—C15—C17	121.82 (13)
C6—C7—H7A	109.5	C11—C16—H16A	109.5
C6—C7—H7B	109.5	C11—C16—H16B	109.5
H7A—C7—H7B	109.5	H16A—C16—H16B	109.5
C6—C7—H7C	109.5	C11—C16—H16C	109.5
H7A—C7—H7C	109.5	H16A—C16—H16C	109.5

H7B—C7—H7C	109.5	H16B—C16—H16C	109.5
N2—C8—C9	125.99 (12)	C15—C17—H17A	109.5
N2—C8—C5	116.51 (12)	C15—C17—H17B	109.5
C9—C8—C5	117.47 (12)	H17A—C17—H17B	109.5
C8—C9—H9A	109.5	C15—C17—H17C	109.5
C8—C9—H9B	109.5	H17A—C17—H17C	109.5
H9A—C9—H9B	109.5	H17B—C17—H17C	109.5
C8—C9—H9C	109.5		

C5—N1—C1—C2	0.26 (19)	N1—C5—C8—C9	1.94 (17)
C5—N1—C1—C6	−178.75 (11)	C4—C5—C8—C9	179.65 (12)
N1—C1—C2—C3	0.7 (2)	C8—N2—C10—C11	−104.44 (15)
C6—C1—C2—C3	179.71 (13)	C8—N2—C10—C15	80.74 (18)
C1—C2—C3—C4	−0.9 (2)	C15—C10—C11—C12	−0.5 (2)
C2—C3—C4—C5	0.2 (2)	N2—C10—C11—C12	−175.34 (13)
C1—N1—C5—C4	−1.06 (19)	C15—C10—C11—C16	−179.67 (15)
C1—N1—C5—C8	176.62 (10)	N2—C10—C11—C16	5.5 (2)
C3—C4—C5—N1	0.9 (2)	C10—C11—C12—C13	0.7 (2)
C3—C4—C5—C8	−176.71 (12)	C16—C11—C12—C13	179.82 (18)
N1—C1—C6—O1	173.71 (12)	C11—C12—C13—C14	−0.5 (3)
C2—C1—C6—O1	−5.3 (2)	C12—C13—C14—C15	0.1 (3)
N1—C1—C6—C7	−6.63 (18)	C13—C14—C15—C10	0.0 (3)
C2—C1—C6—C7	174.33 (13)	C13—C14—C15—C17	179.49 (18)
C10—N2—C8—C9	−2.1 (2)	C11—C10—C15—C14	0.2 (2)
C10—N2—C8—C5	176.01 (11)	N2—C10—C15—C14	174.78 (15)
N1—C5—C8—N2	−176.33 (11)	C11—C10—C15—C17	−179.28 (15)
C4—C5—C8—N2	1.38 (18)	N2—C10—C15—C17	−4.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.64	3.459 (2)	147
C9—H9*C*···O1^{ii}	0.96	2.59	3.366 (2)	138

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