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(*E*)-*N*′-(4-Hydroxybenzylidene)-2-methoxybenzohydrazide

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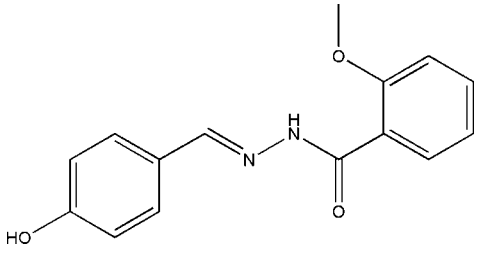
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.136; data-to-parameter ratio = 15.6.

The title compound, $C_{15}H_{14}N_2O_3$, exists in the *E* configuration with respect to the central methylidene unit. The dihedral angle between the two substituted benzene rings is 22.0 (2)°. Within the molecule there is an intramolecular N—H···O hydrogen bond involving the hydrozide H atom and the O atom of the methoxy substituent on the adjacent phenyl ring. In the crystal structure, molecules are linked through intermolecular O—H···O hydrogen bonds, forming zigzag chains along the *b* direction.

Related literature

For bond-length data, see: Allen *et al.* (1987). For background on the biological properties of hydrazones, see: El-Tabl *et al.* (2008); Chen *et al.* (2008); Alvarez *et al.* (2008); Ventura & Martins (2008); Kalinowski *et al.* (2008). For related structures, see: Diao & Yu (2006); Shan *et al.* (2008); Fun *et al.* (2008); Yehye *et al.* (2008); Ejsmont *et al.* (2008); Han *et al.* (2006); Lu *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{14}N_2O_3$
M_r = 270.28
Orthorhombic, *Pbca*
a = 13.113 (3) Å
b = 9.189 (2) Å
c = 22.110 (4) Å
V = 2664.2 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.10 × 0.10 × 0.08 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.991, T_{max} = 0.992
20705 measured reflections
2899 independent reflections
1656 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.136
S = 1.02
2899 reflections
186 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3	0.895 (10)	1.91 (2)	2.620 (2)	135 (2)
O1—H1···O2^{i}	0.82	1.90	2.700 (2)	164

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2061).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Alvarez, C., Alvarez, R., Corchete, P., Lopez, J. L., Perez-Melero, C., Pelaez, R. & Medarde, M. (2008). *Bioorg. Med. Chem.* **16**, 5952–5961.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, J., Liu, F., Song, B.-A., Yang, S., Hu, D.-Y., Jin, H.-H., Chen, Z. & Xue, W. (2008). *Chin. J. Org. Chem.* **28**, 894–898.
Diao, C.-H. & Yu, M. (2006). *Acta Cryst.* E**62**, o5278–o5279.
Ejsmont, K., Zareef, M., Arfan, M., Bashir, S. A. & Zaleski, J. (2008). *Acta Cryst.* E**64**, o1128.
El-Tabl, A. S., El-Saied, F. A. & Al-Hakimi, A. N. (2008). *J. Coord. Chem.* **61**, 2380–2401.
Fun, H.-K., Patil, P. S., Rao, J. N., Kalluraya, B. & Chantrapromma, S. (2008). *Acta Cryst.* E**64**, o1707.
Han, J.-R., Wang, X.-F., Zhen, X.-L., Tian, X. & Liu, S.-X. (2006). *Acta Cryst.* E**62**, o5572–o5573.
Kalinowski, D. S., Sharpe, P. C., Bernhardt, P. V. & Richardson, D. R. (2008). *J. Med. Chem.* **51**, 331–344.
Lu, J.-F., Min, S.-T., Ji, X.-H. & Dang, Z.-H. (2008). *Acta Cryst.* E**64**, o1695.
Shan, S., Tian, Y.-L., Wang, S.-H., Wang, W.-L. & Xu, Y.-L. (2008). *Acta Cryst.* E**64**, o1363.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Ventura, C. & Martins, F. (2008). *J. Med. Chem.* **51**, 612–624.
Yehye, W. A., Ariffin, A. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o960.

supporting information

Acta Cryst. (2008). E**64**, o1999 [doi:10.1107/S1600536808029334]

(*E*)-*N*′-(4-Hydroxybenzylidene)-2-methoxybenzohydrazide

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S1. Comment

Hydrazones derived from the reactions of aldehydes with hydrazides show potential biological properties (El-Tabl *et al.*, 2008; Chen *et al.*, 2008; Alvarez *et al.*, 2008; Ventura & Martins, 2008; Kalinowski *et al.*, 2008). In the last few years, a large number of hydrazones have been reported (Diao & Yu, 2006; Shan *et al.*, 2008; Fun *et al.*, 2008; Yehye *et al.*, 2008; Ejsmont *et al.*, 2008). As a continuous study, the crystal structure of the title compound, (I), is reported in this paper.

Compound (I) was prepared by the reaction of 4-hydroxybenzaldehyde and 2-methoxybenzohydrazide in methanol. The molecular structure of compound (I) is illustrated in Fig. 1. The C7—N1 bond length of 1.272 (3) Å indicates the presence of a typical C═N double bond. The molecule exists in the E configuration with respect to the methylidene unit (C7═N1), as observed in similar compounds (Han *et al.*, 2006; Lu *et al.*, 2008). The dihedral angle between the two substituted benzene rings is 22.02 (12)°, indicating that the molecule is not planar. In the 2-methoxyphenyl unit atom C15 deviates slightly from the mean plane of the benzene ring (C9–C14) by 0.097 (3) Å. The bond lengths are in normal ranges (Allen *et al.*, 1987).

In the molecule there is an intramolecular N—H···O hydrogen bond (Table 1), and in the crystal structure symmetry related molecules are linked through intermolecular O—H···O hydrogen bonds (Table 1), forming zig-zag chains along the b direction (Fig. 2).

S2. Experimental

2-Methoxybenzohydrazide (0.166 g, 1 mmol) was dissolved in ethanol (50 ml), then 4-hydroxybenzaldehyde (0.122 g, 1 mmol) was added slowly to the solution, and the mixture was heated at reflux with continuous stirring for 1 h. The solution was cooled to room temperature, yielding colorless crystallites. Recrystallization from absolute ethanol yielded block-like single crytals of compound (I).

S3. Refinement

The NH H-atom (H2A) was located in a difference Fourier map and freely refined, with the N—H distance restrained to 0.90 (1) Å, and U_{iso} = 0.08 Å^2. The remaining OH and C-bound H-atoms were included in calculated positions and treated as riding atoms: O—H = 0.82 Å with U_{iso}(H) = 1.5U_{eq}(O), and C—H = 0.93–0.96 Å, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

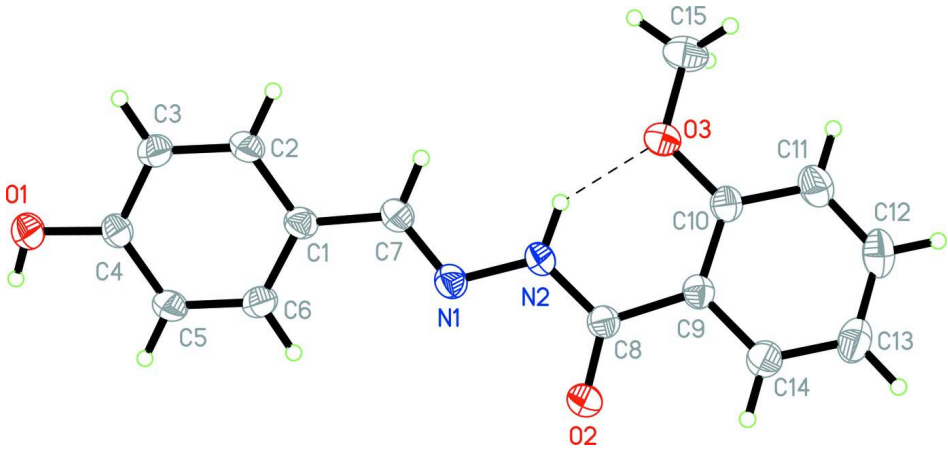

Figure 1

The molecular structure of compound (I), with 30% probability displacement ellipsoids for non-H atoms.

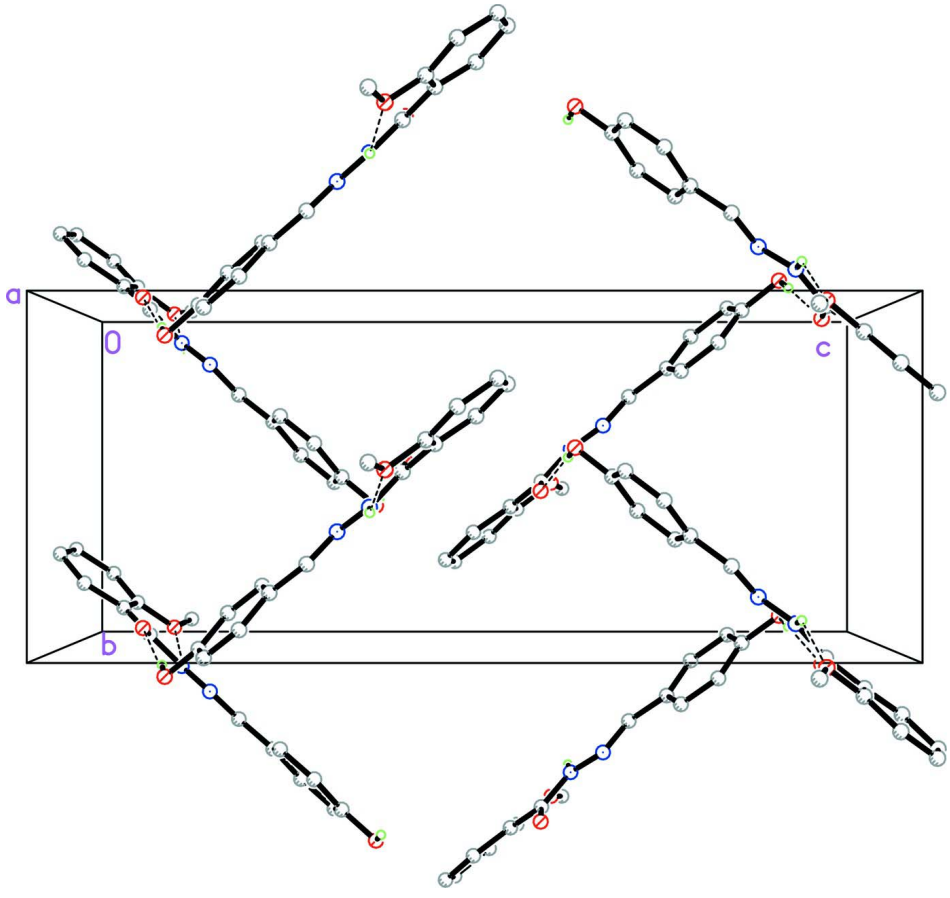

Figure 2

The crystal packing of compound (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

(*E*)-*N*′-(4-Hydroxybenzylidene)-2-methoxybenzohydrazide

Crystal data

$C_{15}H_{14}N_2O_3$
$M_r = 270.28$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.113$ (3) Å
$b = 9.189$ (2) Å
$c = 22.110$ (4) Å
$V = 2664.2$ (10) Å^3
$Z = 8$
$F(000) = 1136$
$D_x = 1.348$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1422 reflections
$\theta = 2.4$–$24.5°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.10 × 0.10 × 0.08 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.991$, $T_{max} = 0.992$
20705 measured reflections
2899 independent reflections
1656 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.8°$
$h = -16 \rightarrow 16$
$k = -11 \rightarrow 11$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.136$
$S = 1.02$
2899 reflections
186 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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.6248P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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	0.05041 (12)	0.41453 (19)	0.87757 (7)	0.0566 (5)
H1	−0.0077	0.4422	0.8850	0.085*
O2	0.12254 (12)	1.04261 (19)	0.58301 (7)	0.0603 (5)
O3	0.43319 (11)	1.01975 (19)	0.60152 (7)	0.0565 (5)

N1	0.18804 (13)	0.8432 (2)	0.66327 (8)	0.0445 (5)
N2	0.25132 (14)	0.9141 (2)	0.62338 (8)	0.0460 (5)
C1	0.18233 (16)	0.6684 (2)	0.74406 (10)	0.0423 (6)
C2	0.23796 (17)	0.5671 (3)	0.77706 (10)	0.0488 (6)
H2	0.3071	0.5555	0.7690	0.059*
C3	0.19308 (17)	0.4837 (3)	0.82142 (10)	0.0493 (6)
H3	0.2319	0.4168	0.8430	0.059*
C4	0.09138 (16)	0.4992 (2)	0.83370 (9)	0.0413 (6)
C5	0.03475 (17)	0.5996 (3)	0.80141 (11)	0.0537 (7)
H5	−0.0343	0.6112	0.8097	0.064*
C6	0.07971 (17)	0.6823 (3)	0.75726 (10)	0.0527 (7)
H6	0.0405	0.7489	0.7358	0.063*
C7	0.23330 (17)	0.7529 (3)	0.69767 (10)	0.0467 (6)
H7	0.3032	0.7404	0.6928	0.056*
C8	0.21358 (17)	1.0145 (2)	0.58522 (9)	0.0415 (5)
C9	0.28755 (16)	1.0927 (2)	0.54622 (9)	0.0409 (5)
C10	0.39297 (17)	1.1018 (3)	0.55572 (10)	0.0440 (6)
C11	0.4525 (2)	1.1908 (3)	0.51948 (11)	0.0585 (7)
H11	0.5224	1.1971	0.5263	0.070*
C12	0.4087 (2)	1.2695 (3)	0.47368 (12)	0.0667 (8)
H12	0.4489	1.3305	0.4501	0.080*
C13	0.3060 (2)	1.2592 (3)	0.46224 (12)	0.0642 (7)
H13	0.2769	1.3110	0.4305	0.077*
C14	0.24661 (19)	1.1715 (3)	0.49838 (10)	0.0532 (6)
H14	0.1771	1.1647	0.4905	0.064*
C15	0.53806 (18)	1.0379 (3)	0.61787 (12)	0.0671 (8)
H15A	0.5805	1.0137	0.5840	0.101*
H15B	0.5540	0.9750	0.6512	0.101*
H15C	0.5499	1.1372	0.6294	0.101*
H2A	0.3188 (8)	0.900 (3)	0.6214 (12)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0478 (10)	0.0620 (11)	0.0600 (10)	0.0031 (9)	0.0133 (8)	0.0151 (9)
O2	0.0392 (10)	0.0760 (13)	0.0656 (11)	0.0092 (9)	0.0079 (8)	0.0192 (10)
O3	0.0400 (9)	0.0684 (12)	0.0611 (10)	−0.0044 (8)	−0.0049 (8)	0.0097 (9)
N1	0.0417 (11)	0.0500 (12)	0.0419 (10)	−0.0011 (9)	0.0048 (9)	0.0008 (10)
N2	0.0366 (10)	0.0537 (13)	0.0477 (11)	0.0013 (10)	0.0096 (9)	0.0093 (10)
C1	0.0372 (12)	0.0498 (14)	0.0400 (12)	0.0021 (11)	0.0026 (10)	−0.0010 (11)
C2	0.0329 (12)	0.0626 (17)	0.0509 (14)	0.0050 (11)	0.0069 (10)	0.0057 (13)
C3	0.0444 (14)	0.0528 (16)	0.0508 (14)	0.0087 (12)	0.0029 (11)	0.0081 (12)
C4	0.0412 (13)	0.0441 (14)	0.0386 (12)	−0.0025 (11)	0.0044 (10)	−0.0017 (11)
C5	0.0340 (12)	0.0695 (18)	0.0575 (15)	0.0055 (12)	0.0067 (11)	0.0122 (13)
C6	0.0430 (14)	0.0646 (18)	0.0506 (14)	0.0104 (12)	0.0004 (11)	0.0132 (13)
C7	0.0394 (13)	0.0546 (16)	0.0460 (13)	0.0040 (12)	0.0080 (10)	0.0026 (12)
C8	0.0407 (13)	0.0460 (14)	0.0377 (12)	0.0023 (11)	0.0025 (10)	−0.0014 (11)
C9	0.0436 (13)	0.0385 (13)	0.0407 (12)	0.0015 (11)	0.0049 (10)	−0.0015 (11)

C10	0.0482 (14)	0.0440 (14)	0.0399 (12)	−0.0019 (11)	0.0030 (10)	−0.0025 (11)
C11	0.0566 (16)	0.0604 (18)	0.0584 (16)	−0.0162 (13)	0.0065 (13)	−0.0018 (14)
C12	0.083 (2)	0.0601 (18)	0.0573 (16)	−0.0179 (16)	0.0138 (15)	0.0089 (15)
C13	0.082 (2)	0.0573 (18)	0.0537 (15)	0.0071 (16)	0.0087 (14)	0.0144 (14)
C14	0.0518 (14)	0.0564 (17)	0.0514 (14)	0.0062 (13)	0.0036 (12)	0.0038 (13)
C15	0.0461 (15)	0.076 (2)	0.0793 (19)	−0.0062 (14)	−0.0128 (14)	−0.0078 (16)

Geometric parameters (Å, º)

O1—C4	1.355 (2)	C5—H5	0.9300
O1—H1	0.8200	C6—H6	0.9300
O2—C8	1.222 (3)	C7—H7	0.9300
O3—C10	1.368 (3)	C8—C9	1.484 (3)
O3—C15	1.432 (3)	C9—C14	1.389 (3)
N1—C7	1.272 (3)	C9—C10	1.401 (3)
N1—N2	1.375 (2)	C10—C11	1.386 (3)
N2—C8	1.344 (3)	C11—C12	1.371 (4)
N2—H2A	0.895 (10)	C11—H11	0.9300
C1—C6	1.383 (3)	C12—C13	1.373 (4)
C1—C2	1.389 (3)	C12—H12	0.9300
C1—C7	1.450 (3)	C13—C14	1.377 (3)
C2—C3	1.377 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.368 (3)	C15—H15A	0.9600
C3—H3	0.9300	C15—H15B	0.9600
C4—C5	1.383 (3)	C15—H15C	0.9600
C5—C6	1.370 (3)		

C4—O1—H1	109.5	O2—C8—N2	122.0 (2)
C10—O3—C15	119.53 (19)	O2—C8—C9	120.8 (2)
C7—N1—N2	114.27 (18)	N2—C8—C9	117.2 (2)
C8—N2—N1	120.36 (19)	C14—C9—C10	117.7 (2)
C8—N2—H2A	115.6 (18)	C14—C9—C8	116.2 (2)
N1—N2—H2A	124.1 (18)	C10—C9—C8	125.9 (2)
C6—C1—C2	117.5 (2)	O3—C10—C11	122.4 (2)
C6—C1—C7	123.3 (2)	O3—C10—C9	117.3 (2)
C2—C1—C7	119.2 (2)	C11—C10—C9	120.3 (2)
C3—C2—C1	121.5 (2)	C12—C11—C10	120.1 (3)
C3—C2—H2	119.2	C12—C11—H11	119.9
C1—C2—H2	119.2	C10—C11—H11	119.9
C4—C3—C2	120.0 (2)	C11—C12—C13	120.8 (3)
C4—C3—H3	120.0	C11—C12—H12	119.6
C2—C3—H3	120.0	C13—C12—H12	119.6
O1—C4—C3	118.0 (2)	C12—C13—C14	119.2 (3)
O1—C4—C5	122.7 (2)	C12—C13—H13	120.4
C3—C4—C5	119.4 (2)	C14—C13—H13	120.4
C6—C5—C4	120.4 (2)	C13—C14—C9	121.9 (2)
C6—C5—H5	119.8	C13—C14—H14	119.0

C4—C5—H5	119.8	C9—C14—H14	119.0
C5—C6—C1	121.2 (2)	O3—C15—H15A	109.5
C5—C6—H6	119.4	O3—C15—H15B	109.5
C1—C6—H6	119.4	H15A—C15—H15B	109.5
N1—C7—C1	123.9 (2)	O3—C15—H15C	109.5
N1—C7—H7	118.1	H15A—C15—H15C	109.5
C1—C7—H7	118.1	H15B—C15—H15C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3	0.90 (1)	1.91 (2)	2.620 (2)	135 (2)
O1—H1···O2^{i}	0.82	1.90	2.700 (2)	164

Symmetry code: (i) $-x, y-1/2, -z+3/2$.