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(*E*)-*N*′-(3-Hydroxy-4-methoxybenzylidene)-4-methoxybenzohydrazide

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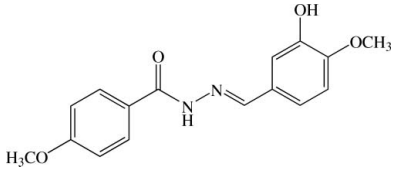
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.109; data-to-parameter ratio = 17.8.

The title molecule, a benzohydrazide derivative, $C_{16}H_{16}N_2O_4$, is twisted with a dihedral angle of 69.97 (5)° between the two benzene rings. An intramolecular O—H···O hydrogen bond generates an S(5) ring motif. In the crystal, molecules are linked by N—H···O and weak C—H···O hydrogen bonds into a chain along the c axis. C—H···π interactions are also present.

Related literature

For bond-length data, see: Allen *et al.* (1987). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Fun *et al.* (2011); Horkaew *et al.* (2011); Promdet *et al.* (2011). For background and applications of benzohydrazide derivatives, see: Bedia *et al.* (2006); Loncle *et al.* (2004); Melnyk *et al.* (2006); Raj *et al.* (2007). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_{16}N_2O_4$
M_r = 300.31
Monoclinic, $P2_1/c$
a = 12.1323 (19) Å
b = 12.9727 (15) Å
c = 9.6714 (12) Å
β = 113.213 (2)°
V = 1398.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.58 × 0.30 × 0.07 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.942, T_{max} = 0.993
14521 measured reflections
3704 independent reflections
3260 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.03
3704 reflections
208 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1*O3*···O4	0.87 (2)	2.18 (2)	2.6692 (13)	115.9 (18)
N1—H1*N1*···O1^{i}	0.887 (18)	1.992 (18)	2.8698 (13)	170.0 (16)
C8—H8*A*···O1^{i}	0.93	2.47	3.2780 (15)	145
C15—H15*C*···*Cg*1^{ii}	0.96	2.72	3.5664 (15)	148
C16—H16*B*···*Cg*1^{iii}	0.96	2.76	3.4366 (16)	128

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5009).

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§ Thomson Reuters ResearcherID: A-5085-2009. Additional correspondence author, e-mail: suchada.c@psu.ac.thl.

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(*E*)-*N*′-(3-Hydroxy-4-methoxybenzylidene)-4-methoxybenzohydrazide

Hoong-Kun Fun, Premrudee Promdet, Suchada Chantrapromma, Jirapa Horkaew and Chatchanok Karalai

S1. Comment

Benzohydrazide derivatives have been reported to possess various biological properties, such as antibacterial and antifungal (Loncle *et al.*, 2004), antitubercular (Bedia *et al.*, 2006), antimalarial (Melnyk *et al.*, 2006) and antiproliferative (Raj *et al.*, 2007) activities. We have previously reported some crystal structures of this type of compounds (Fun *et al.*, 2011; Horkaew *et al.*, 2011; Promdet *et al.*, 2011). The title compound (I) was synthesized in order to study the effect of functional groups to their bioactivities comparing to the closely related structures. (I) was screened for antibacterial and antioxidant activities. Our results show that (I) exhibits moderate antibacterial activity whereas it is inactive for antioxidant activity. The three dimensional structure of (I) was studied in order to gain more details to explain the effect of structure on its bioactivity.

The molecule of the title benzohydrazide derivative (Fig. 1), $C_{16}H_{16}N_2O_4$, exists in a *trans*-configuration with respect to the C8═N2 bond [1.2808 (14) Å] and the torsion angle of N1–N2–C8–C9 is 179.20 (9)°. The molecule is twisted as indicated by the dihedral angle between the two benzene rings being 69.97 (5)°. The middle bridge fragment (O1/C7/N1/N2/C8) is nearly planar with a torsion angle N2–N1–C7–O1 = -0.80 (16)°. The mean plane through this bridge makes dihedral angles of 27.88 (7) and 43.44 (7)° with the C1–C6 and C9–C14 benzene rings, respectively. The methoxy group of 4-methoxyphenyl (at atom C4) is co-planar with its bound benzene ring [torsion angle C15–O2–C4–C5 = -0.76 (16)° and *r.m.s* 0.0131 (1) Å for the seven non H atoms], whereas the methoxy group of the 3-hydroxy-4-methoxyphenyl (at atom C12) is slight deviated with a torsion angle C16–O4–C12–C13 = 10.02 (15)°. An intramolecular O3—H1O3···O4 hydrogen bond generates an S(5) ring motif (Bernstein *et al.*, 1995). Bond distances are of normal values (Allen *et al.*, 1987) and are comparable with the related structures (Fun *et al.*, 2011; Horkaew *et al.*, 2011; Promdet *et al.*, 2011).

In the crystal packing (Fig. 2), the molecules are linked by N—H···O hydrogen bonds and weak C—H···O interactions (Table 1) into chains along the *c* axis. These chains are arranged in a face-to-face manner. The crystal is stabilized by N—H···O hydrogen bonds, weak C—H···O and C—H···π interactions (Table 1).

S2. Experimental

The title compound (I) was prepared by dissolving 4-methoxybenzohydrazide (2 mmol, 0.33 g) in ethanol (10 ml). The solution of 3-hydroxy-4-methoxybenzaldehyde (2 mmol, 0.30 g) in ethanol (10 ml) was then added slowly to the reaction. The mixture was refluxed for around 3 hr. The solution was then cooled to room temperature. Colorless plate-shaped single crystals of the title compound suitable for *X*-ray structure determination were recrystallized from methanol by slow evaporation of the solvent at room temperature after several days (m.p. 491-492 K).

S3. Refinement

Amide and hydroxy H atoms were located in difference maps and refined isotropically [N—H = 0.887 (18) Å and O—H = 0.87 (2) Å]. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å for aromatic and CH and 0.96 Å for CH_3 atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

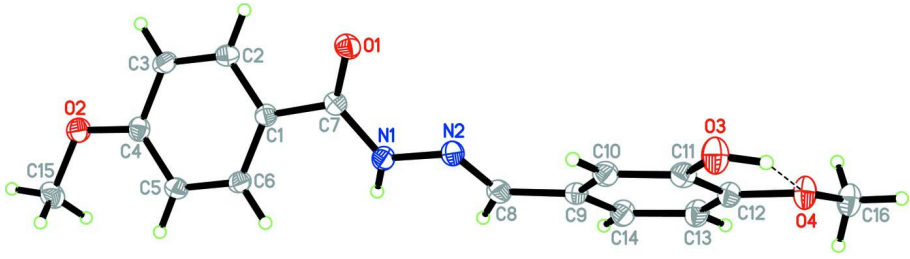

Figure 1

The molecular structure of the title compound, showing 60% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bond was drawn as a dash line.

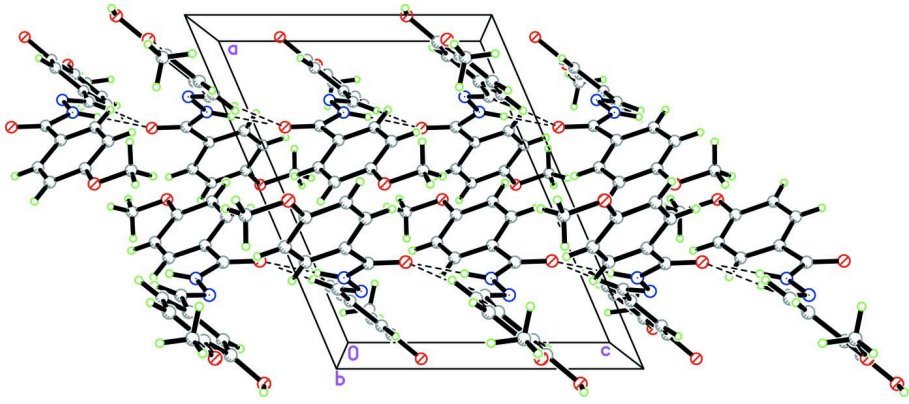

Figure 2

A crystal packing diagram of the title compound viewed along the *b* axis, showing chains running along the *c* axis. Hydrogen bonds were drawn as dashed lines.

(*E*)-*N*′-(3-Hydroxy-4-methoxybenzylidene)-4-methoxybenzohydrazide

Crystal data

$C_{16}H_{16}N_2O_4$
$M_r = 300.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.1323$ (19) Å
$b = 12.9727$ (15) Å
$c = 9.6714$ (12) Å
$\beta = 113.213$ (2)°
$V = 1398.9$ (3) Å^3
$Z = 4$

$F(000) = 632$
$D_x = 1.426$ Mg m^{-3}
Melting point = 491–492 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3704 reflections
$\theta = 1.8$–29.0°
$\mu = 0.10$ mm^{-1}
$T = 100$ K
Plate, colorless
0.58 × 0.30 × 0.07 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.942, T_{max} = 0.993
14521 measured reflections
3704 independent reflections
3260 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 29.0°, θ_{min} = 1.8°
h = −15→16
k = −17→16
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.03
3704 reflections
208 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.5751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.29470 (7)	0.79595 (6)	0.37018 (8)	0.01765 (17)
O2	0.47609 (8)	1.16425 (6)	0.09037 (9)	0.02033 (18)
O3	−0.02649 (8)	0.33066 (7)	0.26553 (10)	0.02208 (19)
H1O3	−0.0427 (18)	0.2655 (17)	0.262 (2)	0.049 (6)*
O4	0.05699 (8)	0.16672 (6)	0.17060 (10)	0.02052 (18)
N1	0.24563 (9)	0.72966 (7)	0.13517 (10)	0.01662 (19)
H1N1	0.2597 (15)	0.7299 (13)	0.0519 (19)	0.027 (4)*
N2	0.20136 (8)	0.63908 (7)	0.16926 (10)	0.01754 (19)
C1	0.33802 (9)	0.89609 (8)	0.19231 (11)	0.0143 (2)
C2	0.42433 (10)	0.95553 (8)	0.30308 (11)	0.0169 (2)
H2A	0.4511	0.9355	0.4033	0.020*
C3	0.47027 (10)	1.04352 (8)	0.26570 (11)	0.0175 (2)
H3A	0.5285	1.0818	0.3403	0.021*
C4	0.42906 (9)	1.07495 (8)	0.11550 (12)	0.0158 (2)

C5	0.34465 (9)	1.01566 (8)	0.00388 (11)	0.0162 (2)
H5A	0.3184	1.0355	−0.0964	0.019*
C6	0.29974 (9)	0.92674 (8)	0.04258 (11)	0.0155 (2)
H6A	0.2434	0.8872	−0.0323	0.019*
C7	0.29096 (9)	0.80337 (8)	0.24151 (11)	0.0143 (2)
C8	0.20399 (10)	0.56293 (9)	0.08631 (12)	0.0174 (2)
H8A	0.2331	0.5735	0.0117	0.021*
C9	0.16289 (9)	0.46024 (8)	0.10510 (11)	0.0167 (2)
C10	0.08516 (9)	0.44367 (8)	0.17847 (11)	0.0170 (2)
H10A	0.0565	0.4994	0.2150	0.020*
C11	0.05118 (9)	0.34488 (8)	0.19644 (12)	0.0168 (2)
C12	0.09594 (9)	0.26028 (8)	0.14405 (12)	0.0167 (2)
C13	0.17260 (10)	0.27633 (9)	0.07125 (12)	0.0192 (2)
H13A	0.2022	0.2205	0.0362	0.023*
C14	0.20503 (10)	0.37620 (9)	0.05082 (12)	0.0192 (2)
H14A	0.2554	0.3869	0.0004	0.023*
C15	0.43662 (11)	1.19826 (9)	−0.06160 (13)	0.0221 (2)
H15A	0.4779	1.2606	−0.0655	0.033*
H15B	0.3518	1.2110	−0.1008	0.033*
H15C	0.4535	1.1461	−0.1208	0.033*
C16	0.11532 (11)	0.07892 (9)	0.14054 (14)	0.0228 (2)
H16A	0.0817	0.0171	0.1624	0.034*
H16B	0.1995	0.0817	0.2025	0.034*
H16C	0.1039	0.0790	0.0365	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0231 (4)	0.0179 (4)	0.0150 (3)	0.0017 (3)	0.0108 (3)	0.0010 (3)
O2	0.0243 (4)	0.0178 (4)	0.0183 (4)	−0.0057 (3)	0.0077 (3)	0.0011 (3)
O3	0.0220 (4)	0.0190 (4)	0.0318 (4)	−0.0008 (3)	0.0175 (3)	0.0007 (3)
O4	0.0227 (4)	0.0151 (4)	0.0284 (4)	−0.0019 (3)	0.0150 (3)	0.0001 (3)
N1	0.0227 (4)	0.0154 (4)	0.0144 (4)	−0.0033 (3)	0.0100 (3)	−0.0004 (3)
N2	0.0195 (4)	0.0164 (4)	0.0166 (4)	−0.0041 (3)	0.0070 (3)	0.0013 (3)
C1	0.0175 (5)	0.0137 (4)	0.0136 (4)	0.0006 (4)	0.0082 (4)	−0.0006 (3)
C2	0.0209 (5)	0.0175 (5)	0.0125 (4)	0.0000 (4)	0.0066 (4)	−0.0009 (4)
C3	0.0197 (5)	0.0172 (5)	0.0147 (4)	−0.0028 (4)	0.0058 (4)	−0.0029 (4)
C4	0.0172 (5)	0.0145 (5)	0.0176 (5)	−0.0006 (4)	0.0088 (4)	0.0002 (4)
C5	0.0183 (5)	0.0170 (5)	0.0130 (4)	−0.0004 (4)	0.0059 (4)	0.0011 (4)
C6	0.0168 (5)	0.0159 (5)	0.0131 (4)	−0.0014 (4)	0.0053 (4)	−0.0014 (3)
C7	0.0144 (4)	0.0150 (5)	0.0148 (4)	0.0015 (4)	0.0071 (4)	0.0006 (3)
C8	0.0190 (5)	0.0183 (5)	0.0149 (4)	−0.0017 (4)	0.0067 (4)	0.0015 (4)
C9	0.0174 (5)	0.0171 (5)	0.0134 (4)	−0.0021 (4)	0.0037 (4)	0.0007 (4)
C10	0.0160 (5)	0.0170 (5)	0.0170 (4)	0.0008 (4)	0.0055 (4)	0.0001 (4)
C11	0.0138 (4)	0.0193 (5)	0.0168 (4)	−0.0004 (4)	0.0057 (4)	0.0007 (4)
C12	0.0164 (5)	0.0155 (5)	0.0176 (4)	−0.0020 (4)	0.0060 (4)	0.0003 (4)
C13	0.0220 (5)	0.0177 (5)	0.0203 (5)	−0.0009 (4)	0.0109 (4)	−0.0020 (4)
C14	0.0229 (5)	0.0196 (5)	0.0186 (5)	−0.0038 (4)	0.0117 (4)	−0.0009 (4)

C15	0.0252 (5)	0.0206 (5)	0.0209 (5)	−0.0015 (4)	0.0096 (4)	0.0056 (4)
C16	0.0274 (6)	0.0153 (5)	0.0298 (6)	−0.0013 (4)	0.0158 (5)	−0.0019 (4)

Geometric parameters (Å, º)

O1—C7	1.2310 (13)	C5—H5A	0.9300
O2—C4	1.3550 (12)	C6—H6A	0.9300
O2—C15	1.4246 (13)	C8—C9	1.4588 (15)
O3—C11	1.3656 (13)	C8—H8A	0.9300
O3—H1O3	0.87 (2)	C9—C14	1.3918 (15)
O4—C12	1.3631 (13)	C9—C10	1.4024 (15)
O4—C16	1.4300 (14)	C10—C11	1.3779 (15)
N1—C7	1.3523 (13)	C10—H10A	0.9300
N1—N2	1.3847 (12)	C11—C12	1.4046 (15)
N1—H1N1	0.887 (17)	C12—C13	1.3858 (15)
N2—C8	1.2808 (14)	C13—C14	1.3906 (15)
C1—C6	1.3930 (14)	C13—H13A	0.9300
C1—C2	1.3980 (14)	C14—H14A	0.9300
C1—C7	1.4877 (14)	C15—H15A	0.9600
C2—C3	1.3796 (15)	C15—H15B	0.9600
C2—H2A	0.9300	C15—H15C	0.9600
C3—C4	1.3978 (14)	C16—H16A	0.9600
C3—H3A	0.9300	C16—H16B	0.9600
C4—C5	1.3907 (14)	C16—H16C	0.9600
C5—C6	1.3888 (14)		
C4—O2—C15	117.11 (9)	C14—C9—C10	119.41 (10)
C11—O3—H1O3	107.6 (13)	C14—C9—C8	118.29 (10)
C12—O4—C16	115.78 (9)	C10—C9—C8	122.28 (10)
C7—N1—N2	119.91 (9)	C11—C10—C9	120.04 (10)
C7—N1—H1N1	121.5 (11)	C11—C10—H10A	120.0
N2—N1—H1N1	116.8 (11)	C9—C10—H10A	120.0
C8—N2—N1	113.42 (9)	O3—C11—C10	119.06 (10)
C6—C1—C2	118.77 (10)	O3—C11—C12	120.68 (10)
C6—C1—C7	123.40 (9)	C10—C11—C12	120.25 (10)
C2—C1—C7	117.83 (9)	O4—C12—C13	125.55 (10)
C3—C2—C1	120.90 (9)	O4—C12—C11	114.57 (9)
C3—C2—H2A	119.6	C13—C12—C11	119.88 (10)
C1—C2—H2A	119.6	C12—C13—C14	119.76 (10)
C2—C3—C4	119.85 (9)	C12—C13—H13A	120.1
C2—C3—H3A	120.1	C14—C13—H13A	120.1
C4—C3—H3A	120.1	C13—C14—C9	120.64 (10)
O2—C4—C5	124.53 (9)	C13—C14—H14A	119.7
O2—C4—C3	115.62 (9)	C9—C14—H14A	119.7
C5—C4—C3	119.85 (10)	O2—C15—H15A	109.5
C6—C5—C4	119.82 (9)	O2—C15—H15B	109.5
C6—C5—H5A	120.1	H15A—C15—H15B	109.5
C4—C5—H5A	120.1	O2—C15—H15C	109.5

C5—C6—C1	120.78 (9)	H15A—C15—H15C	109.5
C5—C6—H6A	119.6	H15B—C15—H15C	109.5
C1—C6—H6A	119.6	O4—C16—H16A	109.5
O1—C7—N1	123.74 (10)	O4—C16—H16B	109.5
O1—C7—C1	121.37 (9)	H16A—C16—H16B	109.5
N1—C7—C1	114.89 (9)	O4—C16—H16C	109.5
N2—C8—C9	122.15 (10)	H16A—C16—H16C	109.5
N2—C8—H8A	118.9	H16B—C16—H16C	109.5
C9—C8—H8A	118.9		

C7—N1—N2—C8	−154.92 (10)	N1—N2—C8—C9	179.20 (9)
C6—C1—C2—C3	0.60 (16)	N2—C8—C9—C14	−158.09 (11)
C7—C1—C2—C3	−178.84 (10)	N2—C8—C9—C10	20.44 (16)
C1—C2—C3—C4	0.97 (17)	C14—C9—C10—C11	0.05 (15)
C15—O2—C4—C5	−0.76 (16)	C8—C9—C10—C11	−178.47 (9)
C15—O2—C4—C3	179.62 (10)	C9—C10—C11—O3	−178.69 (9)
C2—C3—C4—O2	177.65 (10)	C9—C10—C11—C12	1.23 (15)
C2—C3—C4—C5	−2.00 (16)	C16—O4—C12—C13	10.02 (15)
O2—C4—C5—C6	−178.16 (10)	C16—O4—C12—C11	−170.42 (9)
C3—C4—C5—C6	1.45 (16)	O3—C11—C12—O4	−1.02 (14)
C4—C5—C6—C1	0.14 (16)	C10—C11—C12—O4	179.07 (9)
C2—C1—C6—C5	−1.16 (16)	O3—C11—C12—C13	178.58 (10)
C7—C1—C6—C5	178.25 (10)	C10—C11—C12—C13	−1.34 (16)
N2—N1—C7—O1	−0.80 (16)	O4—C12—C13—C14	179.72 (10)
N2—N1—C7—C1	178.78 (9)	C11—C12—C13—C14	0.17 (16)
C6—C1—C7—O1	−155.95 (10)	C12—C13—C14—C9	1.11 (16)
C2—C1—C7—O1	23.46 (15)	C10—C9—C14—C13	−1.22 (16)
C6—C1—C7—N1	24.46 (14)	C8—C9—C14—C13	177.35 (10)
C2—C1—C7—N1	−156.13 (10)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*O*3···O4	0.87 (2)	2.18 (2)	2.6692 (13)	115.9 (18)
N1—H1*N*1···O1^{i}	0.887 (18)	1.992 (18)	2.8698 (13)	170.0 (16)
C8—H8*A*···O1^{i}	0.93	2.47	3.2780 (15)	145
C15—H15*C*···*Cg*1^{ii}	0.96	2.72	3.5664 (15)	148
C16—H16*B*···*Cg*1^{iii}	0.96	2.76	3.4366 (16)	128

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1, −*y*+2, −*z*; (iii) *x*, *y*−1, *z*.