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**(E)-4-Hydroxy-N'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide
N,N-dimethylformamide solvate**

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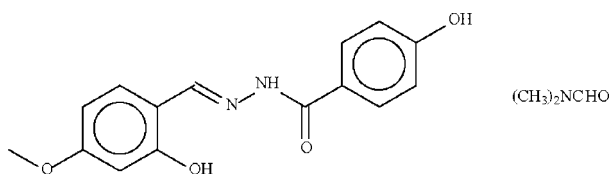
Received 15 December 2008; accepted 16 December 2008

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 16.7.

The Schiff base molecule of the title compound, $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_4 \cdot \text{C}_3\text{H}_7\text{NO}$, adopts a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond; the Schiff base itself is nearly planar (r.m.s. deviation 0.20 Å). The amido N atom is a hydrogen-bond donor to the dimethylformamide solvate molecule. One of the hydroxy groups forms an intramolecular hydrogen bond to the N atom of the $\text{C}=\text{N}$ double bond, whereas the other forms an intermolecular hydrogen bond to the carbonyl group.

Related literature

For the corresponding monohydrate, see: Lair *et al.* (2009).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_4 \cdot \text{C}_3\text{H}_7\text{NO}$

$M_r = 359.38$

Monoclinic, $P2_1/c$
 $a = 11.8273$ (2) Å
 $b = 7.8206$ (2) Å
 $c = 19.4218$ (3) Å
 $\beta = 103.674$ (1)°
 $V = 1745.53$ (6) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 100$ (2) K
 $0.30 \times 0.25 \times 0.15$ mm

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: none
11825 measured reflections

4003 independent reflections
3303 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.104$
 $S = 1.01$
4003 reflections

240 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1}-\text{H1o} \cdots \text{O2}^i$	0.84	1.82	2.656 (1)	174
$\text{O3}-\text{H3o} \cdots \text{N2}$	0.84	1.87	2.607 (1)	145
$\text{N1}-\text{H1n} \cdots \text{O5}$	0.88	1.95	2.787 (1)	157

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2837).

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supporting information

Acta Cryst. (2009). E65, o190 [doi:10.1107/S160053680804289X]

(*E*)-4-Hydroxy-*N'*-(2-hydroxy-4-methoxybenzylidene)benzohydrazide *N,N*-dimethylformamide solvate

Nooraziah Mohd Lair, Hapipah Mohd Ali and Seik Weng Ng

S1. Experimental

2-Hydroxy-3-methoxybenzaldehyde (0.30 g, 2 mmol) and 4-hydroxybenzohydrazide (0.30 g, 2 mmol) were heated in an ethanol-methanol mixture (50 ml) for 2 hours. The solvent was removed and the resulting compound recrystallized from DMF.

S2. Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95–0.98, N–H 0.88, O–H 0.84 Å) and were treated as riding on their parent carbon atoms, with $U(\text{H})$ set to 1.2–1.5 times $U_{\text{eq}}(\text{C}, \text{N}, \text{O})$.

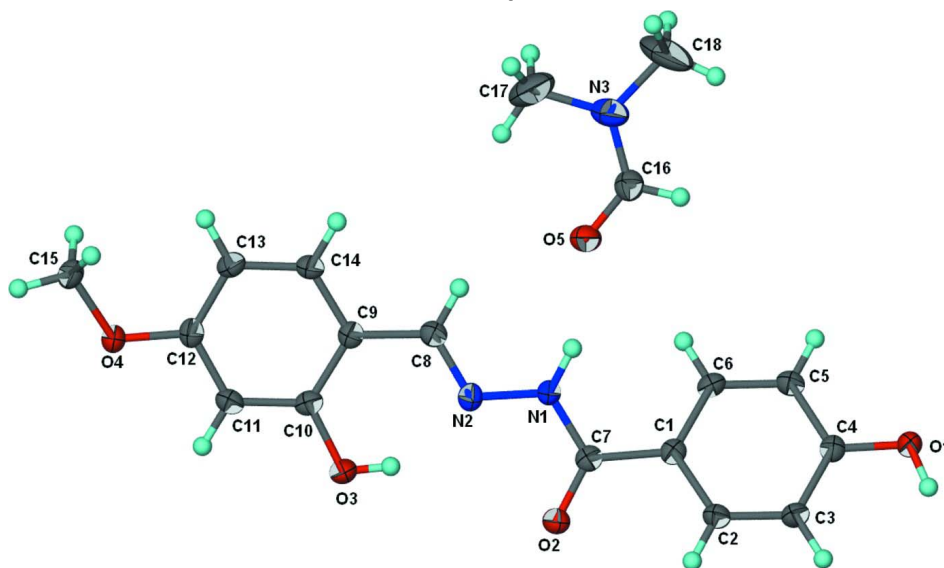


Figure 1

Displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

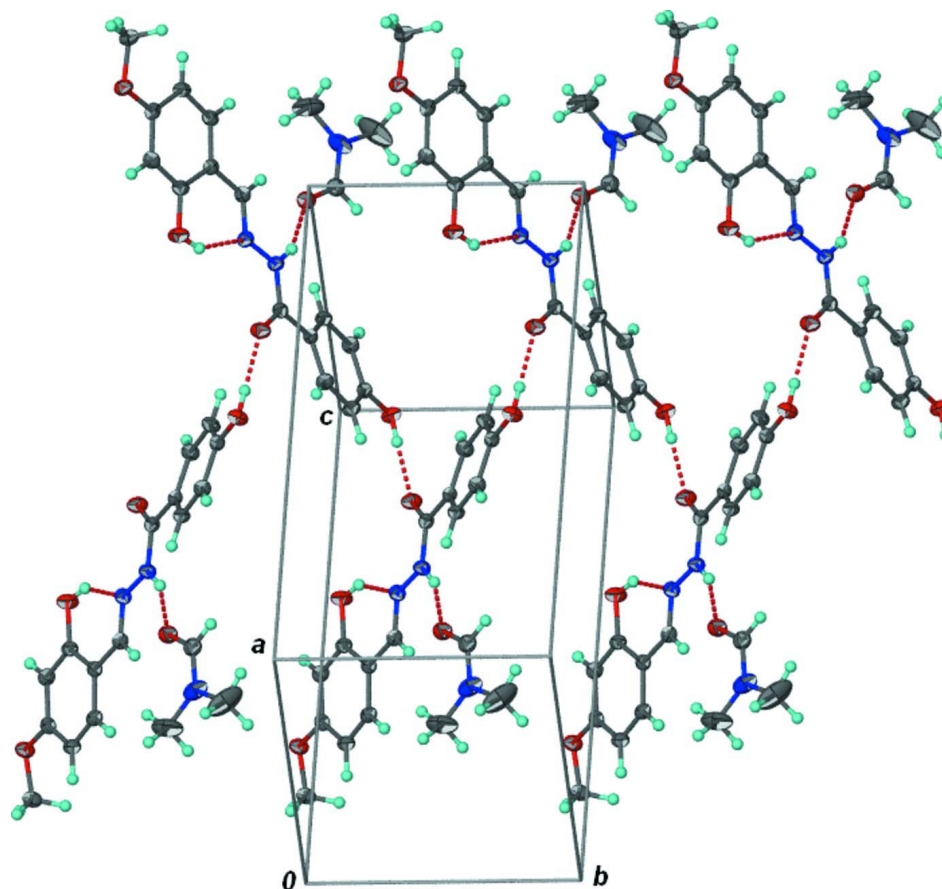


Figure 2

Packing diagram with hydrogen bonds drawn as dashed lines.

(E)-4-Hydroxy-N'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide *N,N*-dimethylformamide solvate

Crystal data

$C_{15}H_{14}N_2O_4 \cdot C_3H_7NO$

$M_r = 359.38$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.8273 (2) \text{ \AA}$

$b = 7.8206 (2) \text{ \AA}$

$c = 19.4218 (3) \text{ \AA}$

$\beta = 103.674 (1)^\circ$

$V = 1745.53 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 760$

$D_x = 1.368 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4180 reflections

$\theta = 2.2\text{--}28.3^\circ$

$\mu = 0.10 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Prism, colorless

$0.30 \times 0.25 \times 0.15 \text{ mm}$

Data collection

Bruker SMART APEX

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

11825 measured reflections

4003 independent reflections

3303 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$

$h = -15 \rightarrow 14$

$k = -10 \rightarrow 8$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.104$

$S = 1.01$

4003 reflections

240 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

$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.678P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.66809 (8)	0.74503 (12)	0.66928 (5)	0.0199 (2)
H1O	0.6979	0.7676	0.7120	0.030*
O2	0.22303 (8)	0.32357 (12)	0.69867 (4)	0.0211 (2)
O3	-0.04810 (8)	0.04690 (13)	0.62396 (5)	0.0228 (2)
H3O	0.0069	0.1161	0.6259	0.034*
O4	-0.40063 (8)	-0.13116 (12)	0.47806 (5)	0.0200 (2)
O5	0.18144 (8)	0.46309 (12)	0.44318 (5)	0.0227 (2)
N1	0.17427 (9)	0.37007 (14)	0.58062 (5)	0.0170 (2)
H1N	0.1888	0.4217	0.5434	0.020*
N2	0.07635 (9)	0.27015 (14)	0.57472 (5)	0.0173 (2)
N3	0.16184 (11)	0.57465 (17)	0.33359 (6)	0.0285 (3)
C1	0.35639 (10)	0.48355 (16)	0.64886 (6)	0.0154 (2)
C2	0.41943 (11)	0.53743 (17)	0.71534 (6)	0.0188 (3)
H2	0.3901	0.5146	0.7559	0.023*
C3	0.52370 (11)	0.62336 (17)	0.72326 (7)	0.0197 (3)
H3	0.5656	0.6584	0.7690	0.024*
C4	0.56747 (11)	0.65871 (16)	0.66420 (6)	0.0164 (3)
C5	0.50566 (11)	0.60607 (16)	0.59728 (6)	0.0179 (3)
H5	0.5351	0.6297	0.5568	0.022*
C6	0.40136 (11)	0.51936 (16)	0.58983 (6)	0.0174 (3)
H6	0.3597	0.4837	0.5441	0.021*
C7	0.24710 (11)	0.38628 (16)	0.64518 (6)	0.0162 (2)
C8	0.00648 (11)	0.25971 (16)	0.51315 (6)	0.0170 (3)
H8	0.0228	0.3201	0.4742	0.020*
C9	-0.09720 (10)	0.15539 (16)	0.50355 (6)	0.0158 (2)
C10	-0.12163 (11)	0.05447 (16)	0.55883 (6)	0.0169 (3)
C11	-0.22325 (11)	-0.04046 (16)	0.54772 (6)	0.0178 (3)
H11	-0.2388	-0.1090	0.5848	0.021*
C12	-0.30237 (11)	-0.03528 (16)	0.48223 (7)	0.0169 (3)
C13	-0.28026 (11)	0.06116 (16)	0.42650 (7)	0.0183 (3)
H13	-0.3341	0.0633	0.3817	0.022*
C14	-0.17781 (11)	0.15370 (16)	0.43817 (6)	0.0173 (3)
H14	-0.1617	0.2186	0.4002	0.021*
C15	-0.49470 (11)	-0.10776 (18)	0.41743 (7)	0.0208 (3)

H15A	-0.5643	-0.1651	0.4252	0.031*
H15B	-0.4739	-0.1568	0.3757	0.031*
H15C	-0.5105	0.0147	0.4098	0.031*
C16	0.21144 (11)	0.56143 (17)	0.40187 (7)	0.0217 (3)
H16	0.2757	0.6343	0.4204	0.026*
C17	0.06495 (16)	0.4656 (3)	0.30112 (9)	0.0449 (5)
H17A	0.0502	0.3839	0.3362	0.067*
H17B	0.0836	0.4033	0.2614	0.067*
H17C	-0.0045	0.5358	0.2837	0.067*
C18	0.20628 (17)	0.6926 (3)	0.28847 (10)	0.0555 (6)
H18A	0.2725	0.7558	0.3170	0.083*
H18B	0.1448	0.7731	0.2665	0.083*
H18C	0.2315	0.6283	0.2514	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0186 (4)	0.0259 (5)	0.0151 (4)	-0.0060 (4)	0.0037 (3)	-0.0012 (4)
O2	0.0185 (4)	0.0274 (5)	0.0168 (4)	-0.0028 (4)	0.0030 (3)	0.0036 (4)
O3	0.0202 (5)	0.0306 (6)	0.0156 (4)	-0.0057 (4)	0.0005 (4)	0.0032 (4)
O4	0.0167 (4)	0.0236 (5)	0.0188 (4)	-0.0051 (4)	0.0026 (4)	0.0005 (4)
O5	0.0268 (5)	0.0235 (5)	0.0173 (4)	-0.0020 (4)	0.0044 (4)	0.0008 (4)
N1	0.0158 (5)	0.0190 (5)	0.0155 (5)	-0.0034 (4)	0.0023 (4)	0.0013 (4)
N2	0.0149 (5)	0.0180 (5)	0.0191 (5)	-0.0012 (4)	0.0040 (4)	-0.0011 (4)
N3	0.0272 (6)	0.0369 (7)	0.0224 (6)	0.0071 (5)	0.0079 (5)	0.0088 (5)
C1	0.0155 (6)	0.0138 (6)	0.0166 (6)	0.0017 (5)	0.0027 (5)	0.0003 (4)
C2	0.0213 (6)	0.0210 (7)	0.0146 (6)	-0.0028 (5)	0.0054 (5)	-0.0002 (5)
C3	0.0224 (6)	0.0220 (7)	0.0140 (6)	-0.0037 (5)	0.0031 (5)	-0.0019 (5)
C4	0.0156 (6)	0.0152 (6)	0.0180 (6)	0.0003 (5)	0.0033 (5)	0.0004 (5)
C5	0.0196 (6)	0.0196 (6)	0.0155 (6)	0.0004 (5)	0.0058 (5)	0.0003 (5)
C6	0.0183 (6)	0.0188 (6)	0.0138 (6)	0.0009 (5)	0.0013 (5)	-0.0008 (5)
C7	0.0157 (6)	0.0159 (6)	0.0168 (6)	0.0021 (5)	0.0032 (5)	-0.0002 (5)
C8	0.0178 (6)	0.0168 (6)	0.0168 (6)	0.0008 (5)	0.0050 (5)	0.0004 (5)
C9	0.0146 (6)	0.0156 (6)	0.0173 (6)	0.0011 (5)	0.0041 (5)	-0.0013 (5)
C10	0.0167 (6)	0.0190 (6)	0.0145 (6)	0.0024 (5)	0.0028 (5)	-0.0008 (5)
C11	0.0195 (6)	0.0189 (6)	0.0161 (6)	0.0009 (5)	0.0064 (5)	0.0018 (5)
C12	0.0151 (6)	0.0160 (6)	0.0203 (6)	-0.0003 (5)	0.0055 (5)	-0.0027 (5)
C13	0.0173 (6)	0.0210 (7)	0.0156 (6)	0.0012 (5)	0.0016 (5)	-0.0002 (5)
C14	0.0189 (6)	0.0179 (6)	0.0151 (6)	0.0012 (5)	0.0042 (5)	0.0022 (5)
C15	0.0163 (6)	0.0252 (7)	0.0198 (6)	-0.0030 (5)	0.0022 (5)	-0.0017 (5)
C16	0.0197 (6)	0.0211 (7)	0.0239 (6)	0.0011 (5)	0.0045 (5)	0.0008 (5)
C17	0.0402 (10)	0.0651 (13)	0.0238 (8)	0.0006 (9)	-0.0040 (7)	-0.0066 (8)
C18	0.0496 (11)	0.0763 (15)	0.0460 (11)	0.0161 (10)	0.0217 (9)	0.0405 (10)

Geometric parameters (Å, °)

O1—C4	1.3514 (15)	C5—H5	0.9500
O1—H1O	0.8400	C6—H6	0.9500

O2—C7	1.2412 (15)	C8—C9	1.4478 (17)
O3—C10	1.3565 (15)	C8—H8	0.9500
O3—H3O	0.8400	C9—C14	1.3962 (17)
O4—C12	1.3693 (15)	C9—C10	1.4162 (17)
O4—C15	1.4278 (15)	C10—C11	1.3855 (17)
O5—C16	1.2229 (16)	C11—C12	1.3901 (17)
N1—C7	1.3489 (15)	C11—H11	0.9500
N1—N2	1.3791 (14)	C12—C13	1.3938 (17)
N1—H1N	0.8800	C13—C14	1.3832 (17)
N2—C8	1.2855 (16)	C13—H13	0.9500
N3—C16	1.3212 (17)	C14—H14	0.9500
N3—C17	1.448 (2)	C15—H15A	0.9800
N3—C18	1.454 (2)	C15—H15B	0.9800
C1—C2	1.3948 (17)	C15—H15C	0.9800
C1—C6	1.4013 (17)	C16—H16	0.9500
C1—C7	1.4870 (17)	C17—H17A	0.9800
C2—C3	1.3808 (18)	C17—H17B	0.9800
C2—H2	0.9500	C17—H17C	0.9800
C3—C4	1.3931 (17)	C18—H18A	0.9800
C3—H3	0.9500	C18—H18B	0.9800
C4—C5	1.3943 (17)	C18—H18C	0.9800
C5—C6	1.3850 (17)		
C4—O1—H1O	109.5	O3—C10—C11	117.60 (11)
C10—O3—H3O	109.5	O3—C10—C9	122.04 (11)
C12—O4—C15	117.61 (10)	C11—C10—C9	120.36 (11)
C7—N1—N2	118.01 (10)	C10—C11—C12	119.89 (11)
C7—N1—H1N	121.0	C10—C11—H11	120.1
N2—N1—H1N	121.0	C12—C11—H11	120.1
C8—N2—N1	117.12 (10)	O4—C12—C11	114.61 (11)
C16—N3—C17	120.60 (13)	O4—C12—C13	124.26 (11)
C16—N3—C18	121.12 (14)	C11—C12—C13	121.13 (11)
C17—N3—C18	118.21 (14)	C14—C13—C12	118.28 (11)
C2—C1—C6	118.28 (11)	C14—C13—H13	120.9
C2—C1—C7	117.86 (11)	C12—C13—H13	120.9
C6—C1—C7	123.83 (11)	C13—C14—C9	122.50 (11)
C3—C2—C1	121.20 (11)	C13—C14—H14	118.7
C3—C2—H2	119.4	C9—C14—H14	118.7
C1—C2—H2	119.4	O4—C15—H15A	109.5
C2—C3—C4	120.06 (12)	O4—C15—H15B	109.5
C2—C3—H3	120.0	H15A—C15—H15B	109.5
C4—C3—H3	120.0	O4—C15—H15C	109.5
O1—C4—C3	122.10 (11)	H15A—C15—H15C	109.5
O1—C4—C5	118.30 (11)	H15B—C15—H15C	109.5
C3—C4—C5	119.60 (11)	O5—C16—N3	125.37 (13)
C6—C5—C4	119.98 (11)	O5—C16—H16	117.3
C6—C5—H5	120.0	N3—C16—H16	117.3
C4—C5—H5	120.0	N3—C17—H17A	109.5

C5—C6—C1	120.89 (11)	N3—C17—H17B	109.5
C5—C6—H6	119.6	H17A—C17—H17B	109.5
C1—C6—H6	119.6	N3—C17—H17C	109.5
O2—C7—N1	121.23 (11)	H17A—C17—H17C	109.5
O2—C7—C1	122.05 (11)	H17B—C17—H17C	109.5
N1—C7—C1	116.72 (11)	N3—C18—H18A	109.5
N2—C8—C9	119.62 (11)	N3—C18—H18B	109.5
N2—C8—H8	120.2	H18A—C18—H18B	109.5
C9—C8—H8	120.2	N3—C18—H18C	109.5
C14—C9—C10	117.80 (11)	H18A—C18—H18C	109.5
C14—C9—C8	119.86 (11)	H18B—C18—H18C	109.5
C10—C9—C8	122.34 (11)		
C7—N1—N2—C8	178.29 (11)	N2—C8—C9—C10	-4.09 (18)
C6—C1—C2—C3	-0.22 (19)	C14—C9—C10—O3	179.47 (11)
C7—C1—C2—C3	177.82 (12)	C8—C9—C10—O3	-1.25 (19)
C1—C2—C3—C4	0.4 (2)	C14—C9—C10—C11	-0.74 (18)
C2—C3—C4—O1	178.84 (12)	C8—C9—C10—C11	178.55 (11)
C2—C3—C4—C5	-0.3 (2)	O3—C10—C11—C12	179.08 (11)
O1—C4—C5—C6	-179.11 (11)	C9—C10—C11—C12	-0.72 (19)
C3—C4—C5—C6	0.07 (19)	C15—O4—C12—C11	168.75 (11)
C4—C5—C6—C1	0.10 (19)	C15—O4—C12—C13	-11.33 (17)
C2—C1—C6—C5	-0.02 (19)	C10—C11—C12—O4	-178.59 (11)
C7—C1—C6—C5	-177.94 (12)	C10—C11—C12—C13	1.49 (19)
N2—N1—C7—O2	-5.05 (18)	O4—C12—C13—C14	179.34 (11)
N2—N1—C7—C1	175.38 (10)	C11—C12—C13—C14	-0.74 (19)
C2—C1—C7—O2	-14.53 (18)	C12—C13—C14—C9	-0.79 (19)
C6—C1—C7—O2	163.40 (12)	C10—C9—C14—C13	1.52 (18)
C2—C1—C7—N1	165.03 (11)	C8—C9—C14—C13	-177.79 (12)
C6—C1—C7—N1	-17.04 (18)	C17—N3—C16—O5	-1.2 (2)
N1—N2—C8—C9	179.42 (11)	C18—N3—C16—O5	-178.22 (15)
N2—C8—C9—C14	175.18 (12)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1o \cdots O2 ⁱ	0.84	1.82	2.656 (1)	174
O3—H3o \cdots N2	0.84	1.87	2.607 (1)	145
N1—H1n \cdots O5	0.88	1.95	2.787 (1)	157

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