organic compounds

(E)-N'-(3,4-Dihydroxybenzylidene)-2,4-dimethylbenzohydrazide monohydrate

Muhammad Taha,[a] Nor Hadiani Ismail,[b] Faridahanim Mohd Jaafar,[b] Ahmad Nazif Aziz[a,c] and Sammer Yousuf[d]*

[a]Atta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA (UiTM), Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor D. E., Malaysia, [b]Faculty of Applied Science, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor D. E., Malaysia, [c]Department of Chemical Sciences, Faculty of Science and Technology, University Malaysia Terengganu, 21030, Kuala Terengganu, Malaysia, and [d]H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan

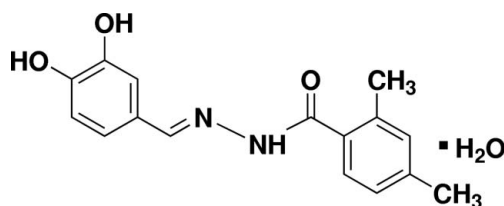Correspondence e-mail: dr.sammer.yousuf@gmail.com

In the title compound, $C_{16}H_{16}N_2O_3 \cdot H_2O$, the dihedral angle between the benzene rings is 30.27 (7)°. In the crystal, the components are linked by N—H⋯O, O—H⋯O and C—H⋯O interactions into a three-dimensional network.

Related literature

For the applications and biological activity of Schiff bases, see: Musharraf *et al.* (2012); Khan *et al.* (2012). For the crystal structures of related compounds, see: Taha *et al.* (2012); Baharudin *et al.* (2012).

Experimental

Crystal data

$C_{16}H_{16}N_2O_3 \cdot H_2O$	c = 13.7886 (5) Å
M_r = 302.32	β = 92.913 (1)°
Monoclinic, $P2_1/n$	V = 1557.87 (10) Å^3
a = 8.1373 (3) Å	Z = 4
b = 13.9025 (5) Å	Mo $K\alpha$ radiation

μ = 0.09 mm^{-1}	0.30 × 0.10 × 0.10 mm
T = 298 K	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	9012 measured reflections
	2897 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	2535 reflections with $I > 2\sigma(I)$
T_{min} = 0.973, T_{max} = 0.991	R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.111	
S = 1.05	
2897 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
221 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1W—H1W1⋯N2[i]	0.87 (2)	2.20 (2)	3.059 (2)	169 (2)
O1W—H2W1⋯O1	0.94 (2)	2.01 (2)	2.935 (2)	173 (2)
N1—H1A⋯O3[ii]	0.91 (2)	2.08 (2)	2.962 (2)	163 (2)
O2—H2A⋯O1[i]	0.88 (2)	1.94 (2)	2.791 (2)	162 (2)
O3—H3A⋯O1W[iii]	0.85 (2)	1.79 (2)	2.629 (2)	172 (2)
C8—H8A⋯O3[ii]	0.93	2.58	3.382 (2)	145
C15—H15B⋯O2[i]	0.96	2.52	3.351 (2)	144

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2622).

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supplementary materials

(*E*)-*N*′-(3,4-Dihydroxybenzylidene)-2,4-dimethylbenzohydrazide monohydrate

Muhammad Taha, Nor Hadiani Ismail, Faridahanim Mohd Jaafar, Ahmad Nazif Aziz and Sammer Yousuf

Comment

Structurally diverse range of benzohydrazides have been extensively studied in order to explore the structural features that may be responsible for different biological activities (Musharraf *et al.*, 2012; Khan *et al.*, 2012). The title compound is yet another benzohydrazide monohydrate, obtained as a part of our ongoing research that has been studied by X-ray crystallographic method and reported in this article.

  In the title compound (Fig. 1) dimethyl and dihydroxy substituted benzene rings (C1–C6 and C9–C14, respectively) are each planner with a dihedral angle 30.27 (7)° between their mean-planes. The azomethine double bond, N2$=$C8 (1.2729 (19) Å) adopts an *E* configuration. The bond lengths and angle are similar to the corresponding bond lengths and angles reported in structurally related benzohydrazide derivatives (Taha *et al.*, 2012; Baharudin *et al.*, 2012). The crystal structure is stabilized by N1—H1A⋯N2, O2—H2A⋯O1, C8—H8A⋯O3 and C15—H15B⋯O2 intermolecular interactions. The ineteractions further extend the structure to a three dimentional network *via* O1W—H2W1⋯O1, O1W—H1A⋯O3 and O3—H3A⋯O1W interactions involving the water of hydration (Table 2 and Fig. 2).

Experimental

The title compound was synthesized by reacting (0.328 g, 2 mmol) 2,4-dimethylbenzohydrazide and (0.276 g, 2 mmol) 3,4-dihydroxybenzaldehyde as starting meterial under the same conditions and solvents as described previously for the synthesis of benzohydrazides (Taha *et al.*, 2012). The title compound was recrystalized by dissolving in methanol to obtain colorless needles (0.499 g, 88% yield). All chemicals were purchased by Sigma Aldrich Germany.

Refinement

H atoms on methyl and benzene ring were positioned geometrically with C—H = 0.96 and 0.93 Å, respectively and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}$(benzene) or $1.5U_{eq}$(methyl). The H atoms on oxygen and nitrogen were located in difference Fourier map and refined isotropically. A rotating group model was applied to the methyl groups.

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); 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* (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).
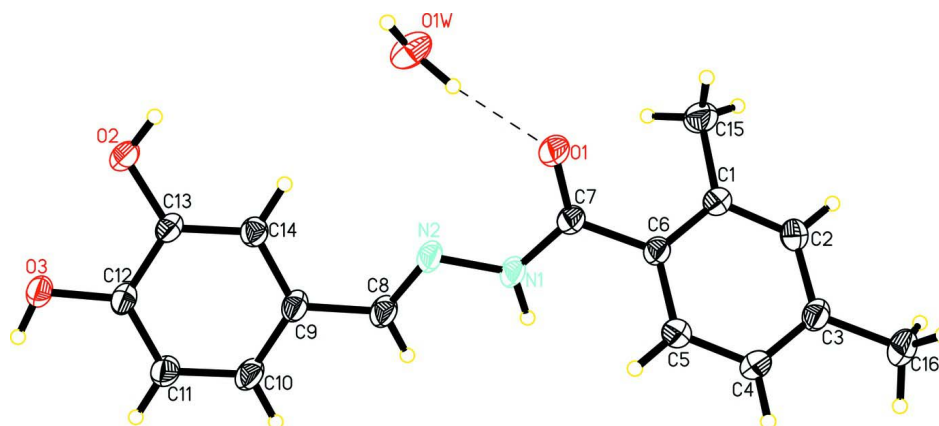
Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at 30% probability level.
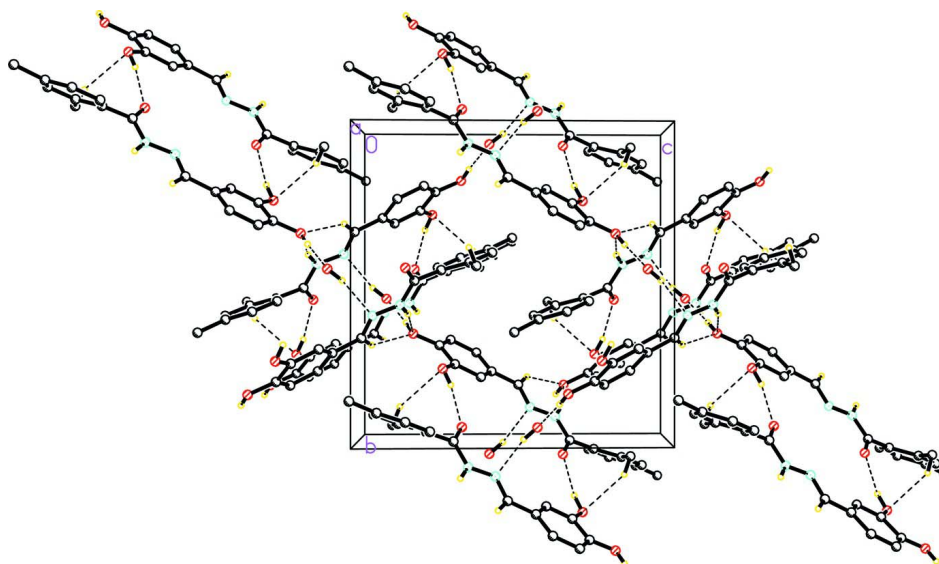
Figure 2

The crystal packing of the title compound. Only hydrogen atoms involved in hydrogen bonding are shown.

(*E*)-*N*′-(3,4-Dihydroxybenzylidene)-2,4-dimethylbenzohydrazide monohydrate

Crystal data

$C_{16}H_{16}N_2O_3 \cdot H_2O$	$F(000) = 640$
$M_r = 302.32$	$D_x = 1.289$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4856 reflections
$a = 8.1373$ (3) Å	$\theta = 2.8$–28.2°
$b = 13.9025$ (5) Å	$\mu = 0.09$ mm^{-1}
$c = 13.7886$ (5) Å	$T = 298$ K
$\beta = 92.913$ (1)°	Block, brown
$V = 1557.87$ (10) Å^3	$0.30 \times 0.10 \times 0.10$ mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	9012 measured reflections
Radiation source: fine-focus sealed tube	2897 independent reflections
Graphite monochromator	2535 reflections with $I > 2\sigma(I)$
ω scan	$R_{int} = 0.016$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{max} = 25.5°$, $\theta_{min} = 2.1°$
	$h = -9 \rightarrow 9$
$T_{min} = 0.973$, $T_{max} = 0.991$	$k = -16 \rightarrow 16$
	$l = -16 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.111$	
$S = 1.05$	H atoms treated by a mixture of independent and constrained refinement
2897 reflections	
221 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.3352P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.19$ e Å^{-3}
	$\Delta\rho_{min} = -0.28$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.15363 (13)	0.55077 (8)	−0.16328 (8)	0.0569 (3)
O1W	−0.12355 (15)	0.45259 (10)	−0.07769 (9)	0.0612 (3)
O2	−0.04800 (12)	0.26761 (9)	0.22605 (8)	0.0505 (3)
O3	0.16469 (13)	0.15980 (8)	0.32684 (7)	0.0460 (3)
N1	0.34634 (15)	0.43523 (9)	−0.14057 (9)	0.0454 (3)
N2	0.28104 (14)	0.40196 (9)	−0.05580 (8)	0.0435 (3)
C1	0.30375 (16)	0.56844 (10)	−0.36100 (10)	0.0395 (3)
C2	0.40413 (18)	0.60048 (11)	−0.43273 (10)	0.0446 (3)
H2C	0.3561	0.6153	−0.4935	0.054*
C3	0.57324 (17)	0.61142 (11)	−0.41767 (10)	0.0435 (3)
C4	0.64410 (17)	0.58608 (11)	−0.32796 (11)	0.0455 (4)
H4A	0.7574	0.5911	−0.3166	0.055*
C5	0.54846 (16)	0.55358 (10)	−0.25556 (10)	0.0423 (3)
H5A	0.5981	0.5371	−0.1956	0.051*
C6	0.37828 (16)	0.54484 (9)	−0.27016 (10)	0.0366 (3)
C7	0.28131 (16)	0.51150 (10)	−0.18789 (10)	0.0397 (3)

C8	0.35766 (18)	0.33077 (11)	−0.01702 (11)	0.0464 (4)
H8A	0.4495	0.3069	−0.0465	0.056*
C9	0.30656 (17)	0.28538 (10)	0.07190 (10)	0.0421 (3)
C10	0.41516 (19)	0.22570 (11)	0.12370 (12)	0.0514 (4)
H10A	0.5192	0.2145	0.1011	0.062*
C11	0.37047 (19)	0.18256 (11)	0.20869 (12)	0.0499 (4)
H11A	0.4448	0.1431	0.2432	0.060*
C12	0.21552 (16)	0.19792 (9)	0.24262 (10)	0.0390 (3)
C13	0.10379 (16)	0.25680 (10)	0.18973 (10)	0.0376 (3)
C14	0.14912 (16)	0.29972 (10)	0.10553 (10)	0.0392 (3)
H14A	0.0745	0.3387	0.0705	0.047*
C15	0.12199 (18)	0.55713 (14)	−0.38483 (12)	0.0571 (4)
H15A	0.1029	0.5506	−0.4538	0.086*
H15B	0.0648	0.6128	−0.3628	0.086*
H15C	0.0825	0.5008	−0.3531	0.086*
C16	0.6765 (2)	0.65068 (14)	−0.49624 (13)	0.0615 (5)
H16A	0.6324	0.6293	−0.5584	0.092*
H16B	0.7875	0.6280	−0.4863	0.092*
H16C	0.6755	0.7197	−0.4941	0.092*
H2A	−0.099 (3)	0.3180 (16)	0.1996 (15)	0.077 (6)*
H1A	0.436 (2)	0.4053 (13)	−0.1634 (13)	0.061 (5)*
H1W1	−0.165 (3)	0.4883 (17)	−0.0335 (16)	0.080 (7)*
H3A	0.239 (2)	0.1248 (15)	0.3533 (15)	0.071 (6)*
H2W1	−0.029 (3)	0.4798 (17)	−0.1022 (16)	0.091 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0495 (6)	0.0633 (7)	0.0601 (7)	0.0209 (5)	0.0261 (5)	0.0182 (5)
O1W	0.0486 (6)	0.0766 (9)	0.0595 (7)	−0.0124 (6)	0.0122 (5)	−0.0274 (6)
O2	0.0399 (5)	0.0578 (7)	0.0557 (7)	0.0085 (5)	0.0200 (5)	0.0140 (5)
O3	0.0453 (6)	0.0499 (6)	0.0442 (6)	0.0056 (5)	0.0153 (5)	0.0141 (5)
N1	0.0462 (6)	0.0506 (7)	0.0414 (7)	0.0134 (6)	0.0227 (5)	0.0112 (5)
N2	0.0453 (6)	0.0477 (7)	0.0393 (6)	0.0066 (5)	0.0194 (5)	0.0077 (5)
C1	0.0360 (7)	0.0429 (7)	0.0400 (7)	0.0004 (5)	0.0051 (6)	0.0011 (6)
C2	0.0478 (8)	0.0505 (8)	0.0358 (7)	0.0008 (6)	0.0041 (6)	0.0062 (6)
C3	0.0437 (7)	0.0430 (8)	0.0448 (8)	−0.0010 (6)	0.0136 (6)	0.0037 (6)
C4	0.0335 (7)	0.0506 (8)	0.0530 (9)	−0.0033 (6)	0.0068 (6)	0.0038 (7)
C5	0.0383 (7)	0.0488 (8)	0.0396 (7)	0.0023 (6)	0.0014 (6)	0.0048 (6)
C6	0.0360 (7)	0.0379 (7)	0.0367 (7)	0.0023 (5)	0.0085 (5)	0.0023 (5)
C7	0.0378 (7)	0.0434 (7)	0.0387 (7)	0.0050 (6)	0.0105 (6)	0.0030 (6)
C8	0.0484 (8)	0.0466 (8)	0.0463 (8)	0.0108 (7)	0.0218 (6)	0.0064 (7)
C9	0.0468 (8)	0.0393 (7)	0.0418 (7)	0.0055 (6)	0.0176 (6)	0.0046 (6)
C10	0.0468 (8)	0.0526 (9)	0.0572 (9)	0.0149 (7)	0.0263 (7)	0.0122 (7)
C11	0.0469 (8)	0.0496 (9)	0.0547 (9)	0.0156 (7)	0.0171 (7)	0.0154 (7)
C12	0.0441 (7)	0.0352 (7)	0.0388 (7)	0.0008 (6)	0.0145 (6)	0.0039 (5)
C13	0.0370 (7)	0.0365 (7)	0.0405 (7)	0.0007 (5)	0.0128 (5)	−0.0002 (5)
C14	0.0420 (7)	0.0361 (7)	0.0401 (7)	0.0036 (6)	0.0082 (6)	0.0034 (6)
C15	0.0401 (8)	0.0788 (12)	0.0521 (9)	−0.0036 (7)	−0.0010 (7)	0.0037 (8)
C16	0.0567 (9)	0.0699 (11)	0.0598 (10)	−0.0030 (8)	0.0225 (8)	0.0146 (9)

Geometric parameters (Å, º)

O1—C7	1.2364 (16)	C5—C6	1.3945 (19)
O1W—H1W1	0.87 (2)	C5—H5A	0.9300
O1W—H2W1	0.94 (2)	C6—C7	1.4884 (18)
O2—C13	1.3645 (15)	C8—C9	1.4581 (19)
O2—H2A	0.88 (2)	C8—H8A	0.9300
O3—C12	1.3599 (16)	C9—C10	1.384 (2)
O3—H3A	0.85 (2)	C9—C14	1.3988 (19)
N1—C7	1.3398 (18)	C10—C11	1.382 (2)
N1—N2	1.3877 (15)	C10—H10A	0.9300
N1—H1A	0.913 (19)	C11—C12	1.3835 (19)
N2—C8	1.2729 (19)	C11—H11A	0.9300
C1—C2	1.3878 (19)	C12—C13	1.4004 (19)
C1—C6	1.4026 (19)	C13—C14	1.3725 (19)
C1—C15	1.5069 (19)	C14—H14A	0.9300
C2—C3	1.390 (2)	C15—H15A	0.9600
C2—H2C	0.9300	C15—H15B	0.9600
C3—C4	1.384 (2)	C15—H15C	0.9600
C3—C16	1.507 (2)	C16—H16A	0.9600
C4—C5	1.373 (2)	C16—H16B	0.9600
C4—H4A	0.9300	C16—H16C	0.9600
H1W1—O1W—H2W1	112 (2)	C10—C9—C14	119.07 (13)
C13—O2—H2A	110.5 (13)	C10—C9—C8	119.44 (12)
C12—O3—H3A	110.4 (13)	C14—C9—C8	121.48 (13)
C7—N1—N2	121.02 (11)	C11—C10—C9	120.62 (13)
C7—N1—H1A	119.8 (11)	C11—C10—H10A	119.7
N2—N1—H1A	119.2 (11)	C9—C10—H10A	119.7
C8—N2—N1	114.37 (11)	C10—C11—C12	120.24 (14)
C2—C1—C6	117.91 (12)	C10—C11—H11A	119.9
C2—C1—C15	119.00 (13)	C12—C11—H11A	119.9
C6—C1—C15	123.05 (12)	O3—C12—C11	123.41 (13)
C1—C2—C3	122.88 (13)	O3—C12—C13	117.06 (11)
C1—C2—H2C	118.6	C11—C12—C13	119.52 (12)
C3—C2—H2C	118.6	O2—C13—C14	123.35 (12)
C4—C3—C2	118.05 (13)	O2—C13—C12	116.69 (12)
C4—C3—C16	120.85 (13)	C14—C13—C12	119.96 (12)
C2—C3—C16	121.10 (13)	C13—C14—C9	120.57 (13)
C5—C4—C3	120.53 (13)	C13—C14—H14A	119.7
C5—C4—H4A	119.7	C9—C14—H14A	119.7
C3—C4—H4A	119.7	C1—C15—H15A	109.5
C4—C5—C6	121.27 (13)	C1—C15—H15B	109.5
C4—C5—H5A	119.4	H15A—C15—H15B	109.5
C6—C5—H5A	119.4	C1—C15—H15C	109.5
C5—C6—C1	119.32 (12)	H15A—C15—H15C	109.5
C5—C6—C7	118.57 (12)	H15B—C15—H15C	109.5
C1—C6—C7	122.11 (12)	C3—C16—H16A	109.5
O1—C7—N1	122.17 (12)	C3—C16—H16B	109.5
O1—C7—C6	123.86 (12)	H16A—C16—H16B	109.5

N1—C7—C6	113.96 (11)	C3—C16—H16C	109.5
N2—C8—C9	122.36 (12)	H16A—C16—H16C	109.5
N2—C8—H8A	118.8	H16B—C16—H16C	109.5
C9—C8—H8A	118.8		
C7—N1—N2—C8	−178.10 (14)	C5—C6—C7—N1	−45.73 (18)
C6—C1—C2—C3	−1.1 (2)	C1—C6—C7—N1	134.90 (14)
C15—C1—C2—C3	−178.87 (15)	N1—N2—C8—C9	−179.45 (13)
C1—C2—C3—C4	2.2 (2)	N2—C8—C9—C10	−163.72 (16)
C1—C2—C3—C16	−177.21 (15)	N2—C8—C9—C14	17.1 (2)
C2—C3—C4—C5	−1.7 (2)	C14—C9—C10—C11	−1.5 (2)
C16—C3—C4—C5	177.66 (15)	C8—C9—C10—C11	179.34 (15)
C3—C4—C5—C6	0.2 (2)	C9—C10—C11—C12	0.6 (3)
C4—C5—C6—C1	0.9 (2)	C10—C11—C12—O3	−178.29 (14)
C4—C5—C6—C7	−178.49 (13)	C10—C11—C12—C13	0.6 (2)
C2—C1—C6—C5	−0.5 (2)	O3—C12—C13—O2	−2.27 (19)
C15—C1—C6—C5	177.23 (14)	C11—C12—C13—O2	178.79 (14)
C2—C1—C6—C7	178.88 (13)	O3—C12—C13—C14	178.14 (12)
C15—C1—C6—C7	−3.4 (2)	C11—C12—C13—C14	−0.8 (2)
N2—N1—C7—O1	−5.9 (2)	O2—C13—C14—C9	−179.69 (13)
N2—N1—C7—C6	172.84 (12)	C12—C13—C14—C9	−0.1 (2)
C5—C6—C7—O1	133.03 (16)	C10—C9—C14—C13	1.3 (2)
C1—C6—C7—O1	−46.3 (2)	C8—C9—C14—C13	−179.59 (14)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···N2[i]	0.87 (2)	2.20 (2)	3.059 (2)	169 (2)
N1—H1A···O3[ii]	0.91 (2)	2.08 (2)	2.962 (2)	163 (2)
O1W—H2W1···O1	0.94 (2)	2.01 (2)	2.935 (2)	173 (2)
O2—H2A···O1[i]	0.88 (2)	1.94 (2)	2.791 (2)	162 (2)
O3—H3A···O1W[iii]	0.85 (2)	1.79 (2)	2.629 (2)	172 (2)
C8—H8A···O3[ii]	0.93	2.58	3.382 (2)	145
C15—H15B···O2[i]	0.96	2.52	3.351 (2)	144

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