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2-{(*E*)-1-[2-(2-Nitrophenyl)hydrazin-1-ylidene]ethyl}benzene-1,3-diol monohydrate

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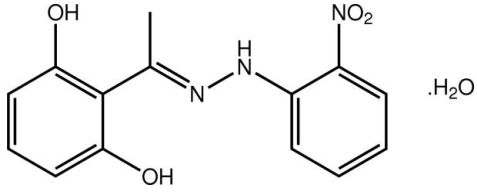
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.194; data-to-parameter ratio = 13.9.

The hydrazone molecule in title monohydrate, $C_{14}H_{13}N_3O_4\cdot H_2O$, is almost coplanar, the dihedral angle between the terminal benzene rings being 3.22 (15)°; the nitro group is coplanar with the benzene ring to which it is bonded [O—N—C—C = −2.8 (4)°]. The hydroxy group forms an intramolecular hydrogen bond with the imine N atom, and the conformation about the imine bond [1.305 (3) Å] is *E*. In the crystal, supramolecular layers in the (203) plane are connected into a double layer *via* water–nitro O—H···O hydrogen bonds, along with π–π interactions [ring centroid–centroid distance = 3.7859 (19) Å].

Related literature

For background on the influence of substituents upon the supramolecular structures of hydrazones, see: Glidewell *et al.* (2004); Ferguson *et al.* (2005); Baddeley *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{13}N_3O_4\cdot H_2O$
M_r = 305.29
Monoclinic, $P2_1/n$
a = 7.6448 (6) Å
b = 21.405 (2) Å
c = 8.5755 (7) Å
β = 106.976 (5)°
V = 1342.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 120 K
0.45 × 0.25 × 0.02 mm

Data collection

Bruker–Nonius Roper CCD camera on κ-goniostat diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.776, T_{max} = 0.998
16295 measured reflections
3068 independent reflections
1492 reflections with $I > 2\sigma(I)$
R_{int} = 0.110

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.194
S = 1.01
3068 reflections
221 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N1	0.85 (2)	1.69 (2)	2.489 (3)	157 (4)
N2—H2N···O3	0.88 (2)	1.93 (2)	2.602 (3)	132 (2)
O2—H2O···O1w^{i}	0.84 (3)	1.90 (3)	2.742 (3)	174 (2)
O1W—H1W···O1^{ii}	0.84 (2)	2.08 (3)	2.910 (3)	169 (3)
O1W—H2W···O4^{iii}	0.85 (3)	2.50 (3)	3.256 (3)	150 (3)
C11—H11···O3^{iv}	0.95	2.52	3.447 (4)	166

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2513).

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supplementary materials

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2-{(*E*)-1-[2-(2-Nitrophenyl)hydrazin-1-ylidene]ethyl}benzene-1,3-diol monohydrate

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Comment

The crystal structure of the title compound (I), has been determined in connection with on-going investigations into the structural chemistry of hydrazones, focusing in particular upon the influence of substituents upon their supramolecular structures, with a special emphasis on derivatives having potential biological activities. These studies have included investigations on substituted phenylhydrazines with substituted benzaldehydes (Glidewell *et al.*, 2004; Ferguson *et al.*, 2005) and 2-hydroxyacetophenone (Baddeley *et al.*, 2009).

In (I) (Fig. 1), the dihedral angle between the benzene rings is 3.22 (15)°, indicating an approximately planar molecule. The nitro group is co-planar with the benzene ring to which it is bonded as seen in the value of the O3—N3—C10—C9 torsion angle of -2.8 (4)°. The hydroxy group forms an intramolecular hydrogen bond with the imine-N1 atom, Table 1. The configuration about the N1═C7 imine bond [1.305 (3) Å] is *E*.

With the exception of the O1w—H2w···O4^{iii} hydrogen bond, all the interactions listed in Table 1 combine to form supramolecular layers parallel to (203). These are connected into double layers *via* the O1w—H2w···O4^{iii} hydrogen bonds and π–π interactions [ring centroid···centroid distance = 3.7859 (19) Å, angle between rings = 3.22 (15)° for *i*: 1 - *x*, -*y*, 1 - *z*]. Layers stack without specific interactions between them (Fig. 2).

Experimental

A solution of 2-nitrophenylhydrazine and 2,6-dihydroxyacetophenone (2 mmol each) in ethanol (20 ml) was refluxed for 1 h, rotary evaporated and the residue recrystallized from methanol, *m*.p. 452–454 K.

Refinement

The *C*-bound H atoms were geometrically placed (C—H = 0.95–0.98 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). The *O*- and *N*-bound H atoms were located from a difference map and refined with the distance restraints O—H = 0.84±0.01 and N—H = 0.88±0.01 Å, and with U_{iso}(H) = zU_{eq}(carrier atom); z = 1.5 for O and z = 1.2 for N.

Computing details

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

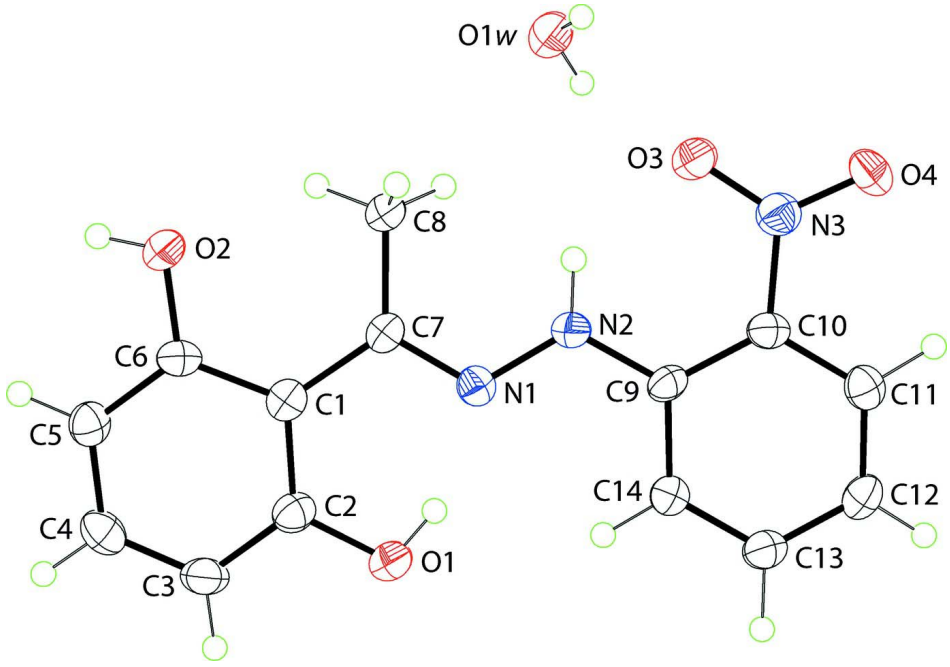

Figure 1

The molecular structures of the constituents of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

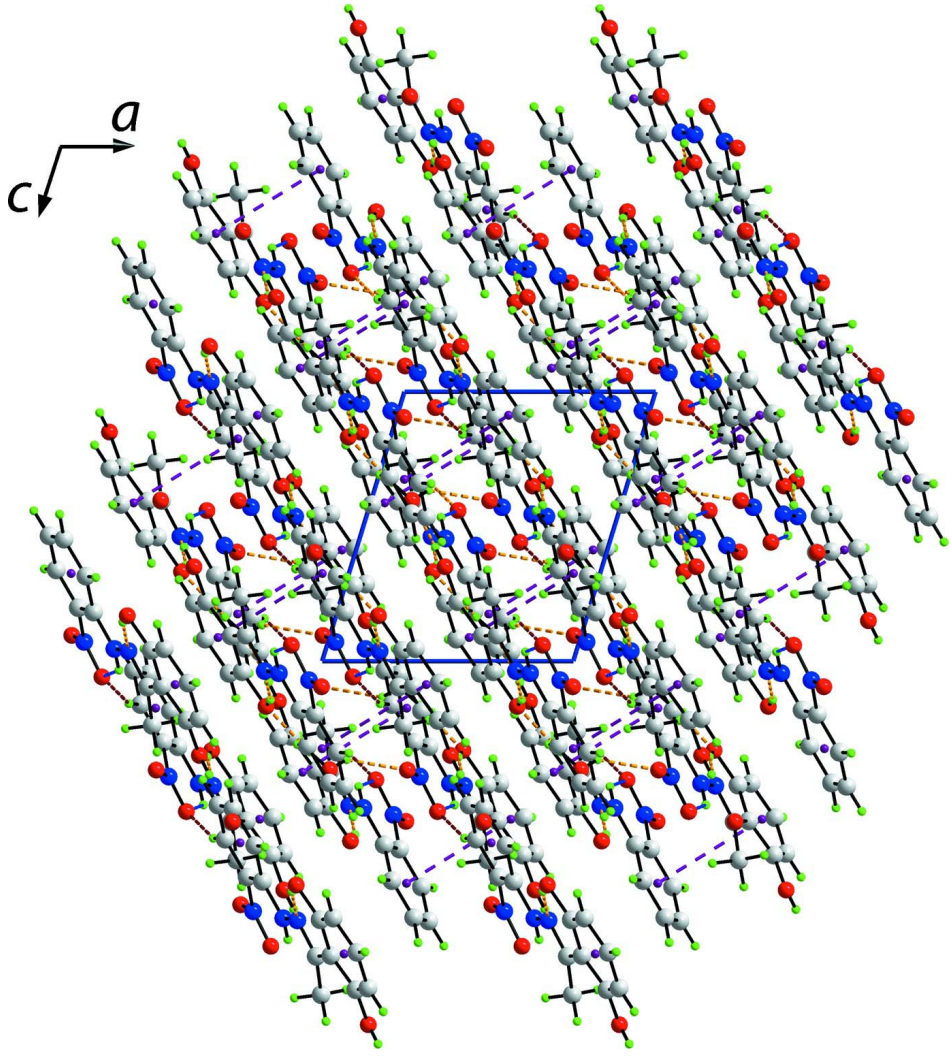

Figure 2

A view in projection down the *b* axis of the packing of supramolecular double layers in (I). The O—H···O (orange), O—H···N (orange), N—H···O (blue), C—H···O (brown) and π–π (purple) interactions are shown as dashed lines.

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Crystal data

$C_{14}H_{13}N_3O_4 \cdot H_2O$
$M_r = 305.29$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.6448$ (6) Å
$b = 21.405$ (2) Å
$c = 8.5755$ (7) Å
$\beta = 106.976$ (5)°
$V = 1342.1$ (2) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.511$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 19763 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.12$ mm^{-1}
$T = 120$ K
Plate, brown
0.45 × 0.25 × 0.02 mm

Data collection

Bruker-Nonius Roper CCD camera on κ-goniostat diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.776, T_{max} = 0.998
16295 measured reflections
3068 independent reflections
1492 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 27.5°, θ_{min} = 2.9°
h = −9→9
k = −27→27
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.194
S = 1.01
3068 reflections
221 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Experimental. IR (KBr, cm^{-1}): *v* 3600–2000 (v br), 3543, 3427, 3340, 1622, 1585, 1525. Anal. Found: C, 54.86; H, 5.03; N, 14.07. Calculated for $C_{14}H_{15}N_3O_5$: C, 55.08; H, 4.95; N, 13.76%.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.6688 (3)	−0.09682 (11)	0.3317 (3)	0.0350 (6)
H1O	0.659 (5)	−0.0590 (7)	0.356 (5)	0.062 (13)*
O2	1.1256 (3)	−0.07064 (10)	0.8502 (3)	0.0340 (6)
H2O	1.189 (4)	−0.0952 (12)	0.921 (3)	0.034 (10)*
O3	0.6421 (3)	0.18198 (10)	0.5589 (3)	0.0353 (6)
O4	0.4717 (3)	0.25227 (10)	0.4047 (3)	0.0411 (7)
N1	0.7166 (3)	0.00802 (11)	0.4628 (3)	0.0247 (6)
N2	0.6577 (3)	0.06852 (12)	0.4550 (3)	0.0272 (6)
H2N	0.702 (4)	0.0956 (11)	0.534 (3)	0.033 (9)*
N3	0.5292 (3)	0.19801 (13)	0.4289 (3)	0.0315 (7)
C1	0.8928 (4)	−0.07782 (14)	0.5935 (4)	0.0238 (7)
C2	0.8060 (4)	−0.11805 (15)	0.4603 (4)	0.0288 (8)
C3	0.8560 (4)	−0.17972 (15)	0.4541 (4)	0.0337 (8)

H3	0.7969	−0.2048	0.3625	0.040*
C4	0.9922 (4)	−0.20473 (15)	0.5816 (4)	0.0322 (8)
H4	1.0262	−0.2473	0.5779	0.039*
C5	1.0795 (4)	−0.16848 (14)	0.7142 (4)	0.0285 (8)
H5	1.1721	−0.1863	0.8019	0.034*
C6	1.0333 (4)	−0.10608 (14)	0.7204 (4)	0.0256 (7)
C7	0.8350 (4)	−0.01181 (14)	0.5962 (3)	0.0228 (7)
C8	0.9016 (4)	0.03103 (14)	0.7387 (4)	0.0314 (8)
H8A	0.9969	0.0584	0.7212	0.043 (10)*
H8B	0.9522	0.0063	0.8380	0.043 (9)*
H8C	0.7996	0.0564	0.7506	0.067 (12)*
C9	0.5300 (4)	0.09005 (14)	0.3180 (3)	0.0246 (7)
C10	0.4639 (4)	0.15195 (14)	0.3020 (3)	0.0252 (7)
C11	0.3303 (4)	0.17195 (15)	0.1615 (4)	0.0285 (8)
H11	0.2881	0.2139	0.1538	0.034*
C12	0.2596 (4)	0.13127 (15)	0.0345 (4)	0.0307 (8)
H12	0.1681	0.1446	−0.0605	0.037*
C13	0.3240 (4)	0.07063 (15)	0.0477 (4)	0.0313 (8)
H13	0.2763	0.0424	−0.0399	0.038*
C14	0.4557 (4)	0.05009 (15)	0.1848 (4)	0.0268 (7)
H14	0.4973	0.0081	0.1895	0.032*
O1W	0.6617 (3)	0.14329 (12)	0.9035 (3)	0.0397 (6)
H1W	0.560 (3)	0.1348 (17)	0.836 (3)	0.060*
H2W	0.714 (4)	0.1722 (13)	0.867 (4)	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0414 (14)	0.0315 (15)	0.0260 (13)	0.0007 (11)	0.0000 (10)	−0.0022 (11)
O2	0.0382 (14)	0.0312 (14)	0.0253 (13)	0.0020 (10)	−0.0021 (11)	−0.0004 (10)
O3	0.0420 (14)	0.0314 (14)	0.0275 (13)	−0.0038 (10)	0.0022 (11)	0.0001 (10)
O4	0.0468 (15)	0.0224 (14)	0.0475 (15)	0.0026 (11)	0.0032 (11)	−0.0025 (11)
N1	0.0256 (14)	0.0238 (15)	0.0257 (14)	−0.0001 (11)	0.0088 (11)	0.0013 (11)
N2	0.0336 (16)	0.0224 (16)	0.0228 (15)	−0.0007 (12)	0.0037 (12)	−0.0022 (12)
N3	0.0348 (17)	0.0299 (17)	0.0292 (16)	−0.0038 (13)	0.0083 (13)	0.0002 (13)
C1	0.0198 (16)	0.0295 (18)	0.0244 (16)	−0.0015 (13)	0.0099 (13)	0.0024 (13)
C2	0.0312 (18)	0.030 (2)	0.0240 (17)	−0.0031 (14)	0.0069 (14)	0.0007 (14)
C3	0.043 (2)	0.029 (2)	0.0288 (18)	−0.0028 (15)	0.0103 (16)	−0.0062 (15)
C4	0.0382 (19)	0.0231 (19)	0.038 (2)	−0.0017 (15)	0.0150 (16)	−0.0007 (15)
C5	0.0317 (18)	0.0274 (19)	0.0275 (18)	0.0004 (14)	0.0103 (14)	0.0044 (14)
C6	0.0298 (18)	0.0255 (19)	0.0225 (16)	−0.0049 (14)	0.0092 (14)	−0.0029 (13)
C7	0.0193 (16)	0.0277 (19)	0.0215 (16)	−0.0010 (13)	0.0062 (13)	0.0021 (13)
C8	0.036 (2)	0.0264 (19)	0.0254 (18)	0.0007 (15)	−0.0015 (15)	−0.0014 (14)
C9	0.0279 (18)	0.0288 (19)	0.0168 (16)	−0.0020 (14)	0.0059 (13)	0.0003 (13)
C10	0.0294 (17)	0.0246 (19)	0.0226 (17)	−0.0046 (14)	0.0092 (14)	−0.0027 (13)
C11	0.0307 (18)	0.0254 (18)	0.0315 (18)	−0.0007 (14)	0.0124 (14)	0.0042 (14)
C12	0.0272 (18)	0.036 (2)	0.0265 (18)	0.0030 (15)	0.0040 (14)	0.0035 (15)
C13	0.0338 (19)	0.035 (2)	0.0239 (18)	0.0005 (15)	0.0061 (14)	−0.0035 (14)
C14	0.0263 (17)	0.0276 (18)	0.0253 (17)	0.0010 (14)	0.0059 (13)	−0.0004 (14)
O1W	0.0406 (15)	0.0385 (16)	0.0343 (14)	−0.0005 (12)	0.0019 (11)	0.0024 (12)

Geometric parameters (Å, º)

O1—C2	1.359 (4)	C5—C6	1.387 (4)
O1—H1O	0.844 (10)	C5—H5	0.9500
O2—C6	1.361 (3)	C7—C8	1.494 (4)
O2—H2O	0.844 (10)	C8—H8A	0.9800
O3—N3	1.242 (3)	C8—H8B	0.9800
O4—N3	1.238 (3)	C8—H8C	0.9800
N1—C7	1.305 (3)	C9—C14	1.407 (4)
N1—N2	1.366 (3)	C9—C10	1.411 (4)
N2—C9	1.370 (4)	C10—C11	1.399 (4)
N2—H2N	0.880 (10)	C11—C12	1.376 (4)
N3—C10	1.445 (4)	C11—H11	0.9500
C1—C6	1.422 (4)	C12—C13	1.381 (4)
C1—C2	1.430 (4)	C12—H12	0.9500
C1—C7	1.483 (4)	C13—C14	1.378 (4)
C2—C3	1.380 (4)	C13—H13	0.9500
C3—C4	1.379 (4)	C14—H14	0.9500
C3—H3	0.9500	O1W—H1W	0.841 (10)
C4—C5	1.377 (4)	O1W—H2W	0.845 (10)
C4—H4	0.9500		

C2—O1—H1O	103 (3)	N1—C7—C8	120.1 (3)
C6—O2—H2O	107 (2)	C1—C7—C8	124.5 (2)
C7—N1—N2	119.1 (3)	C7—C8—H8A	109.5
N1—N2—C9	120.2 (2)	C7—C8—H8B	109.5
N1—N2—H2N	123 (2)	H8A—C8—H8B	109.5
C9—N2—H2N	117 (2)	C7—C8—H8C	109.5
O4—N3—O3	122.0 (3)	H8A—C8—H8C	109.5
O4—N3—C10	119.1 (3)	H8B—C8—H8C	109.5
O3—N3—C10	119.0 (3)	N2—C9—C14	120.6 (3)
C6—C1—C2	115.2 (3)	N2—C9—C10	123.0 (3)
C6—C1—C7	123.8 (3)	C14—C9—C10	116.3 (3)
C2—C1—C7	121.0 (3)	C11—C10—C9	121.5 (3)
O1—C2—C3	116.5 (3)	C11—C10—N3	116.4 (3)
O1—C2—C1	121.0 (3)	C9—C10—N3	122.2 (3)
C3—C2—C1	122.5 (3)	C12—C11—C10	120.5 (3)
C4—C3—C2	119.7 (3)	C12—C11—H11	119.8
C4—C3—H3	120.2	C10—C11—H11	119.8
C2—C3—H3	120.2	C11—C12—C13	118.8 (3)
C3—C4—C5	120.5 (3)	C11—C12—H12	120.6
C3—C4—H4	119.8	C13—C12—H12	120.6
C5—C4—H4	119.8	C14—C13—C12	121.6 (3)
C4—C5—C6	120.5 (3)	C14—C13—H13	119.2
C4—C5—H5	119.8	C12—C13—H13	119.2
C6—C5—H5	119.8	C13—C14—C9	121.3 (3)
O2—C6—C5	119.4 (3)	C13—C14—H14	119.3
O2—C6—C1	118.9 (3)	C9—C14—H14	119.3
C5—C6—C1	121.6 (3)	H1W—O1W—H2W	111 (3)
N1—C7—C1	115.5 (3)		

C7—N1—N2—C9	−178.3 (3)	C6—C1—C7—C8	−7.0 (5)
C6—C1—C2—O1	179.6 (3)	C2—C1—C7—C8	172.1 (3)
C7—C1—C2—O1	0.5 (4)	N1—N2—C9—C14	0.9 (4)
C6—C1—C2—C3	−0.7 (4)	N1—N2—C9—C10	−179.8 (3)
C7—C1—C2—C3	−179.8 (3)	N2—C9—C10—C11	−178.6 (3)
O1—C2—C3—C4	−179.0 (3)	C14—C9—C10—C11	0.7 (4)
C1—C2—C3—C4	1.3 (5)	N2—C9—C10—N3	1.2 (5)
C2—C3—C4—C5	−0.5 (5)	C14—C9—C10—N3	−179.5 (3)
C3—C4—C5—C6	−0.8 (5)	O4—N3—C10—C11	−3.3 (4)
C4—C5—C6—O2	−177.8 (3)	O3—N3—C10—C11	177.0 (3)
C4—C5—C6—C1	1.5 (5)	O4—N3—C10—C9	176.9 (3)
C2—C1—C6—O2	178.6 (3)	O3—N3—C10—C9	−2.8 (4)
C7—C1—C6—O2	−2.3 (4)	C9—C10—C11—C12	0.0 (4)
C2—C1—C6—C5	−0.7 (4)	N3—C10—C11—C12	−179.8 (3)
C7—C1—C6—C5	178.4 (3)	C10—C11—C12—C13	−0.6 (5)
N2—N1—C7—C1	−179.4 (2)	C11—C12—C13—C14	0.4 (5)
N2—N1—C7—C8	1.2 (4)	C12—C13—C14—C9	0.3 (5)
C6—C1—C7—N1	173.6 (3)	N2—C9—C14—C13	178.5 (3)
C2—C1—C7—N1	−7.4 (4)	C10—C9—C14—C13	−0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N1	0.85 (2)	1.69 (2)	2.489 (3)	157 (4)
N2—H2*N*···O3	0.88 (2)	1.93 (2)	2.602 (3)	132 (2)
O2—H2*O*···O1*W*^{i}	0.84 (3)	1.90 (3)	2.742 (3)	174 (2)
O1*W*—H1*W*···O1^{ii}	0.84 (2)	2.08 (3)	2.910 (3)	169 (3)
O1*W*—H2*W*···O4^{iii}	0.85 (3)	2.50 (3)	3.256 (3)	150 (3)
C11—H11···O3^{iv}	0.95	2.52	3.447 (4)	166

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