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Crystal structure and Hirshfeld surface analysis of *N*′-[(1*E*)-1-(3-oxo-3,4-dihydro-2*H*-1,4-benzoxazin-6-yl)ethylidene]benzohydrazide monohydrate

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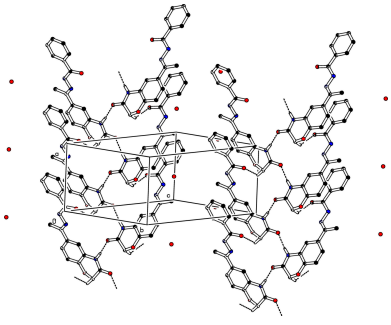
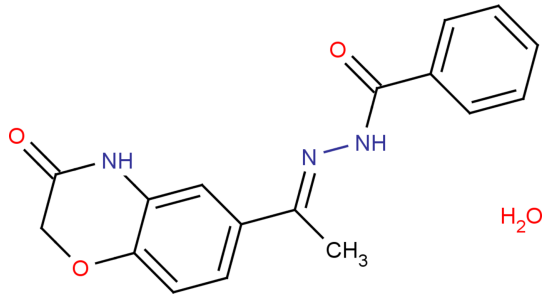
The title compound, $C_{17}H_{15}N_3O_3\cdot H_2O$, a hydrazone derivative, crystallizes with one molecule of water. The morpholine ring adopts a twist-boat conformation. Intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds are responsible for the consolidation of the crystal packing. The intermolecular interactions were quantified using Hirshfeld surface analysis, revealing that H···H interactions contribute most (40.6%) to the crystal packing.

1. Chemical context

Hydrazones, characterized by the —HN—N=C— linkage, are an important class of organic compounds with wide-ranging applications. They are employed as catalysts, bioactive molecules, organic dyes, and liquid crystals, as well as in agriculture as insecticides, sterilants, and herbicides (Meenatchi *et al.*, 2021; Costa *et al.*, 2025; Fuh *et al.*, 2012). Their ability to form hydrogen bonds and coordinate to metal ions enhances their versatility, making them valuable scaffolds in drug design (Karthiga *et al.*, 2025). Hydrazone derivatives also display a wide range of pharmacological activities, including antimicrobial, anticancer, antimalarial, anticonvulsant, and cardioprotective effects, with several already in clinical use. Examples include isoniazid, an essential antitubercular drug, and related analogs such as isocarboxazid, iproniazid, furazolidone, nifuroxazide, nitrofurantoin, and nitrofurazone, which are employed against various diseases. These cases highlight the therapeutic importance of hydrazide/hydrazone derivatives and their relevance in drug discovery (Teneva *et al.*, 2023).





In the context given above, we synthesized a new hydrazone derivative, *N*′-[(1*E*)-1-(3-oxo-3,4-dihydro-2*H*-1,4-benzoxazin-6-yl)ethylidene]benzohydrazide monohydrate, (I), and report

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	1.99	2.847 (3)	173
N3—H3···O1W^{ii}	0.86	2.25	3.037 (3)	152
O1W—H1W···O2^{iii}	0.83 (1)	2.10 (2)	2.925 (3)	169 (5)
O1W—H2W···O3^{iv}	0.83 (1)	2.05 (2)	2.847 (3)	162 (3)
C10—H10B···O1W^{ii}	0.96	2.34	3.200 (3)	150
C17—H17···O1W^{ii}	0.93	2.52	3.228 (3)	133
C1—H1B···O3^{v}	0.97	2.57	3.286 (3)	131
C16—H16···O3^{vi}	0.93	2.58	3.447 (3)	155

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{5}{2}, -z+2$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (iv) $x, y-1, z$; (v) $x-1, y, z$; (vi) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

here its molecular and crystal structure, and the results of a Hirshfeld surface analysis.

2. Structural commentary

The molecular structure of (I) is displayed in Fig. 1. The O2—C2 [1.235 (3) Å], C9—N2 [1.285 (3) Å] and O3—C11 [1.228 (3) Å] bond lengths confirm double-bond character. The morpholine ring adopts a twist-boat conformation with puckering parameters (Cremer & Pople, 1975) q_2 = 0.322 (2) Å, q_3 = 0.141 (2) Å, Q_T = 0.352 (2) Å and φ = 30.8 (3)°. Atom C1 deviates by 0.460 (3) Å from the least-squares plane through the remaining five atoms (O1/C2/N1/C3/C8) of the morpholine ring. The mean-plane calculation of the *N*′-[(1*Z*)-ethyliden]formohydrazide moiety (C9–C10/N2/N3/C11/O3) reveals that the atoms C10 and O3 deviate by 0.1836 (12) and 2.081 (14) Å, respectively, from the plane. This moiety makes a dihedral angle of 2.81 (13)° with respect to the phenyl ring (C12–C17). This phenyl ring and the phenyl ring (C3–C8) fused to the morpholine ring are oriented at a dihedral angle of 5.67 (10)°.

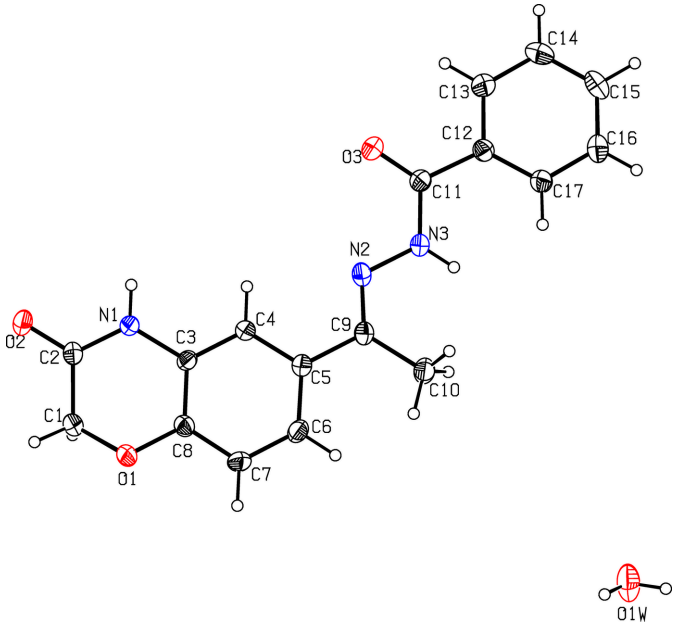

Figure 1
A view of the molecular structure of (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

3. Supramolecular features

In the crystal of (I), the oxygen atom (O1*W*) of the water molecule plays a major role in the crystal packing, acting both as a donor and an acceptor group in intermolecular O—H···O, N—H···O, and C—H···O hydrogen bonds (Table 1). The water molecule O1*W* acts as a trifold acceptor for two C—H···O (C10—H10*B*···O1W^{ii} and C17—H17···O1W^{ii}) and one N3—H3···O1W^{ii} hydrogen bond (Fig. 2). It is a donor for two O—H···O hydrogen bonds (O1*W*—H1*W*···O2^{v} and O1*W*—H2*W*···O3^{vi}; Fig. 3). Molecules associate further into $C(4)$ chains by N1—H1···O2^{i} hydrogen bonds running parallel to [100]. In addition, C16—H16···O3^{iv} hydrogen bonds form $C(6)$ chains running parallel to [110] (Fig. 4).

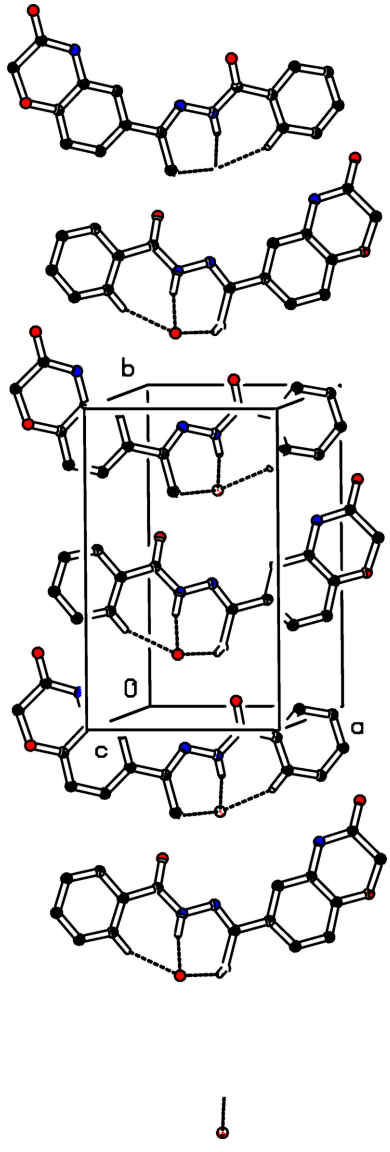

Figure 2
The crystal packing of (I) with N—H···O and C—H···O hydrogen bonds to the solvent water molecule as an acceptor shown as dashed lines. For clarity, H atoms not involved in these hydrogen bonds have been omitted.

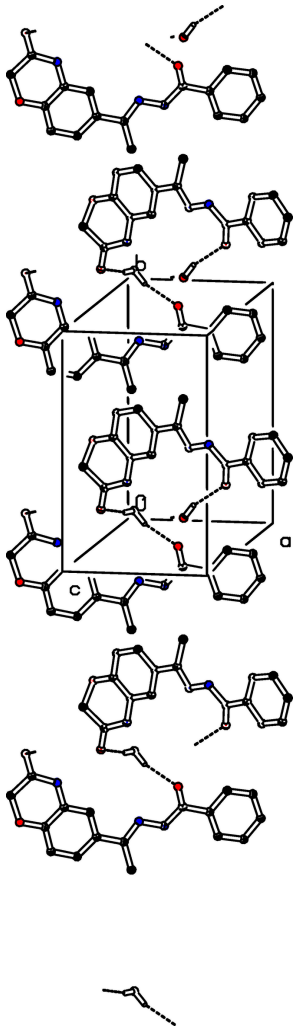

Figure 3
The crystal packing of (I) with O—H···O hydrogen bonds involving the water solvent molecule as a donor shown as dashed lines. For clarity, H atoms not involved in these hydrogen bonds have been omitted.

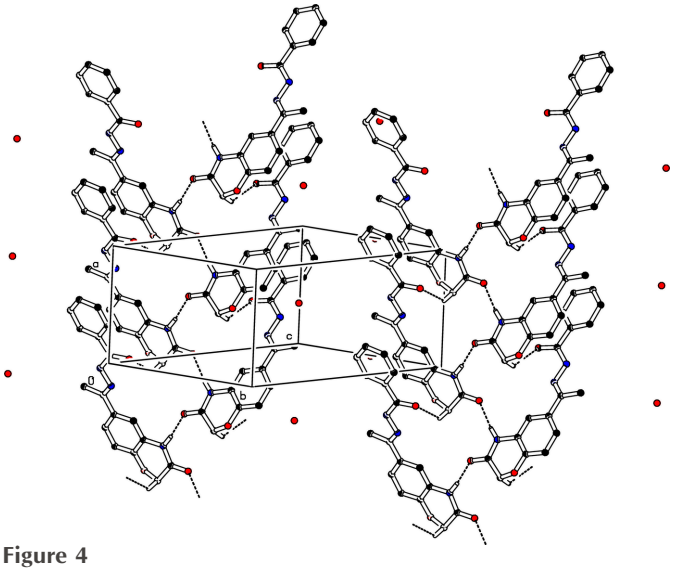

Figure 4
The crystal packing of (I) with N—H···O and C—H···O hydrogen bonds shown as dashed lines. For clarity, H atoms not involved in these hydrogen bonds have been omitted.

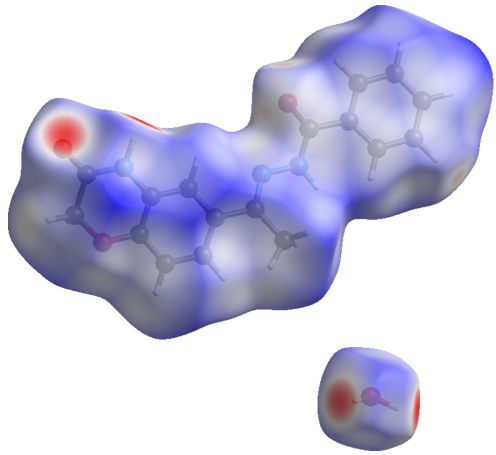

Figure 5
A view of the Hirshfeld surface mapped over d_{norm} for compound (I).

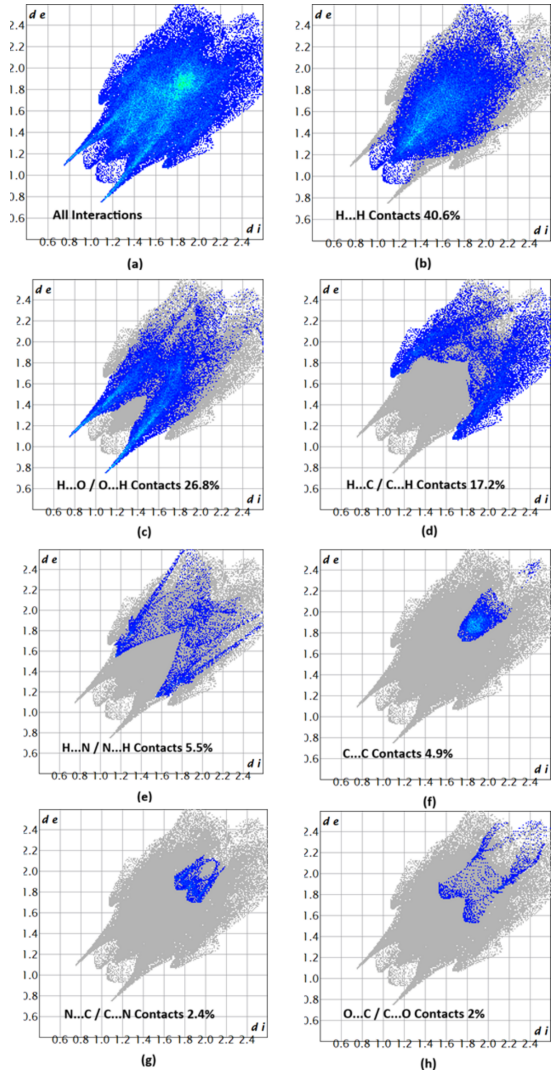

Figure 6
Two-dimensional fingerprint plots for (I), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···O/O···H, (*d*) H···C/C···H, (*e*) H···N/N···H (*f*)C···C, (*g*) N···C/C···N and (*h*) O···C/C···O interactions with the corresponding percentages contribution. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

4. Hirshfeld surface analysis

To further characterize and quantify the intermolecular interactions in the title compound, a Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was carried out using *CrystalExplorer* (Spackman *et al.*, 2021). The HS mapped over d_{norm} is illustrated in Fig. 5 where the deep-red spots at O2, O3, O1*W* and H1 are indicative of the intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds discussed above.

The associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) are displayed in Fig. 6. They provide quantitative information about the non-covalent interactions in the crystal packing in terms of the percentage contribution of the interatomic contacts (Spackman & McKinnon, 2002). The HS analysis revealed that H···H and H···O/O···H contacts are the main contributors to the crystal packing, followed by H···C/C···H, H···N/N···H, C···C, N···C/C···N and O···C/C···O contacts.

5. Synthesis and crystallization

A mixture of 4-benzohydrazide (2 mmol) and 6-acetyl-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one (2 mmol) was dissolved in methanol (25 ml) containing a few drops of glacial acetic acid to obtain a clear solution. The reaction mixture was transferred to a round-bottom flask and refluxed for 3 h with continuous stirring. The progress of the reaction was monitored by thin-layer chromatography (TLC). Upon completion, the solvent was removed under reduced pressure, affording a solid residue. The crude product was collected, washed with cold methanol to remove impurities, and subsequently recrystallized from hot methanol to yield a pure product of (I).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms H1*W* and H2*W* were located in a difference-Fourier map and freely refined. Other H atoms were placed in idealized positions and allowed to ride on their parent atoms with N—H = 0.86 Å and C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C or N) for other H atoms.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{15}N_3O_3{\cdot}H_2O$
M_r	327.33
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	299
a, b, c (Å)	7.4104 (3), 12.2781 (5), 17.3257 (7)
V (Å^3)	1576.39 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.27 × 0.13 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.974, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15825, 3894, 2868
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.111, 1.05
No. of reflections	3894
No. of parameters	226
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.25
Absolute structure	Refined as an inversion twin
Absolute structure parameter	−0.4 (15)

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

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Crystal structure and Hirshfeld surface analysis of *N*′-[(1*E*)-1-(3-oxo-3,4-dihydro-2*H*-1,4-benzoxazin-6-yl)ethylidene]benzohydrazide monohydrate

Sekar Janarthanan, Ganesan Meenambigai, Velayutham Mahalakshmi, Manivel Kavitha, Rajendran Arivu Selvan, Srinivasan Pazhamalai and Sivashanmugam Selvanayagam

Computing details

N′-[(1*E*)-1-(3-Oxo-3,4-dihydro-2*H*-1,4-benzoxazin-6-yl)ethylidene]benzohydrazide monohydrate

Crystal data

$C_{17}H_{15}N_3O_3·H_2O$
M_r = 327.33
Orthorhombic, $P2_12_12_1$
a = 7.4104 (3) Å
b = 12.2781 (5) Å
c = 17.3257 (7) Å
V = 1576.39 (11) Å^3
Z = 4
$F(000)$ = 688
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5917 reflections
θ = 3.0–23.2°
μ = 0.10 mm^{-1}
T = 299 K
Block, colourless
0.27 × 0.13 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: i-mu-s microfocus source
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.974, T_{max} = 0.988
15825 measured reflections
3894 independent reflections
2868 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −9→7
k = −16→16
l = −23→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.05
3894 reflections
226 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: −0.4 (15)

Special details

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. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
H1W	0.377 (7)	0.224 (4)	0.8703 (13)	0.17 (2)*
H2W	0.486 (4)	0.1690 (19)	0.822 (2)	0.080 (11)*
O1	−0.2896 (2)	0.95271 (12)	1.00996 (10)	0.0477 (5)
O2	−0.2428 (2)	1.24134 (13)	1.02249 (10)	0.0469 (5)
O3	0.7149 (2)	1.07637 (13)	0.81266 (10)	0.0495 (5)
N1	−0.0451 (3)	1.11560 (15)	0.98123 (11)	0.0371 (5)
H1	0.041324	1.162300	0.982514	0.044*
N2	0.4543 (3)	0.93097 (16)	0.83363 (11)	0.0398 (5)
N3	0.6079 (3)	0.90671 (16)	0.79078 (12)	0.0408 (5)
H3	0.623173	0.843446	0.770503	0.049*
C1	−0.3546 (3)	1.06120 (19)	0.99967 (15)	0.0414 (6)
H1A	−0.443263	1.076619	1.039357	0.050*
H1B	−0.414913	1.065928	0.950101	0.050*
C2	−0.2091 (3)	1.14674 (18)	1.00297 (12)	0.0347 (5)
C3	−0.0077 (3)	1.00879 (18)	0.95616 (13)	0.0318 (5)
C4	0.1523 (3)	0.98296 (18)	0.91927 (13)	0.0347 (5)
H4	0.235910	1.037560	0.909001	0.042*
C5	0.1897 (3)	0.87617 (17)	0.89736 (12)	0.0327 (5)
C6	0.0621 (4)	0.79616 (19)	0.91380 (14)	0.0397 (6)
H6	0.085751	0.724151	0.900581	0.048*
C7	−0.1005 (4)	0.82224 (19)	0.94971 (14)	0.0413 (6)
H7	−0.185698	0.768344	0.959433	0.050*
C8	−0.1339 (3)	0.92836 (19)	0.97067 (13)	0.0350 (5)
C9	0.3590 (3)	0.84945 (18)	0.85609 (12)	0.0334 (5)
C10	0.4065 (4)	0.73195 (19)	0.84311 (15)	0.0502 (7)
H10A	0.314605	0.686455	0.865158	0.075*
H10B	0.414957	0.718030	0.788712	0.075*
H10C	0.520253	0.716270	0.867180	0.075*
C11	0.7324 (3)	0.98662 (18)	0.78224 (13)	0.0369 (5)
C12	0.8963 (3)	0.95828 (19)	0.73614 (13)	0.0353 (5)
C13	1.0105 (4)	1.0435 (2)	0.71613 (18)	0.0551 (7)
H13	0.980509	1.114507	0.729847	0.066*
C14	1.1677 (4)	1.0237 (3)	0.6761 (2)	0.0665 (9)
H14	1.242362	1.081437	0.662510	0.080*
C15	1.2150 (4)	0.9196 (3)	0.65617 (15)	0.0544 (7)
H15	1.321087	0.906665	0.628974	0.065*
C16	1.1054 (3)	0.8348 (2)	0.67653 (15)	0.0477 (7)
H16	1.137637	0.763970	0.663540	0.057*

C17	0.9464 (3)	0.85385 (19)	0.71639 (14)	0.0405 (6)
H17	0.872727	0.795578	0.729944	0.049*
O1W	0.4179 (3)	0.22231 (19)	0.82551 (14)	0.0727 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0415 (10)	0.0359 (9)	0.0657 (11)	−0.0009 (8)	0.0243 (9)	0.0007 (8)
O2	0.0432 (11)	0.0365 (9)	0.0609 (11)	0.0090 (8)	0.0028 (9)	−0.0107 (8)
O3	0.0499 (11)	0.0332 (9)	0.0655 (11)	0.0002 (9)	0.0116 (10)	−0.0081 (8)
N1	0.0282 (11)	0.0305 (10)	0.0525 (12)	−0.0007 (8)	0.0022 (9)	−0.0086 (9)
N2	0.0338 (11)	0.0396 (11)	0.0459 (11)	0.0059 (10)	0.0052 (10)	−0.0066 (9)
N3	0.0353 (11)	0.0340 (10)	0.0530 (12)	0.0025 (9)	0.0080 (10)	−0.0084 (9)
C1	0.0320 (12)	0.0417 (13)	0.0505 (14)	0.0008 (11)	0.0068 (12)	−0.0059 (12)
C2	0.0331 (12)	0.0365 (12)	0.0346 (11)	0.0048 (10)	0.0010 (11)	−0.0033 (10)
C3	0.0330 (13)	0.0270 (11)	0.0353 (12)	−0.0004 (10)	−0.0015 (10)	−0.0031 (10)
C4	0.0294 (12)	0.0310 (12)	0.0436 (12)	−0.0006 (10)	0.0015 (11)	−0.0026 (10)
C5	0.0346 (13)	0.0326 (11)	0.0309 (11)	0.0035 (10)	0.0005 (10)	0.0001 (9)
C6	0.0487 (15)	0.0281 (11)	0.0424 (13)	0.0019 (11)	0.0061 (13)	−0.0024 (10)
C7	0.0443 (15)	0.0320 (12)	0.0478 (14)	−0.0075 (12)	0.0078 (12)	0.0027 (10)
C8	0.0339 (13)	0.0364 (12)	0.0347 (11)	0.0008 (11)	0.0056 (10)	0.0005 (10)
C9	0.0359 (12)	0.0348 (12)	0.0294 (11)	0.0058 (11)	0.0008 (10)	−0.0014 (9)
C10	0.0559 (17)	0.0370 (14)	0.0577 (16)	0.0071 (13)	0.0198 (14)	0.0021 (12)
C11	0.0373 (13)	0.0322 (12)	0.0412 (12)	0.0016 (11)	0.0013 (11)	0.0020 (11)
C12	0.0336 (13)	0.0372 (13)	0.0350 (12)	0.0021 (11)	−0.0008 (10)	0.0020 (10)
C13	0.0529 (17)	0.0391 (15)	0.0731 (19)	−0.0037 (13)	0.0170 (16)	−0.0023 (14)
C14	0.0474 (18)	0.0582 (19)	0.094 (2)	−0.0145 (15)	0.0197 (17)	0.0046 (17)
C15	0.0351 (14)	0.073 (2)	0.0551 (16)	0.0064 (15)	0.0101 (13)	0.0020 (15)
C16	0.0444 (15)	0.0497 (15)	0.0492 (15)	0.0128 (14)	0.0014 (13)	−0.0043 (12)
C17	0.0373 (14)	0.0368 (13)	0.0476 (14)	0.0018 (12)	0.0029 (12)	0.0026 (11)
O1W	0.0842 (16)	0.0697 (15)	0.0643 (13)	0.0362 (14)	0.0257 (13)	0.0160 (12)

Geometric parameters (Å, º)

O1—C8	1.373 (3)	C6—H6	0.9300
O1—C1	1.427 (3)	C7—C8	1.375 (3)
O2—C2	1.235 (3)	C7—H7	0.9300
O3—C11	1.228 (3)	C9—C10	1.502 (3)
N1—C2	1.329 (3)	C10—H10A	0.9600
N1—C3	1.409 (3)	C10—H10B	0.9600
N1—H1	0.8600	C10—H10C	0.9600
N2—C9	1.285 (3)	C11—C12	1.495 (3)
N2—N3	1.391 (3)	C12—C17	1.378 (3)
N3—C11	1.355 (3)	C12—C13	1.390 (3)
N3—H3	0.8600	C13—C14	1.378 (4)
C1—C2	1.506 (3)	C13—H13	0.9300
C1—H1A	0.9700	C14—C15	1.369 (4)
C1—H1B	0.9700	C14—H14	0.9300

C3—C8	1.383 (3)	C15—C16	1.367 (4)
C3—C4	1.384 (3)	C15—H15	0.9300
C4—C5	1.393 (3)	C16—C17	1.385 (4)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.393 (3)	C17—H17	0.9300
C5—C9	1.481 (3)	O1W—H1W	0.834 (13)
C6—C7	1.393 (4)	O1W—H2W	0.831 (13)

C8—O1—C1	115.12 (17)	O1—C8—C3	120.2 (2)
C2—N1—C3	122.4 (2)	C7—C8—C3	120.5 (2)
C2—N1—H1	118.8	N2—C9—C5	116.0 (2)
C3—N1—H1	118.8	N2—C9—C10	125.1 (2)
C9—N2—N3	116.36 (18)	C5—C9—C10	118.9 (2)
C11—N3—N2	117.42 (19)	C9—C10—H10A	109.5
C11—N3—H3	121.3	C9—C10—H10B	109.5
N2—N3—H3	121.3	H10A—C10—H10B	109.5
O1—C1—C2	113.9 (2)	C9—C10—H10C	109.5
O1—C1—H1A	108.8	H10A—C10—H10C	109.5
C2—C1—H1A	108.8	H10B—C10—H10C	109.5
O1—C1—H1B	108.8	O3—C11—N3	122.0 (2)
C2—C1—H1B	108.8	O3—C11—C12	121.6 (2)
H1A—C1—H1B	107.7	N3—C11—C12	116.3 (2)
O2—C2—N1	122.2 (2)	C17—C12—C13	118.4 (2)
O2—C2—C1	121.4 (2)	C17—C12—C11	124.6 (2)
N1—C2—C1	116.31 (19)	C13—C12—C11	116.9 (2)
C8—C3—C4	120.0 (2)	C14—C13—C12	120.4 (3)
C8—C3—N1	118.4 (2)	C14—C13—H13	119.8
C4—C3—N1	121.6 (2)	C12—C13—H13	119.8
C3—C4—C5	120.8 (2)	C15—C14—C13	120.6 (3)
C3—C4—H4	119.6	C15—C14—H14	119.7
C5—C4—H4	119.6	C13—C14—H14	119.7
C4—C5—C6	118.2 (2)	C16—C15—C14	119.5 (3)
C4—C5—C9	120.6 (2)	C16—C15—H15	120.2
C6—C5—C9	121.2 (2)	C14—C15—H15	120.2
C7—C6—C5	121.1 (2)	C15—C16—C17	120.4 (2)
C7—C6—H6	119.5	C15—C16—H16	119.8
C5—C6—H6	119.5	C17—C16—H16	119.8
C8—C7—C6	119.4 (2)	C12—C17—C16	120.6 (2)
C8—C7—H7	120.3	C12—C17—H17	119.7
C6—C7—H7	120.3	C16—C17—H17	119.7
O1—C8—C7	119.2 (2)	H1W—O1W—H2W	108 (4)

C9—N2—N3—C11	−164.5 (2)	N1—C3—C8—C7	−177.7 (2)
C8—O1—C1—C2	−43.3 (3)	N3—N2—C9—C5	−176.25 (18)
C3—N1—C2—O2	−177.5 (2)	N3—N2—C9—C10	3.4 (3)
C3—N1—C2—C1	0.2 (3)	C4—C5—C9—N2	−8.7 (3)
O1—C1—C2—O2	−153.8 (2)	C6—C5—C9—N2	169.9 (2)
O1—C1—C2—N1	28.4 (3)	C4—C5—C9—C10	171.7 (2)

C2—N1—C3—C8	−14.6 (3)	C6—C5—C9—C10	−9.7 (3)
C2—N1—C3—C4	166.7 (2)	N2—N3—C11—O3	2.1 (3)
C8—C3—C4—C5	−0.9 (3)	N2—N3—C11—C12	179.84 (18)
N1—C3—C4—C5	177.7 (2)	O3—C11—C12—C17	163.5 (2)
C3—C4—C5—C6	−0.2 (3)	N3—C11—C12—C17	−14.2 (3)
C3—C4—C5—C9	178.4 (2)	O3—C11—C12—C13	−12.5 (3)
C4—C5—C6—C7	1.3 (3)	N3—C11—C12—C13	169.7 (2)
C9—C5—C6—C7	−177.3 (2)	C17—C12—C13—C14	1.3 (4)
C5—C6—C7—C8	−1.3 (4)	C11—C12—C13—C14	177.6 (3)
C1—O1—C8—C7	−153.1 (2)	C12—C13—C14—C15	−0.7 (5)
C1—O1—C8—C3	30.4 (3)	C13—C14—C15—C16	−0.3 (5)
C6—C7—C8—O1	−176.3 (2)	C14—C15—C16—C17	0.6 (4)
C6—C7—C8—C3	0.1 (4)	C13—C12—C17—C16	−1.0 (4)
C4—C3—C8—O1	177.4 (2)	C11—C12—C17—C16	−176.9 (2)
N1—C3—C8—O1	−1.3 (3)	C15—C16—C17—C12	0.0 (4)
C4—C3—C8—C7	1.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	1.99	2.847 (3)	173
N3—H3···O1*W*^{ii}	0.86	2.25	3.037 (3)	152
O1*W*—H1*W*···O2^{iii}	0.83 (1)	2.10 (2)	2.925 (3)	169 (5)
O1*W*—H2*W*···O3^{iv}	0.83 (1)	2.05 (2)	2.847 (3)	162 (3)
C10—H10*B*···O1*W*^{ii}	0.96	2.34	3.200 (3)	150
C17—H17···O1*W*^{ii}	0.93	2.52	3.228 (3)	133
C1—H1*B*···O3^{v}	0.97	2.57	3.286 (3)	131
C16—H16···O3^{vi}	0.93	2.58	3.447 (3)	155

Symmetry codes: (i) *x*+1/2, −*y*+5/2, −*z*+2; (ii) −*x*+1, *y*+1/2, −*z*+3/2; (iii) *x*+1/2, −*y*+3/2, −*z*+2; (iv) *x*, *y*−1, *z*; (v) *x*−1, *y*, *z*; (vi) −*x*+2, *y*−1/2, −*z*+3/2.