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Crystal structure, Hirshfeld surface analysis and DFT studies of 4-amino-*N*′-[(1*E*)-1-(3-hydroxyphenyl)ethylidene]benzohydrazide

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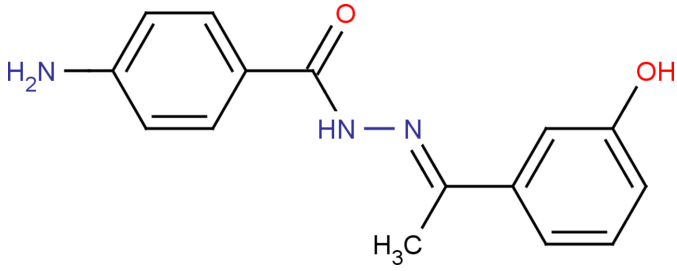
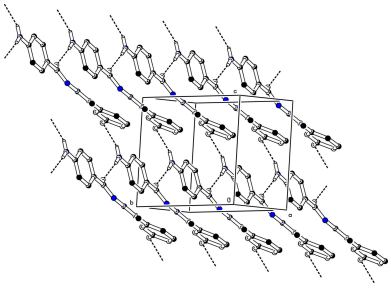
In the title compound, $C_{15}H_{15}N_3O_2$, (**I**), the aniline and phenol rings form a dihedral angle of 62.1 (1)°. Intermolecular N—H···O and O—H···O hydrogen bonds lead to the formation of sheets extending parallel to (010). Intermolecular interactions were quantified and analysed using Hirshfeld surface analysis, revealing that H···H interactions contribute most to the crystal packing (42.2%). The molecular structure was optimized by density functional theory (DFT) at the B3LYP/6–31 G(d,p) level and was compared with the experimentally determined molecular structure in the solid state.

1. Chemical context

Hydrazones have been found to show various biological properties, including antioxidant (Belkheiri *et al.*, 2010), anti-inflammatory (Radwan *et al.*, 2007) and anticancer (Kumar *et al.*, 2012) effects.



In the present work, the synthesis, structural and computational studies of another hydrozone, 4-amino-*N*′-[(1*E*)-1-(3-hydroxyphenyl)ethylidene]benzohydrazide, (**I**), is reported.



2. Structural commentary

The molecular structure of (**I**) is displayed in Fig. 1. The aniline ring (C1–C6/N1) is planar with a maximum deviation of 0.023 (1) Å for atom N1. Likewise, the phenol ring (C10–C15/O2) is planar with a maximum deviation of 0.003 (2) Å for atom C12. These two rings are oriented at a dihedral angle of 62.1 (1)°. The least-squares plane calculation of the *N*′-[(1*E*)-ethylidene]formohydrazide moiety (C7/O1/N2/N3/C8/C9) reveals that this part of the molecule is nearly planar with a maximum deviation of −0.223 (1) Å for atom O1. This moiety forms dihedral angles of 36.5 (1) and 25.6 (1)°, respectively, with respect to the aniline and phenol rings.

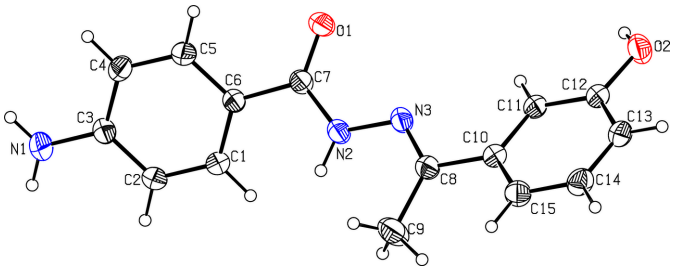


Figure 1
The molecular structure of (**I**) with displacement ellipsoids drawn at the 30% probability level.

3. Supramolecular features

In the crystal, molecules associate pairwise *via* O2—H2···O1^{i} hydrogen bonds (Table 1) into inversion dimers with an R_2^2 (20) graph-set motif (Etter *et al.*, 1990), as shown in Fig. 2.

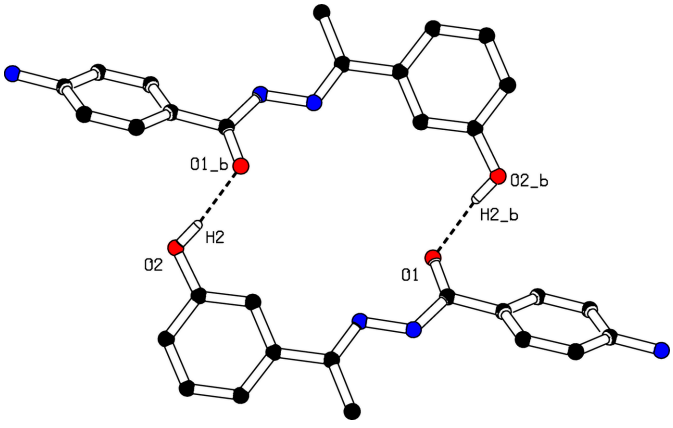


Figure 2
The formation of a centrosymmetric dimer in the crystal structure of (**I**) through O—H···O hydrogen bonds. [Symmetry code: (*b*) $-x+1, -y+2, -z$.]

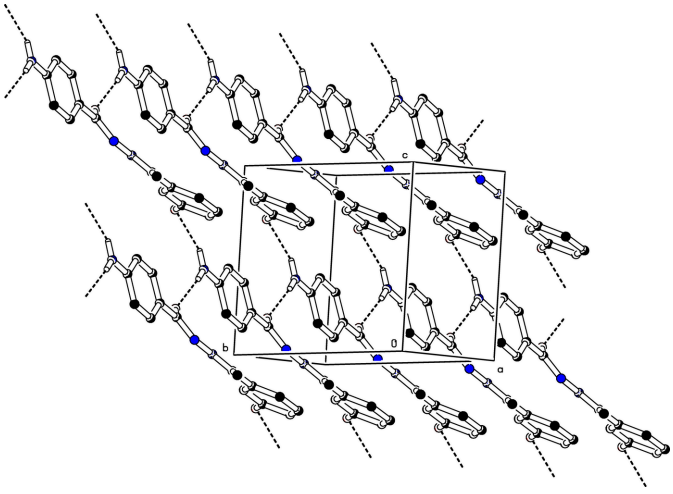


Figure 3
Intermolecular N—H···O and O—H···O hydrogen bonds in (**I**) shown as dashed lines. For clarity, H atoms not involved in these hydrogen bonds have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.88	2.694 (2)	171
N1—H1*B*···O1^{ii}	0.86	2.13	2.958 (2)	162
N1—H1*A*···O2^{iii}	0.86	2.37	3.119 (2)	146

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

Molecules are further linked into a *C*(14) chain motif by N1—H1*A*···O2^{iii} hydrogen bonds running parallel to [100], and by N1—H1*B*···O1^{ii} hydrogen bonds into a *C*(8) chain motif running along [102] (Table 1; Fig. 3). Taken together, these interactions lead to a layered arrangement parallel to (010). It is interesting to note that the amine function (N2—H2*A*) is not involved in any intermolecular interactions.

4. Hirshfeld surface analysis

To further characterize the intermolecular interactions in (**I**), 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. 4, showing the aforementioned hydrogen-bonding interactions as red-colored areas.

The associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) 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 overall two-dimensional fingerprint plot is shown in Fig. 5*a*. The HS analysis reveals that H···H and H···C/C···H contacts are the main contributors to the crystal packing, followed by H···O/O···H, N···H/H···N and C···N/N···C contacts; see Fig. 5*b*–*f*. The HS analysis confirms the importance of H-atom contacts in establishing the packing (Hathwar *et al.*, 2015).

5. DFT Studies

The optimized structure of (**I**) in the gas phase was computed with *Gaussian09W* using the B3LYP/6–31G (d, p) basis set and generated by *GaussView5.0* (Frisch *et al.*, 2009). Comparison of experimentally determined bond lengths and angles (present single-crystal X-ray study) with those of theoretical

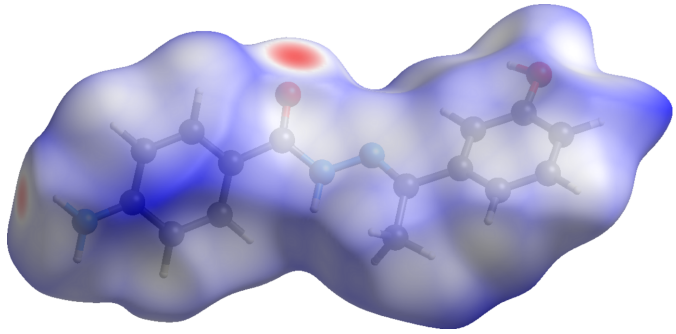


Figure 4
The Hirshfeld surface mapped for (**I**) over d_{norm}.

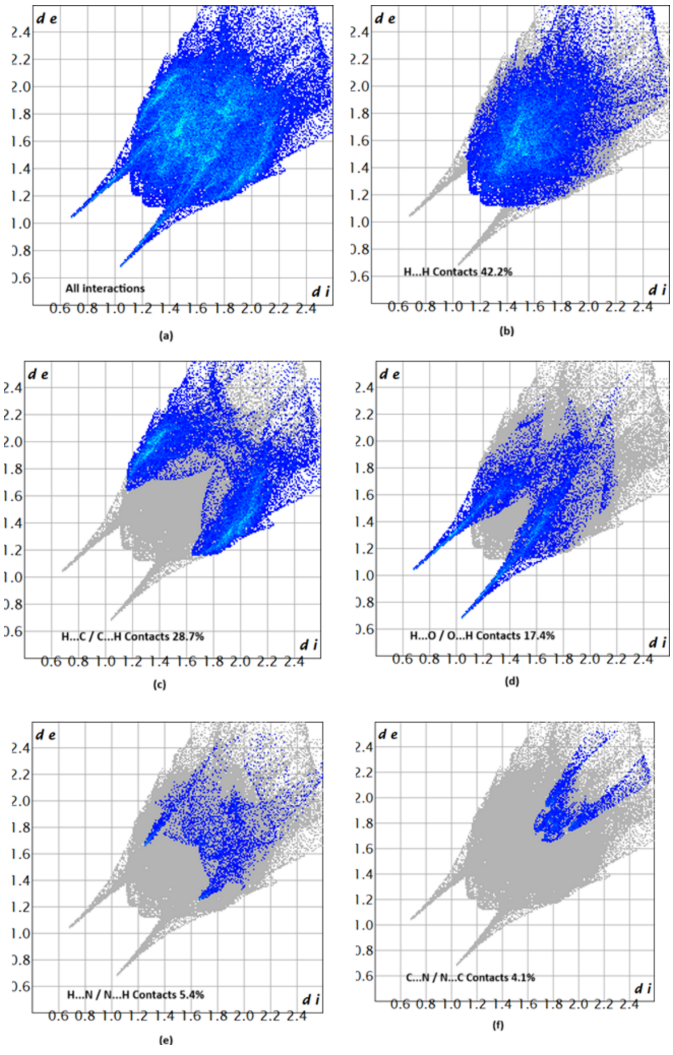


Figure 5
Two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···C/C···H, (*d*) H···O/O···H, (*e*) H···N/N···H and (*f*) N···C/C···N interactions with their relative contributions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

values from the optimized structure showed good agreement [electronic supporting information (ESI), Table S1; the optimized molecular structure of (**I**) is shown in ESI as Fig. S1].

HOMO and LUMO (Fig. 6) were generated and their energies were evaluated from the optimized structure. The biological activity may also be comprehended by using the value of ΔE (Gulsevensidir *et al.*, 2011), which can be used to correlate and understand a decreased toxicity, longer half-life, and sustained activity. Therefore, it is anticipated that molecule (**I**) with ΔE = 4.395 eV might have a strong biological influence with low adverse effects.

The molecular electrostatic potential surface (MEPS; Fig. 7) is used to find the positive and negative electrostatic potential of the molecule, which provides possible information about its reactive sites with regard to chemical processes and binding sites for certain biological entities. The red-colored areas on the MEPS of (**I**) above the carbonyl oxygen atom of the

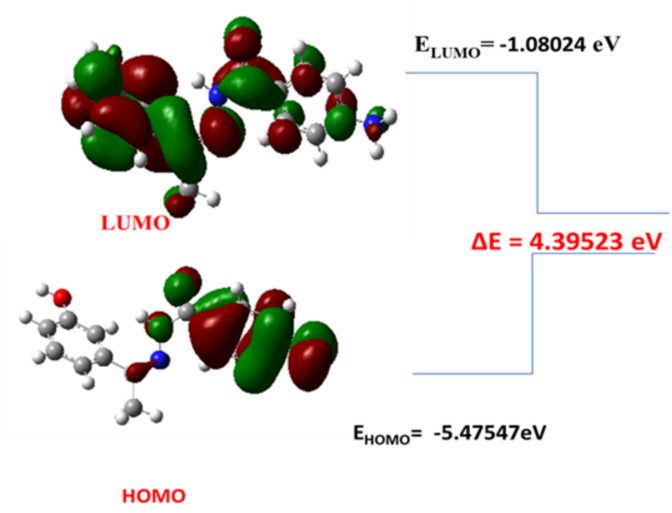


Figure 6
The HOMO/LUMO energy diagram of (**I**).

azonitrile nitrogen moiety, which is likely to undergo electrophilic attack, indicate the electron-rich portion with a partial negative charge. The mild-blue coloration of (**I**) suggests that there are slight electron-deficient regions. The lack of a bright-blue area on the MEPS indicates that the molecule has no potential nucleophilic attack sites. The pale-blue color of the phenyl rings indicate weak electrophilic sites.

6. Synthesis and crystallization

4-Aminobenzohydrazide (2 mmol) and the corresponding substituted aromatic ketone (2 mmol) were dissolved in 25 ml of methanol, along with a few drops of acetic acid, to give a clear solution. The reaction mixture was filled in a round bottom flask and refluxed on a water bath for about 4 h. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction, methanol was removed by vacuum distillation. The solid product was collected, washed, and recrystallized from methanol to obtain a pure product of (**I**).

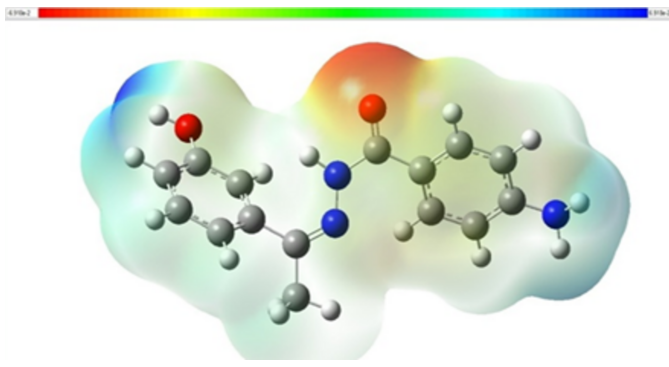


Figure 7
The molecular electrostatic potential surface (MEPS) of (**I**).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atom H2*A* was located from a difference-Fourier map; all other H atoms were placed in idealized positions and allowed to ride on their parent atoms with O—H = 0.82, N—H = 0.86 and C—H = 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C)(C or N or O).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{15}N_3O_2$
M_r	269.30
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	298
a, b, c (Å)	8.3562 (4), 9.2666 (4), 9.9151 (4)
α, β, γ (°)	76.685 (2), 65.316 (1), 84.909 (2)
V (Å^3)	678.83 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.33 × 0.29 × 0.17
Data collection	
Diffractometer	Bruker D8 Quest XRD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13112, 3420, 2620
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.707
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.134, 1.05
No. of reflections	3420
No. of parameters	186
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.15

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

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Crystal structure, Hirshfeld surface analysis and DFT studies of 4-amino-*N*′-[(1*E*)-1-(3-hydroxyphenyl)ethylidene]benzohydrazide

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Computing details

4-Amino-*N*′-[(1*E*)-1-(3-hydroxyphenyl)ethylidene]benzohydrazide

Crystal data

$C_{15}H_{15}N_3O_2$
$M_r = 269.30$
Triclinic, $P\overline{1}$
$a = 8.3562$ (4) Å
$b = 9.2666$ (4) Å
$c = 9.9151$ (4) Å
$\alpha = 76.685$ (2)°
$\beta = 65.316$ (1)°
$\gamma = 84.909$ (2)°
$V = 678.83$ (5) Å^3
$Z = 2$
$F(000) = 284$
$D_x = 1.318$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5917 reflections
$\theta = 2.7$–29.3°
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colorless
0.33 × 0.29 × 0.17 mm

Data collection

Bruker D8 Quest XRD diffractometer
Detector resolution: 7.3910 pixels mm^{-1}
ω and Phi Scans scans
13112 measured reflections
3420 independent reflections
2620 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 30.2°$, $\theta_{min} = 2.7°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.134$
$S = 1.05$
3420 reflections
186 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.2093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.15425 (14)	0.90009 (13)	0.19913 (13)	0.0525 (3)
O2	0.99259 (14)	0.84728 (15)	−0.28575 (16)	0.0642 (4)
H2	0.939270	0.922396	−0.261740	0.096*
N1	−0.67521 (18)	0.83831 (19)	0.41445 (18)	0.0646 (4)
H1A	−0.730474	0.838506	0.509568	0.078*
H1B	−0.733195	0.836403	0.360773	0.078*
N2	0.14917 (16)	0.77285 (15)	0.03196 (16)	0.0470 (3)
N3	0.33033 (15)	0.76091 (14)	−0.03496 (14)	0.0449 (3)
C1	−0.22296 (19)	0.83740 (17)	0.12941 (16)	0.0432 (3)
H1	−0.164218	0.833788	0.027285	0.052*
C2	−0.4043 (2)	0.83844 (17)	0.19445 (17)	0.0456 (3)
H2B	−0.466420	0.837429	0.135719	0.055*
C3	−0.49542 (19)	0.84101 (17)	0.34866 (18)	0.0449 (3)
C4	−0.3979 (2)	0.84413 (19)	0.43329 (17)	0.0490 (4)
H4	−0.456202	0.844926	0.536114	0.059*
C5	−0.2173 (2)	0.84603 (18)	0.36659 (17)	0.0465 (4)
H5	−0.155097	0.850317	0.424490	0.056*
C6	−0.12531 (18)	0.84166 (16)	0.21355 (16)	0.0395 (3)
C7	0.06932 (19)	0.84259 (16)	0.14849 (17)	0.0413 (3)
C8	0.38915 (19)	0.66826 (16)	−0.12234 (17)	0.0430 (3)
C9	0.2747 (2)	0.5749 (3)	−0.1523 (3)	0.0787 (7)
H9A	0.347537	0.514173	−0.221098	0.118*
H9B	0.199464	0.512823	−0.058500	0.118*
H9C	0.204057	0.638171	−0.196627	0.118*
C10	0.58360 (19)	0.65143 (16)	−0.19348 (16)	0.0406 (3)
C11	0.69503 (19)	0.76129 (16)	−0.20501 (16)	0.0417 (3)
H11	0.647841	0.846282	−0.168357	0.050*
C12	0.87624 (19)	0.74403 (17)	−0.27108 (17)	0.0449 (3)
C13	0.9479 (2)	0.61656 (19)	−0.32493 (18)	0.0488 (4)
H13	1.069377	0.604830	−0.368656	0.059*
C14	0.8379 (2)	0.50825 (18)	−0.31303 (19)	0.0507 (4)
H14	0.885554	0.422900	−0.348736	0.061*
C15	0.6570 (2)	0.52448 (17)	−0.24861 (19)	0.0495 (4)
H15	0.584065	0.450565	−0.242003	0.059*
H2A	0.082 (2)	0.730 (2)	0.005 (2)	0.068 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0408 (6)	0.0658 (7)	0.0606 (7)	0.0009 (5)	−0.0226 (5)	−0.0283 (6)
O2	0.0385 (6)	0.0698 (8)	0.0813 (9)	−0.0062 (5)	−0.0078 (6)	−0.0407 (7)
N1	0.0364 (7)	0.0989 (12)	0.0575 (9)	−0.0049 (7)	−0.0141 (6)	−0.0225 (8)
N2	0.0338 (6)	0.0549 (7)	0.0551 (8)	−0.0020 (5)	−0.0144 (6)	−0.0237 (6)
N3	0.0333 (6)	0.0503 (7)	0.0497 (7)	−0.0023 (5)	−0.0125 (5)	−0.0159 (6)
C1	0.0427 (8)	0.0501 (8)	0.0379 (7)	−0.0027 (6)	−0.0150 (6)	−0.0128 (6)

C2	0.0427 (8)	0.0545 (9)	0.0457 (8)	−0.0019 (6)	−0.0219 (6)	−0.0139 (7)
C3	0.0369 (7)	0.0491 (8)	0.0473 (8)	−0.0025 (6)	−0.0150 (6)	−0.0108 (7)
C4	0.0442 (8)	0.0635 (10)	0.0363 (7)	0.0002 (7)	−0.0132 (6)	−0.0110 (7)
C5	0.0429 (8)	0.0586 (9)	0.0420 (8)	0.0002 (7)	−0.0201 (6)	−0.0128 (7)
C6	0.0361 (7)	0.0415 (7)	0.0411 (7)	−0.0018 (5)	−0.0146 (6)	−0.0108 (6)
C7	0.0381 (7)	0.0416 (7)	0.0448 (8)	−0.0014 (6)	−0.0169 (6)	−0.0100 (6)
C8	0.0406 (7)	0.0448 (7)	0.0455 (8)	−0.0011 (6)	−0.0173 (6)	−0.0133 (6)
C9	0.0488 (10)	0.0951 (15)	0.1132 (18)	0.0044 (10)	−0.0324 (11)	−0.0646 (14)
C10	0.0405 (7)	0.0435 (7)	0.0380 (7)	−0.0002 (6)	−0.0148 (6)	−0.0114 (6)
C11	0.0403 (7)	0.0446 (7)	0.0395 (7)	0.0009 (6)	−0.0121 (6)	−0.0163 (6)
C12	0.0403 (8)	0.0535 (8)	0.0409 (7)	−0.0024 (6)	−0.0120 (6)	−0.0181 (7)
C13	0.0397 (8)	0.0589 (9)	0.0464 (8)	0.0053 (7)	−0.0122 (6)	−0.0210 (7)
C14	0.0525 (9)	0.0457 (8)	0.0519 (9)	0.0074 (7)	−0.0159 (7)	−0.0198 (7)
C15	0.0503 (9)	0.0441 (8)	0.0542 (9)	−0.0023 (6)	−0.0176 (7)	−0.0168 (7)

Geometric parameters (Å, º)

O1—C7	1.2360 (17)	C5—C6	1.394 (2)
O2—C12	1.3656 (18)	C5—H5	0.9300
O2—H2	0.8200	C6—C7	1.4782 (19)
N1—C3	1.3652 (19)	C8—C10	1.487 (2)
N1—H1A	0.8600	C8—C9	1.501 (2)
N1—H1B	0.8600	C9—H9A	0.9600
N2—C7	1.3496 (19)	C9—H9B	0.9600
N2—N3	1.3818 (17)	C9—H9C	0.9600
N2—H2A	0.864 (9)	C10—C11	1.394 (2)
N3—C8	1.2811 (19)	C10—C15	1.395 (2)
C1—C2	1.377 (2)	C11—C12	1.387 (2)
C1—C6	1.397 (2)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.392 (2)
C2—C3	1.400 (2)	C13—C14	1.373 (2)
C2—H2B	0.9300	C13—H13	0.9300
C3—C4	1.399 (2)	C14—C15	1.383 (2)
C4—C5	1.371 (2)	C14—H14	0.9300
C4—H4	0.9300	C15—H15	0.9300
C12—O2—H2	109.5	N2—C7—C6	115.58 (12)
C3—N1—H1A	120.0	N3—C8—C10	116.54 (13)
C3—N1—H1B	120.0	N3—C8—C9	124.22 (14)
H1A—N1—H1B	120.0	C10—C8—C9	119.22 (13)
C7—N2—N3	121.26 (12)	C8—C9—H9A	109.5
C7—N2—H2A	117.2 (13)	C8—C9—H9B	109.5
N3—N2—H2A	121.4 (13)	H9A—C9—H9B	109.5
C8—N3—N2	115.54 (12)	C8—C9—H9C	109.5
C2—C1—C6	121.41 (13)	H9A—C9—H9C	109.5
C2—C1—H1	119.3	H9B—C9—H9C	109.5
C6—C1—H1	119.3	C11—C10—C15	119.07 (14)
C1—C2—C3	120.25 (14)	C11—C10—C8	120.63 (13)

C1—C2—H2B	119.9	C15—C10—C8	120.30 (13)
C3—C2—H2B	119.9	C12—C11—C10	120.09 (13)
N1—C3—C4	121.19 (14)	C12—C11—H11	120.0
N1—C3—C2	120.41 (14)	C10—C11—H11	120.0
C4—C3—C2	118.39 (14)	O2—C12—C11	123.02 (13)
C5—C4—C3	120.85 (14)	O2—C12—C13	116.66 (13)
C5—C4—H4	119.6	C11—C12—C13	120.32 (14)
C3—C4—H4	119.6	C14—C13—C12	119.50 (14)
C4—C5—C6	121.19 (14)	C14—C13—H13	120.3
C4—C5—H5	119.4	C12—C13—H13	120.2
C6—C5—H5	119.4	C13—C14—C15	120.83 (14)
C5—C6—C1	117.89 (13)	C13—C14—H14	119.6
C5—C6—C7	118.67 (13)	C15—C14—H14	119.6
C1—C6—C7	123.44 (13)	C14—C15—C10	120.19 (14)
O1—C7—N2	121.81 (13)	C14—C15—H15	119.9
O1—C7—C6	122.59 (13)	C10—C15—H15	119.9

C7—N2—N3—C8	166.52 (15)	N2—N3—C8—C10	−178.92 (13)
C6—C1—C2—C3	−1.2 (2)	N2—N3—C8—C9	−0.7 (2)
C1—C2—C3—N1	−178.36 (15)	N3—C8—C10—C11	−20.1 (2)
C1—C2—C3—C4	0.7 (2)	C9—C8—C10—C11	161.65 (17)
N1—C3—C4—C5	179.65 (16)	N3—C8—C10—C15	159.42 (15)
C2—C3—C4—C5	0.6 (2)	C9—C8—C10—C15	−18.9 (2)
C3—C4—C5—C6	−1.4 (3)	C15—C10—C11—C12	0.3 (2)
C4—C5—C6—C1	0.9 (2)	C8—C10—C11—C12	179.74 (13)
C4—C5—C6—C7	−179.44 (14)	C10—C11—C12—O2	−179.94 (15)
C2—C1—C6—C5	0.4 (2)	C10—C11—C12—C13	−0.6 (2)
C2—C1—C6—C7	−179.23 (14)	O2—C12—C13—C14	179.78 (15)
N3—N2—C7—O1	0.9 (2)	C11—C12—C13—C14	0.4 (2)
N3—N2—C7—C6	−177.49 (13)	C12—C13—C14—C15	0.2 (3)
C5—C6—C7—O1	−27.6 (2)	C13—C14—C15—C10	−0.5 (3)
C1—C6—C7—O1	152.05 (15)	C11—C10—C15—C14	0.3 (2)
C5—C6—C7—N2	150.74 (15)	C8—C10—C15—C14	−179.20 (14)
C1—C6—C7—N2	−29.6 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.88	2.694 (2)	171
N1—H1*B*···O1^{ii}	0.86	2.13	2.958 (2)	162
N1—H1*A*···O2^{iii}	0.86	2.37	3.119 (2)	146

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