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Crystal structure and Hirshfeld surface analysis of (*E*)-4-amino-*N*′-[1-(4-methylphenyl)ethylidene]benzohydrazide

Palaniyappan Sivajeyanthi, Muthaiah Jeevaraj, Bellarmin Edison and Kasthuri Balasubramani*

Department of Chemistry, Government Arts College (Autonomous), Thanthonimalai, Karur 639 005, Tamil Nadu, India. *Correspondence e-mail: manavaibala@gmail.com

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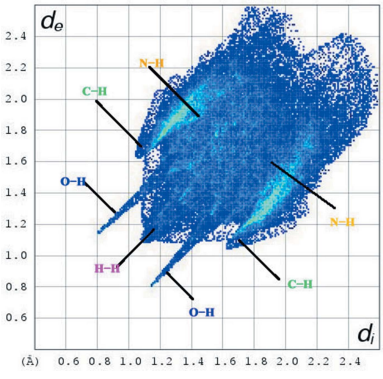
The structure of the title Schiff base, $C_{16}H_{17}N_3O$, displays a *trans* configuration with respect to the C=N double bond, with a dihedral angle of 14.98 (9)° between the benzene rings. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen-bonding interactions, giving sheets extending across the (001) plane. Hirshfeld surface analysis gave fingerprint plots showing enrichment ratios for H···H, O···H, N···H and C···H contacts compared to C···C, N···N and C···N contacts, indicating a high propensity for H···H interactions to form in the crystal.

1. Chemical context

Schiff bases are an important class of compounds in the medicinal and pharmaceutical fields and have played a role in the development of coordination chemistry as they readily form stable complexes with most transition metals. These complexes show interesting properties, *e.g.* their ability to reversibly bind oxygen, catalytic activity in the hydrogenation of olefins and transfer of an amino group, photochromic properties, and complexation ability towards toxic metals (Karthikeyan *et al.*, 2006; Khattab *et al.*, 2005; Küçükgüzel *et al.*, 2006). Hydrazone Schiff base compounds (Cao *et al.*, 2009; Zhou & Yang, 2010; Zhang *et al.*, 2009), derived from the reaction of aldehydes with hydrazines have been shown to possess excellent biological activities, such as anti-bacterial, anti-convulsant and anti-tubercular (Bernhardt *et al.*, 2005; Armstrong *et al.*, 2003). As part of our studies in this area, the title Schiff base compound (*E*)-4-amino-*N*′-(1-(*p*-tolyl)ethylidene)benzohydrazide, was prepared and the crystal structure is reported herein. Hirshfeld surface analysis was also performed for visualizing and quantifying intermolecular interactions in the crystal packing of the compound.



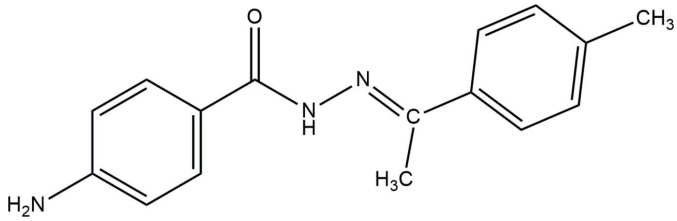


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1*N*3···O1^{i}	0.86	2.10	2.914 (2)	159
C9—H9*A*···O1^{ii}	0.96	2.60	3.475 (3)	152

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

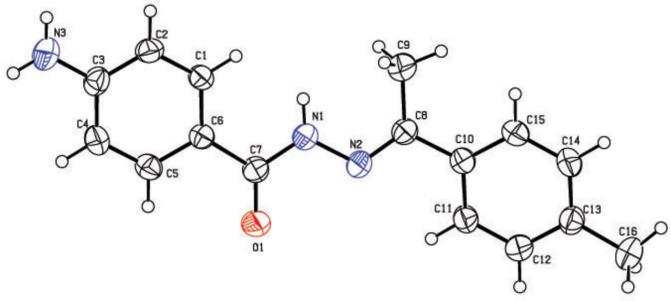


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The asymmetric unit of the title compound contains one independent molecule (Fig. 1), displaying a *trans* conformation with respect to its C=N double bond. The dihedral angle between the benzene rings is 14.98 (9)°. All the bond lengths are within normal ranges. The C8=N2 and C7=O1 bond lengths [1.281 (2) and 1.231 (2) Å, respectively] confirm their double-bond character, whereas the C3—N3, C7—N1 and N1—N2 values [1.365 (3), 1.357 (2) and 1.388 (2) Å, respectively]; these C—N bonds are much shorter than (nominal) isolated C—N bonds (1.46 Å) due to conjugation.

3. Supramolecular features

In the crystal, two types of intermolecular hydrogen-bonding interactions are present (Table 1). The N3—H1*N*3···O1^{i} hydrogen bond between the amino group and a symmetry-related carbonyl group generates zigzag chains extending along the *b*-axis direction, as shown in Fig. 2. The secondary weak methyl C9—H9*A*···O1^{ii} hydrogen-bonding interactions extend the structure across *a* (Fig. 3), generating a layer lying parallel to (001). No reasonable acceptors could be identified for either the second amine N3 H atom or the hydrazide N1 H atom.

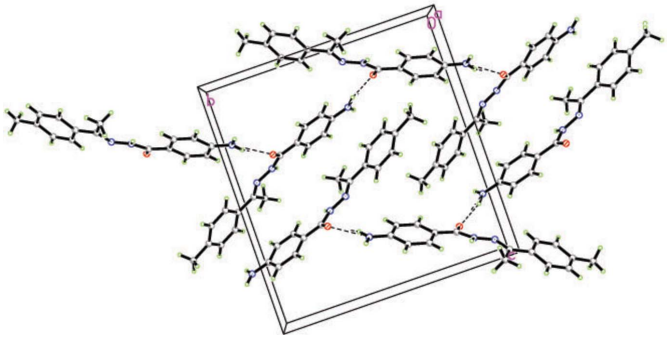


Figure 2
Crystal packing of the title compound in the unit cell, showing molecules linked across *b* *via* N—H···O hydrogen bonds (dashed lines).

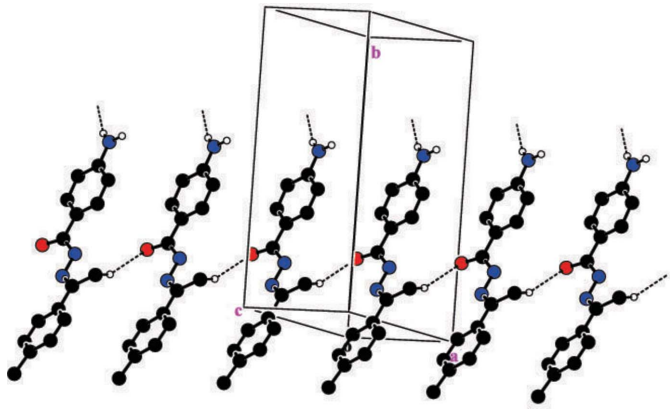


Figure 3
The crystal packing in the title compound in which molecules are linked across *a* *via* weak C—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen-bonding interactions have been omitted.

4. Hirshfeld surface analysis

Hirshfeld surfaces and their associated two-dimensional fingerprint plots (Soman *et al.*, 2014) have been used to quantify the various intermolecular interactions in the title compound. The Hirshfeld surface of a molecule is mapped using the descriptor d_{norm} which encompasses two factors: one is d_e, representing the distance of any surface point nearest to the internal atoms, and the other one is d_i, representing the distance of the surface point nearest to the exterior atoms and also with the van der Waals radii of the atoms (Dalal *et al.*,

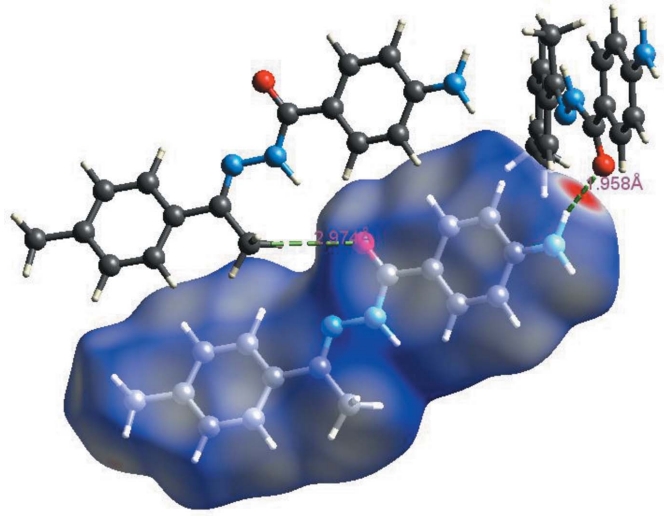


Figure 4
Hirshfeld surfaces mapped over d_{norm} for the title compound.

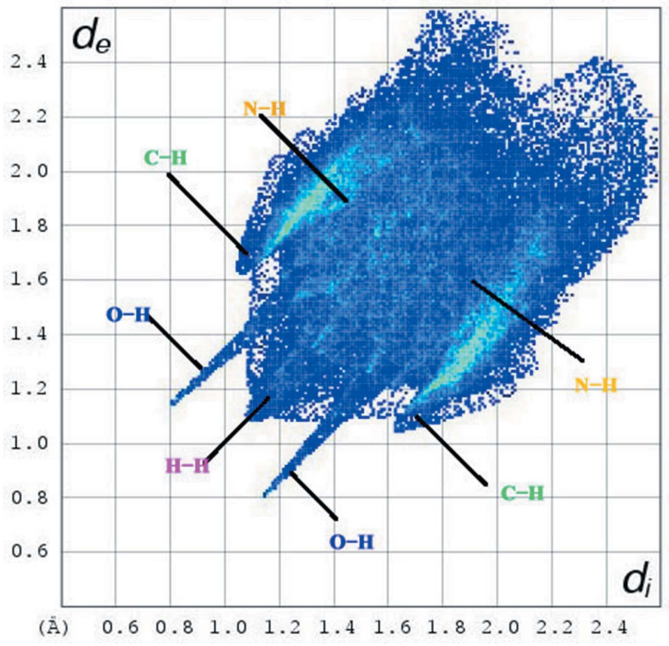


Figure 5
Two-dimensional fingerprint plots of the title compound.

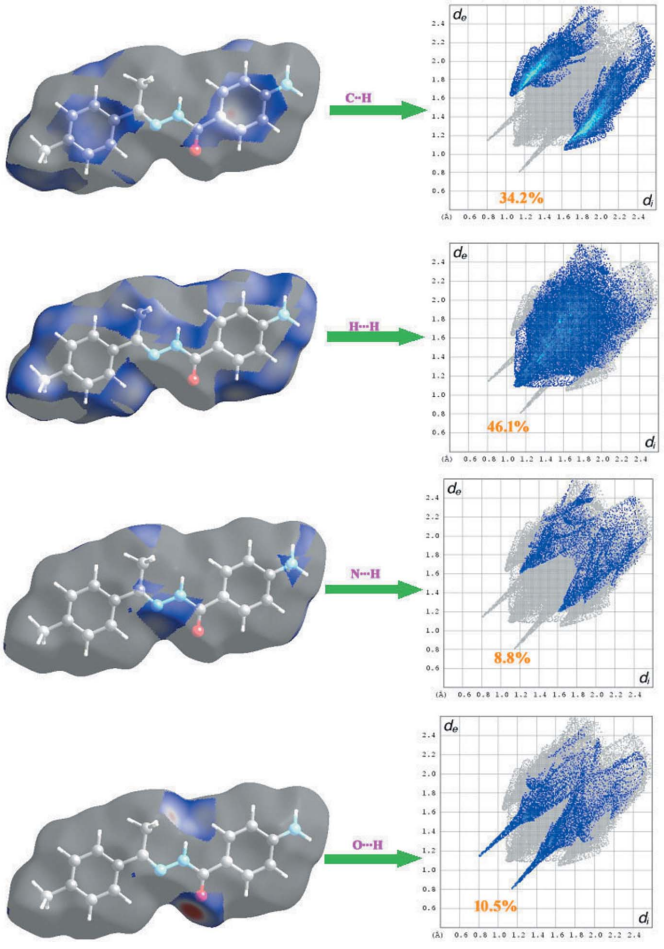


Figure 6
Two-dimensional fingerprint plots with a d_{norm} view of the C···H/H···C (34.2%), H···H (46.1%), N···H/H···N (8.8%) and O···H/H···O (10.5%) contacts in the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}N_3O$
M_r	267.33
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	5.7011 (4), 15.4836 (10), 16.2128 (10)
V (Å^3)	1431.16 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.976, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17427, 3501, 2784
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.141, 1.05
No. of reflections	3501
No. of parameters	182
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.20
Absolute structure	Flack (1983), 1489 Friedel pairs
Absolute structure parameter	0.6 (19)

Computer programs: *APEX2* (Bruker, 2004), *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

2015). The Hirshfeld surfaces mapped over d_{norm} (range of −0.502–1.427 Å) are displayed in Fig. 4. The surfaces are shown as transparent to allow visualization of the molecule. The dominant interaction between oxygen (O) and hydrogen (H) atoms can be observed in the Hirshfeld surface as the red areas (Fig. 4). Other visible spots in the Hirshfeld surfaces correspond to C—H and H—H contacts.

The intermolecular interactions of the title compound are shown in the 2D fingerprint plots shown in Fig. 5. H···H (46.1%) contacts make the largest contribution to the Hirshfeld surfaces. O···H/H···O (10.5%), interactions are represented by left-side blue spikes, top and bottom. The pale yellow N···H/H···N (8.8%) interactions are near the C···H regions while the green C···H/H···C interactions (34.2%) are between the N—H and O—H regions. The whole fingerprint region and all other interactions, which are a combination of d_e and d_i, are displayed in Fig. 6.

5. Synthesis and crystallization

The title compound was synthesized by the reaction of a 1:1 molar ratio mixture of a hot methanolic solution (20 mL) of 4-aminibenzoichydrazide (0.151 mg, Aldrich) and a hot methanolic solution of 4-methylacetophenone (0.134 mg, Aldrich), which was refluxed for 8 h. The solution was then cooled and kept at room temperature after which colourless

block-shaped crystals suitable for the X-ray analysis were obtained in a few days.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically (N—H = 0.86 Å, and C—H = 0.93 or 0.96 Å) and were refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(N, C) or 1.5U_{eq}(methyl C). One reflection (011) was considered to be affected by the beamstop.

Acknowledgements

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

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

Crystal data

$C_{16}H_{17}N_3O$
$M_r = 267.33$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.7011$ (4) Å
$b = 15.4836$ (10) Å
$c = 16.2128$ (10) Å
$V = 1431.16$ (16) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.241$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6816 reflections
$\theta = 5.0$–$49.0°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min} = 0.976$, $T_{max} = 0.984$
17427 measured reflections
3501 independent reflections
2784 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.8°$
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 20$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.141$
$S = 1.05$
3501 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.0847P)^2 + 0.1161P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Absolute structure: Flack (1983), 1489 Friedel pairs

Absolute structure parameter: 0.6 (19)

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2405 (3)	0.16299 (10)	0.88410 (10)	0.0543 (4)
H1N	0.3848	0.1789	0.8871	0.065*
N2	0.1715 (3)	0.08479 (10)	0.91817 (10)	0.0519 (4)
C11	0.0364 (4)	−0.07382 (12)	0.98126 (12)	0.0518 (5)
H11	−0.0509	−0.0504	0.9383	0.062*
O1	−0.1236 (3)	0.19158 (9)	0.83572 (11)	0.0718 (5)
C5	0.0187 (3)	0.35074 (11)	0.77149 (11)	0.0477 (4)
H5	−0.1250	0.3283	0.7548	0.057*
C8	0.3188 (3)	0.04879 (11)	0.96690 (11)	0.0450 (4)
C10	0.2444 (3)	−0.03365 (11)	1.00549 (10)	0.0434 (4)
C12	−0.0420 (4)	−0.14777 (12)	1.02002 (12)	0.0557 (5)
H12	−0.1814	−0.1730	1.0026	0.067*
N3	0.3577 (4)	0.55025 (11)	0.74979 (15)	0.0824 (6)
H2N3	0.4905	0.5709	0.7654	0.099*
H1N3	0.2650	0.5811	0.7201	0.099*
C3	0.2940 (4)	0.46854 (11)	0.77215 (12)	0.0514 (4)
C4	0.0803 (4)	0.43309 (12)	0.74768 (11)	0.0518 (4)
H4	−0.0215	0.4653	0.7151	0.062*
C6	0.1661 (3)	0.30033 (10)	0.81983 (10)	0.0408 (4)
C7	0.0810 (3)	0.21446 (11)	0.84607 (11)	0.0472 (4)
C13	0.0821 (4)	−0.18536 (12)	1.08434 (11)	0.0509 (4)
C16	−0.0112 (5)	−0.26470 (15)	1.12687 (15)	0.0721 (7)
H16A	0.0964	−0.2823	1.1692	0.108*
H16B	−0.0287	−0.3105	1.0874	0.108*
H16C	−0.1608	−0.2519	1.1511	0.108*
C2	0.4428 (3)	0.41823 (12)	0.82025 (13)	0.0527 (4)
H2	0.5868	0.4405	0.8368	0.063*
C1	0.3806 (3)	0.33609 (11)	0.84366 (12)	0.0474 (4)
H1	0.4829	0.3038	0.8759	0.057*
C9	0.5540 (4)	0.08701 (17)	0.98774 (16)	0.0755 (7)
H9A	0.6427	0.0952	0.9380	0.113*
H9B	0.6372	0.0486	1.0238	0.113*
H9C	0.5322	0.1416	1.0147	0.113*

C15	0.3706 (4)	−0.07226 (13)	1.06905 (11)	0.0529 (5)
H15	0.5109	−0.0475	1.0863	0.063*
C14	0.2906 (4)	−0.14736 (14)	1.10736 (13)	0.0574 (5)
H14	0.3796	−0.1722	1.1492	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0503 (8)	0.0419 (7)	0.0706 (10)	−0.0063 (7)	−0.0069 (8)	0.0095 (7)
N2	0.0532 (9)	0.0386 (7)	0.0638 (9)	−0.0062 (7)	−0.0056 (7)	0.0055 (7)
C11	0.0551 (11)	0.0474 (9)	0.0529 (10)	−0.0027 (9)	−0.0118 (9)	0.0072 (8)
O1	0.0552 (9)	0.0525 (8)	0.1078 (12)	−0.0153 (7)	−0.0246 (9)	0.0154 (8)
C5	0.0450 (9)	0.0491 (9)	0.0489 (9)	0.0012 (8)	−0.0064 (8)	−0.0028 (8)
C8	0.0472 (9)	0.0423 (8)	0.0455 (8)	−0.0025 (7)	0.0007 (8)	−0.0019 (7)
C10	0.0446 (9)	0.0428 (8)	0.0429 (8)	0.0027 (8)	−0.0001 (7)	−0.0014 (7)
C12	0.0513 (11)	0.0527 (10)	0.0632 (12)	−0.0089 (9)	−0.0074 (10)	0.0053 (9)
N3	0.0756 (13)	0.0518 (10)	0.1198 (17)	−0.0061 (10)	−0.0042 (13)	0.0306 (11)
C3	0.0549 (11)	0.0407 (9)	0.0585 (10)	0.0024 (8)	0.0096 (9)	0.0037 (8)
C4	0.0553 (11)	0.0483 (9)	0.0518 (10)	0.0099 (8)	−0.0029 (9)	0.0057 (8)
C6	0.0417 (8)	0.0383 (7)	0.0424 (8)	−0.0001 (7)	−0.0012 (7)	−0.0031 (6)
C7	0.0500 (10)	0.0391 (8)	0.0527 (9)	−0.0048 (8)	−0.0078 (8)	−0.0021 (7)
C13	0.0527 (11)	0.0493 (9)	0.0507 (10)	0.0021 (9)	0.0060 (8)	0.0079 (8)
C16	0.0745 (15)	0.0686 (13)	0.0731 (14)	−0.0103 (12)	0.0057 (12)	0.0248 (11)
C2	0.0418 (10)	0.0453 (9)	0.0709 (11)	−0.0054 (8)	−0.0022 (9)	0.0010 (8)
C1	0.0417 (9)	0.0418 (8)	0.0586 (10)	0.0006 (8)	−0.0083 (8)	0.0035 (7)
C9	0.0624 (14)	0.0771 (14)	0.0870 (15)	−0.0209 (13)	−0.0199 (12)	0.0280 (12)
C15	0.0447 (10)	0.0606 (11)	0.0534 (10)	−0.0010 (9)	−0.0079 (8)	0.0058 (9)
C14	0.0545 (12)	0.0640 (12)	0.0536 (10)	0.0040 (10)	−0.0068 (9)	0.0161 (9)

Geometric parameters (Å, º)

N1—C7	1.357 (2)	C3—C2	1.391 (3)
N1—N2	1.388 (2)	C3—C4	1.394 (3)
N1—H1N	0.8600	C4—H4	0.9300
N2—C8	1.281 (2)	C6—C1	1.397 (2)
C11—C12	1.380 (3)	C6—C7	1.478 (2)
C11—C10	1.395 (3)	C13—C14	1.378 (3)
C11—H11	0.9300	C13—C16	1.506 (3)
O1—C7	1.231 (2)	C16—H16A	0.9600
C5—C4	1.378 (2)	C16—H16B	0.9600
C5—C6	1.389 (2)	C16—H16C	0.9600
C5—H5	0.9300	C2—C1	1.374 (3)
C8—C10	1.483 (2)	C2—H2	0.9300
C8—C9	1.504 (3)	C1—H1	0.9300
C10—C15	1.392 (3)	C9—H9A	0.9600
C12—C13	1.388 (3)	C9—H9B	0.9600
C12—H12	0.9300	C9—H9C	0.9600
N3—C3	1.365 (2)	C15—C14	1.395 (3)

N3—H2N3	0.8600	C15—H15	0.9300
N3—H1N3	0.8600	C14—H14	0.9300
C7—N1—N2	120.20 (17)	O1—C7—N1	121.87 (17)
C7—N1—H1N	119.9	O1—C7—C6	122.06 (17)
N2—N1—H1N	119.9	N1—C7—C6	116.05 (16)
C8—N2—N1	116.05 (16)	C14—C13—C12	117.64 (17)
C12—C11—C10	121.11 (18)	C14—C13—C16	121.95 (18)
C12—C11—H11	119.4	C12—C13—C16	120.41 (19)
C10—C11—H11	119.4	C13—C16—H16A	109.5
C4—C5—C6	121.61 (18)	C13—C16—H16B	109.5
C4—C5—H5	119.2	H16A—C16—H16B	109.5
C6—C5—H5	119.2	C13—C16—H16C	109.5
N2—C8—C10	116.57 (16)	H16A—C16—H16C	109.5
N2—C8—C9	123.50 (17)	H16B—C16—H16C	109.5
C10—C8—C9	119.90 (17)	C1—C2—C3	121.04 (17)
C15—C10—C11	117.15 (17)	C1—C2—H2	119.5
C15—C10—C8	122.29 (17)	C3—C2—H2	119.5
C11—C10—C8	120.51 (16)	C2—C1—C6	121.12 (17)
C11—C12—C13	121.66 (19)	C2—C1—H1	119.4
C11—C12—H12	119.2	C6—C1—H1	119.4
C13—C12—H12	119.2	C8—C9—H9A	109.5
C3—N3—H2N3	120.0	C8—C9—H9B	109.5
C3—N3—H1N3	120.0	H9A—C9—H9B	109.5
H2N3—N3—H1N3	120.0	C8—C9—H9C	109.5
N3—C3—C2	120.36 (19)	H9A—C9—H9C	109.5
N3—C3—C4	121.45 (19)	H9B—C9—H9C	109.5
C2—C3—C4	118.18 (16)	C10—C15—C14	121.25 (19)
C5—C4—C3	120.48 (18)	C10—C15—H15	119.4
C5—C4—H4	119.8	C14—C15—H15	119.4
C3—C4—H4	119.8	C13—C14—C15	121.16 (18)
C5—C6—C1	117.57 (15)	C13—C14—H14	119.4
C5—C6—C7	118.01 (16)	C15—C14—H14	119.4
C1—C6—C7	124.35 (15)		
C7—N1—N2—C8	−166.25 (17)	C5—C6—C7—O1	−9.6 (3)
N2—N1—C7—O1	−4.9 (3)	C5—C6—C7—N1	171.91 (16)
N2—N1—C7—C6	173.63 (15)	N2—C8—C10—C11	7.5 (3)
N1—N2—C8—C9	0.2 (3)	N2—C8—C10—C15	−169.65 (18)
N1—N2—C8—C10	178.39 (15)	C9—C8—C10—C11	−174.22 (18)
C6—C1—C2—C3	0.1 (3)	C9—C8—C10—C15	8.6 (3)
C2—C1—C6—C5	0.2 (3)	C8—C10—C11—C12	−176.11 (18)
C2—C1—C6—C7	−176.59 (17)	C15—C10—C11—C12	1.2 (3)
C1—C2—C3—N3	179.6 (2)	C8—C10—C15—C14	176.54 (18)
C1—C2—C3—C4	−0.5 (3)	C11—C10—C15—C14	−0.7 (3)
N3—C3—C4—C5	−179.5 (2)	C10—C11—C12—C13	−0.1 (3)
C2—C3—C4—C5	0.6 (3)	C11—C12—C13—C14	−1.4 (3)
C3—C4—C5—C6	−0.4 (3)	C11—C12—C13—C16	178.4 (2)

C4—C5—C6—C1	−0.1 (3)	C12—C13—C14—C15	1.9 (3)
C4—C5—C6—C7	176.93 (17)	C16—C13—C14—C15	−177.9 (2)
C1—C6—C7—O1	167.14 (18)	C13—C14—C15—C10	−0.9 (3)
C1—C6—C7—N1	−11.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*3···O1^{i}	0.86	2.10	2.914 (2)	159
C9—H9*A*···O1^{ii}	0.96	2.60	3.475 (3)	152

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