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(2*E*)-*N*′-[(*E*)-Benzylidene]-3-phenylprop-2-enohydrazide from synchrotron radiation

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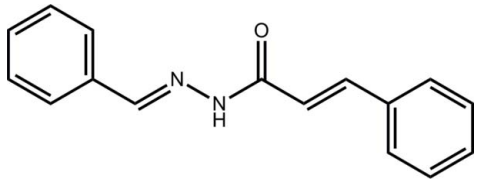
Key indicators: single-crystal synchrotron study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.140; data-to-parameter ratio = 10.7.

In the title compound, $C_{16}H_{14}N_2O$, the dihedral angle between the phenyl rings is 25.48 (12)°. An *E* conformation is found for each of the imine [1.269 (3) Å] and ethylene [1.313 (3) Å] bonds. In the crystal, molecules are linked by N—H···O hydrogen bonds, leading to zigzag chains along [010]. Supramolecular layers in the *ab* plane are formed, whereby the chains are linked by C—H···N and C—H···π interactions.

Related literature

For the biological activity of (*E*)-cinnamoylhydrazone derivatives against Chagas' disease, see: Carvalho *et al.* (2012*b*). For background to Chagas' disease, see: Rassi *et al.* (2010); Soeiro & de Castro (2011). For related structural studies, see: Carvalho *et al.* (2009, 2010*a*,*b*, 2012*a*).



Experimental

Crystal data

$C_{16}H_{14}N_2O$
M_r = 250.30
Orthorhombic, *Pbca*
a = 11.473 (19) Å
b = 7.507 (13) Å
c = 30.50 (5) Å
V = 2627 (8) Å^3
Z = 8
Synchrotron radiation
λ = 0.6943 Å
μ = 0.04 mm^{-1}
T = 120 K
0.12 × 0.03 × 0.02 mm

Data collection

Bruker SMART APEXII CCD diffractometer
14542 measured reflections
1876 independent reflections
1442 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 22.7°

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.140
S = 1.05
1876 reflections
175 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2n···O1^{i}	0.88 (2)	1.93 (2)	2.816 (6)	175 (2)
C5—H5···N1^{ii}	0.95	2.57	3.433 (7)	151
C3—H3···*Cg*1^{iii}	0.95	2.92	3.618 (7)	131
C6—H6···*Cg*1^{iv}	0.95	2.75	3.645 (7)	158

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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: HB6861).

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supplementary materials

Acta Cryst. (2012). E**68**, o2255–o2256 [doi:10.1107/S1600536812028504]

(2*E*)-*N*′-[(*E*)-Benzylidene]-3-phenylprop-2-enohydrazide from synchrotron radiation

Samir A. Carvalho, Edson F. da Silva, Carlos A. M. Fraga, Solange M. S. V. Wardell, James L. Wardell and Edward R. T. Tiekink

Comment

(*E*)-Cinnamoylhydrazone derivatives have recently been shown to be agents against Chagas′ disease (CD) (Carvalho *et al.*, 2012*b*), caused by the parasite *Trypanosoma cruzi*. CD is the major cause of infectious cardiopathy and represents an important public health problem. It affects approximately eight million people in Latin America (Rassi *et al.*, 2010). Neither the two established drugs, Nifurtimox and Benznidazole, is ideal because they present variable results depending on the phase of the disease, the dose and duration of the treatment, the patient's age and endemic region, as well as showing undesirable secondary side-effects (Soeiro & de Castro, 2011). The ArCH═CHCONHN═CHAr′ compounds used in the trypanocidal study (Carvalho *et al.*, 2012*b*) indicated considerable biological potential. Following on from our structural studies on (*E*)-PhCH═CH-CONHNHPh (Carvalho *et al.*, 2009), (*E*)-4-$O_2NC_6H_4$CH═CH-CONHNHCOPh (Carvalho *et al.*, 2010*a*) and (*E*)-PhCH═CH-CONHN═ CHC_6H_4Cl-4.monohydrate (Carvalho *et al.*, 2010*b*), we now wish to report the crystal structure of one of the compounds from the trypanocidal study, namely the title compound, (I).

In (I), Fig. 1, there is a twist in the molecule as seen in the dihedral angle between the phenyl rings of 25.48 (12)°. The greatest deviation from a planar torsion angle is found for C2—C1—C7—N1 of 14.0 (3)°. The conformation about each of the imine [N1═C7 = 1.269 (3) Å] and ethylene [C9═C10 = 1.313 (3) Å] bonds is *E*. In the structure of the 4-chloro-benzylidene derivative (Carvalho *et al.*, 2010*b*), a decidedly more planar arrangement was noted (r.m.s. deviation of the 20 non-H atoms = 0.172 Å). However, a more twisted arrangement was found in the 2-hydroxyl derivative (Carvalho *et al.*, 2012*a*) where the dihedral angle between the benzene rings is 16.67 (8)°.

In the crystal of (I), the molecules are linked by N—H···O hydrogen bonds (Table 1), resulting in zigzag chains along the *b* axis. The chains are linked into a supramolecular layer in the *ab* plane by C—H···N and C—H···π interactions, Fig. 3 and Table 1; the layers inter-digitate along the *c* axis, Fig. 4.

Experimental

The title compound was prepared as reported (Carvalho *et al.*, 2012*b*). The sample used in the crystallographic study was grown from its EtOH solution in the form of small colourless needles.

Refinement

The C-bound H atoms were geometrically placed (C—H = 0.95 Å) and refined as riding with U_{iso}(H) = 1.2U_{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: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); 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).

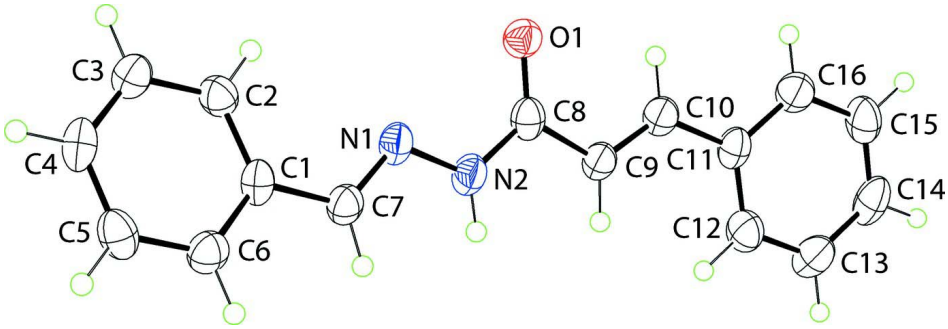

Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

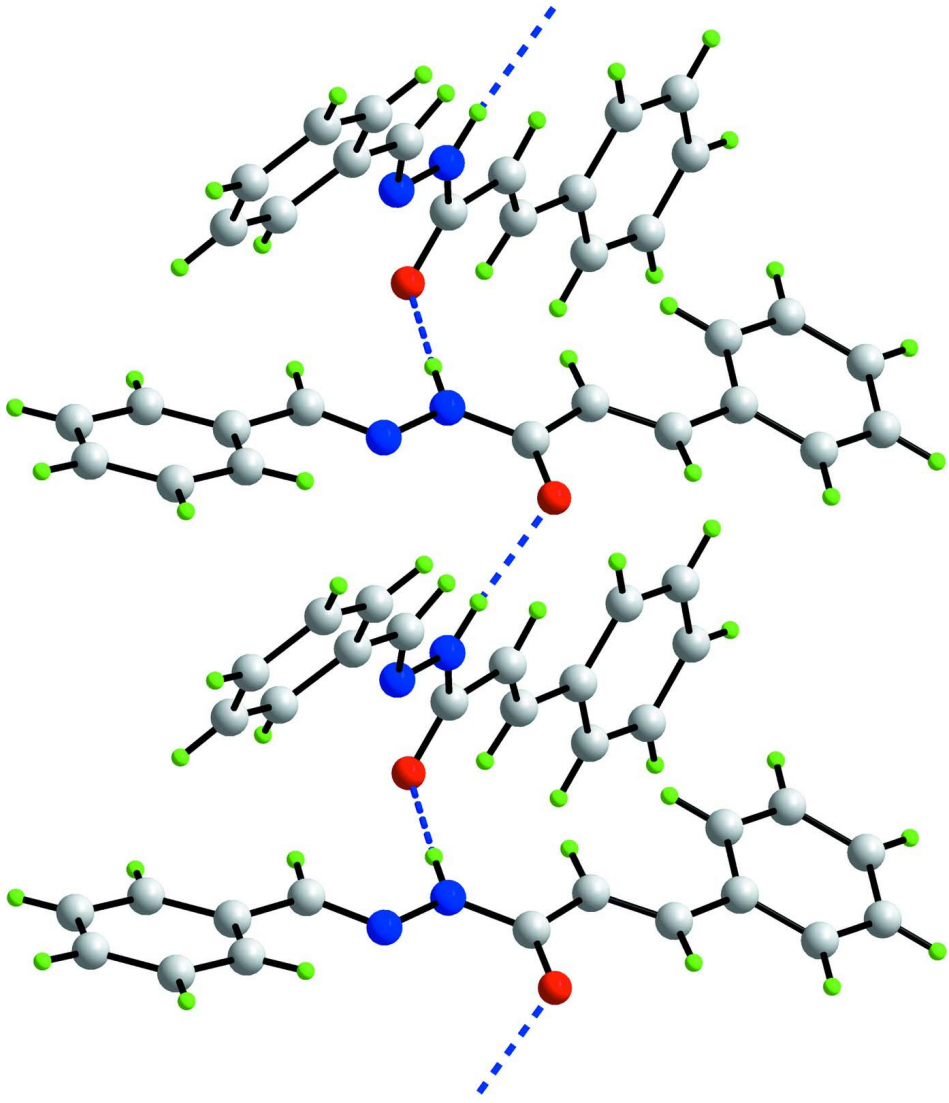

Figure 2

A view of the supramolecular zigzag chain along the *b* axis in (I). The N—H···O hydrogen bonds are shown as blue dashed lines.

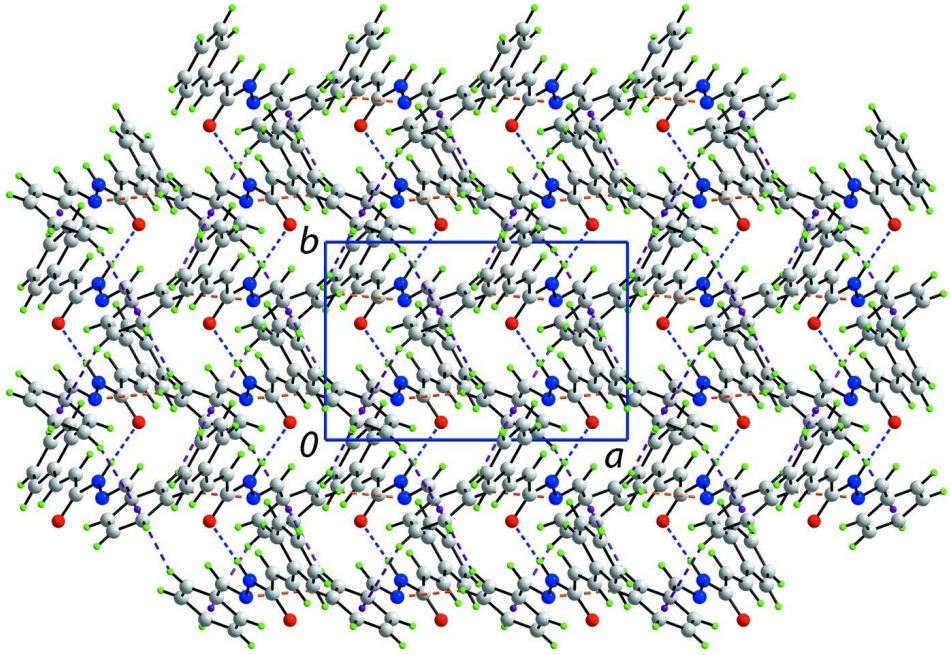

Figure 3

A view of the supramolecular layer in the *ab* plane in (I) sustained by N—H···O, C—H···N and C—H···π interactions, shown as blue, orange and purple dashed lines, respectively.

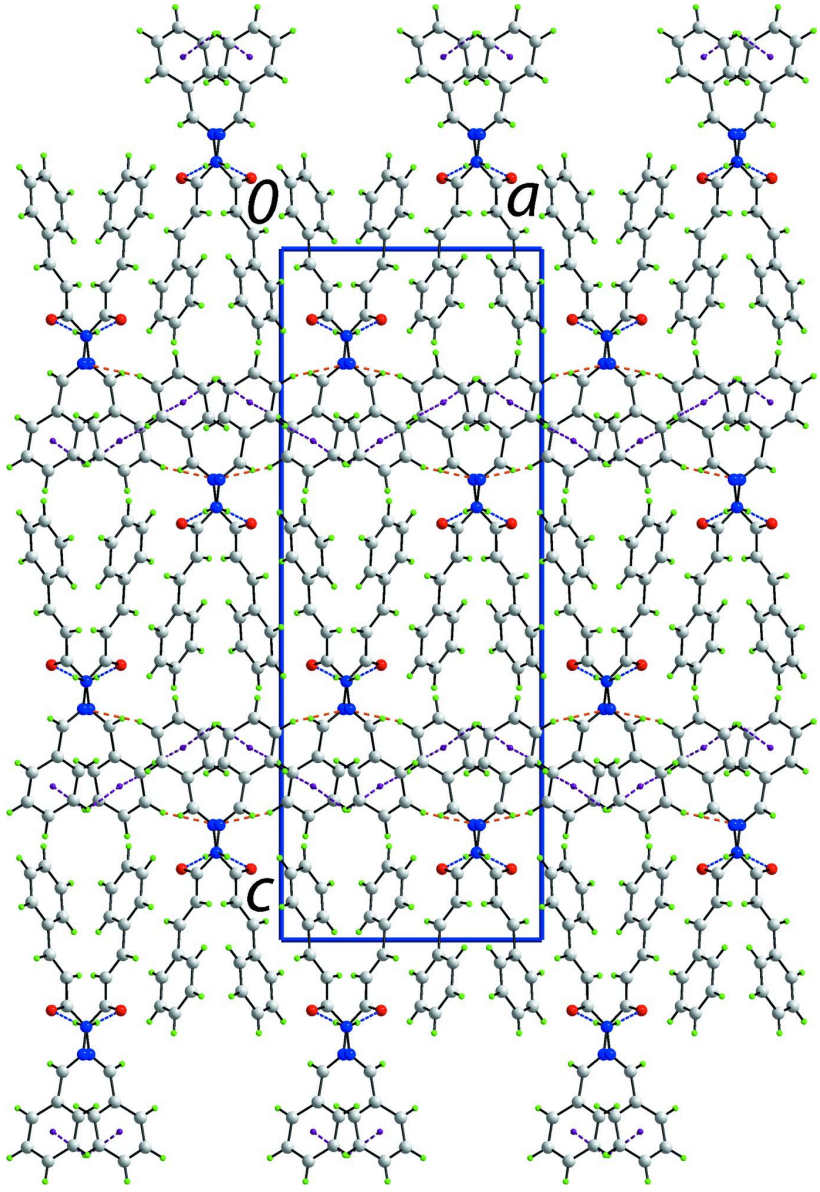

Figure 4

A view in projection down the *b* axis of the unit-cell contents for (I) showing the inter-digitation of layers. The N—H···O, C—H···N and C—H···π interactions, shown as blue, orange and purple dashed lines, respectively.

(2*E*)-*N*′-[(*E*)-Benzylidene]-3-phenylprop-2-enohydrazide

Crystal data

$C_{16}H_{14}N_2O$
M_r = 250.30
Orthorhombic, *Pbca*
Hall symbol: -P 2ybc
a = 11.473 (19) Å
b = 7.507 (13) Å
c = 30.50 (5) Å
V = 2627 (8) Å^3
Z = 8
F(000) = 1056
D_x = 1.266 Mg m^{-3}
Synchrotron radiation, λ = 0.6943 Å
Cell parameters from 996 reflections
θ = 3.2–25.1°
μ = 0.04 mm^{-1}
T = 120 K
Needle, colourless
0.12 × 0.03 × 0.02 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: Daresbury SRS station 9.8
Silicon 111 monochromator
fine–slice ω scans
14542 measured reflections
1876 independent reflections
1442 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 22.7°$, $\theta_{min} = 2.6°$
$h = -12 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.140$
$S = 1.05$
1876 reflections
175 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.9415P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38302 (13)	0.0885 (2)	0.60236 (5)	0.0381 (5)
N1	0.23795 (16)	0.2057 (3)	0.66603 (6)	0.0349 (5)
N2	0.25029 (17)	0.2886 (3)	0.62606 (6)	0.0371 (5)
H2N	0.209 (2)	0.385 (2)	0.6201 (8)	0.045*
C1	0.14001 (19)	0.2034 (3)	0.73493 (7)	0.0338 (6)
C2	0.21991 (19)	0.0947 (3)	0.75586 (7)	0.0373 (6)
H2	0.2886	0.0588	0.7409	0.045*
C3	0.2010 (2)	0.0384 (3)	0.79800 (7)	0.0403 (6)
H3	0.2554	−0.0392	0.8117	0.048*
C4	0.1040 (2)	0.0931 (3)	0.82057 (8)	0.0413 (7)
H4	0.0924	0.0559	0.8500	0.050*
C5	0.0236 (2)	0.2021 (4)	0.80048 (8)	0.0412 (7)
H5	−0.0442	0.2389	0.8159	0.049*
C6	0.0418 (2)	0.2580 (3)	0.75771 (8)	0.0386 (6)
H6	−0.0134	0.3341	0.7439	0.046*
C7	0.15938 (19)	0.2706 (3)	0.69056 (7)	0.0353 (6)
H7	0.1121	0.3649	0.6799	0.042*

C8	0.3245 (2)	0.2246 (3)	0.59613 (7)	0.0357 (6)
C9	0.32566 (19)	0.3248 (3)	0.55473 (7)	0.0344 (6)
H9	0.2785	0.4282	0.5518	0.041*
C10	0.3909 (2)	0.2735 (3)	0.52168 (7)	0.0374 (6)
H10	0.4399	0.1736	0.5268	0.045*
C11	0.39690 (19)	0.3527 (3)	0.47781 (7)	0.0366 (6)
C12	0.3407 (2)	0.5093 (4)	0.46697 (8)	0.0447 (7)
H12	0.2972	0.5710	0.4887	0.054*
C13	0.3468 (2)	0.5770 (4)	0.42517 (9)	0.0501 (7)
H13	0.3079	0.6851	0.4181	0.060*
C14	0.4090 (2)	0.4885 (4)	0.39369 (8)	0.0505 (7)
H14	0.4134	0.5354	0.3648	0.061*
C15	0.4645 (2)	0.3332 (4)	0.40364 (8)	0.0498 (7)
H15	0.5069	0.2716	0.3816	0.060*
C16	0.4593 (2)	0.2651 (4)	0.44565 (8)	0.0437 (7)
H16	0.4988	0.1574	0.4525	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0345 (9)	0.0435 (10)	0.0362 (9)	0.0027 (8)	0.0002 (7)	0.0019 (8)
N1	0.0314 (10)	0.0474 (13)	0.0258 (10)	−0.0017 (9)	−0.0002 (8)	0.0017 (9)
N2	0.0373 (11)	0.0464 (14)	0.0276 (10)	0.0004 (9)	0.0001 (9)	0.0051 (9)
C1	0.0332 (12)	0.0437 (14)	0.0246 (12)	−0.0079 (11)	−0.0008 (10)	−0.0013 (10)
C2	0.0323 (13)	0.0443 (14)	0.0353 (13)	0.0027 (11)	0.0020 (10)	−0.0037 (11)
C3	0.0409 (14)	0.0453 (16)	0.0345 (13)	0.0002 (12)	−0.0052 (11)	0.0027 (11)
C4	0.0493 (16)	0.0497 (16)	0.0249 (12)	−0.0115 (13)	−0.0027 (11)	0.0007 (11)
C5	0.0339 (13)	0.0536 (17)	0.0362 (14)	−0.0068 (12)	0.0071 (11)	−0.0074 (12)
C6	0.0351 (13)	0.0428 (14)	0.0379 (14)	−0.0004 (11)	−0.0053 (11)	−0.0002 (11)
C7	0.0324 (13)	0.0423 (15)	0.0311 (13)	−0.0003 (11)	−0.0039 (10)	−0.0005 (10)
C8	0.0314 (12)	0.0457 (16)	0.0301 (13)	−0.0062 (12)	−0.0013 (10)	−0.0023 (11)
C9	0.0322 (12)	0.0411 (14)	0.0297 (12)	0.0003 (10)	−0.0021 (10)	0.0020 (10)
C10	0.0353 (13)	0.0439 (15)	0.0330 (13)	−0.0003 (11)	−0.0017 (11)	0.0015 (11)
C11	0.0315 (12)	0.0504 (16)	0.0279 (12)	−0.0045 (12)	−0.0002 (10)	0.0028 (11)
C12	0.0419 (14)	0.0579 (17)	0.0344 (14)	0.0029 (13)	0.0071 (11)	0.0013 (13)
C13	0.0423 (15)	0.0629 (19)	0.0449 (16)	0.0034 (13)	−0.0023 (12)	0.0127 (14)
C14	0.0398 (14)	0.081 (2)	0.0312 (14)	−0.0062 (14)	−0.0015 (11)	0.0134 (14)
C15	0.0394 (14)	0.077 (2)	0.0332 (14)	0.0000 (14)	0.0081 (11)	−0.0064 (14)
C16	0.0389 (14)	0.0530 (16)	0.0391 (15)	0.0035 (12)	0.0008 (11)	0.0019 (12)

Geometric parameters (Å, º)

O1—C8	1.238 (3)	C7—H7	0.9500
N1—C7	1.269 (3)	C8—C9	1.470 (4)
N1—N2	1.376 (3)	C9—C10	1.313 (3)
N2—C8	1.338 (3)	C9—H9	0.9500
N2—H2N	0.886 (10)	C10—C11	1.466 (4)
C1—C2	1.383 (3)	C10—H10	0.9500
C1—C6	1.386 (4)	C11—C12	1.381 (4)
C1—C7	1.461 (4)	C11—C16	1.381 (4)

C2—C3	1.370 (4)	C12—C13	1.374 (4)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.371 (4)	C13—C14	1.368 (4)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.377 (4)	C14—C15	1.363 (4)
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.386 (4)	C15—C16	1.381 (4)
C5—H5	0.9500	C15—H15	0.9500
C6—H6	0.9500	C16—H16	0.9500

C7—N1—N2	115.0 (2)	O1—C8—C9	123.4 (2)
C8—N2—N1	120.5 (2)	N2—C8—C9	114.1 (2)
C8—N2—H2N	119.7 (17)	C10—C9—C8	120.9 (2)
N1—N2—H2N	119.8 (17)	C10—C9—H9	119.5
C2—C1—C6	118.8 (2)	C8—C9—H9	119.5
C2—C1—C7	122.0 (2)	C9—C10—C11	127.5 (3)
C6—C1—C7	119.1 (2)	C9—C10—H10	116.3
C3—C2—C1	120.6 (2)	C11—C10—H10	116.3
C3—C2—H2	119.7	C12—C11—C16	118.5 (2)
C1—C2—H2	119.7	C12—C11—C10	122.8 (2)
C2—C3—C4	120.5 (2)	C16—C11—C10	118.7 (3)
C2—C3—H3	119.8	C13—C12—C11	120.9 (2)
C4—C3—H3	119.8	C13—C12—H12	119.6
C3—C4—C5	119.9 (2)	C11—C12—H12	119.6
C3—C4—H4	120.1	C14—C13—C12	119.8 (3)
C5—C4—H4	120.1	C14—C13—H13	120.1
C4—C5—C6	119.8 (2)	C12—C13—H13	120.1
C4—C5—H5	120.1	C15—C14—C13	120.2 (3)
C6—C5—H5	120.1	C15—C14—H14	119.9
C1—C6—C5	120.3 (2)	C13—C14—H14	119.9
C1—C6—H6	119.8	C14—C15—C16	120.2 (3)
C5—C6—H6	119.8	C14—C15—H15	119.9
N1—C7—C1	121.5 (2)	C16—C15—H15	119.9
N1—C7—H7	119.3	C15—C16—C11	120.3 (3)
C1—C7—H7	119.3	C15—C16—H16	119.8
O1—C8—N2	122.5 (2)	C11—C16—H16	119.8

C7—N1—N2—C8	−175.3 (2)	O1—C8—C9—C10	−0.3 (4)
C6—C1—C2—C3	1.6 (4)	N2—C8—C9—C10	−177.4 (2)
C7—C1—C2—C3	178.0 (2)	C8—C9—C10—C11	176.4 (2)
C1—C2—C3—C4	−1.9 (4)	C9—C10—C11—C12	7.2 (4)
C2—C3—C4—C5	1.6 (4)	C9—C10—C11—C16	−171.3 (2)
C3—C4—C5—C6	−0.9 (4)	C16—C11—C12—C13	−0.2 (4)
C2—C1—C6—C5	−0.9 (3)	C10—C11—C12—C13	−178.7 (2)
C7—C1—C6—C5	−177.4 (2)	C11—C12—C13—C14	0.2 (4)
C4—C5—C6—C1	0.6 (4)	C12—C13—C14—C15	0.2 (4)
N2—N1—C7—C1	−176.63 (19)	C13—C14—C15—C16	−0.6 (4)
C2—C1—C7—N1	14.0 (3)	C14—C15—C16—C11	0.6 (4)
C6—C1—C7—N1	−169.6 (2)	C12—C11—C16—C15	−0.2 (4)

N1—N2—C8—O1	1.4 (3)	C10—C11—C16—C15	178.4 (2)
N1—N2—C8—C9	178.50 (19)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2n···O1^{i}	0.88 (2)	1.93 (2)	2.816 (6)	175 (2)
C5—H5···N1^{ii}	0.95	2.57	3.433 (7)	151
C3—H3···*Cg*1^{iii}	0.95	2.92	3.618 (7)	131
C6—H6···*Cg*1^{iv}	0.95	2.75	3.645 (7)	158

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