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(3*Z*)-3-Benzylidene-1*H*-benzimidazo[1,2-*a*]-imidazol-2(3*H*)-one

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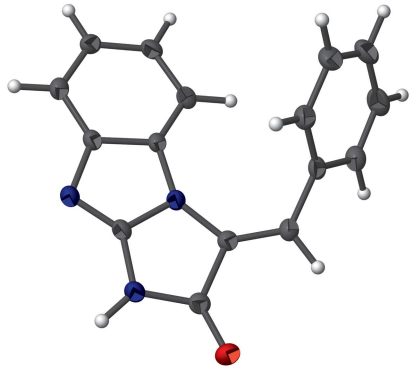
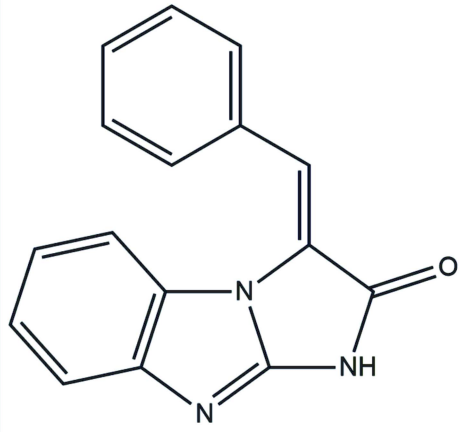
In the title compound, $C_{16}H_{11}N_3O$, the molecular conformation is partially determined by an intramolecular C—H$\cdots\pi$(ring) interaction. In the crystal, pairwise N—H$\cdots$N hydrogen bonds form dimers, which associate into stacks through a combination of C—H$\cdots$O, C—H$\cdots\pi$(ring) and offset π–π stacking interactions.

3D view



Chemical scheme



Structure description

Heterocyclic systems with benzimidazole as a significant component have been widely used in medicinal chemistry and drug development (Wang *et al.*, 2015). They possess antitumor (Soderlin *et al.*, 1999), antifungal (Ke *et al.*, 2014), antiviral (Tonelli *et al.*, 2008) and antidiabetic properties (Bansal & Silakari, 2012). The title compound was obtained by the action of 2-aminobenzimidazole on ethyl glycidate in hot *n*-butanol.

In the title molecule, the tricyclic core is approximately planar with an r.m.s. deviation of 0.062 Å for the 12 non-H atoms making up the ring system. The dihedral angle between the C1–C6 and the central five-membered ring is 4.21 (1)°, while that between the central and outer five-membered rings is 4.1 (1)°. The pendant phenyl group makes a dihedral angle of 52.61 (6)° with the N2/C9/N3/C8/C7 ring, and its orientation appears to be determined in part by an intramolecular C5—H5$\cdots$*Cg*4 contact (Fig. 1 and Table 1).

In the crystal, significant π–π stacking interactions [*Cg*1$\cdots$*Cg*1^{ii} = 3.5537 (12) Å and *Cg*2$\cdots$*Cg*3^{ii} = 3.4421 (12) Å; symmetry code: $-x+1, -y+1, -z$] link adjacent molecules into inversion dimers in a head-to-tail fashion. These dimers are further linked by C—H$\cdots\pi$(ring) contacts (Table 1) into chains of molecules stacked along the *c*-axis direction (Fig. 2). Adjacent chains are connected by C10—H10$\cdots$*Cg*4 contacts, forming sheets of molecules in the *bc* plane. Pairs of N3—H3*A*$\cdots$N1 hydrogen bonds (Table 1) form

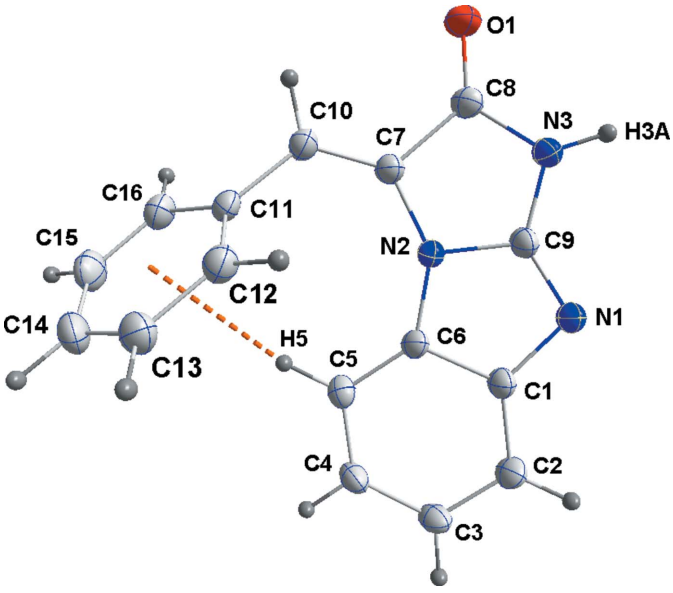


Figure 1
The title molecule with the atom-labeling scheme and 50% probability ellipsoids. The intramolecular C—H···π(ring) interaction is shown by a dotted line.

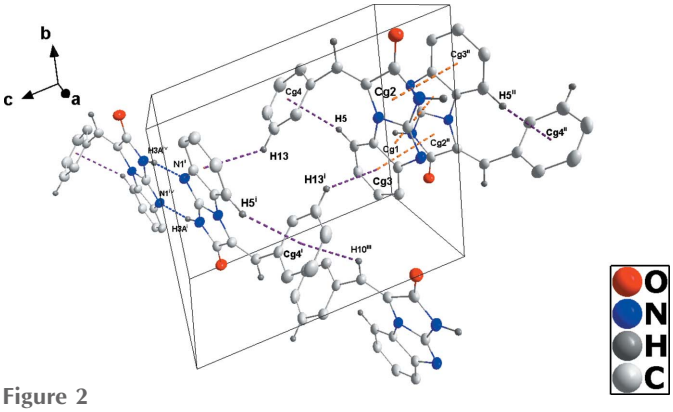


Figure 2
Details of the hydrogen bonding [N—H···N hydrogen bonds are represented by blue dashed lines and C—H···π(ring) interactions are represented by purple dashed lines] and π–π stacking interactions (orange dashed lines). *Cg*1–*Cg*4 are the centroids of the N1/C1/C6/N2/C9, N2/C9/N3/C8/C7, C1–C6 and C11–C16 rings, respectively. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 1-y, -z$; (iii) $x, -1+y, z$; (iv) $-1+x, y, 1+z$.]

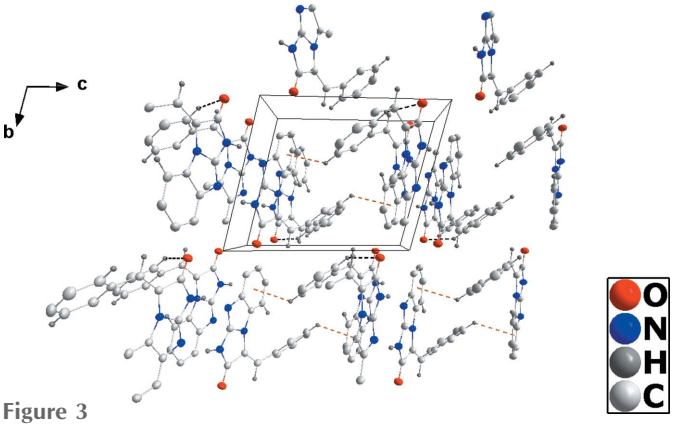


Figure 3
Packing viewed along the *a* axis, with C—H···O and some of the C—H···π(ring) interactions shown, respectively, as black and orange dashed lines.

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

*Cg*3 and *Cg*4 are the centroids of the C1–C6 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1^{i}	0.93 (3)	1.98 (3)	2.876 (2)	162 (3)
C16—H16···O1^{ii}	1.01 (3)	2.58 (3)	3.412 (3)	139 (2)
C5—H5···*Cg*4	1.01 (3)	2.65 (3)	3.512 (2)	143 (3)
C10—H10···*Cg*4^{iii}	1.01 (3)	2.88 (2)	3.606 (2)	129.0 (15)
C13—H13···*Cg*3^{iv}	1.00 (3)	2.73 (3)	3.474 (2)	132 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}N_3O$
M_r	261.28
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	6.6849 (3), 8.9428 (5), 10.7445 (5)
α, β, γ (°)	103.935 (3), 95.015 (4), 96.860 (3)
V (Å^3)	614.44 (5)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	0.74
Crystal size (mm)	0.21 × 0.15 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.83, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4587, 2249, 1810
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.136, 1.09
No. of reflections	2249
No. of parameters	225
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.26

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

inversion dimers with $R_2^2(8)$ rings and, together with C16—H16···O1 hydrogen bonds, stack the molecules along the *a*-axis direction (Fig. 3).

Synthesis and crystallization

A mixture of 2-aminobenzimidazole (0.03 mol) and ethyl glycidate (0.03 mol) was refluxed in 80 ml of *n*-butanol for 48 h. The resulting solution was concentrated under reduced pressure and the crude solid obtained was chromatographed on a silica gel column with a mixture of ethyl acetate/ethanol (80/20) as eluent. The 3-benzylidene-1*H*-benzimidazo[1,2-*a*]-imidazol-2(3*H*)-one obtained was recrystallized from ethanol solution to afford the title compound as colorless crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Three reflections ($5\bar{1}4$, $5\bar{2}8$ and $5\bar{2}7$) were omitted from the final refinement since they fell very close to the edge of a frame and were therefore felt to be poorly recorded.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161908 [https://doi.org/10.1107/S2414314616019088]

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Crystal data

$C_{16}H_{11}N_3O$
M_r = 261.28
Triclinic, $P\overline{1}$
a = 6.6849 (3) Å
b = 8.9428 (5) Å
c = 10.7445 (5) Å
α = 103.935 (3)°
β = 95.015 (4)°
γ = 96.860 (3)°
V = 614.44 (5) Å^3
Z = 2
$F(000)$ = 272
D_x = 1.412 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 3426 reflections
θ = 5.2–72.5°
μ = 0.74 mm^{-1}
T = 150 K
Plate, colourless
0.21 × 0.15 × 0.02 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.83, T_{max} = 0.98
4587 measured reflections
2249 independent reflections
1810 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 72.5°, θ_{min} = 5.2°
h = −8→7
k = −11→9
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.09
2249 reflections
225 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.4943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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.

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}
O1	0.9044 (2)	0.95697 (17)	0.15628 (15)	0.0297 (4)
N1	0.7919 (3)	0.4128 (2)	0.07214 (17)	0.0235 (4)
N2	0.6348 (3)	0.60823 (19)	0.17826 (16)	0.0205 (4)
N3	0.9139 (3)	0.6904 (2)	0.09709 (17)	0.0237 (4)
H3A	1.019 (4)	0.680 (3)	0.047 (3)	0.044 (8)*
C1	0.6146 (3)	0.3508 (2)	0.11504 (19)	0.0215 (4)
C2	0.5370 (3)	0.1964 (2)	0.1005 (2)	0.0245 (5)
H2	0.609 (4)	0.114 (3)	0.058 (3)	0.039 (7)*
C3	0.3508 (3)	0.1635 (2)	0.1428 (2)	0.0262 (5)
H3	0.285 (4)	0.056 (3)	0.127 (3)	0.031 (6)*
C4	0.2429 (3)	0.2818 (3)	0.1978 (2)	0.0267 (5)
H4	0.107 (4)	0.254 (3)	0.222 (2)	0.027 (6)*
C5	0.3203 (3)	0.4385 (2)	0.21698 (19)	0.0223 (4)
H5	0.247 (4)	0.526 (3)	0.260 (3)	0.029 (6)*
C6	0.5095 (3)	0.4707 (2)	0.17753 (19)	0.0212 (4)
C7	0.6545 (3)	0.7717 (2)	0.21504 (19)	0.0219 (4)
C8	0.8346 (3)	0.8244 (2)	0.15278 (19)	0.0232 (5)
C9	0.7924 (3)	0.5630 (2)	0.11100 (19)	0.0216 (4)
C10	0.5593 (3)	0.8678 (2)	0.2973 (2)	0.0234 (5)
H10	0.599 (4)	0.983 (3)	0.307 (2)	0.031 (6)*
C11	0.4150 (3)	0.8193 (2)	0.3810 (2)	0.0232 (5)
C12	0.4692 (4)	0.7249 (3)	0.4607 (2)	0.0273 (5)
H12	0.607 (4)	0.693 (3)	0.460 (3)	0.041 (8)*
C13	0.3346 (4)	0.6764 (3)	0.5388 (2)	0.0333 (5)
H13	0.375 (4)	0.610 (3)	0.596 (3)	0.039 (7)*
C14	0.1420 (4)	0.7199 (3)	0.5370 (2)	0.0373 (6)
H14	0.044 (5)	0.685 (3)	0.592 (3)	0.052 (9)*
C15	0.0887 (4)	0.8166 (3)	0.4608 (3)	0.0365 (6)
H15	−0.049 (5)	0.846 (4)	0.462 (3)	0.057 (9)*
C16	0.2245 (3)	0.8687 (3)	0.3846 (2)	0.0288 (5)
H16	0.189 (4)	0.940 (3)	0.329 (3)	0.039 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0337 (9)	0.0220 (8)	0.0333 (9)	−0.0005 (6)	0.0081 (7)	0.0075 (6)
N1	0.0260 (9)	0.0214 (9)	0.0234 (9)	0.0039 (7)	0.0091 (7)	0.0040 (7)
N2	0.0202 (9)	0.0188 (8)	0.0215 (8)	0.0019 (6)	0.0053 (7)	0.0029 (6)
N3	0.0243 (9)	0.0213 (9)	0.0251 (9)	0.0010 (7)	0.0090 (7)	0.0041 (7)
C1	0.0234 (10)	0.0218 (10)	0.0190 (9)	0.0034 (8)	0.0058 (8)	0.0035 (7)

C2	0.0290 (11)	0.0209 (10)	0.0217 (10)	0.0031 (8)	0.0050 (9)	0.0016 (8)
C3	0.0325 (12)	0.0208 (10)	0.0232 (10)	−0.0019 (9)	0.0064 (9)	0.0033 (8)
C4	0.0272 (12)	0.0281 (11)	0.0241 (11)	−0.0011 (9)	0.0089 (9)	0.0056 (9)
C5	0.0212 (10)	0.0266 (11)	0.0170 (9)	0.0026 (8)	0.0011 (8)	0.0022 (8)
C6	0.0268 (11)	0.0187 (10)	0.0176 (9)	0.0031 (8)	0.0062 (8)	0.0028 (7)
C7	0.0244 (11)	0.0204 (10)	0.0207 (10)	0.0022 (8)	0.0045 (8)	0.0046 (8)
C8	0.0260 (11)	0.0229 (11)	0.0191 (10)	0.0006 (8)	0.0029 (8)	0.0037 (8)
C9	0.0216 (10)	0.0224 (10)	0.0198 (10)	0.0017 (8)	0.0064 (8)	0.0028 (8)
C10	0.0254 (11)	0.0218 (11)	0.0224 (10)	0.0051 (8)	0.0047 (8)	0.0034 (8)
C11	0.0263 (11)	0.0204 (10)	0.0202 (10)	0.0033 (8)	0.0051 (8)	−0.0008 (8)
C12	0.0303 (12)	0.0262 (11)	0.0253 (11)	0.0066 (9)	0.0052 (9)	0.0045 (9)
C13	0.0447 (14)	0.0325 (12)	0.0239 (11)	0.0055 (10)	0.0095 (10)	0.0073 (9)
C14	0.0415 (14)	0.0399 (14)	0.0296 (12)	0.0019 (11)	0.0173 (11)	0.0045 (10)
C15	0.0282 (13)	0.0410 (14)	0.0388 (13)	0.0076 (10)	0.0115 (11)	0.0037 (11)
C16	0.0288 (12)	0.0292 (12)	0.0276 (11)	0.0079 (9)	0.0044 (9)	0.0034 (9)

Geometric parameters (Å, º)

O1—C8	1.212 (3)	C5—C6	1.388 (3)
N1—C9	1.306 (3)	C5—H5	1.01 (3)
N1—C1	1.409 (3)	C7—C10	1.337 (3)
N2—C9	1.375 (3)	C7—C8	1.509 (3)
N2—C6	1.401 (3)	C10—C11	1.472 (3)
N2—C7	1.406 (3)	C10—H10	1.01 (3)
N3—C9	1.365 (3)	C11—C12	1.394 (3)
N3—C8	1.392 (3)	C11—C16	1.397 (3)
N3—H3A	0.93 (3)	C12—C13	1.384 (3)
C1—C2	1.382 (3)	C12—H12	1.00 (3)
C1—C6	1.418 (3)	C13—C14	1.388 (4)
C2—C3	1.386 (3)	C13—H13	1.00 (3)
C2—H2	0.97 (3)	C14—C15	1.382 (4)
C3—C4	1.394 (3)	C14—H14	0.99 (3)
C3—H3	0.98 (3)	C15—C16	1.386 (3)
C4—C5	1.394 (3)	C15—H15	0.98 (3)
C4—H4	0.98 (2)	C16—H16	1.01 (3)
C9—N1—C1	103.06 (16)	O1—C8—N3	126.4 (2)
C9—N2—C6	106.03 (16)	O1—C8—C7	127.33 (19)
C9—N2—C7	109.67 (17)	N3—C8—C7	106.19 (17)
C6—N2—C7	144.18 (18)	N1—C9—N3	134.23 (19)
C9—N3—C8	109.39 (17)	N1—C9—N2	115.54 (18)
C9—N3—H3A	121.3 (18)	N3—C9—N2	110.20 (17)
C8—N3—H3A	128.7 (18)	C7—C10—C11	125.17 (19)
C2—C1—N1	128.60 (19)	C7—C10—H10	116.6 (14)
C2—C1—C6	120.20 (19)	C11—C10—H10	118.1 (14)
N1—C1—C6	111.18 (17)	C12—C11—C16	118.8 (2)
C1—C2—C3	118.06 (19)	C12—C11—C10	119.93 (19)
C1—C2—H2	120.3 (16)	C16—C11—C10	121.3 (2)

C3—C2—H2	121.6 (16)	C13—C12—C11	120.8 (2)
C2—C3—C4	121.4 (2)	C13—C12—H12	120.8 (16)
C2—C3—H3	120.7 (15)	C11—C12—H12	118.5 (16)
C4—C3—H3	117.6 (15)	C12—C13—C14	120.0 (2)
C3—C4—C5	121.7 (2)	C12—C13—H13	120.2 (16)
C3—C4—H4	119.3 (14)	C14—C13—H13	119.7 (16)
C5—C4—H4	119.0 (14)	C15—C14—C13	119.6 (2)
C6—C5—C4	116.56 (19)	C15—C14—H14	119.8 (18)
C6—C5—H5	120.6 (14)	C13—C14—H14	120.6 (18)
C4—C5—H5	122.8 (14)	C14—C15—C16	120.7 (2)
C5—C6—N2	133.96 (19)	C14—C15—H15	117.5 (19)
C5—C6—C1	121.92 (18)	C16—C15—H15	121.8 (19)
N2—C6—C1	104.03 (17)	C15—C16—C11	120.1 (2)
C10—C7—N2	131.17 (19)	C15—C16—H16	121.8 (16)
C10—C7—C8	124.17 (19)	C11—C16—H16	118.1 (16)
N2—C7—C8	104.25 (16)		

C9—N1—C1—C2	179.9 (2)	N2—C7—C8—O1	178.3 (2)
C9—N1—C1—C6	1.4 (2)	C10—C7—C8—N3	167.8 (2)
N1—C1—C2—C3	−175.2 (2)	N2—C7—C8—N3	−5.5 (2)
C6—C1—C2—C3	3.1 (3)	C1—N1—C9—N3	−176.5 (2)
C1—C2—C3—C4	0.5 (3)	C1—N1—C9—N2	1.3 (2)
C2—C3—C4—C5	−2.3 (3)	C8—N3—C9—N1	176.2 (2)
C3—C4—C5—C6	0.5 (3)	C8—N3—C9—N2	−1.6 (2)
C4—C5—C6—N2	179.0 (2)	C6—N2—C9—N1	−3.5 (2)
C4—C5—C6—C1	3.1 (3)	C7—N2—C9—N1	179.52 (17)
C9—N2—C6—C5	−172.6 (2)	C6—N2—C9—N3	174.82 (17)
C7—N2—C6—C5	2.6 (5)	C7—N2—C9—N3	−2.2 (2)
C9—N2—C6—C1	3.9 (2)	N2—C7—C10—C11	5.8 (4)
C7—N2—C6—C1	179.1 (3)	C8—C7—C10—C11	−165.6 (2)
C2—C1—C6—C5	−5.0 (3)	C7—C10—C11—C12	51.9 (3)
N1—C1—C6—C5	173.59 (19)	C7—C10—C11—C16	−129.4 (2)
C2—C1—C6—N2	177.99 (19)	C16—C11—C12—C13	2.1 (3)
N1—C1—C6—N2	−3.4 (2)	C10—C11—C12—C13	−179.1 (2)
C9—N2—C7—C10	−168.0 (2)	C11—C12—C13—C14	1.0 (3)
C6—N2—C7—C10	16.9 (5)	C12—C13—C14—C15	−2.6 (4)
C9—N2—C7—C8	4.7 (2)	C13—C14—C15—C16	1.0 (4)
C6—N2—C7—C8	−170.4 (3)	C14—C15—C16—C11	2.2 (4)
C9—N3—C8—O1	−179.3 (2)	C12—C11—C16—C15	−3.7 (3)
C9—N3—C8—C7	4.5 (2)	C10—C11—C16—C15	177.6 (2)
C10—C7—C8—O1	−8.3 (4)		

Hydrogen-bond geometry (Å, º)

*Cg*3 and *Cg*4 are the centroids of the C1–C6 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1^{i}	0.93 (3)	1.98 (3)	2.876 (2)	162 (3)
C16—H16···O1^{ii}	1.01 (3)	2.58 (3)	3.412 (3)	139 (2)

C5—H5···*Cg*4	1.01 (3)	2.65 (3)	3.512 (2)	143 (3)
C10—H10···*Cg*4^{iii}	1.01 (3)	2.88 (2)	3.606 (2)	129.0 (15)
C13—H13···*Cg*3^{iv}	1.00 (3)	2.73 (3)	3.474 (2)	132 (2)

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