

Crystal structure of 1-benzyl-4-(4-chlorophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]-pyridine-3-carbonitrile

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Received 31 July 2014

Accepted 29 August 2014

Edited by S. Bernès, UANL, México

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Keywords: crystal structure; cycloocta[*b*]pyridine; hydrogen bonding; Schiff bases

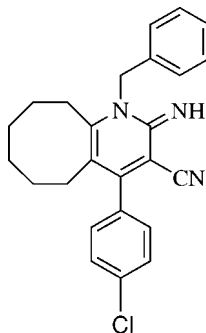
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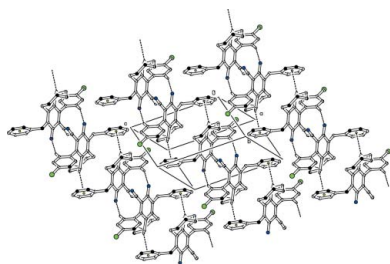
The title compound, C₂₅H₂₄ClN₃, comprises a 2-iminopyridine ring fused with a cyclooctane ring, which adopts a twist boat–chair conformation. In the crystal, C–H···N interactions form R₂²(14) ring motifs and molecules are further connected by weak C–H···π interactions. The resulting supramolecular structure is a two-dimensional framework parallel to the *ab* plane.

1. Chemical context

Schiff bases are compounds carrying an imine or azomethine (–C=N–) functional group. They have gained importance in the medicinal and pharmaceutical fields due to their broad spectrum of biological activity, including anti-inflammatory, analgesic, antimicrobial, anticonvulsant, antitubercular (Aboul-Fadl *et al.*, 2003), anticancer, antioxidant and anti-helminthic, among others. Schiff base derivatives are present in a number of processes, which prompted researchers to design novel heterocyclic/aryl Schiff bases with the aim of developing new environmentally friendly technologies (Bhattacharya *et al.*, 2003). Schiff bases are also used as ligands for catalysts, intermediates in organic synthesis, dyes, pigments, and polymer stabilizers (Dhar & Taploo, 1982).



Iminopyridine complexes can be useful catalysts, and pyridones have been investigated extensively as valuable building blocks for many fused heterocyclic systems (Johns *et al.*, 2003) displaying a wide range of biological and pharmacological activities. They exhibit, for example, antiproliferative and antitubolin activities (Magedov *et al.*, 2008). Many pyridin-2-one and 3-cyano-2-iminopyridine derivatives also exhibit antiproliferative activity (McNamara & Cook, 1987). As part of our studies in this area, the title compound was synthesized



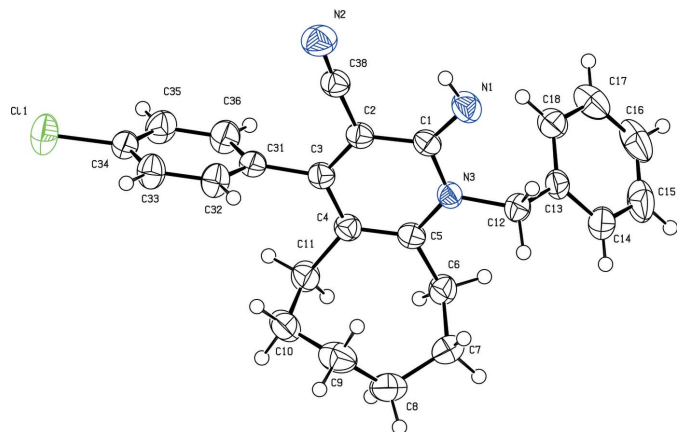


Figure 1
The molecular structure of the title compound, showing 20% probability displacement ellipsoids. All H atoms have been omitted for clarity.

and we report herein on the molecular and crystal structures of this compound.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The cyclooctane ring adopts a twist boat–chair conformation (Wiberg, 2003), as found in similar structures (Vishnupriya *et al.*, 2014*a,b*). As expected, the pyridine ring (atoms C1–C5/N3) is almost planar, with an r.m.s. deviation of 0.002 Å. The chlorobenzene (C31–C36) and phenyl (C13–C18) rings are almost planar, with r.m.s. deviations of 0.005 and 0.004 Å, respectively. The sum of the angles around atom N3 is 359.8°, indicating that atom N3 is sp^2 -hybridized. The C2–C38≡N2 bond angle of 176.07 (19)° shows the linearity of the cyano group, a feature systematically observed in carbonitrile compounds. Nitrile atoms C38 and N2 are displaced from the mean plane of the pyridine ring by 0.0258 (1) and 0.0363 (1) Å, respectively. The imino C1=N1 bond length is 1.286 (2) Å. The imino group is nearly coplanar with the pyridine ring, as indicated by the N1=C1–N3–C5

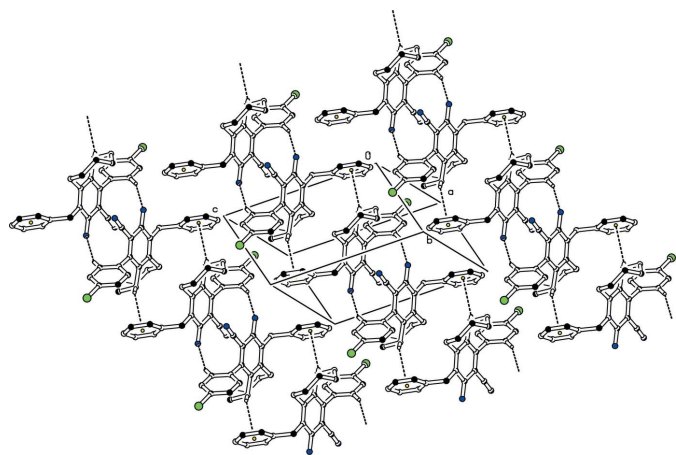


Figure 2
Partial packing diagram of the title compound. Dashed lines represent intermolecular hydrogen bonds and C–H... π contacts. For clarity, H atoms not involved in hydrogen bonding have been omitted.

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

Cg1 is the centroid of the phenyl ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C32–H32...N1 ⁱ	0.93	2.55	3.423 (2)	156
C11–H11B...Cg1 ⁱⁱ	0.97	2.91	3.5642 (2)	126

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

torsion angle of -178.89 (14)°. The chlorobenzene ring is attached to the pyridine ring with a C2=C3–C31=C36 torsion angle of 100.99 (19)°, indicating a (+)antiperiplanar conformation. The C33=C34=C35 bond angle of 121.11 (15)° deviates from 120° due to the presence of the chlorine substituent. The chlorine atom bonded to C34 deviates by 0.0446 (1) Å from the mean plane of the phenyl ring. The chlorine is attached to the benzene ring with a C32=C33=C34–Cl1 torsion angle of 178.95 (13)°. In the pyridine ring, the formal double bonds [C4=C5 = 1.375 (2) and C2=C3 = 1.369 (2) Å] are longer than standard C=C bonds (1.34 Å), while the other bond lengths are slightly shorter than standard C–C and C–N bond lengths, evidencing that there is a homo-conjugation effect for this ring.

3. Supramolecular features

In the crystal, pairs of C–H...N interactions form $R_2^2(14)$ ring motifs (Bernstein *et al.*, 1995), and the resulting dimers are further connected through weak C–H... π interactions involving the phenyl ring as acceptor (Table 1 and Fig. 2). The resulting supramolecular structure is a two-dimensional framework parallel to the crystallographic ab plane.

4. Database survey

Similar structures reported in the literature are 2-methoxy-4-(2-methoxyphenyl)-5,6,7,8,9,10-hexahydrocycloocta[*b*]pyridine-3-carbonitrile (Vishnupriya *et al.*, 2014*a*) and 4-(2-fluorophenyl)-2-methoxy-5,6,7,8,9,10-hexahydrocycloocta[*b*]pyridine-3-carbonitrile (Vishnupriya *et al.*, 2014*b*). In the structure reported here, the twisted conformation of the cyclooctane ring and the planar conformation of the pyridine are similar to those found in the related structures. However, the C=NH functional group present in the title compound allows the formation of C–H...N hydrogen bonds, which are not present in the above-cited compounds. In the title compound, the bond lengths in the central pyridine ring span the range 1.369–1.447 Å, which compares well with the ranges observed in the similar structures (1.314–1.400 Å), but these bonds are systematically longer in the title compound, due to the substitution of the pyridine N atom by a benzyl group.

5. Synthesis and crystallization

Cyclooctanone (1 mmol), 4-chlorobenzaldehyde (1 mmol) and malononitrile (1 mmol) were mixed in ethanol (10 ml),

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₅ H ₂₄ ClN ₃
<i>M_r</i>	401.92
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.2319 (3), 10.5228 (3), 11.7767 (4)
α , β , γ (°)	101.088 (2), 107.524 (2), 114.008 (2)
<i>V</i> (Å ³)	1029.87 (5)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.20
Crystal size (mm)	0.21 × 0.19 × 0.18
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2004)
<i>T_{min}</i> , <i>T_{max}</i>	0.967, 0.974
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	26728, 3842, 3094
<i>R_{int}</i>	0.027
(sin θ/λ) _{max} (Å ⁻¹)	0.606
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.105, 1.05
No. of reflections	3842
No. of parameters	266
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)	0.29, -0.33

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

and *p*-toluenesulfonic acid (0.5 mmol) was added. The reaction mixture was refluxed for 2–3 h. After completion of the reaction (followed by thin-layer chromatography), the mixture was poured into crushed ice and extracted with ethyl acetate. The excess of solvent was removed under reduced pressure and the residue was chromatographed using a petroleum ether/ethyl acetate mixture (97:3 *v/v*) as eluent, to afford the pure product. The product was recrystallized from ethyl acetate, affording colourless crystals (m.p. 493 K; yield 71%).

6. Refinement

C-bound H atoms were placed in calculated positions and allowed to ride on their carrier atoms, with C–H = 0.93 (aromatic CH) or 0.97 Å (methylene CH₂). Imine atom H1 was found in a difference map and refined freely, with the N–H distance restrained to 0.84 (2) Å. Isotropic displacement parameters for H atoms were calculated as *U*_{iso}(H) = 1.2*U*_{eq}(C) for CH and CH₂ groups, while the *U*_{iso} factor for H1 was refined. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

JS and RAN thank the management of The Madura College (Autonomous), Madurai, for their encouragement and support. RRK thanks the University Grants Commission, New Delhi, for funds through Major Research Project F. No. 42–242/2013 (SR).

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supporting information

Acta Cryst. (2014). E70, 167-169 [doi:10.1107/S160053681401962X]

Crystal structure of 1-benzyl-4-(4-chlorophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]pyridine-3-carbonitrile

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

1-Benzyl-4-(4-chlorophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]pyridine-3-carbonitrile

Crystal data

$C_{25}H_{24}ClN_3$	$Z = 2$
$M_r = 401.92$	$F(000) = 424$
Triclinic, $P1$	$D_x = 1.296 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Melting point: 493 K
$a = 10.2319 (3) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 10.5228 (3) \text{ \AA}$	Cell parameters from 2000 reflections
$c = 11.7767 (4) \text{ \AA}$	$\theta = 2-31^\circ$
$\alpha = 101.088 (2)^\circ$	$\mu = 0.20 \text{ mm}^{-1}$
$\beta = 107.524 (2)^\circ$	$T = 293 \text{ K}$
$\gamma = 114.008 (2)^\circ$	Block, colourless
$V = 1029.87 (5) \text{ \AA}^3$	$0.21 \times 0.19 \times 0.18 \text{ mm}$

Data collection

Bruker Kappa APEXII diffractometer	26728 measured reflections
Radiation source: fine-focus sealed tube	3842 independent reflections
Graphite monochromator	3094 reflections with $I > 2\sigma(I)$
Detector resolution: 0 pixels mm^{-1}	$R_{\text{int}} = 0.027$
ω and ϕ scans	$\theta_{\text{max}} = 25.5^\circ$, $\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2004)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.974$	$k = -12 \rightarrow 12$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	2 restraints
Least-squares matrix: full	0 constraints
$R[F^2 > 2\sigma(F^2)] = 0.038$	Primary atom site location: structure-invariant direct methods
$wR(F^2) = 0.105$	Secondary atom site location: difference Fourier map
$S = 1.05$	
3842 reflections	
266 parameters	

Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.4103P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.41432 (18)	0.89760 (17)	0.60601 (14)	0.0337 (3)
C2	0.43550 (18)	0.80064 (17)	0.51697 (14)	0.0335 (3)
C3	0.31232 (18)	0.67411 (17)	0.41791 (14)	0.0333 (3)
C4	0.15512 (18)	0.63430 (17)	0.39917 (14)	0.0353 (3)
C5	0.13131 (18)	0.72425 (17)	0.48236 (14)	0.0335 (3)
C6	-0.03192 (19)	0.6888 (2)	0.46876 (16)	0.0423 (4)
H6A	-0.0265	0.7273	0.5528	0.051*
H6B	-0.0988	0.5812	0.4361	0.051*
C7	-0.1099 (2)	0.7521 (2)	0.38092 (18)	0.0551 (5)
H7A	-0.1975	0.7499	0.3983	0.066*
H7B	-0.0338	0.8559	0.4038	0.066*
C8	-0.1713 (2)	0.6742 (3)	0.23817 (19)	0.0593 (5)
H8A	-0.2427	0.5691	0.2160	0.071*
H8B	-0.2325	0.7141	0.1940	0.071*
C9	-0.0483 (2)	0.6871 (2)	0.18839 (19)	0.0578 (5)
H9A	0.0513	0.7749	0.2484	0.069*
H9B	-0.0788	0.7029	0.1083	0.069*
C10	-0.0220 (2)	0.5534 (2)	0.16653 (17)	0.0557 (5)
H10A	0.0628	0.5763	0.1392	0.067*
H10B	-0.1169	0.4690	0.0970	0.067*
C11	0.0186 (2)	0.50636 (19)	0.28133 (17)	0.0456 (4)
H11A	-0.0733	0.4650	0.2993	0.055*
H11B	0.0448	0.4287	0.2603	0.055*
C12	0.2287 (2)	0.95489 (18)	0.66307 (15)	0.0397 (4)
H12A	0.1371	0.9574	0.6102	0.048*
H12B	0.3189	1.0545	0.6960	0.048*
C13	0.20272 (19)	0.91624 (18)	0.77398 (15)	0.0386 (4)
C14	0.0786 (2)	0.9164 (2)	0.79756 (18)	0.0550 (5)
H14	0.0085	0.9357	0.7426	0.066*
C15	0.0579 (3)	0.8877 (3)	0.9030 (2)	0.0687 (7)
H15	-0.0265	0.8871	0.9179	0.082*
C16	0.1608 (3)	0.8603 (2)	0.98475 (19)	0.0672 (6)
H16	0.1475	0.8427	1.0560	0.081*
C17	0.2835 (2)	0.8589 (2)	0.96164 (18)	0.0570 (5)
H17	0.3531	0.8395	1.0171	0.068*
C18	0.3047 (2)	0.88603 (19)	0.85687 (16)	0.0444 (4)
H18	0.3881	0.8841	0.8417	0.053*
C31	0.34478 (18)	0.57918 (17)	0.33174 (15)	0.0352 (3)
C32	0.3811 (2)	0.61741 (19)	0.23496 (17)	0.0434 (4)
H32	0.3887	0.7054	0.2250	0.052*

C33	0.4064 (2)	0.5266 (2)	0.15252 (17)	0.0458 (4)
H33	0.4291	0.5523	0.0868	0.055*
C34	0.39752 (19)	0.39863 (18)	0.16899 (15)	0.0394 (4)
C35	0.3645 (2)	0.3594 (2)	0.26548 (18)	0.0488 (4)
H35	0.3603	0.2728	0.2764	0.059*
C36	0.3376 (2)	0.4497 (2)	0.34654 (17)	0.0472 (4)
H36	0.3143	0.4229	0.4118	0.057*
C38	0.59554 (19)	0.84653 (18)	0.53780 (15)	0.0384 (4)
N1	0.52304 (18)	1.01684 (16)	0.70223 (14)	0.0466 (4)
N2	0.72609 (18)	0.88953 (19)	0.56079 (16)	0.0557 (4)
N3	0.25617 (15)	0.85167 (14)	0.58174 (11)	0.0328 (3)
Cl1	0.42569 (7)	0.28161 (6)	0.06488 (5)	0.06290 (17)
H1	0.612 (2)	1.031 (2)	0.703 (2)	0.063 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0364 (8)	0.0339 (8)	0.0297 (8)	0.0161 (7)	0.0126 (6)	0.0147 (7)
C2	0.0346 (7)	0.0360 (8)	0.0313 (8)	0.0174 (7)	0.0139 (6)	0.0156 (6)
C3	0.0372 (8)	0.0341 (8)	0.0315 (8)	0.0188 (7)	0.0147 (7)	0.0148 (7)
C4	0.0340 (8)	0.0334 (8)	0.0342 (8)	0.0153 (7)	0.0123 (7)	0.0103 (7)
C5	0.0348 (8)	0.0348 (8)	0.0318 (8)	0.0170 (7)	0.0133 (6)	0.0154 (7)
C6	0.0387 (9)	0.0476 (10)	0.0403 (9)	0.0205 (8)	0.0198 (7)	0.0125 (8)
C7	0.0475 (10)	0.0707 (13)	0.0534 (11)	0.0388 (10)	0.0184 (9)	0.0181 (10)
C8	0.0463 (11)	0.0748 (14)	0.0540 (12)	0.0336 (10)	0.0132 (9)	0.0229 (10)
C9	0.0490 (11)	0.0732 (14)	0.0458 (10)	0.0252 (10)	0.0167 (9)	0.0278 (10)
C10	0.0427 (10)	0.0670 (13)	0.0362 (9)	0.0196 (9)	0.0110 (8)	0.0034 (9)
C11	0.0360 (9)	0.0398 (9)	0.0466 (10)	0.0141 (7)	0.0141 (8)	0.0030 (8)
C12	0.0460 (9)	0.0373 (9)	0.0376 (9)	0.0256 (8)	0.0151 (7)	0.0101 (7)
C13	0.0387 (8)	0.0359 (8)	0.0334 (8)	0.0168 (7)	0.0141 (7)	0.0028 (7)
C14	0.0465 (10)	0.0593 (12)	0.0484 (11)	0.0274 (9)	0.0172 (9)	0.0002 (9)
C15	0.0530 (12)	0.0728 (14)	0.0585 (13)	0.0171 (11)	0.0346 (11)	-0.0048 (11)
C16	0.0625 (13)	0.0677 (14)	0.0382 (10)	0.0069 (11)	0.0264 (10)	0.0034 (10)
C17	0.0534 (11)	0.0595 (12)	0.0379 (10)	0.0146 (9)	0.0149 (9)	0.0155 (9)
C18	0.0399 (9)	0.0479 (10)	0.0389 (9)	0.0179 (8)	0.0162 (7)	0.0127 (8)
C31	0.0320 (8)	0.0351 (8)	0.0345 (8)	0.0160 (7)	0.0117 (7)	0.0099 (7)
C32	0.0541 (10)	0.0374 (9)	0.0494 (10)	0.0248 (8)	0.0291 (8)	0.0203 (8)
C33	0.0572 (11)	0.0464 (10)	0.0460 (10)	0.0272 (9)	0.0319 (9)	0.0211 (8)
C34	0.0371 (8)	0.0394 (9)	0.0397 (9)	0.0203 (7)	0.0152 (7)	0.0090 (7)
C35	0.0627 (11)	0.0458 (10)	0.0535 (11)	0.0357 (9)	0.0273 (9)	0.0245 (9)
C36	0.0631 (11)	0.0526 (11)	0.0452 (10)	0.0362 (9)	0.0304 (9)	0.0270 (8)
C38	0.0372 (8)	0.0421 (9)	0.0357 (8)	0.0188 (7)	0.0153 (7)	0.0162 (7)
N1	0.0411 (8)	0.0414 (8)	0.0408 (8)	0.0139 (7)	0.0126 (7)	0.0049 (7)
N2	0.0407 (9)	0.0659 (11)	0.0566 (10)	0.0236 (8)	0.0201 (7)	0.0214 (8)
N3	0.0374 (7)	0.0333 (7)	0.0289 (6)	0.0190 (6)	0.0136 (5)	0.0112 (5)
Cl1	0.0826 (4)	0.0577 (3)	0.0635 (3)	0.0439 (3)	0.0404 (3)	0.0156 (2)

Geometric parameters (Å, °)

C1—N1	1.286 (2)	C12—N3	1.4786 (19)
C1—N3	1.402 (2)	C12—C13	1.506 (2)
C1—C2	1.447 (2)	C12—H12A	0.9700
C2—C3	1.369 (2)	C12—H12B	0.9700
C2—C38	1.430 (2)	C13—C14	1.380 (2)
C3—C4	1.419 (2)	C13—C18	1.385 (2)
C3—C31	1.490 (2)	C14—C15	1.388 (3)
C4—C5	1.375 (2)	C14—H14	0.9300
C4—C11	1.508 (2)	C15—C16	1.365 (3)
C5—N3	1.379 (2)	C15—H15	0.9300
C5—C6	1.504 (2)	C16—C17	1.368 (3)
C6—C7	1.533 (3)	C16—H16	0.9300
C6—H6A	0.9700	C17—C18	1.377 (2)
C6—H6B	0.9700	C17—H17	0.9300
C7—C8	1.519 (3)	C18—H18	0.9300
C7—H7A	0.9700	C31—C32	1.382 (2)
C7—H7B	0.9700	C31—C36	1.382 (2)
C8—C9	1.510 (3)	C32—C33	1.385 (2)
C8—H8A	0.9700	C32—H32	0.9300
C8—H8B	0.9700	C33—C34	1.367 (2)
C9—C10	1.527 (3)	C33—H33	0.9300
C9—H9A	0.9700	C34—C35	1.369 (2)
C9—H9B	0.9700	C34—C11	1.7387 (16)
C10—C11	1.527 (3)	C35—C36	1.383 (2)
C10—H10A	0.9700	C35—H35	0.9300
C10—H10B	0.9700	C36—H36	0.9300
C11—H11A	0.9700	C38—N2	1.143 (2)
C11—H11B	0.9700	N1—H1	0.861 (15)
N1—C1—N3	118.60 (15)	C10—C11—H11B	109.1
N1—C1—C2	127.15 (15)	H11A—C11—H11B	107.8
N3—C1—C2	114.24 (13)	N3—C12—C13	115.09 (13)
C3—C2—C38	121.37 (14)	N3—C12—H12A	108.5
C3—C2—C1	123.18 (14)	C13—C12—H12A	108.5
C38—C2—C1	115.45 (14)	N3—C12—H12B	108.5
C2—C3—C4	119.51 (14)	C13—C12—H12B	108.5
C2—C3—C31	119.70 (14)	H12A—C12—H12B	107.5
C4—C3—C31	120.79 (13)	C14—C13—C18	118.66 (17)
C5—C4—C3	118.62 (14)	C14—C13—C12	119.81 (16)
C5—C4—C11	121.18 (14)	C18—C13—C12	121.48 (15)
C3—C4—C11	119.80 (14)	C13—C14—C15	120.3 (2)
C4—C5—N3	121.43 (14)	C13—C14—H14	119.9
C4—C5—C6	121.59 (14)	C15—C14—H14	119.9
N3—C5—C6	116.98 (13)	C16—C15—C14	120.32 (19)
C5—C6—C7	114.83 (14)	C16—C15—H15	119.8
C5—C6—H6A	108.6	C14—C15—H15	119.8

C7—C6—H6A	108.6	C15—C16—C17	119.81 (19)
C5—C6—H6B	108.6	C15—C16—H16	120.1
C7—C6—H6B	108.6	C17—C16—H16	120.1
H6A—C6—H6B	107.5	C16—C17—C18	120.5 (2)
C8—C7—C6	116.81 (16)	C16—C17—H17	119.8
C8—C7—H7A	108.1	C18—C17—H17	119.8
C6—C7—H7A	108.1	C17—C18—C13	120.46 (17)
C8—C7—H7B	108.1	C17—C18—H18	119.8
C6—C7—H7B	108.1	C13—C18—H18	119.8
H7A—C7—H7B	107.3	C32—C31—C36	118.56 (15)
C9—C8—C7	116.28 (16)	C32—C31—C3	121.06 (14)
C9—C8—H8A	108.2	C36—C31—C3	120.38 (14)
C7—C8—H8A	108.2	C31—C32—C33	120.92 (15)
C9—C8—H8B	108.2	C31—C32—H32	119.5
C7—C8—H8B	108.2	C33—C32—H32	119.5
H8A—C8—H8B	107.4	C34—C33—C32	119.21 (16)
C8—C9—C10	115.62 (18)	C34—C33—H33	120.4
C8—C9—H9A	108.4	C32—C33—H33	120.4
C10—C9—H9A	108.4	C33—C34—C35	121.11 (15)
C8—C9—H9B	108.4	C33—C34—C11	119.88 (13)
C10—C9—H9B	108.4	C35—C34—C11	119.00 (13)
H9A—C9—H9B	107.4	C34—C35—C36	119.39 (16)
C9—C10—C11	115.86 (15)	C34—C35—H35	120.3
C9—C10—H10A	108.3	C36—C35—H35	120.3
C11—C10—H10A	108.3	C31—C36—C35	120.79 (16)
C9—C10—H10B	108.3	C31—C36—H36	119.6
C11—C10—H10B	108.3	C35—C36—H36	119.6
H10A—C10—H10B	107.4	N2—C38—C2	176.07 (19)
C4—C11—C10	112.58 (15)	C1—N1—H1	107.2 (15)
C4—C11—H11A	109.1	C5—N3—C1	123.00 (13)
C10—C11—H11A	109.1	C5—N3—C12	120.87 (13)
C4—C11—H11B	109.1	C1—N3—C12	115.95 (13)
N1—C1—C2—C3	178.97 (16)	C15—C16—C17—C18	0.5 (3)
N3—C1—C2—C3	-0.5 (2)	C16—C17—C18—C13	0.5 (3)
N1—C1—C2—C38	-1.8 (2)	C14—C13—C18—C17	-0.9 (3)
N3—C1—C2—C38	178.71 (13)	C12—C13—C18—C17	176.46 (16)
C38—C2—C3—C4	-178.72 (14)	C2—C3—C31—C32	-79.6 (2)
C1—C2—C3—C4	0.4 (2)	C4—C3—C31—C32	100.90 (19)
C38—C2—C3—C31	1.8 (2)	C2—C3—C31—C36	100.99 (19)
C1—C2—C3—C31	-179.06 (13)	C4—C3—C31—C36	-78.5 (2)
C2—C3—C4—C5	-0.5 (2)	C36—C31—C32—C33	1.4 (3)
C31—C3—C4—C5	179.02 (14)	C3—C31—C32—C33	-177.97 (15)
C2—C3—C4—C11	172.41 (14)	C31—C32—C33—C34	-1.1 (3)
C31—C3—C4—C11	-8.1 (2)	C32—C33—C34—C35	-0.1 (3)
C3—C4—C5—N3	0.6 (2)	C32—C33—C34—C11	178.95 (13)
C11—C4—C5—N3	-172.17 (14)	C33—C34—C35—C36	0.9 (3)
C3—C4—C5—C6	-179.76 (14)	C11—C34—C35—C36	-178.19 (14)

C11—C4—C5—C6	7.5 (2)	C32—C31—C36—C35	-0.7 (3)
C4—C5—C6—C7	-88.02 (19)	C3—C31—C36—C35	178.75 (16)
N3—C5—C6—C7	91.64 (18)	C34—C35—C36—C31	-0.5 (3)
C5—C6—C7—C8	74.9 (2)	C3—C2—C38—N2	-174 (3)
C6—C7—C8—C9	-67.4 (3)	C1—C2—C38—N2	7 (3)
C7—C8—C9—C10	99.1 (2)	C4—C5—N3—C1	-0.7 (2)
C8—C9—C10—C11	-55.1 (2)	C6—C5—N3—C1	179.62 (13)
C5—C4—C11—C10	88.34 (19)	C4—C5—N3—C12	174.19 (14)
C3—C4—C11—C10	-84.35 (19)	C6—C5—N3—C12	-5.5 (2)
C9—C10—C11—C4	-52.2 (2)	N1—C1—N3—C5	-178.89 (14)
N3—C12—C13—C14	-132.69 (16)	C2—C1—N3—C5	0.6 (2)
N3—C12—C13—C18	49.9 (2)	N1—C1—N3—C12	6.0 (2)
C18—C13—C14—C15	0.4 (3)	C2—C1—N3—C12	-174.52 (12)
C12—C13—C14—C15	-177.01 (17)	C13—C12—N3—C5	86.24 (17)
C13—C14—C15—C16	0.5 (3)	C13—C12—N3—C1	-98.50 (16)
C14—C15—C16—C17	-1.0 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the centroid of the phenyl ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C32—H32 \cdots N1 ⁱ	0.93	2.55	3.423 (2)	156
C11—H11B \cdots Cg1 ⁱⁱ	0.97	2.91	3.5642 (2)	126

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