Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Received 12 September 2014
Accepted 6 October 2014

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; cyclooctapyridine; hydrogen bonding

CCDC references: 1027782; 1027783
Supporting information: this article has supporting information at journals.iucr.org/e

Isotypic crystal structures of 1-benzyl-4-(4-bromophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]pyridine-3-carbonitrile and 1-benzyl-4-(4-fluorophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]pyridine-3-carbonitrile

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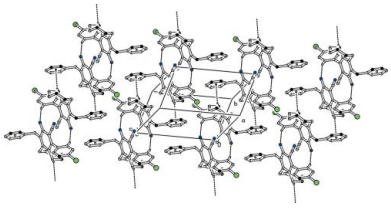
The molecules of the two isotypic title compounds, $C_{25}H_{24}BrN_3$, (I), and $C_{25}H_{24}FN_3$, (II), comprise a 2-iminopyridine ring fused with a cyclooctane ring. In (I), the cyclooctane ring adopts a twisted chair–chair conformation, while in (II), this ring adopts a twisted boat–chair conformation. The dihedral angles between the planes of the pyridine ring and the bromobenzene and phenyl rings are 80.14 (12) and 71.72 (13)°, respectively, in (I). The equivalent angles in (II) are 75.25 (8) and 68.34 (9)°, respectively. In both crystals, inversion dimers linked by pairs of C—H···N interactions generate $R_2^2(14)$ loops, which are further connected by weak C—H···π interactions, generating (110) sheets.

1. Chemical context

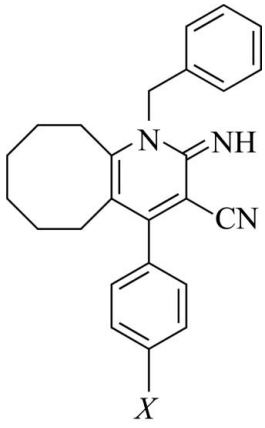
The pyridine skeleton is of great importance to chemists as well as to biologists as it is found in a large variety of naturally occurring compounds and also in clinically useful molecules having diverse biological activities. Its derivatives are known to possess antimicrobial (Jo *et al.*, 2004) and antiviral (Mavel *et al.*, 2002) activities. The heterocyclic 1,4-dihydropyridine ring is a common feature in compounds with various pharmacological activities such as antimicrobial (Hooper *et al.*, 1982) and antithrombotic (Sunkel *et al.*, 1990) activities. The chemistry of imines in particular is of special interest in the literature due to their numerous practical applications (Echevarria *et al.*, 1999). Imines have attracted much attention because of their wide variety of applications in the electronics and photonics fields (Wang *et al.*, 2001). Imines and their complexes have a variety of applications in the biological, clinical and analytical fields (Singh *et al.*, 1975; Patel *et al.*, 1999). Our interest in the preparation of pharmacologically active 2-imino pyridines led us to synthesise the title compounds and we have undertaken the X-ray crystal structure determination of these compounds in order to establish their conformations.



2. Structural commentary

The structures of compounds (I) and (II) are shown in Figs. 1 and 2, respectively. The cyclooctane ring adopts a twisted

chair–chair conformation in compound (I) and twisted boat–chair conformation (Wiberg, 2003) in compound (II).



(I) X = Br
(II) X = F

In both compounds, the imino group is nearly coplanar with the pyridine ring, as indicated by the N1═C1—N3—C5 torsion angle [178.8 (2) for compound (I) and 179.05 (13)° for compound (II)]. Steric hindrances rotate the phenyl (C13–C18) and aromatic (C31–C36) rings out of the plane of the central pyridine ring by 71.72 (13) and 80.14 (12)°, respectively, in compound (I), and by 68.34 (9) and 75.25 (8)°, respectively, in compound (II). Opening up of the N3—C5—C4 angle [121.54 (19)° for compound (I) and 121.29 (13)° for compound (II)] and considerable shortening of the C5—N3 [1.376 (3) Å for compound (I) and 1.3777 (18) Å for compound (II)] bond distance may directly be attributed to the bulky substituents at the *ortho* position C5. The endocyclic angles of the pyridine ring cover the range 114.29 (18)–123.02 (2)° and 118.86 (13)–123.11 (12)° for compounds (I) and (II) respectively. The C1—N3—C5 angle [122.93 (2) for compound (I) and 123.11 (12)° for compound (II)] is expanded as in pyridine itself [123.9 (3)°; Jin *et al.*, 2005].

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

*Cg*1 is the centroid of the C13–C18 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C32—H32···N1^{i}	0.93	2.56	3.421 (3)	154
C11—H11A···Cg1^{ii}	0.97	2.97	3.648 (3)	128

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

*Cg*1 is the centroid of the C13–C18 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C32—H32···N1^{i}	0.93	2.53	3.421 (2)	160
C11—H11A···Cg1^{ii}	0.97	2.93	3.484 (2)	118

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

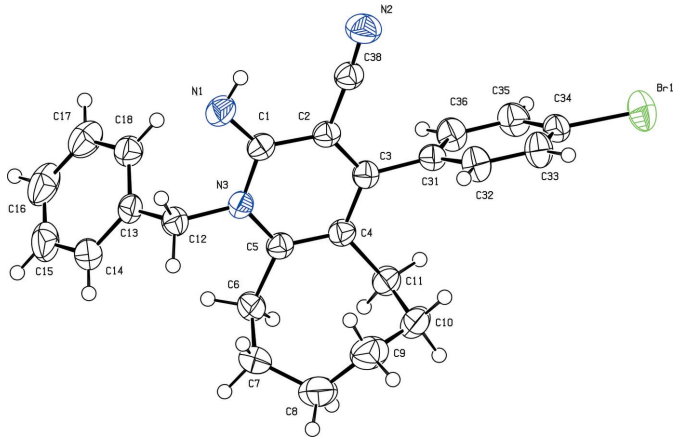


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

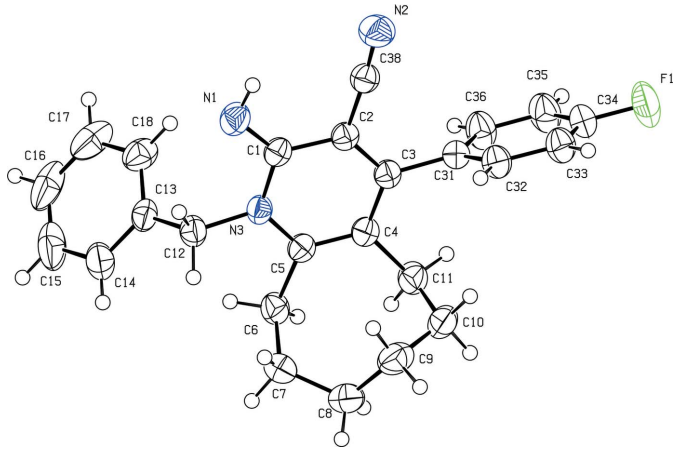


Figure 2
The molecular structure of (II), showing 50% probability displacement ellipsoids.

3. Supramolecular features

In the crystals, 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

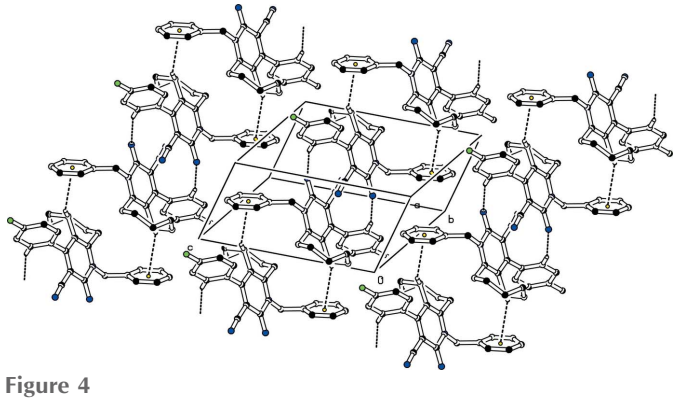


Figure 4
Partial packing diagram of the title compound (II). Dashed lines represent intermolecular hydrogen bonds and C—H···π contacts. For clarity, H atoms not involved in hydrogen bonding have been omitted.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{25}H_{24}BrN_3$	$C_{25}H_{24}FN_3$
M_r	446.38	385.47
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	293	293
a, b, c (Å)	10.2103 (3), 10.7643 (4), 11.6942 (4)	10.1370 (4), 10.2078 (3), 11.8238 (4)
α, β, γ (°)	101.074 (1), 106.726 (1), 115.058 (1)	109.688 (2), 100.309 (2), 111.420 (2)
V (Å^3)	1039.46 (6)	1006.73 (6)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.99	0.08
Crystal size (mm)	0.21 × 0.19 × 0.18	0.21 × 0.19 × 0.18
Data collection		
Diffractometer	Bruker Kappa APEXII	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.967, 0.974	0.967, 0.974
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25106, 4532, 3830	23254, 3752, 2876
R_{int}	0.027	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639	0.606
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.107, 1.03	0.039, 0.109, 1.05
No. of reflections	4532	3752
No. of parameters	266	267
No. of restraints	2	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.93, −0.87	0.17, −0.14

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97*, *SHELXL97* and *SHELXL2014*/6 (Sheldrick, 2008) and *PLATON* (Spek, 2009).

involving the phenyl ring as acceptor (Tables 1 and 2, Figs. 3, 4). In each case, the resulting supramolecular structure is a layer propagating parallel to the (110) 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*). The twisted conformation of the cyclooctane ring of compound (I) is similar to those found in the related structures. However, the

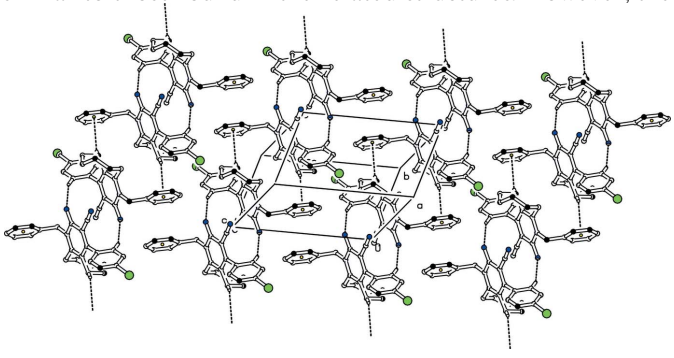


Figure 3
Partial packing diagram of the title compound (I). Dashed lines represent intermolecular hydrogen bonds and C—H···π contacts. For clarity, H atoms not involved in hydrogen bonding have been omitted.

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 compounds, the bond lengths in the central pyridine ring span the range 1.369–1.446 Å, which compare well with the range observed in the similar structures (1.314–1.400 Å), but these bonds are systematically longer in the title compounds, due to the substitution of the pyridine N atom by a benzyl group. The bond length of the nitrile group attached to pyridine ring [N2≡C38 = 1.137 (3) Å in compound (I) and 1.1426 (19) Å in compound (II)] and the linearity of the cyano moiety [N2≡C38—C2 = 176.3 (3) for compound (I) and 175.68 (17)° for compound (II)] have characteristic features that are observed in 3-cyano-2-pyridine derivatives (Hursthouse *et al.*, 1992; Patel *et al.*, 2002).

5. Synthesis and crystallization

The two compounds were prepared in a similar manner using 4-fluoro aldehyde (1 mmol) for compound (I) and 4-bromo aldehyde (1 mmol) for compound (II). A mixture of cyclooctanone (1mmol), respective aldehyde (1 mmol) and malononitrile (1 mmol) were taken in ethanol (10 mL) to which *p*-toluenesulfonic acid (pTSA) (0.5 mmol) was added. The reaction mixture was heated under reflux for 2–3 h. After completion of the reaction (TLC), the reaction mixture was poured into crushed ice and extracted with ethyl acetate. The

excess solvent was removed under vacuum and the residue was subjected to column chromatography using petroleum ether/ethyl acetate mixture (97:3 *v*/*v*) as eluent to afford pure product. The product was recrystallized from ethyl acetate, affording colourless crystals of compounds (I) and (II) [m.p. 493 K; yield 91% for (I) and m.p. 473 K; yield 65% for (II)].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. 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 CH_2). Imine atom H1 was found in a difference map and refined with a distance restraint in both compounds of N—H = 0.86 (10) Å. Isotropic displacement parameters for H atoms were calculated as U_{iso} = 1.5U_{eq}(C) for CH_3 groups and U_{iso} = 1.2U_{eq}(carrier atom) for all other H atoms. The DELU restraint was applied in compound (II).

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). E**70**, 344-347 [doi:10.1107/S1600536814022016]

Isotypic crystal structures of 1-benzyl-4-(4-bromophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocycloocta[*b*]pyridine-3-carbonitrile and 1-benzyl-4-(4-fluorophenyl)-2-imino-1,2,5,6,7,8,9,10-octahydrocyclo-octa[*b*]pyridine-3-carbonitrile

R. A. Nagalakshmi, J. Suresh, S. Maharani, R. Ranjith Kumar and P. L. Nilantha Lakshman

Computing details

For both compounds, data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004). Program(s) used to solve structure: *SHELXL97* (Sheldrick, 2008) for (I); *SHELXS97* (Sheldrick, 2008) for (II). For both compounds, program(s) used to refine structure: *SHELXL2014*/6 (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014*/6 (Sheldrick, 2008).

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

Crystal data

$C_{25}H_{24}BrN_3$
M_r = 446.38
Triclinic, $P\overline{1}$
a = 10.2103 (3) Å
b = 10.7643 (4) Å
c = 11.6942 (4) Å
α = 101.074 (1)°
β = 106.726 (1)°
γ = 115.058 (1)°
V = 1039.46 (6) Å^3
Z = 2
$F(000)$ = 460
D_x = 1.426 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2000 reflections
θ = 3–21°
μ = 1.99 mm^{-1}
T = 293 K
Block, colourless
0.21 × 0.19 × 0.18 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.967, T_{max} = 0.974
25106 measured reflections
4532 independent reflections
3830 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.0°, θ_{min} = 2.2°
h = −13→13
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.03
4532 reflections
266 parameters
2 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.8341P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.93$ e Å^{-3}
$\Delta\rho_{min} = -0.87$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0878 (3)	0.0974 (2)	−0.1085 (2)	0.0341 (4)
C2	0.0659 (2)	0.1930 (2)	−0.0207 (2)	0.0339 (4)
C3	0.1891 (3)	0.3193 (2)	0.0767 (2)	0.0343 (4)
C4	0.3478 (3)	0.3602 (2)	0.0957 (2)	0.0361 (5)
C5	0.3719 (3)	0.2714 (2)	0.0138 (2)	0.0335 (4)
C6	0.5365 (3)	0.3076 (3)	0.0277 (2)	0.0433 (5)
H6A	0.6046	0.4137	0.0602	0.052*
H6B	0.5321	0.2693	−0.0563	0.052*
C7	0.6116 (3)	0.2460 (4)	0.1167 (3)	0.0571 (7)
H7A	0.5328	0.1445	0.0959	0.069*
H7B	0.6983	0.2456	0.0984	0.069*
C8	0.6748 (4)	0.3263 (4)	0.2585 (3)	0.0647 (8)
H8A	0.7358	0.2886	0.3038	0.078*
H8B	0.7475	0.4294	0.2783	0.078*
C9	0.5525 (4)	0.3159 (4)	0.3098 (3)	0.0631 (7)
H9A	0.5835	0.3032	0.3913	0.076*
H9B	0.4517	0.2282	0.2514	0.076*
C10	0.5269 (3)	0.4473 (4)	0.3292 (3)	0.0582 (7)
H10A	0.4425	0.4258	0.3582	0.070*
H10B	0.6230	0.5319	0.3972	0.070*
C11	0.4847 (3)	0.4898 (3)	0.2120 (2)	0.0457 (6)
H11A	0.4572	0.5648	0.2317	0.055*
H11B	0.5770	0.5314	0.1929	0.055*
C12	0.2749 (3)	0.0440 (3)	−0.1662 (2)	0.0404 (5)
H12A	0.1839	−0.0548	−0.1994	0.048*
H12B	0.3668	0.0427	−0.1136	0.048*
C13	0.3020 (3)	0.0841 (2)	−0.2770 (2)	0.0391 (5)
C14	0.4290 (3)	0.0892 (3)	−0.3004 (3)	0.0565 (7)
H14	0.4999	0.0716	−0.2457	0.068*
C15	0.4510 (4)	0.1206 (4)	−0.4053 (3)	0.0710 (10)
H15	0.5369	0.1244	−0.4205	0.085*
C16	0.3473 (4)	0.1460 (4)	−0.4863 (3)	0.0700 (9)
H16	0.3617	0.1658	−0.5571	0.084*
C17	0.2225 (4)	0.1422 (3)	−0.4632 (3)	0.0583 (7)
H17	0.1522	0.1601	−0.5181	0.070*

C18	0.1998 (3)	0.1120 (3)	−0.3591 (2)	0.0444 (5)
H18	0.1147	0.1105	−0.3440	0.053*
C31	0.1563 (3)	0.4135 (2)	0.1609 (2)	0.0357 (5)
C32	0.1211 (3)	0.3808 (3)	0.2607 (2)	0.0450 (5)
H32	0.1141	0.2962	0.2740	0.054*
C33	0.0962 (3)	0.4725 (3)	0.3411 (2)	0.0468 (6)
H33	0.0739	0.4506	0.4089	0.056*
C34	0.1048 (3)	0.5954 (2)	0.3197 (2)	0.0393 (5)
C35	0.1356 (3)	0.6289 (3)	0.2198 (3)	0.0485 (6)
H35	0.1389	0.7119	0.2053	0.058*
C36	0.1620 (3)	0.5377 (3)	0.1406 (2)	0.0463 (6)
H36	0.1838	0.5601	0.0728	0.056*
C38	−0.0952 (3)	0.1466 (3)	−0.0413 (2)	0.0385 (5)
N1	−0.0211 (3)	−0.0218 (2)	−0.2039 (2)	0.0465 (5)
N2	−0.2259 (3)	0.1036 (3)	−0.0637 (2)	0.0552 (6)
N3	0.2469 (2)	0.14417 (19)	−0.08436 (17)	0.0335 (4)
Br1	0.07794 (4)	0.72595 (3)	0.43133 (3)	0.06264 (13)
H1	−0.1109 (16)	−0.035 (3)	−0.205 (3)	0.056 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0355 (11)	0.0344 (10)	0.0315 (10)	0.0164 (9)	0.0131 (9)	0.0148 (9)
C2	0.0328 (10)	0.0360 (11)	0.0326 (10)	0.0164 (9)	0.0132 (9)	0.0150 (9)
C3	0.0369 (11)	0.0338 (10)	0.0338 (11)	0.0182 (9)	0.0158 (9)	0.0134 (9)
C4	0.0321 (11)	0.0341 (11)	0.0351 (11)	0.0137 (9)	0.0123 (9)	0.0092 (9)
C5	0.0337 (10)	0.0360 (11)	0.0313 (10)	0.0170 (9)	0.0136 (9)	0.0147 (9)
C6	0.0362 (12)	0.0488 (13)	0.0427 (12)	0.0200 (10)	0.0193 (10)	0.0118 (10)
C7	0.0480 (15)	0.0759 (19)	0.0521 (15)	0.0418 (15)	0.0150 (12)	0.0165 (14)
C8	0.0502 (16)	0.083 (2)	0.0582 (18)	0.0363 (16)	0.0152 (14)	0.0260 (16)
C9	0.0573 (17)	0.0820 (19)	0.0501 (16)	0.0335 (16)	0.0207 (13)	0.0317 (15)
C10	0.0444 (14)	0.0706 (17)	0.0350 (13)	0.0202 (13)	0.0104 (11)	0.0020 (12)
C11	0.0350 (12)	0.0391 (12)	0.0448 (13)	0.0130 (10)	0.0120 (10)	0.0008 (10)
C12	0.0451 (12)	0.0382 (12)	0.0383 (12)	0.0252 (10)	0.0148 (10)	0.0092 (9)
C13	0.0386 (12)	0.0360 (11)	0.0335 (11)	0.0168 (10)	0.0132 (9)	0.0022 (9)
C14	0.0437 (14)	0.0648 (17)	0.0473 (15)	0.0264 (13)	0.0162 (12)	−0.0001 (13)
C15	0.0487 (16)	0.077 (2)	0.0569 (18)	0.0142 (15)	0.0312 (15)	−0.0062 (15)
C16	0.0627 (19)	0.072 (2)	0.0415 (15)	0.0080 (16)	0.0276 (14)	0.0068 (14)
C17	0.0597 (17)	0.0588 (17)	0.0408 (14)	0.0189 (14)	0.0188 (13)	0.0175 (12)
C18	0.0421 (12)	0.0481 (13)	0.0387 (12)	0.0202 (11)	0.0176 (10)	0.0124 (10)
C31	0.0320 (10)	0.0362 (11)	0.0357 (11)	0.0165 (9)	0.0131 (9)	0.0103 (9)
C32	0.0579 (15)	0.0379 (12)	0.0519 (14)	0.0270 (11)	0.0314 (12)	0.0218 (11)
C33	0.0585 (15)	0.0462 (13)	0.0466 (13)	0.0277 (12)	0.0317 (12)	0.0204 (11)
C34	0.0354 (11)	0.0359 (11)	0.0423 (12)	0.0184 (10)	0.0147 (10)	0.0071 (9)
C35	0.0604 (15)	0.0455 (13)	0.0546 (15)	0.0347 (12)	0.0264 (13)	0.0253 (12)
C36	0.0595 (15)	0.0517 (14)	0.0451 (13)	0.0348 (13)	0.0281 (12)	0.0263 (11)
C38	0.0378 (12)	0.0416 (12)	0.0357 (11)	0.0194 (10)	0.0147 (9)	0.0161 (10)
N1	0.0399 (11)	0.0401 (11)	0.0406 (11)	0.0132 (9)	0.0104 (9)	0.0041 (9)

N2	0.0392 (12)	0.0662 (15)	0.0572 (14)	0.0244 (11)	0.0198 (10)	0.0227 (12)
N3	0.0369 (9)	0.0332 (9)	0.0295 (9)	0.0181 (8)	0.0131 (7)	0.0105 (7)
Br1	0.0776 (2)	0.05343 (18)	0.0665 (2)	0.04027 (16)	0.03763 (17)	0.01234 (14)

Geometric parameters (Å, º)

C1—N1	1.286 (3)	C12—N3	1.477 (3)
C1—N3	1.401 (3)	C12—C13	1.504 (3)
C1—C2	1.444 (3)	C12—H12A	0.9700
C2—C3	1.364 (3)	C12—H12B	0.9700
C2—C38	1.430 (3)	C13—C18	1.379 (4)
C3—C4	1.421 (3)	C13—C14	1.382 (3)
C3—C31	1.485 (3)	C14—C15	1.387 (5)
C4—C5	1.370 (3)	C14—H14	0.9300
C4—C11	1.509 (3)	C15—C16	1.363 (5)
C5—N3	1.376 (3)	C15—H15	0.9300
C5—C6	1.505 (3)	C16—C17	1.363 (5)
C6—C7	1.532 (4)	C16—H16	0.9300
C6—H6A	0.9700	C17—C18	1.374 (4)
C6—H6B	0.9700	C17—H17	0.9300
C7—C8	1.508 (4)	C18—H18	0.9300
C7—H7A	0.9700	C31—C32	1.380 (3)
C7—H7B	0.9700	C31—C36	1.383 (3)
C8—C9	1.507 (4)	C32—C33	1.385 (3)
C8—H8A	0.9700	C32—H32	0.9300
C8—H8B	0.9700	C33—C34	1.365 (3)
C9—C10	1.531 (5)	C33—H33	0.9300
C9—H9A	0.9700	C34—C35	1.368 (4)
C9—H9B	0.9700	C34—Br1	1.892 (2)
C10—C11	1.529 (4)	C35—C36	1.382 (4)
C10—H10A	0.9700	C35—H35	0.9300
C10—H10B	0.9700	C36—H36	0.9300
C11—H11A	0.9700	C38—N2	1.137 (3)
C11—H11B	0.9700	N1—H1	0.8600 (10)
N1—C1—N3	118.5 (2)	C10—C11—H11B	109.1
N1—C1—C2	127.2 (2)	H11A—C11—H11B	107.9
N3—C1—C2	114.29 (18)	N3—C12—C13	114.51 (18)
C3—C2—C38	121.2 (2)	N3—C12—H12A	108.6
C3—C2—C1	123.2 (2)	C13—C12—H12A	108.6
C38—C2—C1	115.60 (19)	N3—C12—H12B	108.6
C2—C3—C4	119.6 (2)	C13—C12—H12B	108.6
C2—C3—C31	119.77 (19)	H12A—C12—H12B	107.6
C4—C3—C31	120.68 (19)	C18—C13—C14	118.6 (2)
C5—C4—C3	118.5 (2)	C18—C13—C12	121.5 (2)
C5—C4—C11	121.4 (2)	C14—C13—C12	119.9 (2)
C3—C4—C11	119.8 (2)	C13—C14—C15	120.1 (3)
C4—C5—N3	121.54 (19)	C13—C14—H14	120.0

C4—C5—C6	121.5 (2)	C15—C14—H14	120.0
N3—C5—C6	116.91 (19)	C16—C15—C14	120.3 (3)
C5—C6—C7	114.3 (2)	C16—C15—H15	119.8
C5—C6—H6A	108.7	C14—C15—H15	119.8
C7—C6—H6A	108.7	C17—C16—C15	119.8 (3)
C5—C6—H6B	108.7	C17—C16—H16	120.1
C7—C6—H6B	108.7	C15—C16—H16	120.1
H6A—C6—H6B	107.6	C16—C17—C18	120.4 (3)
C8—C7—C6	116.4 (2)	C16—C17—H17	119.8
C8—C7—H7A	108.2	C18—C17—H17	119.8
C6—C7—H7A	108.2	C17—C18—C13	120.7 (3)
C8—C7—H7B	108.2	C17—C18—H18	119.6
C6—C7—H7B	108.2	C13—C18—H18	119.6
H7A—C7—H7B	107.3	C32—C31—C36	118.7 (2)
C9—C8—C7	116.1 (3)	C32—C31—C3	121.5 (2)
C9—C8—H8A	108.3	C36—C31—C3	119.8 (2)
C7—C8—H8A	108.3	C31—C32—C33	120.8 (2)
C9—C8—H8B	108.3	C31—C32—H32	119.6
C7—C8—H8B	108.3	C33—C32—H32	119.6
H8A—C8—H8B	107.4	C34—C33—C32	119.1 (2)
C8—C9—C10	115.9 (3)	C34—C33—H33	120.5
C8—C9—H9A	108.3	C32—C33—H33	120.5
C10—C9—H9A	108.3	C33—C34—C35	121.4 (2)
C8—C9—H9B	108.3	C33—C34—Br1	120.00 (18)
C10—C9—H9B	108.3	C35—C34—Br1	118.56 (18)
H9A—C9—H9B	107.4	C34—C35—C36	119.2 (2)
C11—C10—C9	116.2 (2)	C34—C35—H35	120.4
C11—C10—H10A	108.2	C36—C35—H35	120.4
C9—C10—H10A	108.2	C35—C36—C31	120.7 (2)
C11—C10—H10B	108.2	C35—C36—H36	119.6
C9—C10—H10B	108.2	C31—C36—H36	119.6
H10A—C10—H10B	107.4	N2—C38—C2	176.3 (3)
C4—C11—C10	112.3 (2)	C1—N1—H1	107.0 (19)
C4—C11—H11A	109.1	C5—N3—C1	122.93 (18)
C10—C11—H11A	109.1	C5—N3—C12	120.97 (18)
C4—C11—H11B	109.1	C1—N3—C12	116.00 (18)

N1—C1—C2—C3	−178.7 (2)	C14—C15—C16—C17	0.8 (5)
N3—C1—C2—C3	0.8 (3)	C15—C16—C17—C18	−0.4 (5)
N1—C1—C2—C38	1.7 (3)	C16—C17—C18—C13	−0.5 (4)
N3—C1—C2—C38	−178.73 (18)	C14—C13—C18—C17	1.0 (4)
C38—C2—C3—C4	178.7 (2)	C12—C13—C18—C17	−177.1 (2)
C1—C2—C3—C4	−0.8 (3)	C2—C3—C31—C32	80.6 (3)
C38—C2—C3—C31	−2.0 (3)	C4—C3—C31—C32	−100.0 (3)
C1—C2—C3—C31	178.55 (19)	C2—C3—C31—C36	−99.9 (3)
C2—C3—C4—C5	0.8 (3)	C4—C3—C31—C36	79.4 (3)
C31—C3—C4—C5	−178.6 (2)	C36—C31—C32—C33	−1.7 (4)
C2—C3—C4—C11	−172.9 (2)	C3—C31—C32—C33	177.7 (2)

C31—C3—C4—C11	7.7 (3)	C31—C32—C33—C34	0.9 (4)
C3—C4—C5—N3	−0.7 (3)	C32—C33—C34—C35	0.7 (4)
C11—C4—C5—N3	172.8 (2)	C32—C33—C34—Br1	−178.0 (2)
C3—C4—C5—C6	179.9 (2)	C33—C34—C35—C36	−1.4 (4)
C11—C4—C5—C6	−6.5 (3)	Br1—C34—C35—C36	177.4 (2)
C4—C5—C6—C7	88.6 (3)	C34—C35—C36—C31	0.5 (4)
N3—C5—C6—C7	−90.8 (3)	C32—C31—C36—C35	1.1 (4)
C5—C6—C7—C8	−76.6 (3)	C3—C31—C36—C35	−178.4 (2)
C6—C7—C8—C9	68.4 (4)	C4—C5—N3—C1	0.8 (3)
C7—C8—C9—C10	−98.9 (3)	C6—C5—N3—C1	−179.84 (19)
C8—C9—C10—C11	55.3 (3)	C4—C5—N3—C12	−175.6 (2)
C5—C4—C11—C10	−88.0 (3)	C6—C5—N3—C12	3.8 (3)
C3—C4—C11—C10	85.5 (3)	N1—C1—N3—C5	178.8 (2)
C9—C10—C11—C4	51.2 (3)	C2—C1—N3—C5	−0.7 (3)
N3—C12—C13—C18	−50.3 (3)	N1—C1—N3—C12	−4.7 (3)
N3—C12—C13—C14	131.6 (2)	C2—C1—N3—C12	175.76 (18)
C18—C13—C14—C15	−0.6 (4)	C13—C12—N3—C5	−85.2 (2)
C12—C13—C14—C15	177.5 (3)	C13—C12—N3—C1	98.2 (2)
C13—C14—C15—C16	−0.3 (5)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C13–C18 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C32—H32···N1^{i}	0.93	2.56	3.421 (3)	154
C11—H11*A*···*Cg*1^{ii}	0.97	2.97	3.648 (3)	128

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

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

Crystal data

$C_{25}H_{24}FN_3$
M_r = 385.47
Triclinic, $P\overline{1}$
a = 10.1370 (4) Å
b = 10.2078 (3) Å
c = 11.8238 (4) Å
α = 109.688 (2)°
β = 100.309 (2)°
γ = 111.420 (2)°
V = 1006.73 (6) Å^3

Z = 2
F(000) = 408
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2000 reflections
θ = 2–31°
μ = 0.08 mm^{-1}
T = 293 K
Block, colourless
0.21 × 0.19 × 0.18 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.967, T_{max} = 0.974
23254 measured reflections

3752 independent reflections
2876 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −12→12
k = −12→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.109$
$S = 1.05$
3752 reflections
267 parameters
2 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.3339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL2014*/6 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.38640 (16)	0.41969 (17)	0.59999 (13)	0.0347 (3)
C2	0.28977 (16)	0.44165 (16)	0.50992 (13)	0.0343 (3)
C3	0.16525 (16)	0.32042 (16)	0.40896 (13)	0.0341 (3)
C4	0.12688 (16)	0.16454 (17)	0.39051 (13)	0.0366 (3)
C5	0.21646 (16)	0.13987 (16)	0.47452 (13)	0.0345 (3)
C6	0.18252 (19)	−0.02211 (18)	0.46013 (15)	0.0442 (4)
H6A	0.0738	−0.0860	0.4268	0.053*
H6B	0.2196	−0.0159	0.5442	0.053*
C7	0.2506 (2)	−0.1046 (2)	0.37256 (17)	0.0562 (5)
H7A	0.3563	−0.0323	0.3975	0.067*
H7B	0.2469	−0.1927	0.3887	0.067*
C8	0.1783 (2)	−0.1646 (2)	0.22930 (17)	0.0583 (5)
H8A	0.2219	−0.2277	0.1857	0.070*
H8B	0.0716	−0.2328	0.2046	0.070*
C9	0.1946 (2)	−0.0406 (2)	0.18178 (17)	0.0570 (5)
H9A	0.2813	0.0570	0.2441	0.068*
H9B	0.2155	−0.0717	0.1026	0.068*
C10	0.0585 (2)	−0.0109 (2)	0.15827 (15)	0.0564 (5)
H10A	−0.0238	−0.1036	0.0864	0.068*
H10B	0.0830	0.0743	0.1337	0.068*
C11	0.00304 (18)	0.02948 (18)	0.27088 (15)	0.0475 (4)
H11A	−0.0777	0.0557	0.2488	0.057*
H11B	−0.0377	−0.0616	0.2872	0.057*
C12	0.44774 (17)	0.23479 (19)	0.65601 (14)	0.0411 (4)
H12A	0.5478	0.3219	0.6876	0.049*
H12B	0.4517	0.1414	0.6027	0.049*
C13	0.41019 (17)	0.21501 (18)	0.76831 (14)	0.0409 (4)
C14	0.4226 (2)	0.0975 (2)	0.79530 (17)	0.0578 (5)

H14	0.4469	0.0274	0.7406	0.069*
C15	0.3991 (2)	0.0836 (3)	0.9035 (2)	0.0756 (7)
H15	0.4071	0.0040	0.9208	0.091*
C16	0.3641 (3)	0.1865 (3)	0.98465 (19)	0.0782 (7)
H16	0.3500	0.1780	1.0580	0.094*
C17	0.3499 (2)	0.3013 (2)	0.95823 (17)	0.0694 (6)
H17	0.3251	0.3706	1.0133	0.083*
C18	0.3719 (2)	0.31600 (19)	0.85034 (16)	0.0521 (4)
H18	0.3609	0.3944	0.8328	0.063*
C31	0.07281 (16)	0.35321 (17)	0.31963 (13)	0.0371 (3)
C32	0.12480 (18)	0.39428 (18)	0.22997 (15)	0.0435 (4)
H32	0.2186	0.4033	0.2270	0.052*
C33	0.0391 (2)	0.4221 (2)	0.14484 (16)	0.0491 (4)
H33	0.0734	0.4484	0.0839	0.059*
C34	−0.09671 (19)	0.4101 (2)	0.15238 (16)	0.0494 (4)
C35	−0.1521 (2)	0.3707 (2)	0.23943 (18)	0.0586 (5)
H35	−0.2454	0.3637	0.2424	0.070*
C36	−0.06628 (19)	0.3413 (2)	0.32320 (17)	0.0526 (4)
H36	−0.1027	0.3133	0.3827	0.063*
C38	0.33469 (17)	0.60054 (18)	0.53208 (14)	0.0395 (3)
N1	0.50412 (15)	0.52710 (17)	0.69710 (13)	0.0485 (4)
N2	0.37721 (18)	0.73047 (17)	0.55698 (14)	0.0572 (4)
N3	0.34211 (13)	0.26298 (14)	0.57514 (11)	0.0346 (3)
F1	−0.18123 (13)	0.43791 (15)	0.06937 (11)	0.0758 (4)
H1	0.520 (2)	0.6177 (14)	0.7008 (19)	0.065 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0340 (7)	0.0397 (8)	0.0314 (7)	0.0162 (6)	0.0147 (6)	0.0157 (6)
C2	0.0359 (7)	0.0374 (7)	0.0328 (7)	0.0173 (6)	0.0154 (6)	0.0167 (6)
C3	0.0353 (7)	0.0403 (8)	0.0326 (7)	0.0194 (6)	0.0157 (6)	0.0181 (6)
C4	0.0347 (8)	0.0383 (8)	0.0350 (8)	0.0157 (6)	0.0112 (6)	0.0158 (6)
C5	0.0360 (7)	0.0376 (8)	0.0322 (7)	0.0162 (6)	0.0153 (6)	0.0167 (6)
C6	0.0515 (9)	0.0422 (8)	0.0411 (8)	0.0199 (7)	0.0139 (7)	0.0238 (7)
C7	0.0739 (12)	0.0487 (10)	0.0532 (10)	0.0376 (9)	0.0180 (9)	0.0221 (8)
C8	0.0773 (13)	0.0448 (9)	0.0506 (10)	0.0314 (9)	0.0204 (9)	0.0156 (8)
C9	0.0743 (12)	0.0491 (10)	0.0431 (9)	0.0251 (9)	0.0243 (9)	0.0169 (8)
C10	0.0729 (12)	0.0428 (9)	0.0354 (9)	0.0186 (9)	0.0039 (8)	0.0135 (7)
C11	0.0421 (9)	0.0407 (8)	0.0467 (9)	0.0137 (7)	0.0027 (7)	0.0172 (7)
C12	0.0405 (8)	0.0499 (9)	0.0373 (8)	0.0251 (7)	0.0112 (6)	0.0204 (7)
C13	0.0387 (8)	0.0425 (8)	0.0324 (7)	0.0133 (7)	0.0039 (6)	0.0164 (7)
C14	0.0618 (11)	0.0604 (11)	0.0516 (10)	0.0290 (9)	0.0076 (9)	0.0299 (9)
C15	0.0747 (14)	0.0776 (14)	0.0661 (13)	0.0202 (12)	0.0013 (11)	0.0504 (12)
C16	0.0799 (15)	0.0760 (15)	0.0375 (10)	−0.0012 (12)	0.0042 (10)	0.0284 (10)
C17	0.0788 (14)	0.0539 (11)	0.0429 (10)	0.0053 (10)	0.0240 (10)	0.0117 (9)
C18	0.0616 (11)	0.0412 (9)	0.0427 (9)	0.0140 (8)	0.0192 (8)	0.0164 (7)
C31	0.0391 (8)	0.0378 (8)	0.0346 (8)	0.0190 (6)	0.0110 (6)	0.0156 (6)

C32	0.0418 (8)	0.0477 (9)	0.0451 (9)	0.0207 (7)	0.0159 (7)	0.0246 (7)
C33	0.0565 (10)	0.0548 (10)	0.0469 (9)	0.0266 (8)	0.0200 (8)	0.0319 (8)
C34	0.0564 (10)	0.0532 (10)	0.0450 (9)	0.0318 (8)	0.0102 (8)	0.0250 (8)
C35	0.0529 (10)	0.0847 (13)	0.0617 (11)	0.0458 (10)	0.0251 (9)	0.0396 (10)
C36	0.0530 (10)	0.0756 (12)	0.0524 (10)	0.0389 (9)	0.0266 (8)	0.0389 (9)
C38	0.0427 (8)	0.0410 (8)	0.0368 (8)	0.0197 (7)	0.0155 (7)	0.0178 (7)
N1	0.0435 (8)	0.0441 (8)	0.0426 (8)	0.0135 (7)	0.0039 (6)	0.0149 (6)
N2	0.0693 (10)	0.0438 (8)	0.0571 (9)	0.0241 (7)	0.0215 (8)	0.0230 (7)
N3	0.0360 (6)	0.0407 (7)	0.0299 (6)	0.0189 (5)	0.0114 (5)	0.0168 (5)
F1	0.0799 (8)	0.1045 (9)	0.0715 (7)	0.0590 (7)	0.0180 (6)	0.0556 (7)

Geometric parameters (Å, º)

C1—N1	1.2847 (19)	C12—N3	1.4790 (18)
C1—N3	1.3994 (18)	C12—C13	1.501 (2)
C1—C2	1.446 (2)	C12—H12A	0.9700
C2—C3	1.369 (2)	C12—H12B	0.9700
C2—C38	1.428 (2)	C13—C18	1.381 (2)
C3—C4	1.419 (2)	C13—C14	1.382 (2)
C3—C31	1.4896 (19)	C14—C15	1.385 (3)
C4—C5	1.3737 (19)	C14—H14	0.9300
C4—C11	1.505 (2)	C15—C16	1.366 (3)
C5—N3	1.3777 (18)	C15—H15	0.9300
C5—C6	1.502 (2)	C16—C17	1.358 (3)
C6—C7	1.533 (2)	C16—H16	0.9300
C6—H6A	0.9700	C17—C18	1.381 (2)
C6—H6B	0.9700	C17—H17	0.9300
C7—C8	1.520 (2)	C18—H18	0.9300
C7—H7A	0.9700	C31—C36	1.380 (2)
C7—H7B	0.9700	C31—C32	1.384 (2)
C8—C9	1.518 (2)	C32—C33	1.382 (2)
C8—H8A	0.9700	C32—H32	0.9300
C8—H8B	0.9700	C33—C34	1.358 (2)
C9—C10	1.517 (3)	C33—H33	0.9300
C9—H9A	0.9700	C34—F1	1.3570 (18)
C9—H9B	0.9700	C34—C35	1.363 (2)
C10—C11	1.525 (2)	C35—C36	1.382 (2)
C10—H10A	0.9700	C35—H35	0.9300
C10—H10B	0.9700	C36—H36	0.9300
C11—H11A	0.9700	C38—N2	1.1426 (19)
C11—H11B	0.9700	N1—H1	0.864 (9)
N1—C1—N3	118.86 (13)	C10—C11—H11B	109.2
N1—C1—C2	126.92 (14)	H11A—C11—H11B	107.9
N3—C1—C2	114.22 (12)	N3—C12—C13	115.71 (12)
C3—C2—C38	121.57 (13)	N3—C12—H12A	108.4
C3—C2—C1	123.31 (13)	C13—C12—H12A	108.4
C38—C2—C1	115.11 (13)	N3—C12—H12B	108.4

C2—C3—C4	119.20 (13)	C13—C12—H12B	108.4
C2—C3—C31	119.87 (13)	H12A—C12—H12B	107.4
C4—C3—C31	120.92 (13)	C18—C13—C14	118.55 (15)
C5—C4—C3	118.86 (13)	C18—C13—C12	122.21 (14)
C5—C4—C11	120.91 (13)	C14—C13—C12	119.14 (15)
C3—C4—C11	119.70 (13)	C13—C14—C15	120.31 (19)
C4—C5—N3	121.29 (13)	C13—C14—H14	119.8
C4—C5—C6	121.54 (13)	C15—C14—H14	119.8
N3—C5—C6	117.16 (12)	C16—C15—C14	120.2 (2)
C5—C6—C7	115.02 (13)	C16—C15—H15	119.9
C5—C6—H6A	108.5	C14—C15—H15	119.9
C7—C6—H6A	108.5	C17—C16—C15	119.92 (19)
C5—C6—H6B	108.5	C17—C16—H16	120.0
C7—C6—H6B	108.5	C15—C16—H16	120.0
H6A—C6—H6B	107.5	C16—C17—C18	120.6 (2)
C8—C7—C6	117.39 (15)	C16—C17—H17	119.7
C8—C7—H7A	108.0	C18—C17—H17	119.7
C6—C7—H7A	108.0	C17—C18—C13	120.41 (18)
C8—C7—H7B	108.0	C17—C18—H18	119.8
C6—C7—H7B	108.0	C13—C18—H18	119.8
H7A—C7—H7B	107.2	C36—C31—C32	118.80 (14)
C9—C8—C7	116.07 (15)	C36—C31—C3	121.03 (13)
C9—C8—H8A	108.3	C32—C31—C3	120.16 (13)
C7—C8—H8A	108.3	C33—C32—C31	120.83 (15)
C9—C8—H8B	108.3	C33—C32—H32	119.6
C7—C8—H8B	108.3	C31—C32—H32	119.6
H8A—C8—H8B	107.4	C34—C33—C32	118.37 (15)
C10—C9—C8	115.10 (16)	C34—C33—H33	120.8
C10—C9—H9A	108.5	C32—C33—H33	120.8
C8—C9—H9A	108.5	F1—C34—C33	118.67 (15)
C10—C9—H9B	108.5	F1—C34—C35	118.52 (16)
C8—C9—H9B	108.5	C33—C34—C35	122.81 (15)
H9A—C9—H9B	107.5	C34—C35—C36	118.38 (16)
C9—C10—C11	115.73 (14)	C34—C35—H35	120.8
C9—C10—H10A	108.3	C36—C35—H35	120.8
C11—C10—H10A	108.3	C31—C36—C35	120.80 (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	175.68 (17)
C4—C11—C10	112.25 (13)	C1—N1—H1	109.5 (13)
C4—C11—H11A	109.2	C5—N3—C1	123.11 (12)
C10—C11—H11A	109.2	C5—N3—C12	120.92 (12)
C4—C11—H11B	109.2	C1—N3—C12	115.68 (12)

N1—C1—C2—C3	−179.54 (14)	C14—C15—C16—C17	1.1 (3)
N3—C1—C2—C3	0.16 (19)	C15—C16—C17—C18	−0.6 (3)
N1—C1—C2—C38	1.5 (2)	C16—C17—C18—C13	−0.6 (3)
N3—C1—C2—C38	−178.81 (12)	C14—C13—C18—C17	1.4 (3)

C38—C2—C3—C4	179.19 (13)	C12—C13—C18—C17	−174.81 (16)
C1—C2—C3—C4	0.3 (2)	C2—C3—C31—C36	−105.63 (18)
C38—C2—C3—C31	−0.3 (2)	C4—C3—C31—C36	74.87 (19)
C1—C2—C3—C31	−179.22 (13)	C2—C3—C31—C32	75.25 (18)
C2—C3—C4—C5	−0.2 (2)	C4—C3—C31—C32	−104.25 (17)
C31—C3—C4—C5	179.26 (13)	C36—C31—C32—C33	−0.4 (2)
C2—C3—C4—C11	−172.00 (13)	C3—C31—C32—C33	178.75 (14)
C31—C3—C4—C11	7.5 (2)	C31—C32—C33—C34	0.8 (2)
C3—C4—C5—N3	−0.3 (2)	C32—C33—C34—F1	179.75 (15)
C11—C4—C5—N3	171.40 (13)	C32—C33—C34—C35	−0.6 (3)
C3—C4—C5—C6	−179.76 (13)	F1—C34—C35—C36	179.53 (16)
C11—C4—C5—C6	−8.1 (2)	C33—C34—C35—C36	−0.2 (3)
C4—C5—C6—C7	87.41 (18)	C32—C31—C36—C35	−0.4 (3)
N3—C5—C6—C7	−92.12 (16)	C3—C31—C36—C35	−179.49 (16)
C5—C6—C7—C8	−73.7 (2)	C34—C35—C36—C31	0.6 (3)
C6—C7—C8—C9	67.0 (2)	C4—C5—N3—C1	0.7 (2)
C7—C8—C9—C10	−99.2 (2)	C6—C5—N3—C1	−179.73 (12)
C8—C9—C10—C11	54.5 (2)	C4—C5—N3—C12	−172.79 (13)
C5—C4—C11—C10	−89.02 (17)	C6—C5—N3—C12	6.73 (19)
C3—C4—C11—C10	82.57 (17)	N1—C1—N3—C5	179.05 (13)
C9—C10—C11—C4	53.53 (19)	C2—C1—N3—C5	−0.67 (18)
N3—C12—C13—C18	−47.2 (2)	N1—C1—N3—C12	−7.09 (19)
N3—C12—C13—C14	136.67 (15)	C2—C1—N3—C12	173.18 (11)
C18—C13—C14—C15	−0.9 (3)	C13—C12—N3—C5	−88.06 (16)
C12—C13—C14—C15	175.42 (16)	C13—C12—N3—C1	97.94 (15)
C13—C14—C15—C16	−0.3 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C13–C18 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C32—H32···N1^{i}	0.93	2.53	3.421 (2)	160
C11—H11*A*···*Cg*1^{ii}	0.97	2.93	3.484 (2)	118

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