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1-[6-(1*H*-Indol-1-yl)pyridin-2-yl]-1*H*-indole-3-carbaldehyde

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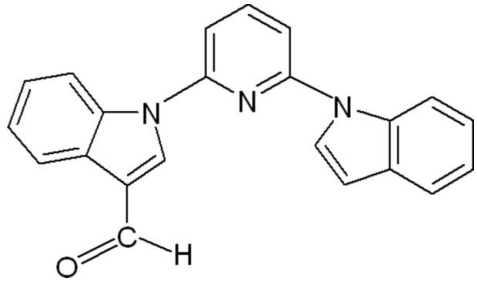
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.118; data-to-parameter ratio = 15.0.

In the title compound, $C_{22}H_{15}N_3O$, the dihedral angle between the two indole units is 33.72 (3)°. The molecular structure features a weak intramolecular C—H···N interaction. In the crystal, weak C—H···O and C—H···π interactions, forming a two-dimensional network parallel to the *bc* plane.

Related literature

For the biological activity of indole derivatives, see: Macor *et al.* (1992); Andreani *et al.* (2001); Quetin-Leclercq (1994); Mukhopadhyay *et al.* (1981); Singh *et al.* (2000). For related structures see: Dileep *et al.* (2012); Wu *et al.* (2012)



Experimental

Crystal data

$C_{22}H_{15}N_3O$
M_r = 337.37
Orthorhombic, *Pnna*
a = 18.2208 (7) Å
b = 15.7672 (9) Å
c = 11.7034 (7) Å
V = 3362.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.987
11189 measured reflections
3521 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.118
S = 1.00
3521 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

*Cg*5 is the centroid of the C16–C21 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.50	3.227 (3)	135
C12—H12···N1	0.93	2.41	2.931 (2)	116
C2—H2···*Cg*5^{ii}	0.93	2.73	3.554 (2)	148

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5369).

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supporting information

Acta Cryst. (2014). E**70**, o106 [doi:10.1107/S1600536813034375]

1-[6-(1*H*-Indol-1-yl)pyridin-2-yl]-1*H*-indole-3-carbaldehyde

C. Ramathilagam, P. R. Umarani, N. Venkatesan, P. Rajakumar, B. Gunasekaran and V. Manivannan

S1. Comment

The chemistry of indole has been of increasing interest, since several compounds of this type possess diverse biological activities (Macor *et al.*, 1992). These derivatives exhibit antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). Some of the indole alkaloids extracted from plants possess interesting cytotoxic and antiparasitic properties (Quetin-Leclercq, 1994; Mukhopadhyay *et al.*, 1981).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Dileep *et al.*, 2012; Wu *et al.*, 2012). The dihedral angle between the two indole moieties is 33.72 (3) °. The molecular structure is stabilized by weak intramolecular C—H···N interaction and the crystal packing is controlled by weak intermolecular C—H···O and C—H···π [C2—H2···*Cg*5(*x*, 1/2 - *y*, 1/2 - *z*) distance of 3.554 (2) Å, (*Cg*5 is the centroid of the ring defined by the atoms C16—C21)] interactions.

S2. Experimental

To a stirred solution of dimethylformamide (2.10g, 28.70 mmol) at 0°C, added phosphorous oxycholoride (1.10g, 7.17 mmol) drop wise under nitrogen atmosphere. 2,6-bis(*N*-indolyl)pyridine (1.0g, 3.23 mmol) in dimethylformamide was then added to the reaction at 0°C to 10°C. After the completion of addition, the reaction mixture was allow to attain room temperature and then stirred for additional one hour at 35°C. The reaction was then quenched by adding crushed ice (100 g) and further water (100 ml). Then the reaction mixture was then treated thrice with NaOH solution (1*M*). The reaction mixture was heated after adding one portion of NaOH solution and the rest of the two portions were added later with stirring. The reaction mixture was then kept in refrigerator overnight. The precipitate obtained was collected by filtration and then dissolved in chloroform (2 *x* 100 ml). The organic layer was then dried over (Na_2SO_4), filtered and solvent was evaporated under reduced pressure to give the residue which was then chromatographed over SiO_2 using hexane: chloroform (1:4) as eluting solvent to give the mono aldehyde(27%) as a colourless solid and further elution with $CHCl_3$: methanol (99:1) afforded the corresponding dialdehyde (55%).

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H.

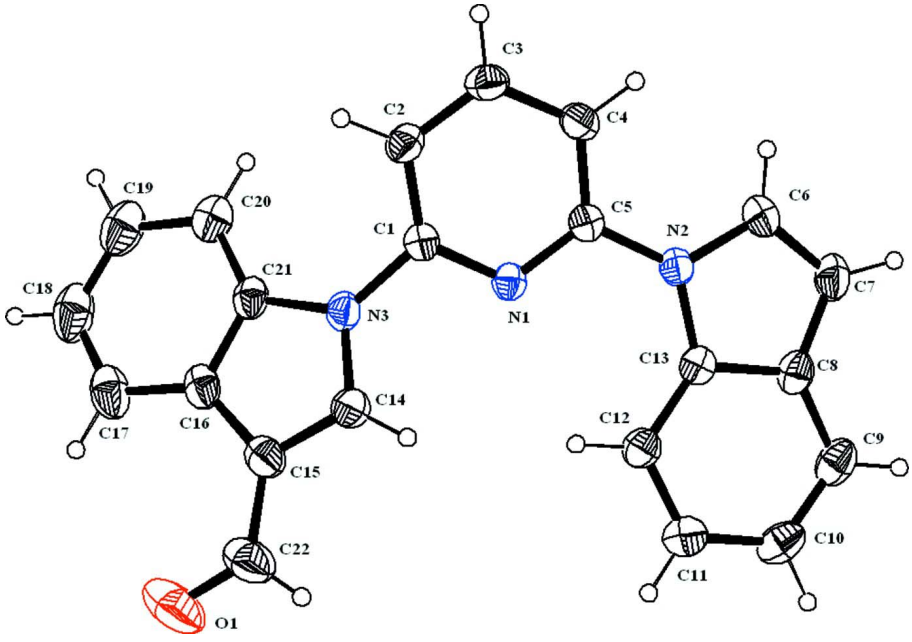

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

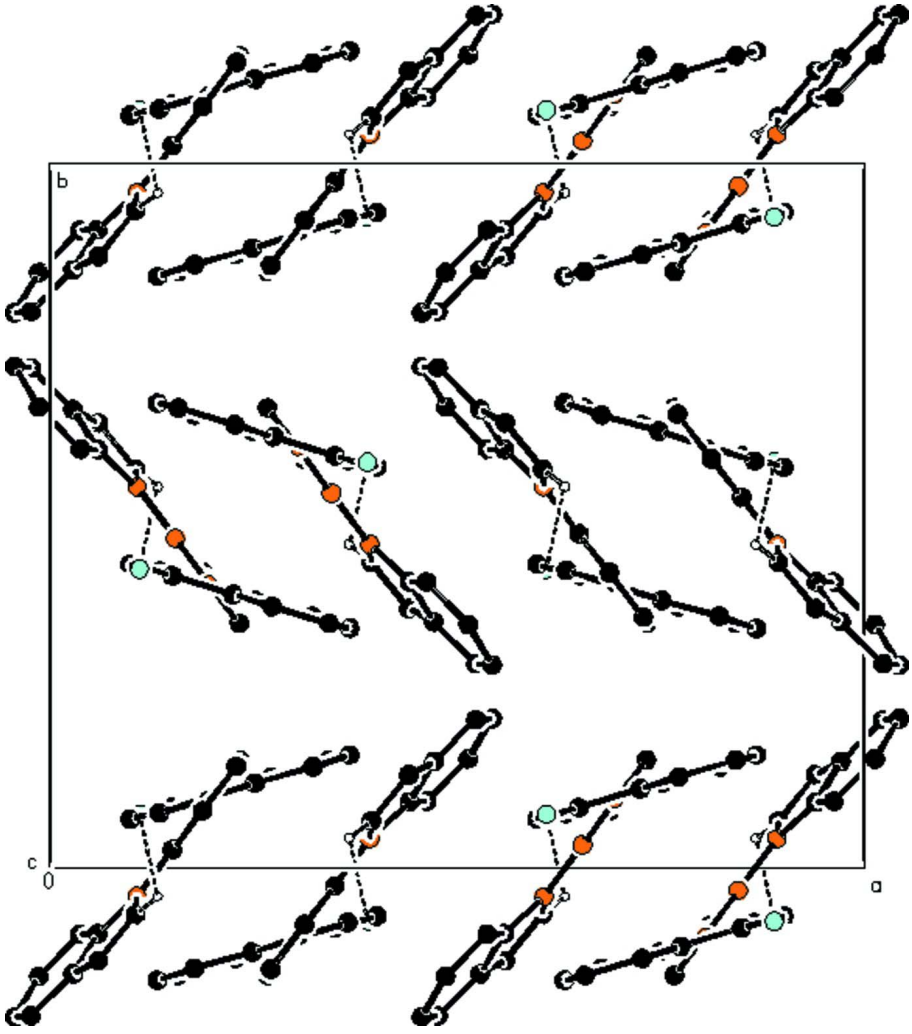

Figure 2

The packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{22}H_{15}N_3O$
$M_r = 337.37$
Orthorhombic, *Pnna*
Hall symbol: -P 2a 2bc
$a = 18.2208\ (7)$ Å
$b = 15.7672\ (9)$ Å
$c = 11.7034\ (7)$ Å
$V = 3362.3\ (3)$ Å^3
$Z = 8$
$F(000) = 1408$
$D_x = 1.333$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3755 reflections
$\theta = 2.0–26.6°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.987
11189 measured reflections
3521 independent reflections
2072 reflections with $I > 2\sigma(I)$

R_{int} = 0.031
θ_{max} = 26.7°, θ_{min} = 2.1°
h = −14→22
k = −19→13
l = −14→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.118
S = 1.00
3521 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.3404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.19452 (8)	0.09535 (11)	0.38032 (14)	0.0407 (4)
C2	0.23265 (9)	0.15297 (11)	0.44461 (16)	0.0493 (5)
H2	0.2599	0.1961	0.4109	0.059*
C3	0.22882 (10)	0.14407 (12)	0.56135 (16)	0.0541 (5)
H3	0.2545	0.1812	0.6083	0.065*
C4	0.18729 (10)	0.08067 (12)	0.60890 (15)	0.0506 (5)
H4	0.1840	0.0745	0.6877	0.061*
C5	0.15023 (8)	0.02580 (10)	0.53543 (14)	0.0408 (4)
C6	0.10521 (10)	−0.06632 (14)	0.69106 (16)	0.0595 (5)
H6	0.1322	−0.0413	0.7495	0.071*
C7	0.05930 (11)	−0.13186 (14)	0.70475 (18)	0.0658 (6)
H7	0.0495	−0.1599	0.7730	0.079*
C8	0.02821 (9)	−0.15088 (12)	0.59656 (16)	0.0510 (5)
C9	−0.02337 (10)	−0.21026 (13)	0.55946 (19)	0.0619 (6)
H9	−0.0439	−0.2484	0.6109	0.074*
C10	−0.04334 (10)	−0.21191 (13)	0.4474 (2)	0.0639 (6)
H10	−0.0771	−0.2520	0.4222	0.077*
C11	−0.01383 (10)	−0.15451 (13)	0.37027 (18)	0.0598 (5)
H11	−0.0286	−0.1565	0.2943	0.072*
C12	0.03711 (9)	−0.09435 (12)	0.40377 (16)	0.0500 (5)
H12	0.0564	−0.0557	0.3518	0.060*
C13	0.05850 (9)	−0.09360 (10)	0.51763 (15)	0.0417 (4)
C14	0.13419 (11)	0.07765 (11)	0.19300 (16)	0.0528 (5)
H14	0.0891	0.0604	0.2220	0.063*
C15	0.15005 (12)	0.08533 (11)	0.07958 (16)	0.0579 (5)
C16	0.22504 (11)	0.11196 (11)	0.07240 (16)	0.0530 (5)
C17	0.27264 (15)	0.12907 (13)	−0.01922 (19)	0.0745 (7)
H17	0.2566	0.1241	−0.0943	0.089*

C18	0.34277 (16)	0.15310 (15)	0.0044 (2)	0.0852 (8)
H18	0.3745	0.1651	−0.0557	0.102*
C19	0.36810 (13)	0.16008 (14)	0.1154 (2)	0.0807 (7)
H19	0.4164	0.1765	0.1283	0.097*
C20	0.32270 (11)	0.14309 (12)	0.20799 (19)	0.0610 (5)
H20	0.3396	0.1470	0.2828	0.073*
C21	0.25168 (10)	0.12027 (10)	0.18389 (15)	0.0489 (5)
C22	0.09838 (16)	0.06891 (14)	−0.0091 (2)	0.0804 (7)
H22	0.0518	0.0513	0.0129	0.096*
N1	0.15424 (7)	0.03227 (8)	0.42256 (11)	0.0408 (4)
N2	0.10689 (7)	−0.04099 (9)	0.57769 (11)	0.0438 (4)
N3	0.19390 (8)	0.09876 (9)	0.25834 (12)	0.0464 (4)
O1	0.10984 (12)	0.07594 (11)	−0.11088 (14)	0.1121 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0422 (9)	0.0379 (10)	0.0420 (10)	0.0049 (8)	0.0027 (8)	0.0014 (8)
C2	0.0513 (11)	0.0412 (10)	0.0555 (12)	−0.0061 (9)	0.0021 (9)	−0.0001 (9)
C3	0.0583 (12)	0.0485 (11)	0.0555 (12)	−0.0063 (10)	−0.0070 (9)	−0.0080 (10)
C4	0.0599 (11)	0.0518 (12)	0.0402 (11)	−0.0027 (10)	−0.0033 (9)	−0.0020 (9)
C5	0.0404 (9)	0.0405 (10)	0.0415 (10)	0.0049 (8)	0.0026 (8)	0.0004 (8)
C6	0.0656 (12)	0.0715 (14)	0.0415 (11)	−0.0075 (11)	0.0011 (9)	0.0080 (10)
C7	0.0693 (13)	0.0733 (15)	0.0548 (13)	−0.0130 (12)	0.0074 (10)	0.0201 (11)
C8	0.0455 (10)	0.0474 (11)	0.0600 (12)	0.0034 (9)	0.0045 (9)	0.0108 (10)
C9	0.0523 (12)	0.0494 (13)	0.0841 (16)	−0.0028 (10)	0.0022 (11)	0.0159 (11)
C10	0.0525 (12)	0.0461 (13)	0.0930 (18)	−0.0048 (10)	−0.0075 (12)	0.0009 (12)
C11	0.0575 (12)	0.0569 (13)	0.0650 (13)	−0.0005 (11)	−0.0078 (10)	−0.0025 (11)
C12	0.0501 (10)	0.0461 (11)	0.0537 (12)	−0.0003 (9)	0.0010 (9)	0.0014 (9)
C13	0.0378 (9)	0.0380 (10)	0.0493 (11)	0.0060 (8)	0.0033 (8)	0.0006 (9)
C14	0.0634 (12)	0.0436 (11)	0.0515 (12)	−0.0067 (10)	−0.0049 (10)	0.0035 (9)
C15	0.0851 (15)	0.0409 (11)	0.0476 (12)	−0.0030 (11)	−0.0051 (11)	0.0012 (9)
C16	0.0813 (14)	0.0307 (10)	0.0469 (12)	0.0023 (10)	0.0109 (10)	0.0005 (9)
C17	0.117 (2)	0.0508 (13)	0.0559 (14)	0.0038 (14)	0.0237 (14)	−0.0006 (10)
C18	0.100 (2)	0.0672 (16)	0.088 (2)	−0.0025 (15)	0.0469 (16)	0.0001 (14)
C19	0.0740 (15)	0.0641 (15)	0.104 (2)	−0.0029 (12)	0.0309 (15)	−0.0014 (14)
C20	0.0591 (12)	0.0508 (12)	0.0729 (14)	0.0022 (10)	0.0118 (11)	0.0007 (10)
C21	0.0614 (12)	0.0323 (10)	0.0530 (12)	−0.0003 (9)	0.0097 (10)	0.0017 (9)
C22	0.125 (2)	0.0581 (14)	0.0584 (15)	−0.0025 (14)	−0.0222 (14)	−0.0043 (12)
N1	0.0427 (8)	0.0375 (8)	0.0422 (9)	0.0005 (7)	0.0031 (6)	0.0023 (7)
N2	0.0475 (8)	0.0438 (9)	0.0400 (9)	−0.0009 (7)	0.0039 (7)	0.0025 (7)
N3	0.0538 (9)	0.0405 (9)	0.0448 (9)	−0.0051 (7)	0.0049 (7)	0.0043 (7)
O1	0.189 (2)	0.0900 (13)	0.0577 (12)	0.0140 (13)	−0.0299 (12)	−0.0115 (9)

Geometric parameters (Å, º)

C1—N1	1.331 (2)	C11—H11	0.9300
C1—C2	1.369 (2)	C12—C13	1.388 (2)

C1—N3	1.429 (2)	C12—H12	0.9300
C2—C3	1.375 (2)	C13—N2	1.400 (2)
C2—H2	0.9300	C14—C15	1.364 (2)
C3—C4	1.372 (2)	C14—N3	1.371 (2)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.394 (2)	C15—C22	1.425 (3)
C4—H4	0.9300	C15—C16	1.432 (3)
C5—N1	1.3269 (19)	C16—C21	1.398 (2)
C5—N2	1.406 (2)	C16—C17	1.405 (3)
C6—C7	1.339 (3)	C17—C18	1.361 (3)
C6—N2	1.386 (2)	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.383 (3)
C7—C8	1.419 (3)	C18—H18	0.9300
C7—H7	0.9300	C19—C20	1.390 (3)
C8—C9	1.396 (3)	C19—H19	0.9300
C8—C13	1.405 (2)	C20—C21	1.372 (3)
C9—C10	1.362 (3)	C20—H20	0.9300
C9—H9	0.9300	C21—N3	1.408 (2)
C10—C11	1.386 (3)	C22—O1	1.215 (3)
C10—H10	0.9300	C22—H22	0.9300
C11—C12	1.384 (3)		

N1—C1—C2	124.85 (16)	C12—C13—C8	121.02 (17)
N1—C1—N3	113.26 (15)	N2—C13—C8	107.35 (16)
C2—C1—N3	121.88 (16)	C15—C14—N3	110.69 (17)
C1—C2—C3	116.90 (17)	C15—C14—H14	124.7
C1—C2—H2	121.5	N3—C14—H14	124.7
C3—C2—H2	121.5	C14—C15—C22	123.6 (2)
C4—C3—C2	120.36 (17)	C14—C15—C16	106.58 (17)
C4—C3—H3	119.8	C22—C15—C16	129.9 (2)
C2—C3—H3	119.8	C21—C16—C17	118.7 (2)
C3—C4—C5	117.99 (17)	C21—C16—C15	107.70 (16)
C3—C4—H4	121.0	C17—C16—C15	133.6 (2)
C5—C4—H4	121.0	C18—C17—C16	118.6 (2)
N1—C5—C4	122.65 (16)	C18—C17—H17	120.7
N1—C5—N2	116.02 (15)	C16—C17—H17	120.7
C4—C5—N2	121.32 (16)	C17—C18—C19	121.7 (2)
C7—C6—N2	110.53 (17)	C17—C18—H18	119.1
C7—C6—H6	124.7	C19—C18—H18	119.1
N2—C6—H6	124.7	C18—C19—C20	121.2 (2)
C6—C7—C8	107.79 (17)	C18—C19—H19	119.4
C6—C7—H7	126.1	C20—C19—H19	119.4
C8—C7—H7	126.1	C21—C20—C19	116.9 (2)
C9—C8—C13	119.42 (18)	C21—C20—H20	121.6
C9—C8—C7	133.48 (18)	C19—C20—H20	121.6
C13—C8—C7	107.10 (17)	C20—C21—C16	122.93 (17)
C10—C9—C8	119.50 (19)	C20—C21—N3	129.86 (18)
C10—C9—H9	120.2	C16—C21—N3	107.17 (16)

C8—C9—H9	120.2	O1—C22—C15	125.7 (3)
C9—C10—C11	120.73 (19)	O1—C22—H22	117.1
C9—C10—H10	119.6	C15—C22—H22	117.1
C11—C10—H10	119.6	C5—N1—C1	117.23 (14)
C12—C11—C10	121.54 (19)	C6—N2—C13	107.22 (14)
C12—C11—H11	119.2	C6—N2—C5	124.40 (15)
C10—C11—H11	119.2	C13—N2—C5	128.38 (14)
C11—C12—C13	117.77 (17)	C14—N3—C21	107.86 (15)
C11—C12—H12	121.1	C14—N3—C1	123.68 (14)
C13—C12—H12	121.1	C21—N3—C1	128.43 (15)
C12—C13—N2	131.59 (16)		

N1—C1—C2—C3	0.3 (3)	C19—C20—C21—N3	179.32 (18)
N3—C1—C2—C3	179.43 (15)	C17—C16—C21—C20	−1.1 (3)
C1—C2—C3—C4	−1.1 (3)	C15—C16—C21—C20	178.44 (17)
C2—C3—C4—C5	0.6 (3)	C17—C16—C21—N3	−179.34 (16)
C3—C4—C5—N1	0.6 (2)	C15—C16—C21—N3	0.19 (19)
C3—C4—C5—N2	179.67 (16)	C14—C15—C22—O1	179.0 (2)
N2—C6—C7—C8	−0.6 (2)	C16—C15—C22—O1	−0.8 (4)
C6—C7—C8—C9	−178.4 (2)	C4—C5—N1—C1	−1.4 (2)
C6—C7—C8—C13	0.5 (2)	N2—C5—N1—C1	179.54 (13)
C13—C8—C9—C10	0.2 (3)	C2—C1—N1—C5	0.9 (2)
C7—C8—C9—C10	178.9 (2)	N3—C1—N1—C5	−178.30 (13)
C8—C9—C10—C11	−1.0 (3)	C7—C6—N2—C13	0.6 (2)
C9—C10—C11—C12	0.6 (3)	C7—C6—N2—C5	−179.48 (16)
C10—C11—C12—C13	0.6 (3)	C12—C13—N2—C6	177.36 (18)
C11—C12—C13—N2	−178.68 (16)	C8—C13—N2—C6	−0.26 (18)
C11—C12—C13—C8	−1.3 (3)	C12—C13—N2—C5	−2.6 (3)
C9—C8—C13—C12	1.0 (3)	C8—C13—N2—C5	179.79 (15)
C7—C8—C13—C12	−178.03 (16)	N1—C5—N2—C6	169.29 (16)
C9—C8—C13—N2	178.90 (15)	C4—C5—N2—C6	−9.8 (2)
C7—C8—C13—N2	−0.11 (19)	N1—C5—N2—C13	−10.8 (2)
N3—C14—C15—C22	−179.03 (18)	C4—C5—N2—C13	170.11 (16)
N3—C14—C15—C16	0.8 (2)	C15—C14—N3—C21	−0.7 (2)
C14—C15—C16—C21	−0.6 (2)	C15—C14—N3—C1	−178.77 (16)
C22—C15—C16—C21	179.2 (2)	C20—C21—N3—C14	−177.78 (18)
C14—C15—C16—C17	178.8 (2)	C16—C21—N3—C14	0.30 (19)
C22—C15—C16—C17	−1.4 (4)	C20—C21—N3—C1	0.2 (3)
C21—C16—C17—C18	0.0 (3)	C16—C21—N3—C1	178.24 (16)
C15—C16—C17—C18	−179.4 (2)	N1—C1—N3—C14	34.4 (2)
C16—C17—C18—C19	0.7 (3)	C2—C1—N3—C14	−144.83 (17)
C17—C18—C19—C20	−0.3 (4)	N1—C1—N3—C21	−143.23 (16)
C18—C19—C20—C21	−0.8 (3)	C2—C1—N3—C21	37.5 (3)
C19—C20—C21—C16	1.5 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*5 is the centroid of the C16–C21 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{i}	0.93	2.50	3.227 (3)	135
C12—H12···N1	0.93	2.41	2.931 (2)	116
C2—H2···*Cg*5^{ii}	0.93	2.73	3.554 (2)	148

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