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Crystal structure of (*E*)-4-[*N*-(7-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-carboximidoyl]phenol

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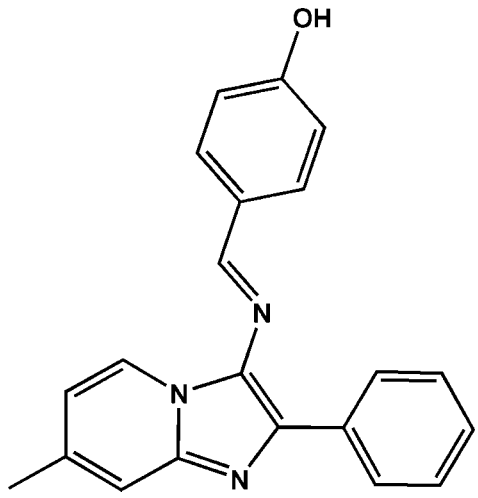
The molecule of the title compound, $C_{21}H_{17}N_3O$, is built up from fused five- and six-membered rings connected to a methyl group, a phenyl ring and an (iminomethyl)phenol group. The fused ring system is almost planar (r.m.s. deviation = 0.031 Å) and forms dihedral angles of 64.97 (7) and 18.52 (6)° with the phenyl ring and the (iminomethyl)phenol group, respectively. In the crystal, centrosymmetric molecules are linked by pairs of C—H···π interactions into dimeric units, which are further connected by O–H···N hydrogen bonds to form layers parallel to (101).

Keywords: crystal structure; imidazo[1,2a]pyridine derivative; hydrogen bonding; C—H···π interactions.

CCDC reference: 1426925

1. Related literature

For the biological activities of imidazo[1,2*a*]pyridine derivatives, see: Solomons *et al.* (1997); Bhandari *et al.* (2008); Ertl *et al.* (2000). For the synthesis of related compounds, see: Radi *et al.* (2015); Elaatiaoui *et al.* (2014).



2. Experimental

2.1. Crystal data

$C_{21}H_{17}N_3O$
M_r = 327.38
Monoclinic $P2_1/n$
a = 12.295 (3) Å
b = 9.587 (2) Å
c = 14.977 (4) Å
β = 101.548 (1)°
V = 1729.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.42 × 0.31 × 0.26 mm

2.2. Data collection

Bruker X8 APEX Diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.673, T_{max} = 0.746
26727 measured reflections
4126 independent reflections
2970 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.140
S = 1.02
4126 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of the C15–C20 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···*Cg*1^{i}	0.93	2.74	3.6705 (18)	175
O1—H1···N1^{ii}	0.82	1.86	2.6699 (17)	170

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RZ5169).

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supporting information

Acta Cryst. (2015). E**71**, o803–o804 [doi:10.1107/S2056989015017843]

Crystal structure of (*E*)-4-[*N*-(7-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)carboximidoyl]phenol

Abdelmalik Elaatiaoui, Rafik Saddik, Noureddine Benchat, Mohamed Saadi and Lahcen El Ammari

S1. Comment

Our interest on imidazo[1,2a]pyridine derivatives allowed us to investigate on the synthesis with a good yield of novel Schiff base compounds from this series by using acetic acid as catalyst (Radi *et al.*, 2015). Schiff bases are known for their important therapeutic properties (Solomons *et al.*, 1997; Bhandari *et al.*, 2008; Ertl *et al.*, 2000). The present paper is a continuation of our research work devoted to the development of imidazo[1,2a]pyridine derivatives with potential pharmacological activities (Elaatiaoui *et al.*, 2014).

The molecular structure of the title compound is shown in Fig. 1. The fused five- and six-membered rings are almost coplanar, with a maximum deviation of 0.054 (2) Å for atom C4. The mean plane through the fused ring system makes dihedral angles of 64.97 (7)° and 18.52 (6)° with the phenyl ring (C8–C13) and the (iminomethyl)phenol group (N3/C14–C20), respectively. The dihedral angle between the two aromatic rings C8–C13 and C15–C20 is 69.25 (7)°. The cohesion of the crystal structure is ensured by C—H···π interactions (Table 1) linking centrosymmetrically-related molecules into dimeric units, which are further connected by O—H···N hydrogen bonds (Table 1) to form layers parallel to the (1 0 1) plane as shown in Fig. 2.

S2. Experimental

To 7-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-amine (2.39 mmol) dissolved in 20 ml of dry diethyl ether two drops of acetic acid as catalyst (0.3 ml) were added, and the solution was stirred for 15–20 minutes at room temperature. Then 4-hydroxybenzaldehyde (2.39 mmol) was added and the reaction mixture stirred for 24 h at room temperature. The reaction was monitored by TLC. The formed product was filtered and washed with dry ether. The final purification was performed by recrystallization from hot methanol to give a crystalline powder. The powder was recrystallized from methanol and after 3 days the formed green crystals were filtered on Hotman paper (Yield 92.15%).

Spectral data. R_f = 0.50 (silica, CH2Cl2/CH3OH: 9/1). ^{1}HNMR (300 MHz, DMSO, δ p.p.m.): 8.659 (s, 1H, HC18=N); 8.322 (d, 1H, C3H, J= 6.99 Hz); 7.842 (d, 2H, C12H C16H, J=7.29 Hz); 7.654 (d, 2H, C15H + C13H, J=22,2 Hz); 7.35 (q, 4H, C6H + C14H, C24H + C20H); 6.75 (d, 3H, C2H + C23H + C21H, J = 6.09 Hz); 2.41 (s, 3H, C17H). ^{13}C NMR (75 MHz, DMSO, δ p.p.m.): 171.94; 160.87; 158.06; 142.28; 135.41; 134.78; 132.47; 130.38; 128.55; 128.48; 127.54; 127.26; 123.04; 115.80; 115.22; 115.02; 20.76. m/*z* (*M*+): 328.00. IR: ν (CH═N, imine) = 1655 cm^{-1}; ν(OH)=3450 cm^{-1}.

S3. Refinement

H atoms were located in a difference map and treated as riding with C–H = 0.93-0.96 Å, O–H = 0.82 Å, and with U_{iso}(H) = 1.5 U_{eq}(C, O) for methyl and hydroxide H atoms and U_{iso}(H) = 1.2 U_{eq}(C) for aromatic H atoms. One reflection ($\bar{1}$ 0 1) affected by beamstop was removed during the last cycles of refinement.

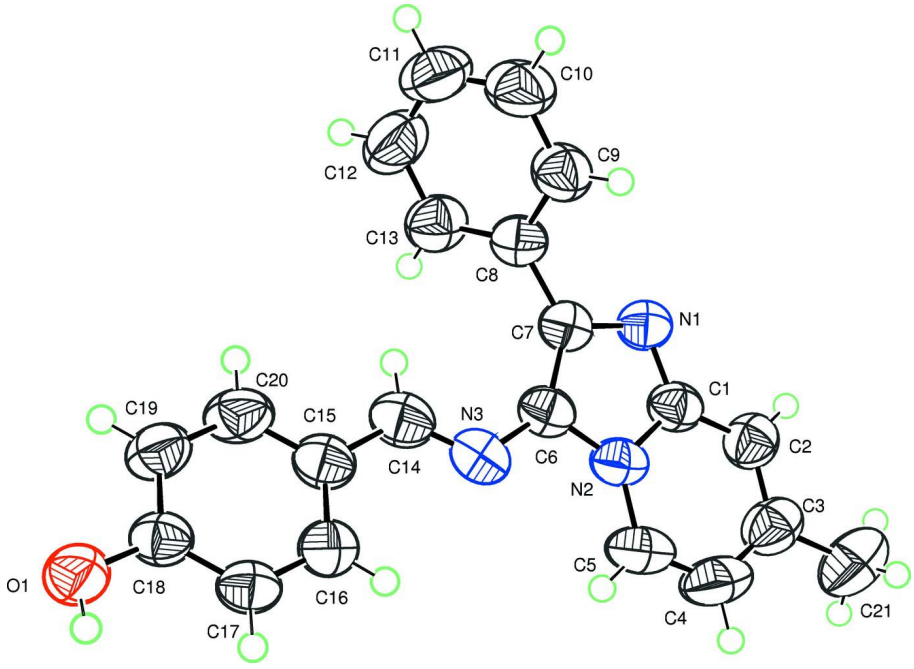

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small circles of arbitrary radius.

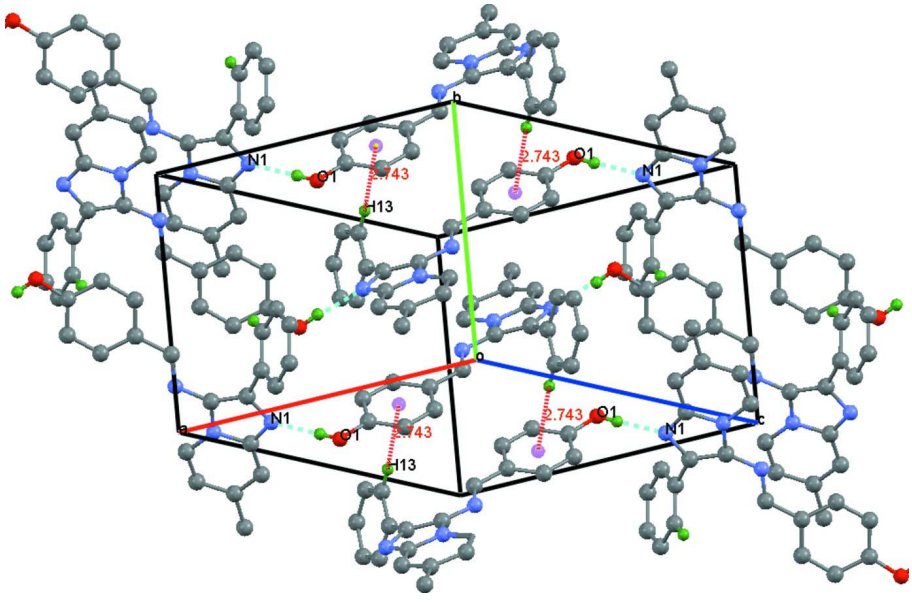

Figure 2

Packing diagram of the title compound showing the fornation of a layer parallel to the (1 0 1) plane by O—H···N hydrogen bonds cyan dotted lines) and C—H···π hydrogen interactions (red dotted lines). Hydrogen atoms not invoolved in hydrogen bonding are omitted.

(*E*)-4-[*N*-(7-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)carboximidoyl]phenol

Crystal data

$C_{21}H_{17}N_3O$
$M_r = 327.38$
Monoclinic, $P2_1/n$
$a = 12.295$ (3) Å
$b = 9.587$ (2) Å
$c = 14.977$ (4) Å
$\beta = 101.548$ (1)°
$V = 1729.6$ (7) Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.257$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4126 reflections
$\theta = 2.4$–27.9°
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, green
0.42 × 0.31 × 0.26 mm

Data collection

Bruker X8 APEX Diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.673$, $T_{max} = 0.746$
26727 measured reflections
4126 independent reflections
2970 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.4°$
$h = -16 \rightarrow 16$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.140$
$S = 1.02$
4126 reflections
226 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.4096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.54952 (12)	0.49279 (15)	0.29735 (10)	0.0451 (3)
C2	0.50833 (14)	0.40312 (17)	0.22392 (11)	0.0535 (4)
H2	0.5552	0.3713	0.1867	0.064*
C3	0.39967 (15)	0.36297 (19)	0.20743 (12)	0.0615 (4)
C4	0.33099 (15)	0.4141 (2)	0.26548 (14)	0.0695 (5)
H4	0.2572	0.3858	0.2555	0.083*
C5	0.36876 (13)	0.5026 (2)	0.33486 (13)	0.0620 (5)
H5	0.3219	0.5349	0.3719	0.074*
C6	0.53862 (12)	0.62960 (16)	0.41673 (10)	0.0452 (3)
C7	0.64653 (12)	0.62297 (15)	0.40304 (9)	0.0418 (3)

C8	0.75103 (12)	0.68006 (16)	0.45771 (9)	0.0436 (3)
C9	0.83189 (14)	0.58748 (19)	0.50032 (11)	0.0561 (4)
H9	0.8193	0.4920	0.4940	0.067*
C10	0.93079 (16)	0.6352 (2)	0.55190 (12)	0.0696 (5)
H10	0.9839	0.5719	0.5805	0.083*
C11	0.95080 (16)	0.7758 (3)	0.56102 (14)	0.0751 (6)
H11	1.0170	0.8079	0.5964	0.090*
C12	0.87302 (17)	0.8688 (2)	0.51789 (14)	0.0727 (5)
H12	0.8872	0.9641	0.5232	0.087*
C13	0.77345 (14)	0.82168 (18)	0.46638 (12)	0.0579 (4)
H13	0.7212	0.8856	0.4374	0.069*
C14	0.52384 (14)	0.78868 (19)	0.52891 (12)	0.0562 (4)
H14	0.5941	0.8193	0.5237	0.067*
C15	0.47106 (12)	0.85783 (17)	0.59525 (10)	0.0484 (4)
C16	0.36939 (12)	0.81542 (16)	0.61444 (10)	0.0470 (3)
H16	0.3318	0.7408	0.5826	0.056*
C17	0.32421 (12)	0.88222 (16)	0.67956 (10)	0.0464 (3)
H17	0.2574	0.8511	0.6924	0.056*
C18	0.37814 (12)	0.99643 (16)	0.72644 (10)	0.0457 (3)
C19	0.47875 (13)	1.04114 (19)	0.70700 (11)	0.0556 (4)
H19	0.5152	1.1177	0.7373	0.067*
C20	0.52369 (13)	0.9715 (2)	0.64294 (11)	0.0586 (4)
H20	0.5914	1.0013	0.6311	0.070*
C21	0.3546 (2)	0.2628 (2)	0.13212 (16)	0.0885 (7)
H21A	0.2772	0.2469	0.1308	0.133*
H21B	0.3636	0.3014	0.0749	0.133*
H21C	0.3942	0.1761	0.1425	0.133*
N1	0.65214 (10)	0.53861 (13)	0.32982 (8)	0.0456 (3)
N2	0.47802 (10)	0.54401 (13)	0.34959 (8)	0.0465 (3)
N3	0.48107 (11)	0.68926 (14)	0.47735 (9)	0.0506 (3)
O1	0.33670 (9)	1.06880 (13)	0.78932 (7)	0.0589 (3)
H1	0.2777	1.0339	0.7953	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0404 (7)	0.0465 (8)	0.0483 (8)	0.0019 (6)	0.0084 (6)	0.0070 (6)
C2	0.0550 (9)	0.0524 (9)	0.0513 (9)	−0.0014 (7)	0.0063 (7)	0.0013 (7)
C3	0.0577 (10)	0.0605 (10)	0.0600 (10)	−0.0065 (8)	−0.0028 (8)	0.0048 (8)
C4	0.0408 (9)	0.0817 (13)	0.0793 (13)	−0.0094 (9)	−0.0039 (8)	0.0051 (10)
C5	0.0361 (8)	0.0752 (11)	0.0742 (11)	0.0034 (8)	0.0096 (8)	0.0066 (9)
C6	0.0412 (8)	0.0482 (8)	0.0463 (8)	0.0044 (6)	0.0095 (6)	0.0059 (6)
C7	0.0411 (7)	0.0428 (7)	0.0422 (7)	0.0013 (6)	0.0096 (6)	0.0064 (6)
C8	0.0408 (7)	0.0510 (8)	0.0399 (7)	−0.0002 (6)	0.0106 (6)	0.0044 (6)
C9	0.0544 (9)	0.0591 (9)	0.0527 (9)	0.0081 (8)	0.0053 (7)	0.0004 (7)
C10	0.0537 (10)	0.0908 (14)	0.0582 (10)	0.0154 (10)	−0.0031 (8)	−0.0059 (10)
C11	0.0495 (10)	0.1046 (16)	0.0673 (12)	−0.0103 (11)	0.0020 (8)	−0.0204 (11)
C12	0.0654 (12)	0.0690 (12)	0.0826 (13)	−0.0206 (10)	0.0119 (10)	−0.0095 (10)

C13	0.0540 (9)	0.0538 (9)	0.0642 (10)	−0.0036 (8)	0.0078 (8)	0.0086 (8)
C14	0.0481 (9)	0.0665 (10)	0.0577 (9)	0.0027 (8)	0.0193 (7)	0.0031 (8)
C15	0.0444 (8)	0.0551 (9)	0.0469 (8)	0.0026 (7)	0.0121 (6)	0.0052 (7)
C16	0.0457 (8)	0.0453 (8)	0.0497 (8)	0.0000 (6)	0.0092 (6)	0.0052 (6)
C17	0.0381 (7)	0.0524 (8)	0.0500 (8)	−0.0015 (6)	0.0118 (6)	0.0073 (7)
C18	0.0406 (8)	0.0560 (8)	0.0403 (7)	0.0008 (6)	0.0077 (6)	0.0037 (6)
C19	0.0467 (8)	0.0688 (10)	0.0520 (9)	−0.0129 (8)	0.0116 (7)	−0.0071 (8)
C20	0.0435 (8)	0.0778 (11)	0.0576 (9)	−0.0110 (8)	0.0180 (7)	−0.0022 (8)
C21	0.0867 (15)	0.0875 (15)	0.0824 (14)	−0.0259 (12)	−0.0044 (12)	−0.0115 (12)
N1	0.0410 (6)	0.0489 (7)	0.0476 (7)	−0.0011 (5)	0.0108 (5)	0.0019 (5)
N2	0.0366 (6)	0.0509 (7)	0.0513 (7)	0.0028 (5)	0.0068 (5)	0.0054 (6)
N3	0.0474 (7)	0.0553 (8)	0.0508 (7)	0.0083 (6)	0.0139 (6)	0.0045 (6)
O1	0.0498 (6)	0.0726 (8)	0.0577 (7)	−0.0102 (5)	0.0184 (5)	−0.0137 (6)

Geometric parameters (Å, º)

C1—N1	1.3326 (19)	C11—H11	0.9300
C1—N2	1.3789 (19)	C12—C13	1.386 (3)
C1—C2	1.408 (2)	C12—H12	0.9300
C2—C3	1.364 (2)	C13—H13	0.9300
C2—H2	0.9300	C14—N3	1.272 (2)
C3—C4	1.415 (3)	C14—C15	1.451 (2)
C3—C21	1.500 (3)	C14—H14	0.9300
C4—C5	1.350 (3)	C15—C20	1.390 (2)
C4—H4	0.9300	C15—C16	1.398 (2)
C5—N2	1.375 (2)	C16—C17	1.374 (2)
C5—H5	0.9300	C16—H16	0.9300
C6—N3	1.3818 (19)	C17—C18	1.395 (2)
C6—C7	1.384 (2)	C17—H17	0.9300
C6—N2	1.393 (2)	C18—O1	1.3491 (18)
C7—N1	1.3753 (19)	C18—C19	1.394 (2)
C7—C8	1.483 (2)	C19—C20	1.372 (2)
C8—C13	1.386 (2)	C19—H19	0.9300
C8—C9	1.389 (2)	C20—H20	0.9300
C9—C10	1.382 (2)	C21—H21A	0.9600
C9—H9	0.9300	C21—H21B	0.9600
C10—C11	1.372 (3)	C21—H21C	0.9600
C10—H10	0.9300	O1—H1	0.8200
C11—C12	1.371 (3)		
N1—C1—N2	109.89 (13)	C12—C13—C8	120.56 (17)
N1—C1—C2	130.74 (14)	C12—C13—H13	119.7
N2—C1—C2	119.36 (14)	C8—C13—H13	119.7
C3—C2—C1	119.98 (16)	N3—C14—C15	124.79 (16)
C3—C2—H2	120.0	N3—C14—H14	117.6
C1—C2—H2	120.0	C15—C14—H14	117.6
C2—C3—C4	118.30 (16)	C20—C15—C16	117.76 (14)
C2—C3—C21	121.16 (19)	C20—C15—C14	118.96 (14)

C4—C3—C21	120.50 (18)	C16—C15—C14	123.28 (15)
C5—C4—C3	122.34 (16)	C17—C16—C15	121.05 (15)
C5—C4—H4	118.8	C17—C16—H16	119.5
C3—C4—H4	118.8	C15—C16—H16	119.5
C4—C5—N2	118.64 (17)	C16—C17—C18	120.29 (14)
C4—C5—H5	120.7	C16—C17—H17	119.9
N2—C5—H5	120.7	C18—C17—H17	119.9
N3—C6—C7	138.47 (15)	O1—C18—C19	117.56 (14)
N3—C6—N2	116.61 (13)	O1—C18—C17	123.18 (13)
C7—C6—N2	104.84 (12)	C19—C18—C17	119.25 (14)
N1—C7—C6	110.35 (13)	C20—C19—C18	119.66 (16)
N1—C7—C8	118.76 (12)	C20—C19—H19	120.2
C6—C7—C8	130.65 (13)	C18—C19—H19	120.2
C13—C8—C9	118.18 (15)	C19—C20—C15	121.97 (15)
C13—C8—C7	123.17 (14)	C19—C20—H20	119.0
C9—C8—C7	118.62 (14)	C15—C20—H20	119.0
C10—C9—C8	120.95 (17)	C3—C21—H21A	109.5
C10—C9—H9	119.5	C3—C21—H21B	109.5
C8—C9—H9	119.5	H21A—C21—H21B	109.5
C11—C10—C9	120.06 (18)	C3—C21—H21C	109.5
C11—C10—H10	120.0	H21A—C21—H21C	109.5
C9—C10—H10	120.0	H21B—C21—H21C	109.5
C12—C11—C10	119.85 (18)	C1—N1—C7	106.85 (12)
C12—C11—H11	120.1	C5—N2—C1	121.28 (14)
C10—C11—H11	120.1	C5—N2—C6	130.54 (14)
C11—C12—C13	120.37 (19)	C1—N2—C6	108.05 (12)
C11—C12—H12	119.8	C14—N3—C6	120.33 (14)
C13—C12—H12	119.8	C18—O1—H1	109.5

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C15–C20 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*1^{i}	0.93	2.74	3.6705 (18)	175
O1—H1···N1^{ii}	0.82	1.86	2.6699 (17)	170

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