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(2-Hydroxyphenyl)(4,2′:4′,4″-terpyridin-6′-yl)-methanone

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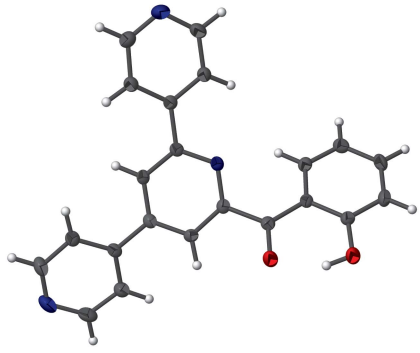
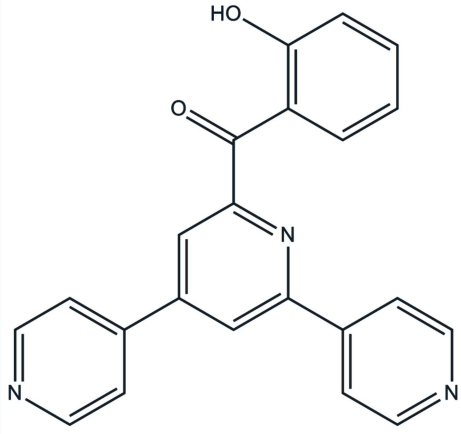
The title compound, $C_{22}H_{15}N_3O_2$, can be described as a ketone with a phenol substituent and a terpyridine ligand coordinated to the carbonyl group. The three six-membered rings of the terpyridine ligand are not coplanar. The dihedral angles between the mean planes of the central ring and the external pyridine ligands are 22.77 (9) and 26.77 (7)°. The central ring of the terpyridine ligand is also not coplanar with the *o*-hydroxy phenyl ring, the dihedral angle being 39.72 (5)°. An intramolecular O—H···O hydrogen bond occurs. The crystal structure of the title compound is consolidated by C—H···O and C—H···N hydrogen bonding interactions.

3D view



Chemical scheme



Structure description

Pyridine and derivatives play critical roles in the biochemical field. The hydrazone derivatives of benzoylpyridines exhibit cytotoxic activity towards tumor cell lines (Santos *et al.*, 2018) and show excellent antiproliferative activity (Kalinowski *et al.*, 2007). The quest for an efficient method for the preparation of such pyridine derivatives is ongoing. Herein, we report a novel method for the preparation of a 2-benzoylpyridine derivative in a one-pot reaction of 3-aminocoumarin with 4-acetylpyridine. The structural elucidation of the compound by spectroscopic investigation and single-crystal analysis has been performed.

The molecular structure of the title compound is shown in Fig. 1. It crystallizes in the orthorhombic crystal system in $P2_12_12_1$ space group with one molecule in the asymmetric unit. The compound can be described as a ketone with a phenol substituent and a terpyridine ligand coordinated to the carbonyl group. The dihedral angle between the mean planes of the central ring of the terpyridine ligand and the *o*-hydroxy phenyl ring is

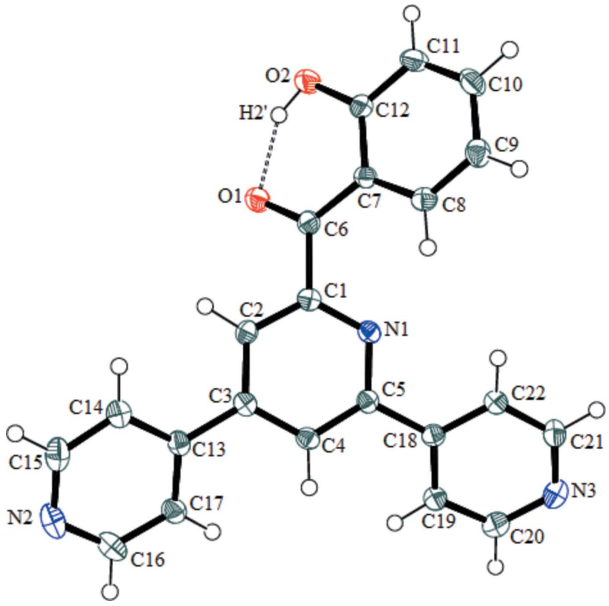


Figure 1
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

39.72 (5)°. The three six-membered rings of the terpyridine ligand are not coplanar. The dihedral angles between the mean planes of the central ring and the external pyridine ligands are 22.77 (9) and 26.77 (7)° (for C13–C17/N2 and C18–C22/N3, respectively). A strong intramolecular O—H···O hydrogen bond (O2—H2′···O1) exists between the O1 and O2 atoms of the phenol ring (Table 1).

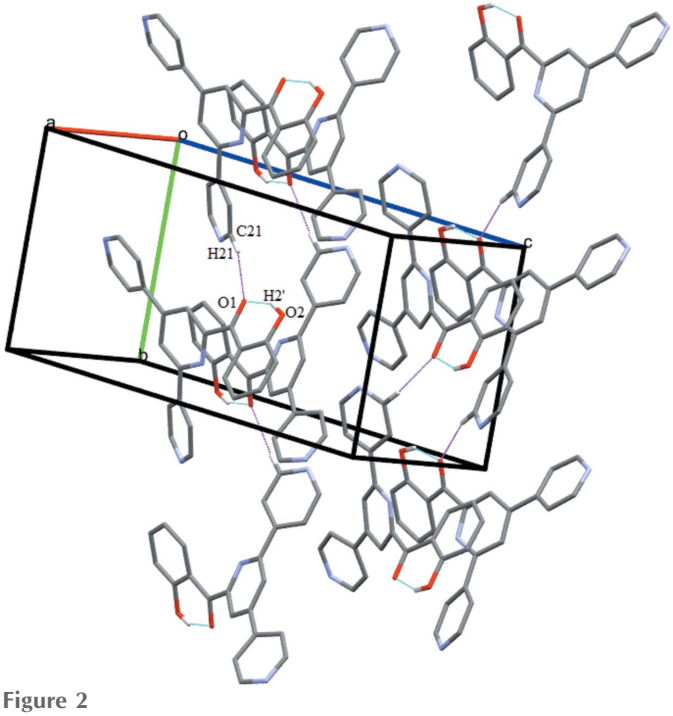


Figure 2
Unit-cell packing of the title compound showing intramolecular O—H···O and intermolecular C—H···O interactions as dotted lines. H atoms not involved in hydrogen bonding have been excluded.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2′···O1	0.87 (4)	1.73 (4)	2.527 (3)	152 (3)
C16—H16···O2^{i}	0.95	2.59	3.309 (3)	132
C17—H17···N2^{ii}	0.95	2.49	3.344 (3)	150
C21—H21···O1^{iii}	0.95	2.45	3.380 (3)	165

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

The crystal packing features the C21—H21···O1 interaction along the crystallographic *a* axis. The O1 atom of the phenol group is involves in both intra- and inter-molecular hydrogen bonding (Table 1, Fig. 2). The crystal structure is further stabilized by the following intermolecular interactions: C17—H17···N2^{ii} [symmetry code: (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$], which connects the molecules in a zigzag pattern, and C16—H16···O2^{i} [symmetry code: (i) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$], which forms molecular chains along the crystallographic *b* and *a* axes, respectively (Fig. 3). In addition, a weak π–π stacking interaction exhibiting a centroid–centroid distance of 3.7919 (15) Å between C7–C12 and C13–C17/N2 rings is observed (Fig. 4).

Synthesis and crystallization

A mixture of 3-amino-4-hydroxycoumarin (10 mmol, 1.0 equiv.), 4-acetylpyridine (22 mmol, 2.2 equiv.) and a few drops of TEA (0.2 equiv.) in toluene (25 ml) was refluxed under nitrogen for 4 h. The progress of the reaction was monitored by TLC. The reaction mixture was allowed to attain room temperature and the solvent was dried using a rotary evaporator. The crude product was purified by flash column chromatography to obtain a yellowish brown solid with 67%

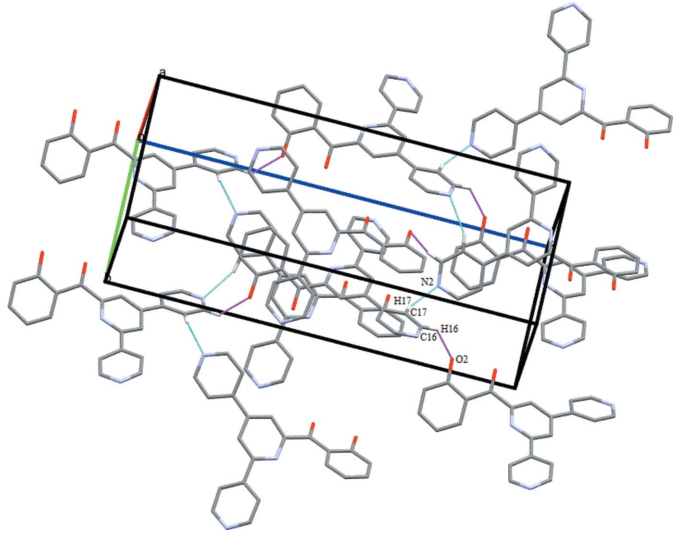


Figure 3
Unit-cell packing of the title compound showing intermolecular C—H···N and C—H···O interactions as dotted lines. H atoms not involved in hydrogen bonding have been excluded.

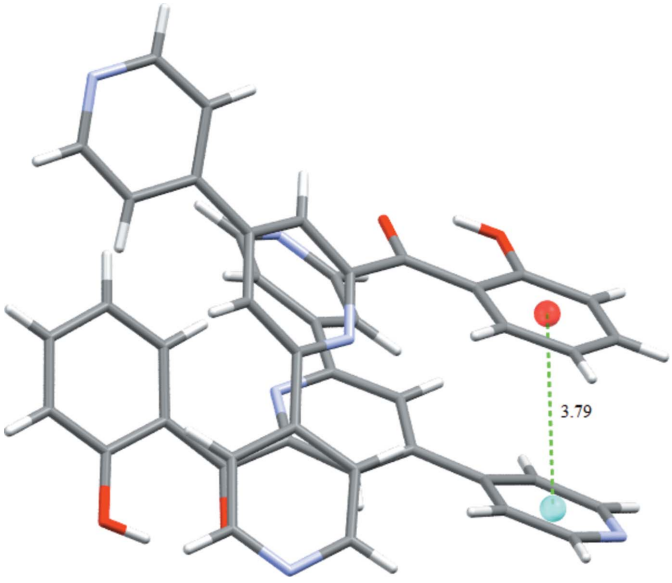


Figure 4
Unit-cell packing depicting the intermolecular π–π stacking interactions as dotted lines.

yield, R_f = 0.10 (5% DCM/MeOH), m.p. 190–192°C. The compound was recrystallized from ethanol solution. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 12.13 (*s*, 1H), 8.84 (*d*, *J* = 6.4 Hz, 2H), 8.81 (*d*, *J* = 6.4 Hz, 2H), 8.25 (*dd*, *J* = 8.0, 1.2 Hz, 1H), 8.22 (*d*, *J* = 1.2 Hz, 1H), 8.19 (*d*, *J* = 1.2 Hz, 1H), 8.01 (*dd*, *J* = 4.8, 1.6 Hz, 2H), 7.66 (*dd*, *J* = 3.2, 1.6 Hz, 2H), 7.58 (*t*, *J* = 7.6 Hz, 1H), 7.12 (*d*, *J* = 8.4–0 Hz, 1H), 6.96 (*t*, *J* = 7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 196.7, 164.9, 156.6, 154.4, 150.9, 150.8, 150.7, 148.7, 144.8, 144.6, 137.1, 134.2, 122.3, 121.4, 121.1, 120.4, 118.9, 118.5.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{15}N_3O_2$
M_r	353.37
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, *b*, *c* (Å)	7.2994 (2), 9.6105 (3), 23.9296 (8)
V (Å^3)	1678.68 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.48 × 0.25 × 0.18
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1998)
T_{min}, T_{max}	0.879, 0.928
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23873, 3416, 3003
R_{int}	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.088, 1.10
No. of reflections	3416
No. of parameters	248
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.23

Computer programs: *SMART* and *SAINT* (Bruker, 1998), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015) and *ORTEP-3 for Windows* (Farrugia, 2012).

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full crystallographic data

IUCrData (2020). **5**, x200857 [https://doi.org/10.1107/S2414314620008573]

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(2-Hydroxyphenyl)(4,2′:4′,4′′-terpyridin-6′-yl)methanone

Crystal data

$C_{22}H_{15}N_3O_2$
M_r = 353.37
Orthorhombic, $P2_12_12_1$
a = 7.2994 (2) Å
b = 9.6105 (3) Å
c = 23.9296 (8) Å
V = 1678.68 (9) Å^3
Z = 4
F(000) = 736
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9903 reflections
θ = 2.9–26.3°
μ = 0.09 mm^{-1}
T = 150 K
Parallelepiped, yellow
0.48 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.879, T_{max} = 0.928
23873 measured reflections
3416 independent reflections
3003 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 26.4°, θ_{min} = 3.3°
h = −9→8
k = −12→11
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.088
S = 1.10
3416 reflections
248 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 0.4435P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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. The hydroxy H atom was located in the Fourier maps and freyly refined, while all other H atoms were fixed geometrically and allow to ride on their parent carbon atoms, with a C—H distance of 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6864 (3)	0.49905 (18)	1.05784 (7)	0.0296 (4)
O2	0.7035 (3)	0.49051 (18)	1.16325 (7)	0.0321 (4)
H2′	0.706 (5)	0.522 (3)	1.1292 (14)	0.051 (10)*
N1	0.6398 (3)	0.18406 (19)	0.98997 (7)	0.0195 (4)
N2	0.3663 (3)	0.6191 (2)	0.76383 (9)	0.0348 (6)
N3	0.8135 (4)	−0.2862 (2)	0.91678 (9)	0.0367 (6)
C1	0.6004 (3)	0.3190 (2)	0.99800 (9)	0.0193 (5)
C2	0.5477 (3)	0.4093 (2)	0.95579 (9)	0.0201 (5)
H2	0.525464	0.504644	0.963740	0.024*
C3	0.5278 (3)	0.3587 (2)	0.90164 (9)	0.0197 (5)
C4	0.5690 (3)	0.2187 (2)	0.89279 (9)	0.0199 (5)
H4	0.557492	0.179870	0.856446	0.024*
C5	0.6269 (3)	0.1354 (2)	0.93715 (9)	0.0194 (5)
C6	0.6289 (3)	0.3781 (2)	1.05576 (9)	0.0211 (5)
C7	0.5894 (3)	0.2996 (2)	1.10698 (9)	0.0195 (5)
C8	0.5071 (3)	0.1676 (2)	1.10724 (10)	0.0220 (5)
H8	0.476367	0.124708	1.072717	0.026*
C9	0.4699 (3)	0.0988 (3)	1.15652 (10)	0.0263 (5)
H9	0.414255	0.009436	1.155914	0.032*
C10	0.5147 (4)	0.1617 (3)	1.20729 (10)	0.0296 (6)
H10	0.490145	0.114222	1.241306	0.036*
C11	0.5937 (4)	0.2912 (3)	1.20868 (10)	0.0294 (6)
H11	0.623645	0.332654	1.243546	0.035*
C12	0.6301 (3)	0.3618 (2)	1.15932 (10)	0.0230 (5)
C13	0.4716 (3)	0.4501 (2)	0.85454 (9)	0.0208 (5)
C14	0.3732 (4)	0.5721 (3)	0.86268 (10)	0.0281 (6)
H14	0.339665	0.600640	0.899286	0.034*
C15	0.3244 (4)	0.6518 (3)	0.81667 (11)	0.0350 (6)
H15	0.256962	0.734852	0.823080	0.042*
C16	0.4630 (4)	0.5027 (3)	0.75683 (11)	0.0315 (6)
H16	0.496579	0.477605	0.719817	0.038*
C17	0.5177 (3)	0.4161 (3)	0.79977 (10)	0.0248 (5)
H17	0.586121	0.334272	0.792006	0.030*
C18	0.6840 (3)	−0.0113 (2)	0.92905 (9)	0.0205 (5)
C19	0.7538 (3)	−0.0593 (3)	0.87856 (10)	0.0252 (5)
H19	0.759270	0.000724	0.847051	0.030*
C20	0.8152 (4)	−0.1948 (3)	0.87460 (11)	0.0333 (6)
H20	0.861862	−0.225112	0.839599	0.040*
C21	0.7440 (4)	−0.2392 (3)	0.96517 (11)	0.0321 (6)
H21	0.739621	−0.301578	0.995929	0.039*
C22	0.6785 (4)	−0.1058 (2)	0.97307 (10)	0.0250 (5)
H22	0.630106	−0.078786	1.008290	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0424 (11)	0.0236 (9)	0.0228 (9)	−0.0076 (8)	−0.0032 (8)	0.0015 (7)
O2	0.0489 (12)	0.0263 (10)	0.0212 (9)	−0.0064 (8)	−0.0069 (8)	−0.0005 (8)
N1	0.0189 (10)	0.0212 (10)	0.0183 (10)	−0.0016 (8)	0.0001 (7)	0.0018 (8)
N2	0.0347 (13)	0.0338 (13)	0.0360 (13)	0.0014 (11)	−0.0033 (10)	0.0151 (10)
N3	0.0515 (15)	0.0219 (12)	0.0366 (13)	0.0032 (11)	−0.0013 (11)	−0.0022 (9)
C1	0.0161 (11)	0.0223 (12)	0.0195 (11)	−0.0022 (9)	0.0010 (9)	−0.0001 (9)
C2	0.0198 (11)	0.0175 (12)	0.0231 (12)	−0.0018 (9)	0.0003 (9)	−0.0004 (9)
C3	0.0155 (11)	0.0227 (12)	0.0208 (11)	−0.0013 (9)	−0.0003 (9)	0.0024 (9)
C4	0.0187 (11)	0.0230 (12)	0.0179 (11)	−0.0019 (9)	−0.0020 (9)	0.0001 (9)
C5	0.0178 (11)	0.0194 (12)	0.0211 (11)	−0.0033 (9)	0.0003 (9)	0.0017 (9)
C6	0.0202 (12)	0.0213 (12)	0.0217 (12)	0.0020 (10)	−0.0021 (9)	0.0004 (10)
C7	0.0187 (11)	0.0215 (12)	0.0183 (11)	0.0040 (9)	−0.0014 (9)	−0.0001 (9)
C8	0.0196 (11)	0.0247 (13)	0.0217 (11)	0.0013 (9)	0.0007 (9)	−0.0017 (10)
C9	0.0253 (12)	0.0242 (13)	0.0294 (13)	−0.0001 (10)	0.0057 (11)	0.0035 (10)
C10	0.0345 (14)	0.0326 (14)	0.0217 (12)	0.0038 (12)	0.0047 (11)	0.0075 (11)
C11	0.0375 (15)	0.0333 (14)	0.0175 (12)	0.0053 (12)	−0.0012 (10)	−0.0018 (11)
C12	0.0262 (12)	0.0211 (12)	0.0218 (12)	0.0030 (10)	−0.0012 (10)	−0.0008 (10)
C13	0.0183 (11)	0.0207 (11)	0.0232 (11)	−0.0019 (9)	−0.0035 (9)	0.0032 (10)
C14	0.0312 (13)	0.0259 (13)	0.0272 (13)	0.0026 (11)	−0.0017 (11)	0.0020 (10)
C15	0.0371 (15)	0.0257 (14)	0.0423 (16)	0.0063 (12)	−0.0035 (13)	0.0064 (12)
C16	0.0299 (14)	0.0412 (16)	0.0235 (13)	−0.0002 (12)	−0.0019 (11)	0.0080 (12)
C17	0.0243 (13)	0.0267 (14)	0.0233 (12)	0.0018 (10)	−0.0031 (10)	0.0010 (10)
C18	0.0195 (12)	0.0209 (12)	0.0209 (11)	−0.0032 (10)	−0.0040 (9)	−0.0004 (9)
C19	0.0304 (13)	0.0226 (12)	0.0226 (12)	−0.0020 (10)	−0.0026 (10)	0.0011 (10)
C20	0.0436 (15)	0.0279 (14)	0.0283 (13)	0.0019 (12)	0.0018 (12)	−0.0040 (11)
C21	0.0444 (17)	0.0220 (13)	0.0299 (13)	−0.0020 (12)	−0.0046 (12)	0.0047 (11)
C22	0.0315 (13)	0.0227 (13)	0.0208 (12)	−0.0013 (10)	−0.0006 (10)	0.0011 (9)

Geometric parameters (Å, º)

O1—C6	1.237 (3)	C9—C10	1.396 (3)
O2—C12	1.351 (3)	C9—H9	0.9500
O2—H2′	0.87 (3)	C10—C11	1.372 (4)
N1—C1	1.342 (3)	C10—H10	0.9500
N1—C5	1.351 (3)	C11—C12	1.388 (3)
N2—C16	1.334 (3)	C11—H11	0.9500
N2—C15	1.338 (3)	C13—C14	1.389 (3)
N3—C20	1.338 (3)	C13—C17	1.392 (3)
N3—C21	1.343 (3)	C14—C15	1.388 (3)
C1—C2	1.386 (3)	C14—H14	0.9500
C1—C6	1.509 (3)	C15—H15	0.9500
C2—C3	1.392 (3)	C16—C17	1.381 (3)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.395 (3)	C17—H17	0.9500
C3—C13	1.487 (3)	C18—C19	1.390 (3)

C4—C5	1.395 (3)	C18—C22	1.391 (3)
C4—H4	0.9500	C19—C20	1.380 (3)
C5—C18	1.484 (3)	C19—H19	0.9500
C6—C7	1.467 (3)	C20—H20	0.9500
C7—C8	1.404 (3)	C21—C22	1.381 (4)
C7—C12	1.419 (3)	C21—H21	0.9500
C8—C9	1.379 (3)	C22—H22	0.9500
C8—H8	0.9500		

C12—O2—H2′	105 (2)	C10—C11—H11	119.9
C1—N1—C5	116.96 (19)	C12—C11—H11	119.9
C16—N2—C15	115.9 (2)	O2—C12—C11	117.7 (2)
C20—N3—C21	115.7 (2)	O2—C12—C7	122.0 (2)
N1—C1—C2	124.1 (2)	C11—C12—C7	120.3 (2)
N1—C1—C6	117.72 (19)	C14—C13—C17	117.1 (2)
C2—C1—C6	118.1 (2)	C14—C13—C3	122.4 (2)
C1—C2—C3	119.3 (2)	C17—C13—C3	120.6 (2)
C1—C2—H2	120.4	C15—C14—C13	119.2 (2)
C3—C2—H2	120.4	C15—C14—H14	120.4
C2—C3—C4	117.1 (2)	C13—C14—H14	120.4
C2—C3—C13	121.9 (2)	N2—C15—C14	124.1 (2)
C4—C3—C13	120.9 (2)	N2—C15—H15	117.9
C3—C4—C5	120.2 (2)	C14—C15—H15	117.9
C3—C4—H4	119.9	N2—C16—C17	124.4 (2)
C5—C4—H4	119.9	N2—C16—H16	117.8
N1—C5—C4	122.3 (2)	C17—C16—H16	117.8
N1—C5—C18	115.6 (2)	C16—C17—C13	119.3 (2)
C4—C5—C18	122.1 (2)	C16—C17—H17	120.3
O1—C6—C7	121.0 (2)	C13—C17—H17	120.3
O1—C6—C1	115.9 (2)	C19—C18—C22	116.9 (2)
C7—C6—C1	123.0 (2)	C19—C18—C5	122.1 (2)
C8—C7—C12	117.8 (2)	C22—C18—C5	120.9 (2)
C8—C7—C6	123.5 (2)	C20—C19—C18	119.4 (2)
C12—C7—C6	118.7 (2)	C20—C19—H19	120.3
C9—C8—C7	121.4 (2)	C18—C19—H19	120.3
C9—C8—H8	119.3	N3—C20—C19	124.4 (2)
C7—C8—H8	119.3	N3—C20—H20	117.8
C8—C9—C10	119.4 (2)	C19—C20—H20	117.8
C8—C9—H9	120.3	N3—C21—C22	124.2 (2)
C10—C9—H9	120.3	N3—C21—H21	117.9
C11—C10—C9	120.8 (2)	C22—C21—H21	117.9
C11—C10—H10	119.6	C21—C22—C18	119.5 (2)
C9—C10—H10	119.6	C21—C22—H22	120.3
C10—C11—C12	120.2 (2)	C18—C22—H22	120.3

C5—N1—C1—C2	0.2 (3)	C6—C7—C12—O2	0.1 (3)
C5—N1—C1—C6	−175.1 (2)	C8—C7—C12—C11	1.9 (3)
N1—C1—C2—C3	2.1 (3)	C6—C7—C12—C11	179.6 (2)

C6—C1—C2—C3	177.4 (2)	C2—C3—C13—C14	−24.2 (3)
C1—C2—C3—C4	−2.1 (3)	C4—C3—C13—C14	158.0 (2)
C1—C2—C3—C13	180.0 (2)	C2—C3—C13—C17	155.4 (2)
C2—C3—C4—C5	0.1 (3)	C4—C3—C13—C17	−22.4 (3)
C13—C3—C4—C5	178.0 (2)	C17—C13—C14—C15	0.8 (4)
C1—N1—C5—C4	−2.3 (3)	C3—C13—C14—C15	−179.6 (2)
C1—N1—C5—C18	175.8 (2)	C16—N2—C15—C14	−0.8 (4)
C3—C4—C5—N1	2.2 (3)	C13—C14—C15—N2	−0.1 (4)
C3—C4—C5—C18	−175.8 (2)	C15—N2—C16—C17	1.0 (4)
N1—C1—C6—O1	143.3 (2)	N2—C16—C17—C13	−0.3 (4)
C2—C1—C6—O1	−32.3 (3)	C14—C13—C17—C16	−0.7 (3)
N1—C1—C6—C7	−37.6 (3)	C3—C13—C17—C16	179.7 (2)
C2—C1—C6—C7	146.9 (2)	N1—C5—C18—C19	−151.7 (2)
O1—C6—C7—C8	173.4 (2)	C4—C5—C18—C19	26.4 (3)
C1—C6—C7—C8	−5.7 (3)	N1—C5—C18—C22	24.9 (3)
O1—C6—C7—C12	−4.2 (3)	C4—C5—C18—C22	−157.0 (2)
C1—C6—C7—C12	176.7 (2)	C22—C18—C19—C20	−0.7 (4)
C12—C7—C8—C9	−1.3 (3)	C5—C18—C19—C20	176.0 (2)
C6—C7—C8—C9	−178.9 (2)	C21—N3—C20—C19	0.9 (4)
C7—C8—C9—C10	0.1 (3)	C18—C19—C20—N3	−0.3 (4)
C8—C9—C10—C11	0.5 (4)	C20—N3—C21—C22	−0.5 (4)
C9—C10—C11—C12	0.1 (4)	N3—C21—C22—C18	−0.4 (4)
C10—C11—C12—O2	178.2 (2)	C19—C18—C22—C21	1.1 (4)
C10—C11—C12—C7	−1.3 (4)	C5—C18—C22—C21	−175.7 (2)
C8—C7—C12—O2	−177.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2′···O1	0.87 (4)	1.73 (4)	2.527 (3)	152 (3)
C16—H16···O2^{i}	0.95	2.59	3.309 (3)	132
C17—H17···N2^{ii}	0.95	2.49	3.344 (3)	150
C21—H21···O1^{iii}	0.95	2.45	3.380 (3)	165

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