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4'-(3,4-Dimethoxyphenyl)-2,2':6',2''-terpyridine

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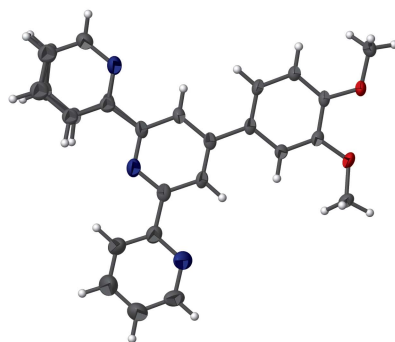
Keywords: crystal structure; terpyridine; dimethoxyphenyl substituent; hydrogen bonds; π - π contacts.

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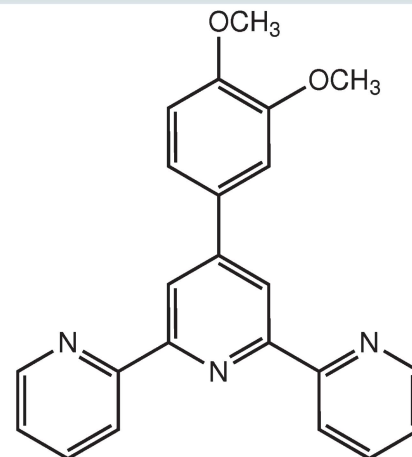
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{19}N_3O_2$, the terpyridine unit has a dimethoxyphenyl substituent at the 4-position of the central pyridyl ring. The three pyridyl rings are in a *transoid* conformation with respect to the interannular C—C bonds. In addition, the pendant dimethoxyphenyl substituent is almost coplanar with the terpyridyl unit; the dihedral angle between the central pyridyl ring and the benzene ring is $7.14(11)^\circ$, which is much smaller than that found in the structural isomer with a 2,5-dimethoxyphenyl substituent. The C—C and C—N bond lengths within the aromatic rings are normal. One of the terminal pyridyl rings is disordered over two sets of sites with an occupancy ratio of 0.744 (7):0.256 (7). The orientation of the two methoxy groups at the 3- and 4-positions is such that the methyl groups point away from each other in opposite directions. In the crystal structure, C—H \cdots N hydrogen bonds form chains along *b* while C—H \cdots O contacts form inversion dimers, creating double chains. These combine with C—H \cdots π contacts and π \cdots π interactions, with a centroid-centroid distance of $3.858(4)$ Å, to stack molecules along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Polypyridines display unique photophysical and redox properties (Winter *et al.*, 2011). Terpyridine analogs are also known to act as tridentate ligands using all three of the N-donor atoms.

Although the title compound, $C_{23}H_{19}N_3O_2$, has been obtained previously by a standard Kröhnke-type synthesis (Whittle *et al.*, 1995), we have prepared it by a direct condensation reaction between 2-acetylpyridine and 3,4-dimethoxybenzaldehyde, according to a procedure reported earlier for a similar compound (Storrier *et al.*, 1998).

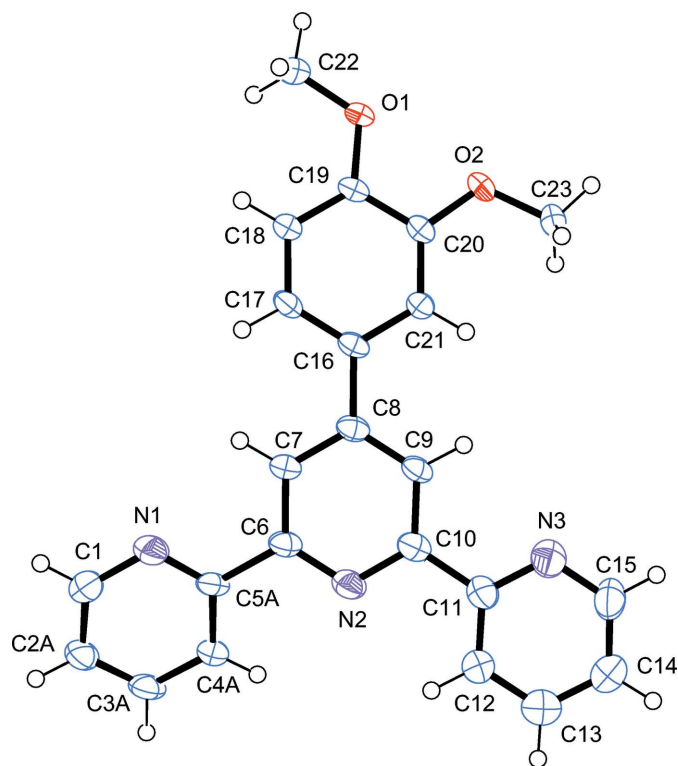


Figure 1
The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms. Only the major component of the disordered pyridyl ring is shown.

In the molecule (Fig. 1), the terpyridine unit has a dimethoxyphenyl substituent at the 4-position of the central pyridyl ring. The three pyridyl rings adopt the expected *transoid* conformation with respect to the interannular C–C bonds. The pendant dimethoxyphenyl substituent lies close to the plane of the terpyridyl unit with a dihedral angle of

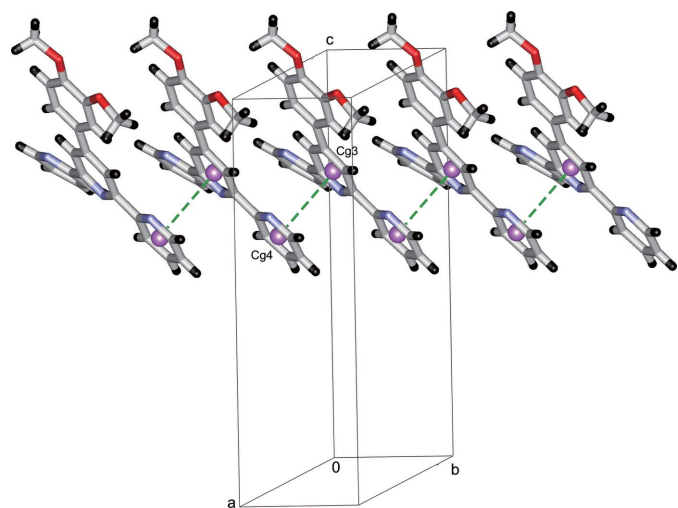


Figure 2
 π – π contacts in the crystal packing of the title compound. Only the major component of the disordered pyridyl ring is shown.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$Cg1$ and $Cg5$ are the centroids of the $N1/C1$ – $C5A$ and $C16$ – $C21$ rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C3A-H3A\cdots N3^i$	0.95	2.43	3.285 (7)	149
$C23-H18\cdots O1^{ii}$	0.98	2.53	3.511 (5)	174
$C18-H12\cdots Cg5^{iii}$	0.95	2.87	3.648 (5)	139
$C23-H17\cdots Cg1^{iv}$	0.98	2.90	3.432 (5)	115
$C23-H19\cdots Cg5^v$	0.98	2.89	3.724 (5)	143

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

7.14 (11°) between the $N2/C6$ – $C10$ and $C16$ – $C21$ ring planes. This is comparable to that found for the related compound with a phenyl substituent (10.9° ; Constable *et al.*, 1990) but distinct from that of the corresponding 2,5-dimethoxyphenyl structural isomer (50.2° ; Storrier *et al.*, 1998). This difference can be ascribed in part to the intramolecular steric interactions between the *ortho*-substituents (either $-\text{OCH}_3$ or $-\text{H}$) on the phenyl ring and the 3- or 5-protons on the central pyridine ring. One of the terminal pyridyl rings is disordered over two sets of sites with an occupancy ratio of 0.744 (7): 0.256 (7). The orientation of the two methoxy groups at the 3- and 4-positions is such that the methyl groups point away from each other in opposite directions.

In the crystal structure, a π – π contact between $Cg3$ and $Cg4$, 3.858 (4) \AA , ($Cg3$ and $Cg4$ are the centroids of the $N2/C6$ – $C10$ and $N3/C11$ – $C15$ rings respectively; symmetry operation $x, -1 + y, z$) stack molecules along the b -axis direction, Fig. 2. $C18-H12\cdots\pi$ and $C23-H19\cdots\pi$ hydrogen bonds (Table 1) also contribute to this stacking. In addition $C3A-H3A\cdots N3$ hydrogen bonds form $C(10)$ chains along a while $C23-H18\cdots O3$ contacts form inversion dimers and, together with a $C23-H17\cdots\pi$ contact, generate a double chain of molecules along a . The overall effect, Fig. 3, sees sheets of molecules stacked along the b -axis direction.

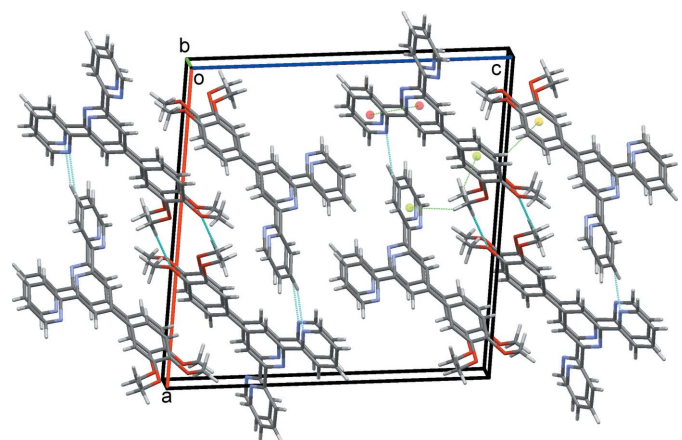


Figure 3
Overall packing of the title compound viewed along b . Hydrogen bonds are drawn as blue dashed lines with representative π – π and $C-H\cdots\pi$ contacts shown as green dotted lines. Ring centroids are shown as coloured spheres.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₃ H ₁₉ N ₃ O ₂
<i>M_r</i>	369.42
Crystal system, space group	Monoclinic, <i>P2₁/a</i>
Temperature (K)	93
<i>a</i> , <i>b</i> , <i>c</i> (Å)	18.280 (14), 5.493 (4), 18.298 (14)
β (°)	96.020 (6)
<i>V</i> (Å ³)	1827 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.20 × 0.15 × 0.08
Data collection	
Diffractometer	Rigaku Saturn724
Absorption correction	Multi-scan (<i>REQAB</i> ; Rigaku, 1998)
<i>T_{min}</i> , <i>T_{max}</i>	0.881, 0.993
No. of measured, independent and observed [<i>F</i> ² > 2.0 σ (<i>F</i> ²)] reflections	17670, 4118, 2937
<i>R_{int}</i>	0.075
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.648
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.100, 0.224, 1.14
No. of reflections	4118
No. of parameters	270
No. of restraints	18
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.44, -0.43

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *CrystalStructure* (Rigaku, 2010), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

Synthesis and crystallization

The title compound was prepared by a direct condensation reaction between 2-acetylpyridine and 3,4-dimethoxy-

benzaldehyde in ammonium acetate–acetamide to afford a pale-yellow solid in 23% yield, which is a modification of a literature method (Storrier *et al.*, 1998). The crude product was purified by column chromatography and then recrystallized from a chloroform–diethyl ether (1/40) mixture at ambient temperature to give good quality crystals suitable for X-ray diffraction.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The carbon atoms of one of the pyridyl rings were disordered over two sites and refined as (C2A, C3A, C4A, C5A) and (C2B, C3B, C4B, C5B) with occupancies that sum to unity. This disorder model converged with an occupancy ratio 0.744 (7):0.256 (7).

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full crystallographic data

IUCrData (2016). **1**, x160950 [doi:10.1107/S2414314616009500]

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Crystal data

$C_{23}H_{19}N_3O_2$

$M_r = 369.42$

Monoclinic, $P2_1/a$

Hall symbol: -P 2yab

$a = 18.280$ (14) Å

$b = 5.493$ (4) Å

$c = 18.298$ (14) Å

$\beta = 96.020$ (6)°

$V = 1827$ (3) Å³

$Z = 4$

$F(000) = 776.00$

$D_x = 1.343$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 3564 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 0.09$ mm⁻¹

$T = 93$ K

Block, colorless

$0.20 \times 0.15 \times 0.08$ mm

Data collection

Rigaku Saturn724
diffractometer

Detector resolution: 28.944 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*REQAB*; Rigaku, 1998)

$T_{\min} = 0.881$, $T_{\max} = 0.993$

17670 measured reflections

4118 independent reflections

2937 reflections with $F^2 > 2.0\sigma(F^2)$

$R_{\text{int}} = 0.075$

$\theta_{\max} = 27.4$ °

$h = -23 \rightarrow 23$

$k = -7 \rightarrow 6$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.100$

$wR(F^2) = 0.224$

$S = 1.14$

4118 reflections

270 parameters

18 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

$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 2.0174P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.44$ e Å⁻³

$\Delta\rho_{\min} = -0.43$ e Å⁻³

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2 . R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R-factor (gt).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.40936 (11)	0.0742 (5)	1.03502 (12)	0.0328 (6)	
O2	0.42133 (12)	0.4172 (5)	0.94160 (13)	0.0373 (6)	
N1	0.01717 (16)	-0.3469 (7)	0.74911 (17)	0.0458 (9)	
N2	0.09106 (15)	0.1770 (6)	0.66251 (15)	0.0391 (8)	
N3	0.21225 (16)	0.6651 (6)	0.61704 (18)	0.0458 (9)	
C1	-0.0454 (2)	-0.4808 (8)	0.7454 (2)	0.0482 (10)	
C2B	-0.0955 (12)	-0.468 (4)	0.6835 (11)	0.045 (6)*	0.256 (7)
C2A	-0.1103 (4)	-0.4111 (14)	0.7073 (4)	0.0463 (16)	0.744 (7)
C3B	-0.0833 (9)	-0.324 (3)	0.6262 (9)	0.045 (5)*	0.256 (7)
C3A	-0.1108 (3)	-0.1923 (11)	0.6710 (3)	0.0416 (15)	0.744 (7)
C4B	-0.0222 (8)	-0.173 (3)	0.6330 (8)	0.033 (4)*	0.256 (7)
C4A	-0.0474 (3)	-0.0582 (9)	0.6719 (3)	0.0343 (13)	0.744 (7)
C5B	0.0254 (16)	-0.171 (6)	0.6961 (14)	0.031 (7)*	0.256 (7)
C5A	0.0166 (5)	-0.1472 (17)	0.7106 (5)	0.0294 (17)	0.744 (7)
C6	0.08608 (17)	0.0020 (7)	0.71429 (17)	0.0312 (8)	
C7	0.13976 (16)	-0.0289 (6)	0.77322 (17)	0.0282 (7)	
C8	0.20105 (16)	0.1251 (6)	0.78114 (16)	0.0282 (7)	
C9	0.20605 (16)	0.3003 (6)	0.72868 (17)	0.0290 (7)	
C10	0.15111 (18)	0.3231 (7)	0.66967 (17)	0.0327 (8)	
C11	0.1539 (2)	0.5164 (8)	0.6129 (2)	0.0419 (9)	
C12	0.0988 (4)	0.5414 (11)	0.5584 (3)	0.096 (2)	
C13	0.1006 (4)	0.7274 (14)	0.5080 (4)	0.127 (3)	
C14	0.1603 (3)	0.8778 (11)	0.5112 (3)	0.0791 (17)	
C15	0.2144 (3)	0.8425 (8)	0.5668 (3)	0.0509 (11)	
C16	0.25678 (16)	0.1036 (6)	0.84759 (17)	0.0271 (7)	
C17	0.25191 (17)	-0.0796 (7)	0.89922 (18)	0.0314 (8)	
C18	0.30174 (17)	-0.0968 (7)	0.96230 (18)	0.0307 (8)	
C19	0.35774 (16)	0.0731 (6)	0.97494 (16)	0.0274 (7)	
C20	0.36432 (16)	0.2606 (6)	0.92346 (17)	0.0269 (7)	
C21	0.31479 (16)	0.2735 (6)	0.86080 (17)	0.0270 (7)	
C22	0.4094 (2)	-0.1284 (7)	1.0841 (2)	0.0459 (10)	
C23	0.43971 (19)	0.5865 (7)	0.88633 (19)	0.0376 (9)	
H1	-0.0441	-0.6320	0.7708	0.0578*	
H2A	-0.1532	-0.5095	0.7060	0.0556*	0.744 (7)
H2B	-0.1392	-0.5629	0.6811	0.0545*	0.256 (7)
H3A	-0.1551	-0.1337	0.6452	0.0499*	0.744 (7)
H3B	-0.1159	-0.3268	0.5822	0.0543*	0.256 (7)
H4A	-0.0473	0.0928	0.6467	0.0411*	0.744 (7)
H4B	-0.0133	-0.0686	0.5934	0.0391*	0.256 (7)
H5	0.1348	-0.1544	0.8081	0.0338*	
H6	0.2471	0.4072	0.7323	0.0348*	
H7	0.0587	0.4306	0.5547	0.1153*	
H8	0.0605	0.7506	0.4712	0.1520*	
H9	0.1638	1.0028	0.4759	0.0949*	
H10	0.2558	0.9482	0.5703	0.0611*	

H11	0.2136	-0.1965	0.8914	0.0377*
H12	0.2973	-0.2247	0.9965	0.0368*
H13	0.3199	0.3991	0.8260	0.0324*
H14	0.4415	-0.0927	1.1291	0.0551*
H15	0.4275	-0.2734	1.0605	0.0551*
H16	0.3593	-0.1579	1.0964	0.0551*
H17	0.4553	0.4966	0.8444	0.0452*
H18	0.4798	0.6925	0.9070	0.0452*
H19	0.3965	0.6857	0.8700	0.0452*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0254 (12)	0.0376 (14)	0.0326 (12)	-0.0081 (10)	-0.0100 (9)	0.0043 (11)
O2	0.0285 (12)	0.0427 (15)	0.0385 (13)	-0.0161 (11)	-0.0062 (10)	0.0035 (11)
N1	0.0304 (16)	0.064 (3)	0.0415 (17)	-0.0086 (15)	-0.0048 (13)	0.0096 (17)
N2	0.0261 (15)	0.052 (2)	0.0378 (16)	-0.0039 (14)	-0.0017 (12)	0.0015 (15)
N3	0.0301 (16)	0.048 (2)	0.060 (2)	0.0081 (14)	0.0083 (15)	0.0105 (17)
C1	0.043 (3)	0.058 (3)	0.042 (2)	-0.007 (2)	-0.0024 (17)	0.016 (2)
C2A	0.032 (3)	0.073 (5)	0.034 (3)	-0.018 (3)	0.000 (3)	0.007 (4)
C3A	0.023 (3)	0.067 (4)	0.033 (3)	-0.004 (3)	-0.0054 (19)	0.003 (3)
C4A	0.026 (3)	0.040 (3)	0.035 (3)	-0.002 (2)	-0.0054 (19)	0.004 (3)
C5A	0.020 (3)	0.048 (5)	0.020 (4)	-0.000 (3)	-0.000 (3)	-0.002 (3)
C6	0.0226 (15)	0.040 (2)	0.0302 (16)	0.0030 (14)	-0.0024 (13)	-0.0003 (15)
C7	0.0229 (15)	0.0327 (18)	0.0277 (16)	0.0018 (13)	-0.0026 (13)	-0.0017 (14)
C8	0.0203 (15)	0.0366 (19)	0.0273 (16)	0.0044 (13)	0.0011 (12)	-0.0050 (14)
C9	0.0179 (14)	0.0382 (19)	0.0306 (16)	-0.0011 (14)	0.0005 (13)	-0.0037 (15)
C10	0.0267 (17)	0.041 (2)	0.0302 (16)	-0.0003 (15)	0.0017 (13)	-0.0059 (15)
C11	0.0333 (19)	0.052 (3)	0.041 (2)	-0.0086 (17)	0.0034 (16)	0.0035 (18)
C12	0.096 (4)	0.114 (5)	0.068 (3)	-0.069 (4)	-0.038 (3)	0.048 (3)
C13	0.112 (5)	0.156 (6)	0.098 (4)	-0.079 (5)	-0.057 (4)	0.072 (4)
C14	0.072 (4)	0.097 (4)	0.065 (3)	-0.027 (3)	-0.012 (3)	0.040 (3)
C15	0.039 (3)	0.048 (3)	0.067 (3)	0.0001 (19)	0.013 (2)	0.019 (3)
C16	0.0172 (14)	0.0338 (18)	0.0298 (16)	0.0015 (13)	-0.0004 (12)	-0.0046 (14)
C17	0.0216 (15)	0.0337 (19)	0.0374 (18)	-0.0064 (14)	-0.0039 (13)	-0.0006 (15)
C18	0.0250 (16)	0.0332 (18)	0.0324 (17)	-0.0043 (14)	-0.0038 (13)	0.0032 (15)
C19	0.0199 (15)	0.0332 (18)	0.0280 (16)	-0.0006 (13)	-0.0032 (12)	-0.0040 (14)
C20	0.0194 (14)	0.0299 (18)	0.0312 (16)	-0.0018 (13)	0.0019 (12)	-0.0032 (14)
C21	0.0216 (15)	0.0301 (18)	0.0291 (16)	-0.0008 (13)	0.0014 (12)	0.0009 (14)
C22	0.043 (2)	0.046 (3)	0.044 (2)	-0.0116 (18)	-0.0174 (17)	0.0109 (18)
C23	0.0342 (18)	0.041 (2)	0.0372 (19)	-0.0146 (16)	0.0027 (15)	0.0059 (16)

Geometric parameters (Å, °)

O1—C19	1.372 (4)	C14—C15	1.357 (7)
O1—C22	1.430 (5)	C16—C17	1.390 (5)
O2—C20	1.365 (4)	C16—C21	1.414 (5)
O2—C23	1.439 (5)	C17—C18	1.397 (5)

N1—C1	1.356 (6)	C18—C19	1.387 (5)
N1—C5B	1.39 (3)	C19—C20	1.409 (5)
N1—C5A	1.303 (10)	C20—C21	1.386 (5)
N2—C6	1.360 (5)	C1—H1	0.950
N2—C10	1.355 (5)	C2B—H2B	0.950
N3—C11	1.340 (5)	C2A—H2A	0.950
N3—C15	1.344 (6)	C3B—H3B	0.950
C1—C2B	1.38 (2)	C3A—H3A	0.950
C1—C2A	1.366 (7)	C4B—H4B	0.950
C2B—C3B	1.35 (3)	C4A—H4A	0.950
C2A—C3A	1.373 (9)	C7—H5	0.950
C3B—C4B	1.39 (2)	C9—H6	0.950
C3A—C4A	1.371 (7)	C12—H7	0.950
C4B—C5B	1.37 (3)	C13—H8	0.950
C4A—C5A	1.392 (9)	C14—H9	0.950
C5B—C6	1.47 (3)	C15—H10	0.950
C5A—C6	1.51 (1)	C17—H11	0.950
C6—C7	1.390 (5)	C18—H12	0.950
C7—C8	1.399 (5)	C21—H13	0.950
C8—C9	1.369 (5)	C22—H14	0.980
C8—C16	1.507 (4)	C22—H15	0.980
C9—C10	1.401 (5)	C22—H16	0.980
C10—C11	1.490 (6)	C23—H17	0.980
C11—C12	1.348 (7)	C23—H18	0.980
C12—C13	1.379 (9)	C23—H19	0.980
C13—C14	1.365 (9)		
C19—O1—C22	117.0 (3)	C2B—C1—H1	115.146
C20—O2—C23	117.7 (3)	C2A—C1—H1	118.101
C1—N1—C5B	119.7 (12)	C1—C2B—H2B	119.442
C1—N1—C5A	118.1 (5)	C3B—C2B—H2B	119.434
C6—N2—C10	117.7 (3)	C1—C2A—H2A	121.526
C11—N3—C15	119.0 (4)	C3A—C2A—H2A	121.510
N1—C1—C2B	119.8 (10)	C2B—C3B—H3B	120.699
N1—C1—C2A	123.8 (5)	C4B—C3B—H3B	120.704
C1—C2B—C3B	121.1 (17)	C2A—C3A—H3A	119.945
C1—C2A—C3A	117.0 (6)	C4A—C3A—H3A	119.929
C2B—C3B—C4B	118.6 (15)	C3B—C4B—H4B	119.525
C2A—C3A—C4A	120.1 (5)	C5B—C4B—H4B	119.544
C3B—C4B—C5B	120.9 (17)	C3A—C4A—H4A	120.592
C3A—C4A—C5A	118.8 (6)	C5A—C4A—H4A	120.568
N1—C5B—C4B	118 (3)	C6—C7—H5	120.034
N1—C5A—C4A	121.9 (7)	C8—C7—H5	120.028
N2—C6—C7	122.2 (3)	C8—C9—H6	119.727
C6—C7—C8	119.9 (3)	C10—C9—H6	119.732
C7—C8—C9	117.6 (3)	C11—C12—H7	119.902
C7—C8—C16	120.2 (3)	C13—C12—H7	119.894
C9—C8—C16	122.1 (3)	C12—C13—H8	120.215

C8—C9—C10	120.5 (3)	C14—C13—H8	120.221
N2—C10—C9	122.0 (3)	C13—C14—H9	121.201
N2—C10—C11	116.2 (3)	C15—C14—H9	121.188
C9—C10—C11	121.8 (3)	N3—C15—H10	118.484
N3—C11—C10	118.7 (3)	C14—C15—H10	118.487
N3—C11—C12	120.5 (4)	C16—C17—H11	119.063
C10—C11—C12	120.8 (4)	C18—C17—H11	119.048
C11—C12—C13	120.2 (6)	C17—C18—H12	120.059
C12—C13—C14	119.6 (6)	C19—C18—H12	120.051
C13—C14—C15	117.6 (6)	C16—C21—H13	119.310
N3—C15—C14	123.0 (4)	C20—C21—H13	119.313
C8—C16—C17	121.3 (3)	O1—C22—H14	109.474
C8—C16—C21	121.2 (3)	O1—C22—H15	109.477
C17—C16—C21	117.5 (3)	O1—C22—H16	109.470
C16—C17—C18	121.9 (3)	H14—C22—H15	109.474
C17—C18—C19	119.9 (3)	H14—C22—H16	109.461
O1—C19—C18	124.8 (3)	H15—C22—H16	109.471
O1—C19—C20	115.6 (3)	O2—C23—H17	109.476
C18—C19—C20	119.6 (3)	O2—C23—H18	109.480
O2—C20—C19	114.5 (3)	O2—C23—H19	109.465
O2—C20—C21	125.8 (3)	H17—C23—H18	109.468
C19—C20—C21	119.7 (3)	H17—C23—H19	109.463
C16—C21—C20	121.4 (3)	H18—C23—H19	109.475
N1—C1—H1	118.105		
C22—O1—C19—C18	6.5 (5)	C7—C8—C16—C17	5.0 (5)
C22—O1—C19—C20	-173.2 (3)	C7—C8—C16—C21	-173.1 (3)
C23—O2—C20—C19	169.3 (3)	C9—C8—C16—C17	-178.2 (3)
C23—O2—C20—C21	-10.8 (5)	C9—C8—C16—C21	3.6 (5)
C1—N1—C5B—C4B	-14 (3)	C16—C8—C9—C10	-176.5 (3)
C5B—N1—C1—C2B	9.9 (15)	C8—C9—C10—N2	0.8 (5)
C5B—N1—C1—C2A	-20.7 (15)	C8—C9—C10—C11	178.2 (3)
C1—N1—C5A—C4A	6.1 (10)	N2—C10—C11—N3	-179.6 (3)
C5A—N1—C1—C2B	26.3 (7)	N2—C10—C11—C12	0.4 (5)
C5A—N1—C1—C2A	-4.3 (7)	C9—C10—C11—N3	2.9 (5)
C6—N2—C10—C9	-1.1 (5)	C9—C10—C11—C12	-177.1 (3)
C6—N2—C10—C11	-178.6 (3)	N3—C11—C12—C13	-2.8 (8)
C10—N2—C6—C7	0.3 (5)	C10—C11—C12—C13	177.3 (4)
C11—N3—C15—C14	-0.6 (6)	C11—C12—C13—C14	3.5 (10)
C15—N3—C11—C10	-178.8 (4)	C12—C13—C14—C15	-2.8 (9)
C15—N3—C11—C12	1.3 (6)	C13—C14—C15—N3	1.3 (8)
N1—C1—C2B—C3B	-0 (2)	C8—C16—C17—C18	-177.8 (3)
N1—C1—C2A—C3A	0.2 (8)	C8—C16—C21—C20	177.2 (3)
C2B—C1—C2A—C3A	-89 (2)	C17—C16—C21—C20	-1.0 (5)
C2A—C1—C2B—C3B	107 (3)	C21—C16—C17—C18	0.4 (5)
C1—C2B—C3B—C4B	-5 (3)	C16—C17—C18—C19	0.4 (5)
C1—C2A—C3A—C4A	2.1 (8)	C17—C18—C19—O1	179.7 (3)
C2B—C3B—C4B—C5B	1 (3)	C17—C18—C19—C20	-0.7 (5)

C2A—C3A—C4A—C5A	-0.4 (8)	O1—C19—C20—O2	-0.4 (4)
C3B—C4B—C5B—N1	9 (4)	O1—C19—C20—C21	179.7 (3)
C3A—C4A—C5A—N1	-3.9 (10)	C18—C19—C20—O2	179.9 (3)
N2—C6—C7—C8	0.8 (5)	C18—C19—C20—C21	0.0 (5)
C6—C7—C8—C9	-1.1 (5)	O2—C20—C21—C16	-179.1 (3)
C6—C7—C8—C16	175.8 (3)	C19—C20—C21—C16	0.8 (5)
C7—C8—C9—C10	0.3 (5)		

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

Cg1 and Cg5 are the centroids of the N1,C1–C5A and C16–C21 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3A—H3A \cdots N3 ⁱ	0.95	2.43	3.285 (7)	149
C23—H18 \cdots O1 ⁱⁱ	0.98	2.53	3.511 (5)	174
C18—H12 \cdots Cg5 ⁱⁱⁱ	0.95	2.87	3.648 (5)	139
C23—H17 \cdots Cg1 ^{iv}	0.98	2.90	3.432 (5)	115
C23—H19 \cdots Cg5 ^v	0.98	2.89	3.724 (5)	143

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