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# 4′-(2-Methoxyphenyl)-2,2′:6′,2″-terpyridine

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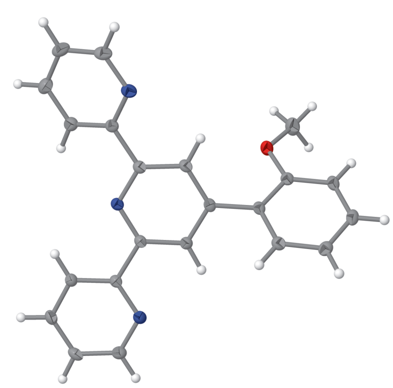
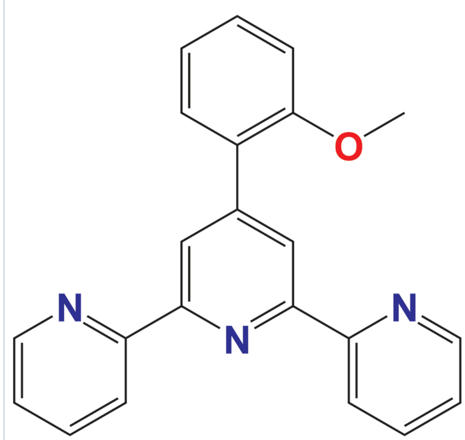
In the title compound, $C_{22}H_{17}N_3O$, the N atoms of the pyridine rings exhibit a typical *trans–trans* arrangement: the dihedral angles between the central pyridine ring and the peripheral rings are 22.24 (4) and 2.38 (4)°. In the crystal, pairwise C—H⋯N hydrogen bonds form inversion dimers described by an $R_2^2(6)$ graph set descriptor, which further interact through C—H⋯$\pi$ and $\pi$–$\pi$ interactions, creating a two-dimensional supramolecular network propagating in the *bc* plane.

**3D view**



**Chemical scheme**




## Structure description

Terpyridines are *N*,*N*,*N*-type pincer ligands that provide tight chelation with various metal cations in a nearly planar *cis–cis* geometry of their pyridine N atoms (Wei *et al.*, 2019). This conformation allows for a good conjugation between the aromatic rings and the metal cation making terpyridine a 'non-innocent' ligand, capable of stabilizing low-valency metal ions (García–Domínguez *et al.*, 2017). The ligand exhibits two possible coordination modes: mono-terpyridine pincer complexes and bis-terpyridine complexes depending on the number of coordinating terpyridine ligands (Taniya *et al.*, 2021). The transition-metal complexes of 4′-aryl-substituted-2,2′:6′,2"-terpyridines possess rich supramolecular chemistry (Wei *et al.*, 2019) as well as biological, DNA binding, and electrochemical properties, which render them as useful candidates for applications in the fields of medicine and molecular biology (Lazić *et al.*, 2016). The substituent groups on the ligands may be used to tailor the properties of the resulting coordination complexes (Shi *et al.*, 2006).

The title compound, $C_{22}H_{17}N_3O$ (**I**), is a terpyridine derivative with a 2-methoxyphenyl substituent at the third carbon atom of the central pyridine ring. The crystal structure of the compound contains one molecule in the asymmetric unit in space group $P2_1/c$. As is typical for a non-coordinated terpyridine, the structure exhibits a *trans–trans* arrangement of the pyridine N atoms [N1—C3—C4—N2 = 158.59 (10)°;

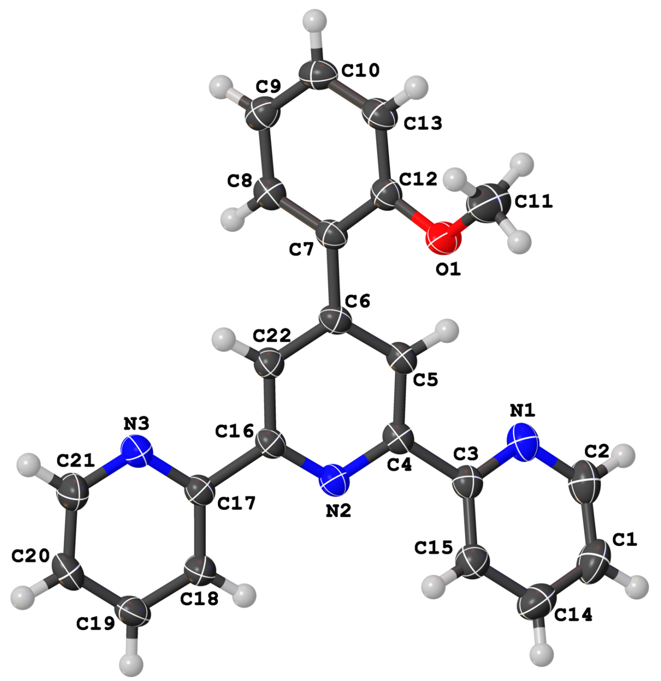



**Figure 1**
The molecular structure of (**I**) showing displacement ellipsoids drawn at the 50% probability level.

N3—C17—C16—N2 = −179.09 (10)°], as illustrated in Fig. 1. The peripheral pyridine rings subtend dihedral angles of 22.24 (4)° (N1 ring) and 2.38 (4)° (N3 ring) with the central pyridine ring. The methoxyphenyl ring is significantly twisted away from the central pyridine ring, with a dihedral angle of 48.93 (4)°. All other geometrical parameters for (**I**) are comparable with those of 4′-(2,4-dimethoxyphenyl)-2,2′:6′,2′′-terpyridine (Cambridge Structural Database refcode: JEYHED; Demircioğlu *et al.*, 2018).

In the extended structure of (**I**), weak C—H···N hydrogen bonds connect the molecules (Fig. 2, Table 1). These interactions form hydrogen-bonded cyclic dimers, described by an $R_2^2(6)$ graph set descriptor. The hydrogen-bonded dimers interact through C—H···π interactions, where C8—H8 interacts with the centroid of one of the peripheral pyridine rings and C13—H13 interacts with the centroid of the methoxy-substituted ring. These interactions link neighbouring dimers along the *b*-axis direction forming a zigzag pattern, as shown in Fig. 3. The planarity of the molecules facilitates π–π interactions between the central pyridine ring and the other pyridine ring not involved in the C—H···π intermolecular interaction, with the shortest centroid–centroid separation being 3.5864 (6) Å. The C—H···π and π–π interactions

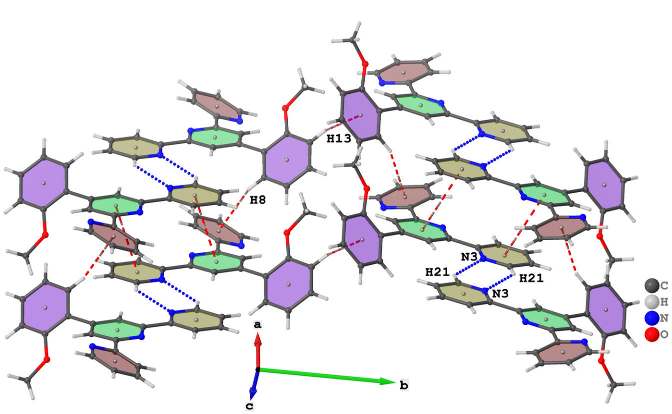



**Figure 2**
Illustration of intermolecular C—H···N interactions in the extended structure of (**I**) depicted as blue dotted lines and C—H···π and π–π interactions represented by red dashed lines.

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

*Cg*1 and *Cg*4 are the centroids of the N1/C1–3/C14/C15 and C7–C12 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C21—H21···N3$^{i}$ | 0.95 | 2.66 | 3.4138 (16) | 137 |
| C8—H8···*Cg*1$^{ii}$ | 0.95 | 2.68 | 3.5698 (12) | 155 |
| C13—H13···*Cg*4$^{iii}$ | 0.95 | 2.77 | 3.5182 (12) | 136 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{22}H_{17}N_3O$ |
| $M_r$ | 339.38 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 100 |
| *a*, *b*, *c* (Å) | 7.7366 (3), 29.5787 (10), 7.3852 (3) |
| β (°) | 91.962 (2) |
| *V* (Å$^3$) | 1689.03 (11) |
| *Z* | 4 |
| Radiation type | Mo *K*α |
| μ (mm$^{-1}$) | 0.08 |
| Crystal size (mm) | 0.43 × 0.28 × 0.26 |
| | |
| Data collection | |
| Diffractometer | Bruker *SMART APEX2* area detector |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.955, 0.988 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 36956, 4227, 3728 |
| $R_{int}$ | 0.024 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.670 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.041, 0.119, 1.03 |
| No. of reflections | 4227 |
| No. of parameters | 236 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.37, −0.24 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXS* (Sheldrick, 2008), *SHELXL2019/3* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

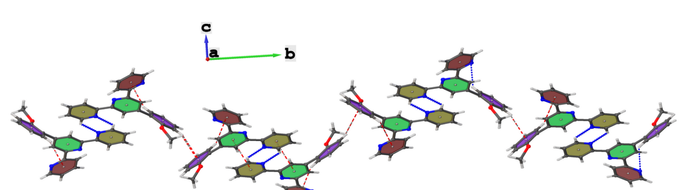



**Figure 3**
Representation of zigzag propagation patterns of the hydrogen bonded dimers along the crystallographic *b*-axis direction.

combine to form a two-dimensional supramolecular arrangement extending over the crystallographic *bc* plane.

## Synthesis and crystallization

The title compound was synthesized using a method modified from Winter *et al.* (2006): 2-methoxybenzaldehyde (10 mmol) was dissolved in ethanol (30 ml), cooled to 0 °C, and treated with a 2-acetylpyridine/NaOH solution. After stirring for 2 h at 0 °C, 25% aqueous ammonia (30 ml) was added, and the reaction was stirred at room temperature for 18 h. The precipitate was filtered, washed with water and 1:1 water–ethanol, dried under vacuum, and recrystallized from methanol solution to yield X-ray-quality crystals.

## Refinement

Crystallographic data and structure refinement details are summarized in Table 2.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2024). **9**, x241143 [https://doi.org/10.1107/S241431462401143X]

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### 4′-(2-Methoxyphenyl)-2,2′:6′,2′′-terpyridine

*Crystal data*

$C_{22}H_{17}N_3O$
$M_r$ = 339.38
Monoclinic, $P2_1/c$
$a$ = 7.7366 (3) Å
$b$ = 29.5787 (10) Å
$c$ = 7.3852 (3) Å
$\beta$ = 91.962 (2)°
$V$ = 1689.03 (11) Å$^3$
$Z$ = 4
$F(000)$ = 712
$D_x$ = 1.335 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9871 reflections
$\theta$ = 2.6–28.4°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 100 K
Block, yellow
0.43 × 0.28 × 0.26 mm

*Data collection*

Bruker SMART APEX2 area detector diffractometer
Radiation source: microfocus sealed X-ray tube, Incoatec I$\mu$s
Graphite monochromator
Detector resolution: 7.9 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min}$ = 0.955, $T_{max}$ = 0.988
36956 measured reflections
4227 independent reflections
3728 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 28.4°, $\theta_{min}$ = 2.6°
$h = -10 \rightarrow 10$
$k = -39 \rightarrow 39$
$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.119
$S$ = 1.03
4227 reflections
236 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.47285 (11) | 0.30543 (3) | 1.08916 (12) | 0.02170 (19) |
| N1 | 0.14529 (13) | 0.35669 (3) | 0.52813 (13) | 0.0196 (2) |
| N2 | 0.41380 (12) | 0.44519 (3) | 0.71159 (13) | 0.01598 (19) |
| N3 | 0.78678 (13) | 0.50369 (3) | 0.89892 (14) | 0.0217 (2) |
| C1 | −0.12572 (16) | 0.38731 (5) | 0.41546 (18) | 0.0264 (3) |
| H1 | −0.231198 | 0.382780 | 0.348239 | 0.032* |
| C2 | −0.00699 (16) | 0.35250 (4) | 0.43771 (17) | 0.0235 (2) |
| H2 | −0.035260 | 0.323951 | 0.385741 | 0.028* |
| C3 | 0.18315 (14) | 0.39749 (4) | 0.59943 (15) | 0.0167 (2) |
| C4 | 0.35441 (14) | 0.40258 (3) | 0.69551 (14) | 0.0158 (2) |
| C5 | 0.44371 (14) | 0.36519 (3) | 0.76556 (15) | 0.0166 (2) |
| H5 | 0.397404 | 0.335618 | 0.750921 | 0.020* |
| C6 | 0.60216 (14) | 0.37190 (3) | 0.85748 (14) | 0.0156 (2) |
| C7 | 0.70993 (14) | 0.33454 (3) | 0.93456 (14) | 0.0158 (2) |
| C8 | 0.88534 (14) | 0.33331 (4) | 0.89734 (15) | 0.0181 (2) |
| H8 | 0.932059 | 0.356180 | 0.823112 | 0.022* |
| C9 | 0.99367 (15) | 0.29944 (4) | 0.96611 (16) | 0.0196 (2) |
| H9 | 1.112894 | 0.299176 | 0.939317 | 0.024* |
| C10 | 0.92535 (15) | 0.26616 (4) | 1.07407 (16) | 0.0199 (2) |
| H10 | 0.997718 | 0.242459 | 1.119075 | 0.024* |
| C11 | 0.41225 (17) | 0.27917 (5) | 1.23632 (19) | 0.0307 (3) |
| H11A | 0.407983 | 0.247215 | 1.201421 | 0.046* |
| H11B | 0.296187 | 0.289352 | 1.266515 | 0.046* |
| H11C | 0.490993 | 0.282929 | 1.342035 | 0.046* |
| C12 | 0.64395 (14) | 0.30124 (3) | 1.04914 (15) | 0.0169 (2) |
| C13 | 0.75168 (15) | 0.26701 (4) | 1.11749 (15) | 0.0188 (2) |
| H13 | 0.706583 | 0.244292 | 1.193593 | 0.023* |
| C14 | −0.08713 (16) | 0.42885 (4) | 0.49347 (18) | 0.0252 (3) |
| H14 | −0.166839 | 0.453225 | 0.483221 | 0.030* |
| C15 | 0.07000 (15) | 0.43416 (4) | 0.58670 (16) | 0.0206 (2) |
| H15 | 0.100200 | 0.462304 | 0.641067 | 0.025* |
| C16 | 0.56678 (14) | 0.45144 (3) | 0.79773 (14) | 0.0153 (2) |
| C17 | 0.63187 (14) | 0.49871 (3) | 0.81402 (14) | 0.0155 (2) |
| C18 | 0.53607 (15) | 0.53500 (4) | 0.74648 (16) | 0.0196 (2) |
| H18 | 0.427971 | 0.530273 | 0.684452 | 0.024* |
| C19 | 0.60155 (15) | 0.57845 (4) | 0.77145 (17) | 0.0209 (2) |
| H19 | 0.538544 | 0.603934 | 0.727027 | 0.025* |
| C20 | 0.75910 (15) | 0.58400 (4) | 0.86153 (16) | 0.0199 (2) |
| H20 | 0.805831 | 0.613325 | 0.882233 | 0.024* |
| C21 | 0.84764 (16) | 0.54583 (4) | 0.92113 (18) | 0.0238 (3) |
| H21 | 0.957322 | 0.549703 | 0.980925 | 0.029* |
| C22 | 0.66411 (14) | 0.41587 (4) | 0.87251 (15) | 0.0164 (2) |
| H22 | 0.772010 | 0.421713 | 0.933282 | 0.020* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0192 (4) | 0.0219 (4) | 0.0242 (4) | 0.0007 (3) | 0.0036 (3) | 0.0082 (3) |
| N1 | 0.0222 (5) | 0.0204 (5) | 0.0163 (5) | −0.0044 (3) | 0.0005 (4) | −0.0007 (3) |
| N2 | 0.0178 (4) | 0.0157 (4) | 0.0146 (4) | −0.0014 (3) | 0.0013 (3) | 0.0004 (3) |
| N3 | 0.0207 (5) | 0.0164 (4) | 0.0276 (5) | −0.0017 (3) | −0.0043 (4) | 0.0011 (4) |
| C1 | 0.0196 (6) | 0.0363 (7) | 0.0230 (6) | −0.0054 (5) | −0.0042 (4) | 0.0016 (5) |
| C2 | 0.0249 (6) | 0.0264 (6) | 0.0193 (6) | −0.0081 (4) | −0.0002 (4) | −0.0026 (4) |
| C3 | 0.0179 (5) | 0.0180 (5) | 0.0140 (5) | −0.0023 (4) | 0.0008 (4) | 0.0019 (4) |
| C4 | 0.0182 (5) | 0.0156 (5) | 0.0139 (5) | −0.0010 (4) | 0.0015 (4) | −0.0004 (4) |
| C5 | 0.0196 (5) | 0.0138 (5) | 0.0163 (5) | −0.0016 (4) | 0.0010 (4) | −0.0003 (4) |
| C6 | 0.0183 (5) | 0.0144 (5) | 0.0144 (5) | 0.0012 (4) | 0.0023 (4) | 0.0008 (4) |
| C7 | 0.0195 (5) | 0.0131 (4) | 0.0147 (5) | 0.0001 (4) | −0.0011 (4) | −0.0008 (4) |
| C8 | 0.0207 (5) | 0.0169 (5) | 0.0168 (5) | −0.0014 (4) | 0.0008 (4) | −0.0001 (4) |
| C9 | 0.0185 (5) | 0.0217 (5) | 0.0186 (5) | 0.0017 (4) | −0.0011 (4) | −0.0029 (4) |
| C10 | 0.0240 (5) | 0.0178 (5) | 0.0176 (5) | 0.0041 (4) | −0.0035 (4) | −0.0014 (4) |
| C11 | 0.0263 (6) | 0.0348 (7) | 0.0315 (7) | 0.0028 (5) | 0.0078 (5) | 0.0155 (5) |
| C12 | 0.0186 (5) | 0.0162 (5) | 0.0158 (5) | −0.0009 (4) | −0.0003 (4) | −0.0011 (4) |
| C13 | 0.0249 (5) | 0.0157 (5) | 0.0156 (5) | −0.0002 (4) | −0.0015 (4) | 0.0021 (4) |
| C14 | 0.0200 (6) | 0.0298 (6) | 0.0255 (6) | 0.0028 (4) | −0.0014 (5) | 0.0035 (5) |
| C15 | 0.0205 (5) | 0.0207 (5) | 0.0205 (6) | −0.0007 (4) | −0.0007 (4) | 0.0009 (4) |
| C16 | 0.0176 (5) | 0.0139 (5) | 0.0144 (5) | −0.0008 (4) | 0.0020 (4) | 0.0007 (4) |
| C17 | 0.0173 (5) | 0.0148 (5) | 0.0144 (5) | −0.0007 (4) | 0.0018 (4) | 0.0006 (4) |
| C18 | 0.0185 (5) | 0.0169 (5) | 0.0232 (6) | −0.0007 (4) | −0.0020 (4) | 0.0029 (4) |
| C19 | 0.0231 (6) | 0.0153 (5) | 0.0246 (6) | 0.0013 (4) | 0.0020 (4) | 0.0035 (4) |
| C20 | 0.0255 (6) | 0.0147 (5) | 0.0199 (6) | −0.0046 (4) | 0.0043 (4) | −0.0008 (4) |
| C21 | 0.0226 (6) | 0.0207 (6) | 0.0277 (6) | −0.0043 (4) | −0.0054 (5) | 0.0004 (4) |
| C22 | 0.0165 (5) | 0.0161 (5) | 0.0167 (5) | −0.0009 (4) | −0.0002 (4) | 0.0010 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.4279 (14) | C9—H9 | 0.9500 |
| O1—C12 | 1.3718 (14) | C9—C10 | 1.3832 (17) |
| N1—C2 | 1.3400 (15) | C10—H10 | 0.9500 |
| N1—C3 | 1.3449 (14) | C10—C13 | 1.3922 (16) |
| N2—C4 | 1.3454 (13) | C11—H11A | 0.9800 |
| N2—C16 | 1.3372 (14) | C11—H11B | 0.9800 |
| N3—C17 | 1.3415 (14) | C11—H11C | 0.9800 |
| N3—C21 | 1.3403 (14) | C12—C13 | 1.3949 (15) |
| C1—H1 | 0.9500 | C13—H13 | 0.9500 |
| C1—C2 | 1.3858 (18) | C14—H14 | 0.9500 |
| C1—C14 | 1.3855 (18) | C14—C15 | 1.3854 (16) |
| C2—H2 | 0.9500 | C15—H15 | 0.9500 |
| C3—C4 | 1.4891 (15) | C16—C17 | 1.4896 (14) |
| C3—C15 | 1.3949 (15) | C16—C22 | 1.3965 (14) |
| C4—C5 | 1.3942 (15) | C17—C18 | 1.3874 (15) |
| C5—H5 | 0.9500 | C18—H18 | 0.9500 |

| | | | |
|---|---|---|---|
| C5—C6 | 1.3950 (15) | C18—C19 | 1.3915 (15) |
| C6—C7 | 1.4858 (14) | C19—H19 | 0.9500 |
| C6—C22 | 1.3893 (14) | C19—C20 | 1.3783 (16) |
| C7—C8 | 1.3943 (15) | C20—H20 | 0.9500 |
| C7—C12 | 1.4060 (15) | C20—C21 | 1.3848 (16) |
| C8—H8 | 0.9500 | C21—H21 | 0.9500 |
| C8—C9 | 1.3909 (15) | C22—H22 | 0.9500 |

| | | | |
|---|---|---|---|
| C12—O1—C11 | 117.34 (9) | H11A—C11—H11B | 109.5 |
| C2—N1—C3 | 117.01 (10) | H11A—C11—H11C | 109.5 |
| C16—N2—C4 | 117.74 (9) | H11B—C11—H11C | 109.5 |
| C21—N3—C17 | 117.64 (10) | O1—C12—C7 | 116.06 (9) |
| C2—C1—H1 | 120.8 | O1—C12—C13 | 123.82 (10) |
| C14—C1—H1 | 120.8 | C13—C12—C7 | 120.11 (10) |
| C14—C1—C2 | 118.50 (11) | C10—C13—C12 | 119.95 (10) |
| N1—C2—C1 | 123.94 (11) | C10—C13—H13 | 120.0 |
| N1—C2—H2 | 118.0 | C12—C13—H13 | 120.0 |
| C1—C2—H2 | 118.0 | C1—C14—H14 | 120.7 |
| N1—C3—C4 | 117.10 (9) | C15—C14—C1 | 118.69 (11) |
| N1—C3—C15 | 122.92 (10) | C15—C14—H14 | 120.7 |
| C15—C3—C4 | 119.97 (10) | C3—C15—H15 | 120.5 |
| N2—C4—C3 | 115.62 (9) | C14—C15—C3 | 118.91 (11) |
| N2—C4—C5 | 123.16 (10) | C14—C15—H15 | 120.5 |
| C5—C4—C3 | 121.21 (9) | N2—C16—C17 | 117.35 (9) |
| C4—C5—H5 | 120.5 | N2—C16—C22 | 122.72 (9) |
| C4—C5—C6 | 118.93 (9) | C22—C16—C17 | 119.93 (10) |
| C6—C5—H5 | 120.5 | N3—C17—C16 | 115.79 (9) |
| C5—C6—C7 | 123.57 (9) | N3—C17—C18 | 122.73 (10) |
| C22—C6—C5 | 117.84 (9) | C18—C17—C16 | 121.48 (10) |
| C22—C6—C7 | 118.56 (9) | C17—C18—H18 | 120.7 |
| C8—C7—C6 | 118.76 (9) | C17—C18—C19 | 118.64 (10) |
| C8—C7—C12 | 118.43 (10) | C19—C18—H18 | 120.7 |
| C12—C7—C6 | 122.76 (10) | C18—C19—H19 | 120.5 |
| C7—C8—H8 | 119.2 | C20—C19—C18 | 119.08 (10) |
| C9—C8—C7 | 121.69 (10) | C20—C19—H19 | 120.5 |
| C9—C8—H8 | 119.2 | C19—C20—H20 | 120.8 |
| C8—C9—H9 | 120.5 | C19—C20—C21 | 118.42 (10) |
| C10—C9—C8 | 119.06 (11) | C21—C20—H20 | 120.8 |
| C10—C9—H9 | 120.5 | N3—C21—C20 | 123.46 (11) |
| C9—C10—H10 | 119.6 | N3—C21—H21 | 118.3 |
| C9—C10—C13 | 120.71 (10) | C20—C21—H21 | 118.3 |
| C13—C10—H10 | 119.6 | C6—C22—C16 | 119.59 (10) |
| O1—C11—H11A | 109.5 | C6—C22—H22 | 120.2 |
| O1—C11—H11B | 109.5 | C16—C22—H22 | 120.2 |
| O1—C11—H11C | 109.5 | | |

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|---|---|---|---|
| O1—C12—C13—C10 | −178.02 (10) | C7—C8—C9—C10 | 0.04 (17) |
| N1—C3—C4—N2 | 158.59 (10) | C7—C12—C13—C10 | 0.84 (16) |

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|---|---|---|---|
| N1—C3—C4—C5 | −22.36 (15) | C8—C7—C12—O1 | 176.60 (9) |
| N1—C3—C15—C14 | −1.38 (17) | C8—C7—C12—C13 | −2.34 (16) |
| N2—C4—C5—C6 | 0.20 (17) | C8—C9—C10—C13 | −1.61 (17) |
| N2—C16—C17—N3 | −179.09 (10) | C9—C10—C13—C12 | 1.18 (17) |
| N2—C16—C17—C18 | 1.50 (16) | C11—O1—C12—C7 | −165.58 (11) |
| N2—C16—C22—C6 | 0.33 (16) | C11—O1—C12—C13 | 13.32 (16) |
| N3—C17—C18—C19 | −1.50 (18) | C12—C7—C8—C9 | 1.92 (16) |
| C1—C14—C15—C3 | −0.31 (18) | C14—C1—C2—N1 | −1.13 (19) |
| C2—N1—C3—C4 | −178.33 (10) | C15—C3—C4—N2 | −21.48 (15) |
| C2—N1—C3—C15 | 1.75 (16) | C15—C3—C4—C5 | 157.57 (11) |
| C2—C1—C14—C15 | 1.48 (18) | C16—N2—C4—C3 | 179.67 (9) |
| C3—N1—C2—C1 | −0.47 (17) | C16—N2—C4—C5 | 0.65 (16) |
| C3—C4—C5—C6 | −178.77 (10) | C16—C17—C18—C19 | 177.86 (10) |
| C4—N2—C16—C17 | 179.69 (9) | C17—N3—C21—C20 | 0.10 (19) |
| C4—N2—C16—C22 | −0.92 (16) | C17—C16—C22—C6 | 179.71 (10) |
| C4—C3—C15—C14 | 178.70 (10) | C17—C18—C19—C20 | 0.23 (17) |
| C4—C5—C6—C7 | −178.80 (10) | C18—C19—C20—C21 | 1.09 (17) |
| C4—C5—C6—C22 | −0.78 (16) | C19—C20—C21—N3 | −1.31 (19) |
| C5—C6—C7—C8 | 131.01 (11) | C21—N3—C17—C16 | −178.07 (10) |
| C5—C6—C7—C12 | −51.41 (16) | C21—N3—C17—C18 | 1.33 (17) |
| C5—C6—C22—C16 | 0.53 (16) | C22—C6—C7—C8 | −46.99 (14) |
| C6—C7—C8—C9 | 179.61 (10) | C22—C6—C7—C12 | 130.59 (11) |
| C6—C7—C12—O1 | −0.99 (15) | C22—C16—C17—N3 | 1.50 (15) |
| C6—C7—C12—C13 | −179.93 (10) | C22—C16—C17—C18 | −177.91 (10) |
| C7—C6—C22—C16 | 178.65 (10) | | |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 and *Cg*4 are the centroids of the N1/C1–3/C14/C15 and C7–C12 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C21—H21···N3$^{i}$ | 0.95 | 2.66 | 3.4138 (16) | 137 |
| C8—H8···*Cg*1$^{ii}$ | 0.95 | 2.68 | 3.5698 (12) | 155 |
| C13—H13···*Cg*4$^{iii}$ | 0.95 | 2.77 | 3.5182 (12) | 136 |

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