Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (2*E*)-3-(2-Chlorobenzo[*h*]quinolin-3-yl)-1-(2-methyl-4-phenylquinolin-3-yl)prop-2-en-1-one

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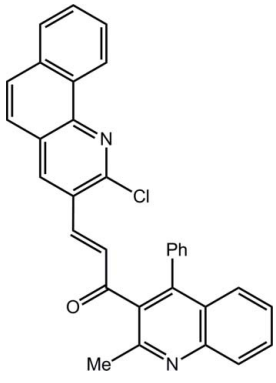
Received 28 July 2013; accepted 1 August 2013

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.034; $wR$ factor = 0.095; data-to-parameter ratio = 14.9.

In the title compound, $C_{32}H_{21}ClN_2O$, an almost planar (r.m.s. deviation = 0.033 Å) prop-2-en-1-one bridge links quinolinyl and benzoquinolinyl residues; the latter are twisted out of the plane of the bridge [dihedral angles = 75.94 (5) and 20.20 (5)°, respectively]. In the crystal, a three-dimensional architecture arises as a result of C—H···O, C—H···$\pi$ and $\pi$–$\pi$ [centroid–centroid distances involving pyridine rings = 3.5806 (7)–3.7537 (7) Å] interactions.

## Related literature

For biological applications of quinoline derivatives, see: Jörg *et al.* (2007); Prasath *et al.* (2013*a*). For a related structure, see: Prasath *et al.* (2013*b*).




## Experimental

### Crystal data

$C_{32}H_{21}ClN_2O$ $M_r$ = 484.96
Triclinic, $P\overline{1}$
$a$ = 7.1354 (3) Å
$b$ = 10.1627 (5) Å
$c$ = 17.0127 (8) Å
$\alpha$ = 78.758 (4)°
$\beta$ = 79.544 (4)°
$\gamma$ = 84.042 (4)°
$V$ = 1186.91 (9) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 1.65 mm$^{-1}$
$T$ = 100 K
0.30 × 0.25 × 0.20 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min}$ = 0.870, $T_{max}$ = 1.000
8673 measured reflections
4849 independent reflections
4433 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
$S$ = 1.04
4849 reflections
326 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

*Cg*1 is the centroid of the N1-pyridyl ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10*C*···O1$^{i}$ | 0.98 | 2.54 | 3.4116 (18) | 148 |
| C15—H15···*Cg*1$^{ii}$ | 0.95 | 2.65 | 3.4695 (15) | 145 |

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

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

RP gratefully acknowledges the Council of Scientific and Industrial Research (CSIR), India, for a Senior Research Fellowship (09/919/(0014)/2012 EMR-I). We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR-MOHE/SC/03).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2642).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o1393 [doi:10.1107/S1600536813021545]

## (2*E*)-3-(2-Chlorobenzo[*h*]quinolin-3-yl)-1-(2-methyl-4-phenylquinolin-3-yl)prop-2-en-1-one

**R. Prasath, S. Sarveswari, Seik Weng Ng and Edward R. T. Tiekink**

### 1. Comment

In connection with the biological potential of quinolinyl derivatives (Jörg *et al.* 2007; Prasath *et al.* 2013*a*), the title compound (I) was prepared and subjected to a crystallographic study.

The molecular structure of (I) (Fig. 1), sees two somewhat splayed [dihedral angle = 61.60 (3)°] quinolinyl and benzoquinolinyl residues connected by the ends of a planar (r.m.s. deviation = 0.033 Å) prop-2-en-1-one bridge. The quinolinyl, especially, and benzoquinolinyl residues are twisted out of the plane of the prop-2-en-1-one bridge forming dihedral angles of 75.94 (5) and 20.20 (5)°, respectively. The phenyl ring is inclined with respect to the quinolinyl residue to which it is attached, forming a dihedral angle of 73.76 (5)°. Finally, the conformation about the ethylene bond [C18═C19 = 1.3351 (18) Å] is *E*.

A similar conformation was reported recently for a related structure having two quinolinyl residues bridged by a prop-2-en-1-one residue, namely (*2E*)-3-(2-chloro-8-methylquinolin-3-yl)-1-(5,7-dimethylquinolin-6-yl)prop-2-en-1-one (Prasath *et al.*, 2013*b*) where the dihedral angle between the quinolinyl residues was 83.72 (4)°.

In the crystal packing methyl-*C*—*H*···*O* (carbonyl) interactions (Table 1), link molecules into centrosymmetric dimers which are connected into a three dimensional architecture by phenyl-C—H···$\pi$(N1-pyridyl) (Table 1), and $\pi$–$\pi$ interactions [inter-centroid distances: *Cg*(N1-pyridyl)···*Cg*(C1–C6)$^{i}$ = 3.7537 (7) Å, *Cg*(N2-pyridyl)···*Cg*(C22—C23,C28–C31)$^{ii,iii}$ = 3.5806 (7) and 3.7286 (7) Å for *i* - *x*, 1 - *y*, 2 - *z*, *ii* 1 - *x*, -*y*, 1 - *z*, *iii* -*x*, -*y*, 1 - *z*] (Fig. 2).

### 2. Experimental

A mixture of 3-acetyl-2-methyl-4-phenylquinoline (260 mg, 0.001 *M*) and 2-chlorobenzoquinoline-3-carbaldehyde (240 mg, 0.001 *M*) in methanol (20 ml) containing potassium hydroxide (0.2 g) was stirred at room temperature for 12 h. After this, the reaction mixture was neutralized with dilute acetic acid and the resultant solid was filtered, dried and purified by column chromatography using an ethyl acetate - hexane (4:1) mixture to afford the title compound, (I). Re-crystallization was by slow evaporation of an acetone solution of (I), which yielded colourless blocks in 80% yield; *M*.pt: 460–462 K.

### 3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95–0.98 Å, $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND*

(Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

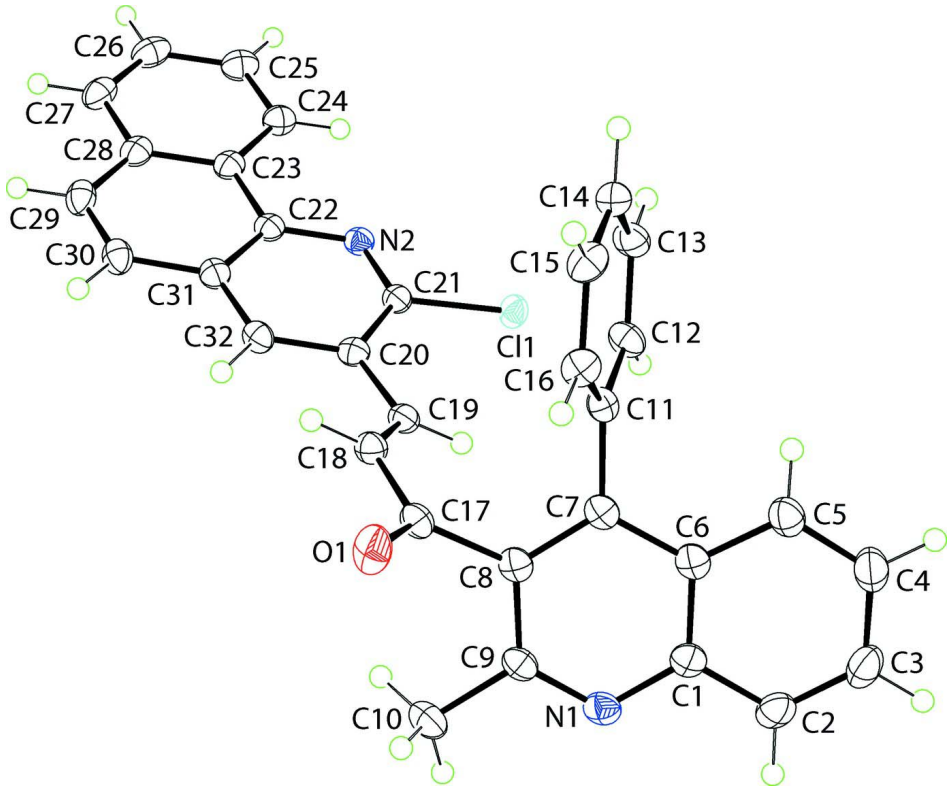


**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

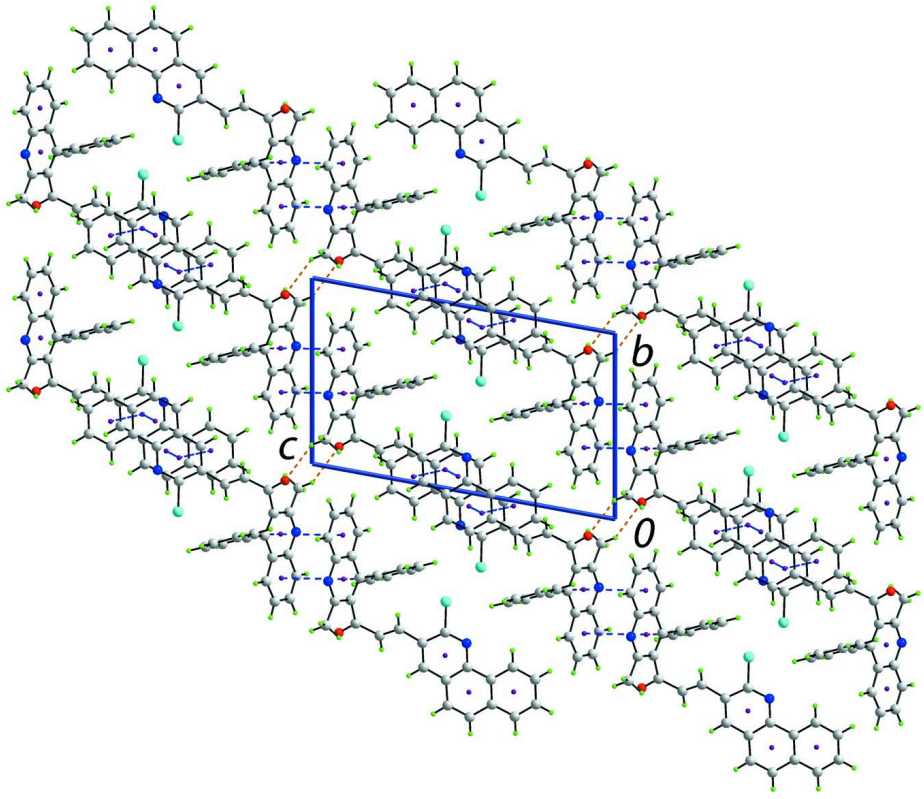


**Figure 2**

View in projection down the *a* axis of the unit-cell contents of (I). The C—H···O, C—H···$\pi$ and $\pi$—$\pi$ interactions are shown as orange, purple and blue dashed lines, respectively.

**(2*E*)-3-(2-Chlorobenzo[*h*]quinolin-3-yl)-1-(2-methyl-4-phenylquinolin-3-yl)prop-2-en-1-one**

*Crystal data*

$C_{32}H_{21}ClN_2O$
$M_r$ = 484.96
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 7.1354 (3) Å
$b$ = 10.1627 (5) Å
$c$ = 17.0127 (8) Å
$\alpha$ = 78.758 (4)°
$\beta$ = 79.544 (4)°
$\gamma$ = 84.042 (4)°
$V$ = 1186.91 (9) Å$^3$
$Z$ = 2
$F(000)$ = 504
$D_x$ = 1.357 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 5174 reflections
$\theta$ = 2.7–76.5°
$\mu$ = 1.65 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.30 × 0.25 × 0.20 mm

*Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min}$ = 0.870, $T_{max}$ = 1.000
8673 measured reflections
4849 independent reflections
4433 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

$\theta_{max}$ = 76.6°, $\theta_{min}$ = 2.7°
$h$ = −7→8
$k$ = −10→12
$l$ = −15→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
$S$ = 1.04
4849 reflections
326 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
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.2928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.32862 (4) | 0.39004 (3) | 0.557615 (17) | 0.02330 (9) |
| O1 | −0.10222 (16) | 0.11751 (11) | 0.91090 (6) | 0.0351 (3) |
| N1 | 0.29529 (16) | 0.38332 (11) | 0.94697 (6) | 0.0245 (2) |
| N2 | 0.31428 (15) | 0.18592 (10) | 0.48984 (6) | 0.0194 (2) |
| C1 | 0.22372 (19) | 0.51192 (13) | 0.92151 (7) | 0.0228 (3) |
| C2 | 0.2945 (2) | 0.61806 (15) | 0.94820 (8) | 0.0295 (3) |
| H2 | 0.3912 | 0.5989 | 0.9814 | 0.035* |
| C3 | 0.2242 (2) | 0.74768 (15) | 0.92635 (9) | 0.0348 (3) |
| H3 | 0.2719 | 0.8182 | 0.9447 | 0.042* |
| C4 | 0.0813 (2) | 0.77789 (15) | 0.87687 (9) | 0.0346 (3) |
| H4 | 0.0311 | 0.8682 | 0.8634 | 0.042* |
| C5 | 0.0143 (2) | 0.67797 (14) | 0.84801 (8) | 0.0283 (3) |
| H5 | −0.0798 | 0.6997 | 0.8136 | 0.034* |
| C6 | 0.08475 (18) | 0.54237 (13) | 0.86931 (7) | 0.0217 (3) |
| C7 | 0.01900 (18) | 0.43308 (13) | 0.84298 (7) | 0.0204 (2) |
| C8 | 0.08610 (18) | 0.30408 (13) | 0.87255 (7) | 0.0208 (3) |
| C9 | 0.22715 (18) | 0.28343 (13) | 0.92474 (7) | 0.0225 (3) |
| C10 | 0.3081 (2) | 0.14360 (14) | 0.95496 (9) | 0.0308 (3) |
| H10A | 0.4311 | 0.1487 | 0.9718 | 0.046* |
| H10B | 0.3267 | 0.0908 | 0.9114 | 0.046* |
| H10C | 0.2192 | 0.1004 | 1.0014 | 0.046* |
| C11 | −0.11840 (18) | 0.46154 (12) | 0.78448 (8) | 0.0210 (2) |
| C12 | −0.05441 (19) | 0.51971 (13) | 0.70407 (8) | 0.0246 (3) |
| H12 | 0.0762 | 0.5378 | 0.6873 | 0.029* |

| | | | | |
|---|---|---|---|---|
| C13 | −0.1793 (2) | 0.55154 (14) | 0.64831 (8) | 0.0262 (3) |
| H13 | −0.1337 | 0.5896 | 0.5934 | 0.031* |
| C14 | −0.3710 (2) | 0.52756 (13) | 0.67300 (8) | 0.0259 (3) |
| H14 | −0.4576 | 0.5513 | 0.6353 | 0.031* |
| C15 | −0.43578 (19) | 0.46909 (14) | 0.75253 (9) | 0.0273 (3) |
| H15 | −0.5668 | 0.4523 | 0.7693 | 0.033* |
| C16 | −0.30955 (19) | 0.43462 (14) | 0.80842 (8) | 0.0250 (3) |
| H16 | −0.3543 | 0.3929 | 0.8627 | 0.030* |
| C17 | 0.00319 (19) | 0.18359 (13) | 0.85606 (8) | 0.0224 (3) |
| C18 | 0.04774 (18) | 0.14195 (13) | 0.77665 (8) | 0.0217 (3) |
| H18 | −0.0178 | 0.0691 | 0.7701 | 0.026* |
| C19 | 0.17108 (18) | 0.19583 (12) | 0.71255 (8) | 0.0202 (2) |
| H19 | 0.2367 | 0.2702 | 0.7168 | 0.024* |
| C20 | 0.20927 (17) | 0.14471 (13) | 0.63586 (7) | 0.0194 (2) |
| C21 | 0.28047 (17) | 0.22343 (12) | 0.56031 (8) | 0.0190 (2) |
| C22 | 0.27867 (17) | 0.05826 (12) | 0.48717 (7) | 0.0190 (2) |
| C23 | 0.31445 (17) | 0.01556 (13) | 0.40911 (8) | 0.0211 (3) |
| C24 | 0.38163 (19) | 0.10284 (14) | 0.33679 (8) | 0.0246 (3) |
| H24 | 0.4041 | 0.1927 | 0.3385 | 0.030* |
| C25 | 0.4152 (2) | 0.05881 (15) | 0.26338 (9) | 0.0288 (3) |
| H25 | 0.4604 | 0.1183 | 0.2148 | 0.035* |
| C26 | 0.3824 (2) | −0.07406 (16) | 0.26052 (9) | 0.0297 (3) |
| H26 | 0.4060 | −0.1041 | 0.2099 | 0.036* |
| C27 | 0.31638 (19) | −0.16072 (15) | 0.33042 (9) | 0.0279 (3) |
| H27 | 0.2949 | −0.2503 | 0.3277 | 0.033* |
| C28 | 0.28016 (18) | −0.11821 (13) | 0.40624 (8) | 0.0230 (3) |
| C29 | 0.20946 (19) | −0.20770 (13) | 0.47966 (9) | 0.0256 (3) |
| H29 | 0.1870 | −0.2972 | 0.4772 | 0.031* |
| C30 | 0.17442 (18) | −0.16655 (13) | 0.55216 (9) | 0.0243 (3) |
| H30 | 0.1267 | −0.2272 | 0.5998 | 0.029* |
| C31 | 0.20836 (17) | −0.03237 (13) | 0.55800 (8) | 0.0209 (2) |
| C32 | 0.17548 (17) | 0.01381 (13) | 0.63202 (8) | 0.0208 (2) |
| H32 | 0.1292 | −0.0454 | 0.6806 | 0.025* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.03021 (17) | 0.01941 (15) | 0.02004 (15) | −0.00805 (11) | −0.00196 (11) | −0.00167 (11) |
| O1 | 0.0475 (6) | 0.0300 (5) | 0.0246 (5) | −0.0175 (5) | 0.0085 (4) | −0.0029 (4) |
| N1 | 0.0274 (6) | 0.0271 (6) | 0.0169 (5) | −0.0041 (4) | −0.0017 (4) | 0.0003 (4) |
| N2 | 0.0178 (5) | 0.0207 (5) | 0.0196 (5) | −0.0021 (4) | −0.0038 (4) | −0.0022 (4) |
| C1 | 0.0258 (6) | 0.0256 (6) | 0.0150 (6) | −0.0046 (5) | 0.0015 (5) | −0.0015 (5) |
| C2 | 0.0380 (8) | 0.0324 (7) | 0.0184 (6) | −0.0089 (6) | −0.0022 (5) | −0.0045 (5) |
| C3 | 0.0529 (10) | 0.0289 (7) | 0.0241 (7) | −0.0119 (7) | −0.0008 (6) | −0.0091 (6) |
| C4 | 0.0515 (10) | 0.0225 (7) | 0.0276 (7) | 0.0001 (6) | −0.0015 (6) | −0.0050 (5) |
| C5 | 0.0343 (7) | 0.0245 (7) | 0.0234 (6) | 0.0005 (5) | −0.0012 (5) | −0.0028 (5) |
| C6 | 0.0232 (6) | 0.0226 (6) | 0.0160 (6) | −0.0029 (5) | 0.0032 (5) | −0.0010 (5) |
| C7 | 0.0196 (6) | 0.0223 (6) | 0.0162 (5) | −0.0027 (5) | 0.0026 (4) | −0.0004 (4) |
| C8 | 0.0215 (6) | 0.0222 (6) | 0.0160 (6) | −0.0038 (5) | 0.0024 (4) | −0.0005 (4) |
| C9 | 0.0239 (6) | 0.0232 (6) | 0.0170 (6) | −0.0031 (5) | −0.0001 (5) | 0.0021 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0349 (8) | 0.0256 (7) | 0.0288 (7) | −0.0013 (6) | −0.0074 (6) | 0.0041 (5) |
| C11 | 0.0222 (6) | 0.0186 (6) | 0.0209 (6) | −0.0011 (5) | −0.0019 (5) | −0.0019 (5) |
| C12 | 0.0224 (6) | 0.0242 (6) | 0.0237 (6) | −0.0028 (5) | −0.0021 (5) | 0.0025 (5) |
| C13 | 0.0299 (7) | 0.0252 (6) | 0.0215 (6) | −0.0033 (5) | −0.0048 (5) | 0.0017 (5) |
| C14 | 0.0275 (7) | 0.0239 (6) | 0.0281 (7) | 0.0002 (5) | −0.0097 (5) | −0.0058 (5) |
| C15 | 0.0211 (6) | 0.0328 (7) | 0.0296 (7) | −0.0053 (5) | −0.0012 (5) | −0.0099 (6) |
| C16 | 0.0240 (7) | 0.0290 (7) | 0.0211 (6) | −0.0045 (5) | 0.0003 (5) | −0.0047 (5) |
| C17 | 0.0239 (6) | 0.0205 (6) | 0.0200 (6) | −0.0029 (5) | −0.0009 (5) | 0.0014 (5) |
| C18 | 0.0217 (6) | 0.0216 (6) | 0.0212 (6) | −0.0039 (5) | −0.0039 (5) | −0.0010 (5) |
| C19 | 0.0204 (6) | 0.0198 (6) | 0.0199 (6) | −0.0023 (5) | −0.0051 (5) | −0.0003 (5) |
| C20 | 0.0152 (6) | 0.0227 (6) | 0.0200 (6) | −0.0024 (4) | −0.0032 (4) | −0.0021 (5) |
| C21 | 0.0165 (6) | 0.0192 (6) | 0.0212 (6) | −0.0031 (4) | −0.0041 (4) | −0.0012 (5) |
| C22 | 0.0141 (5) | 0.0215 (6) | 0.0214 (6) | −0.0013 (4) | −0.0039 (4) | −0.0027 (5) |
| C23 | 0.0153 (6) | 0.0240 (6) | 0.0250 (6) | 0.0002 (5) | −0.0049 (5) | −0.0059 (5) |
| C24 | 0.0230 (6) | 0.0274 (6) | 0.0238 (6) | −0.0003 (5) | −0.0046 (5) | −0.0055 (5) |
| C25 | 0.0259 (7) | 0.0367 (8) | 0.0244 (7) | −0.0003 (6) | −0.0047 (5) | −0.0073 (6) |
| C26 | 0.0239 (7) | 0.0413 (8) | 0.0276 (7) | 0.0011 (6) | −0.0055 (5) | −0.0157 (6) |
| C27 | 0.0214 (6) | 0.0316 (7) | 0.0350 (7) | 0.0007 (5) | −0.0081 (5) | −0.0150 (6) |
| C28 | 0.0153 (6) | 0.0261 (6) | 0.0293 (7) | 0.0001 (5) | −0.0053 (5) | −0.0086 (5) |
| C29 | 0.0201 (6) | 0.0218 (6) | 0.0363 (7) | −0.0024 (5) | −0.0054 (5) | −0.0073 (5) |
| C30 | 0.0205 (6) | 0.0210 (6) | 0.0304 (7) | −0.0037 (5) | −0.0025 (5) | −0.0023 (5) |
| C31 | 0.0162 (6) | 0.0215 (6) | 0.0246 (6) | −0.0014 (5) | −0.0039 (5) | −0.0029 (5) |
| C32 | 0.0179 (6) | 0.0207 (6) | 0.0217 (6) | −0.0038 (5) | −0.0014 (5) | 0.0007 (5) |

*Geometric parameters (Å, º)*

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| Cl1—C21 | 1.7526 (12) | C14—C15 | 1.383 (2) |
| O1—C17 | 1.2219 (16) | C14—H14 | 0.9500 |
| N1—C9 | 1.3149 (17) | C15—C16 | 1.3976 (19) |
| N1—C1 | 1.3703 (17) | C15—H15 | 0.9500 |
| N2—C21 | 1.3019 (16) | C16—H16 | 0.9500 |
| N2—C22 | 1.3585 (16) | C17—C18 | 1.4643 (18) |
| C1—C2 | 1.4187 (19) | C18—C19 | 1.3351 (18) |
| C1—C6 | 1.4200 (18) | C18—H18 | 0.9500 |
| C2—C3 | 1.366 (2) | C19—C20 | 1.4671 (17) |
| C2—H2 | 0.9500 | C19—H19 | 0.9500 |
| C3—C4 | 1.410 (2) | C20—C32 | 1.3923 (17) |
| C3—H3 | 0.9500 | C20—C21 | 1.4130 (17) |
| C4—C5 | 1.372 (2) | C22—C31 | 1.4127 (18) |
| C4—H4 | 0.9500 | C22—C23 | 1.4477 (17) |
| C5—C6 | 1.4180 (18) | C23—C24 | 1.4067 (19) |
| C5—H5 | 0.9500 | C23—C28 | 1.4176 (18) |
| C6—C7 | 1.4257 (18) | C24—C25 | 1.3801 (19) |
| C7—C8 | 1.3788 (18) | C24—H24 | 0.9500 |
| C7—C11 | 1.4895 (18) | C25—C26 | 1.406 (2) |
| C8—C9 | 1.4328 (18) | C25—H25 | 0.9500 |
| C8—C17 | 1.5075 (17) | C26—C27 | 1.373 (2) |
| C9—C10 | 1.5067 (18) | C26—H26 | 0.9500 |
| C10—H10A | 0.9800 | C27—C28 | 1.4108 (19) |
| C10—H10B | 0.9800 | C27—H27 | 0.9500 |

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| C10—H10C | 0.9800 | C28—C29 | 1.437 (2) |
| C11—C16 | 1.3905 (18) | C29—C30 | 1.351 (2) |
| C11—C12 | 1.3940 (18) | C29—H29 | 0.9500 |
| C12—C13 | 1.3877 (19) | C30—C31 | 1.4347 (17) |
| C12—H12 | 0.9500 | C30—H30 | 0.9500 |
| C13—C14 | 1.389 (2) | C31—C32 | 1.4005 (18) |
| C13—H13 | 0.9500 | C32—H32 | 0.9500 |

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| C9—N1—C1 | 118.65 (12) | C11—C16—H16 | 120.1 |
| C21—N2—C22 | 117.81 (11) | C15—C16—H16 | 120.1 |
| N1—C1—C2 | 117.88 (12) | O1—C17—C18 | 118.97 (12) |
| N1—C1—C6 | 122.75 (12) | O1—C17—C8 | 119.05 (12) |
| C2—C1—C6 | 119.37 (12) | C18—C17—C8 | 121.98 (11) |
| C3—C2—C1 | 120.19 (14) | C19—C18—C17 | 126.68 (12) |
| C3—C2—H2 | 119.9 | C19—C18—H18 | 116.7 |
| C1—C2—H2 | 119.9 | C17—C18—H18 | 116.7 |
| C2—C3—C4 | 120.63 (13) | C18—C19—C20 | 122.60 (11) |
| C2—C3—H3 | 119.7 | C18—C19—H19 | 118.7 |
| C4—C3—H3 | 119.7 | C20—C19—H19 | 118.7 |
| C5—C4—C3 | 120.53 (14) | C32—C20—C21 | 114.63 (11) |
| C5—C4—H4 | 119.7 | C32—C20—C19 | 122.08 (11) |
| C3—C4—H4 | 119.7 | C21—C20—C19 | 123.29 (11) |
| C4—C5—C6 | 120.27 (14) | N2—C21—C20 | 126.73 (11) |
| C4—C5—H5 | 119.9 | N2—C21—Cl1 | 114.54 (9) |
| C6—C5—H5 | 119.9 | C20—C21—Cl1 | 118.72 (9) |
| C5—C6—C1 | 118.95 (12) | N2—C22—C31 | 121.81 (11) |
| C5—C6—C7 | 123.36 (12) | N2—C22—C23 | 118.37 (11) |
| C1—C6—C7 | 117.66 (12) | C31—C22—C23 | 119.83 (11) |
| C8—C7—C6 | 118.52 (12) | C24—C23—C28 | 119.61 (12) |
| C8—C7—C11 | 122.21 (11) | C24—C23—C22 | 121.87 (12) |
| C6—C7—C11 | 119.26 (11) | C28—C23—C22 | 118.53 (12) |
| C7—C8—C9 | 119.66 (12) | C25—C24—C23 | 120.44 (13) |
| C7—C8—C17 | 121.10 (12) | C25—C24—H24 | 119.8 |
| C9—C8—C17 | 119.07 (11) | C23—C24—H24 | 119.8 |
| N1—C9—C8 | 122.61 (12) | C24—C25—C26 | 120.01 (14) |
| N1—C9—C10 | 116.89 (12) | C24—C25—H25 | 120.0 |
| C8—C9—C10 | 120.48 (12) | C26—C25—H25 | 120.0 |
| C9—C10—H10A | 109.5 | C27—C26—C25 | 120.43 (13) |
| C9—C10—H10B | 109.5 | C27—C26—H26 | 119.8 |
| H10A—C10—H10B | 109.5 | C25—C26—H26 | 119.8 |
| C9—C10—H10C | 109.5 | C26—C27—C28 | 120.74 (13) |
| H10A—C10—H10C | 109.5 | C26—C27—H27 | 119.6 |
| H10B—C10—H10C | 109.5 | C28—C27—H27 | 119.6 |
| C16—C11—C12 | 119.22 (12) | C27—C28—C23 | 118.77 (13) |
| C16—C11—C7 | 121.74 (11) | C27—C28—C29 | 121.20 (12) |
| C12—C11—C7 | 119.03 (11) | C23—C28—C29 | 120.03 (12) |
| C13—C12—C11 | 120.78 (12) | C30—C29—C28 | 121.05 (12) |
| C13—C12—H12 | 119.6 | C30—C29—H29 | 119.5 |
| C11—C12—H12 | 119.6 | C28—C29—H29 | 119.5 |

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| C12—C13—C14 | 119.79 (13) | C29—C30—C31 | 120.81 (13) |
| C12—C13—H13 | 120.1 | C29—C30—H30 | 119.6 |
| C14—C13—H13 | 120.1 | C31—C30—H30 | 119.6 |
| C15—C14—C13 | 119.88 (13) | C32—C31—C22 | 117.68 (11) |
| C15—C14—H14 | 120.1 | C32—C31—C30 | 122.58 (12) |
| C13—C14—H14 | 120.1 | C22—C31—C30 | 119.74 (12) |
| C14—C15—C16 | 120.41 (12) | C20—C32—C31 | 121.34 (12) |
| C14—C15—H15 | 119.8 | C20—C32—H32 | 119.3 |
| C16—C15—H15 | 119.8 | C31—C32—H32 | 119.3 |
| C11—C16—C15 | 119.90 (12) | | |

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| C9—N1—C1—C2 | 178.03 (12) | C9—C8—C17—C18 | −109.35 (14) |
| C9—N1—C1—C6 | −2.71 (18) | O1—C17—C18—C19 | −174.33 (14) |
| N1—C1—C2—C3 | −178.22 (12) | C8—C17—C18—C19 | 4.6 (2) |
| C6—C1—C2—C3 | 2.5 (2) | C17—C18—C19—C20 | 178.53 (12) |
| C1—C2—C3—C4 | −0.3 (2) | C18—C19—C20—C32 | −22.79 (19) |
| C2—C3—C4—C5 | −1.8 (2) | C18—C19—C20—C21 | 156.45 (12) |
| C3—C4—C5—C6 | 1.5 (2) | C22—N2—C21—C20 | −0.07 (19) |
| C4—C5—C6—C1 | 0.7 (2) | C22—N2—C21—Cl1 | −179.46 (9) |
| C4—C5—C6—C7 | 178.69 (13) | C32—C20—C21—N2 | 0.69 (19) |
| N1—C1—C6—C5 | 178.07 (12) | C19—C20—C21—N2 | −178.60 (11) |
| C2—C1—C6—C5 | −2.69 (18) | C32—C20—C21—Cl1 | −179.95 (9) |
| N1—C1—C6—C7 | −0.04 (18) | C19—C20—C21—Cl1 | 0.76 (16) |
| C2—C1—C6—C7 | 179.20 (12) | C21—N2—C22—C31 | −0.37 (17) |
| C5—C6—C7—C8 | −174.86 (12) | C21—N2—C22—C23 | 179.59 (11) |
| C1—C6—C7—C8 | 3.16 (17) | N2—C22—C23—C24 | −0.97 (18) |
| C5—C6—C7—C11 | 5.43 (19) | C31—C22—C23—C24 | 179.00 (11) |
| C1—C6—C7—C11 | −176.55 (11) | N2—C22—C23—C28 | 179.08 (11) |
| C6—C7—C8—C9 | −3.58 (18) | C31—C22—C23—C28 | −0.95 (17) |
| C11—C7—C8—C9 | 176.12 (11) | C28—C23—C24—C25 | −0.35 (19) |
| C6—C7—C8—C17 | 171.82 (11) | C22—C23—C24—C25 | 179.70 (12) |
| C11—C7—C8—C17 | −8.49 (18) | C23—C24—C25—C26 | −0.1 (2) |
| C1—N1—C9—C8 | 2.33 (19) | C24—C25—C26—C27 | 0.2 (2) |
| C1—N1—C9—C10 | −179.25 (11) | C25—C26—C27—C28 | 0.1 (2) |
| C7—C8—C9—N1 | 0.84 (19) | C26—C27—C28—C23 | −0.46 (19) |
| C17—C8—C9—N1 | −174.65 (11) | C26—C27—C28—C29 | 179.43 (12) |
| C7—C8—C9—C10 | −177.52 (12) | C24—C23—C28—C27 | 0.59 (18) |
| C17—C8—C9—C10 | 6.99 (18) | C22—C23—C28—C27 | −179.45 (11) |
| C8—C7—C11—C16 | 73.14 (17) | C24—C23—C28—C29 | −179.29 (12) |
| C6—C7—C11—C16 | −107.17 (14) | C22—C23—C28—C29 | 0.66 (18) |
| C8—C7—C11—C12 | −108.44 (14) | C27—C28—C29—C30 | −179.82 (12) |
| C6—C7—C11—C12 | 71.26 (16) | C23—C28—C29—C30 | 0.07 (19) |
| C16—C11—C12—C13 | 0.4 (2) | C28—C29—C30—C31 | −0.5 (2) |
| C7—C11—C12—C13 | −178.03 (12) | N2—C22—C31—C32 | 0.16 (18) |
| C11—C12—C13—C14 | 1.2 (2) | C23—C22—C31—C32 | −179.81 (11) |
| C12—C13—C14—C15 | −1.6 (2) | N2—C22—C31—C30 | −179.50 (11) |
| C13—C14—C15—C16 | 0.4 (2) | C23—C22—C31—C30 | 0.53 (18) |
| C12—C11—C16—C15 | −1.64 (19) | C29—C30—C31—C32 | −179.43 (12) |
| C7—C11—C16—C15 | 176.78 (12) | C29—C30—C31—C22 | 0.21 (19) |

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| C14—C15—C16—C11 | 1.3 (2) | C21—C20—C32—C31 | −0.87 (18) |
| C7—C8—C17—O1 | −105.83 (15) | C19—C20—C32—C31 | 178.43 (11) |
| C9—C8—C17—O1 | 69.59 (17) | C22—C31—C32—C20 | 0.50 (18) |
| C7—C8—C17—C18 | 75.23 (16) | C30—C31—C32—C20 | −179.85 (12) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the N1-pyridyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10*C*···O1$^{i}$ | 0.98 | 2.54 | 3.4116 (18) | 148 |
| C15—H15···*Cg*1$^{ii}$ | 0.95 | 2.65 | 3.4695 (15) | 145 |

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