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# 2-[4,5-Diphenyl-2-(pyridin-2-yl)-1*H*-imidazol-1-yl]-3-phenylpropan-1-ol

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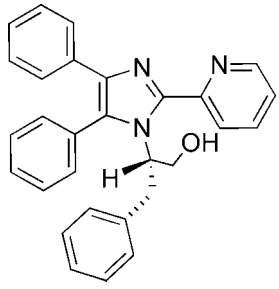
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.038; $wR$ factor = 0.102; data-to-parameter ratio = 14.3.

In the title compound, $C_{29}H_{25}N_3O$, the central imidazole ring forms dihedral angles of 64.7 (3), 33.5 (3) and 81.2 (2)° with the pyridyl and two phenyl substituents, respectively. An intramolecular C—H···N hydrogen bond is observed. In the crystal, O—H···N and C—H···O hydrogen bonds link the molecules into chains parallel to the *a* axis.

## Related literature

For the synthesis and properties of chiral ionic liquids, see: Ding & Armstrong (2005); Bwambok *et al.* (2008); Mao *et al.* (2010). For a related structure, see: Xiao *et al.* (2012).




## Experimental

### Crystal data

$C_{29}H_{25}N_3O$
$M_r$ = 431.52
Orthorhombic, $P2_12_12_1$
$a$ = 9.2695 (4) Å
$b$ = 15.8818 (6) Å
$c$ = 16.0498 (6) Å
$V$ = 2362.79 (16) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.58 mm$^{-1}$
$T$ = 291 K
0.38 × 0.28 × 0.25 mm

### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min}$ = 0.809, $T_{max}$ = 0.868
9413 measured reflections
4442 independent reflections
3981 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
$S$ = 1.04
4442 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.13 e Å$^{-3}$
Absolute structure: Flack (1983), 1871 Friedel pairs
Flack parameter: 0.2 (4)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C27—H27$A$···N3 | 0.97 | 2.42 | 3.277 (2) | 146 |
| C22—H22···O1$^{i}$ | 0.93 | 2.54 | 3.350 (3) | 146 |
| O1—H1···N1$^{ii}$ | 0.85 (3) | 1.94 (3) | 2.789 (2) | 174 (3) |

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

Data collection: *CrysAlis PRO* (Agilent, 2011); 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: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2739).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1670 [doi:10.1107/S1600536812018703]

## 2-[4,5-Diphenyl-2-(pyridin-2-yl)-1*H*-imidazol-1-yl]-3-phenylpropan-1-ol

**Liangru Yang, Yongmei Xiao, Kun He, Jinwei Yuan and Pu Mao**

### Comment

Our group is interested in the synthesis of chiral imidazole derivatives from natural precursors through a convenient four component–one pot synthetic protocol using an aldehyde, glyoxal, ammonia, and an amine (Mao *et al.*, 2010). During our studies we observed that by carefully choosing the four components, a number of different imidazole derivatives could be obtained easily (Xiao *et al.*, 2012). The condensation of *L*-phenylalaninol, dibenzoyl, 2-formyl pyridine and ammonium acetate afforded the title compound. This compound may serve as a starting material for the research of imidazolium based chiral ionic liquids in catalysis, chiral recognization and separation (Ding & Armstrong, 2005; Bwambok *et al.*, 2008).

The molecular structure of the title compound is shown in Figure 1. As expected, the imidazole core (N1, C7, C8, N2, C15) is essentially planar, featuring an average deviation smaller than 0.6 (2) Å. The dihedral angle between the pyridyl and imidazole rings is 64.7 (3) °, and the dihedral angles between the two phenyl substituents and the imidazole ring are 33.5 (3)° and 81.2 (2)°, respectively. The chiral C28 atom maintains the *S* configuration of the *L*-phenylalaninol. The molecular conformation is enforced by an intramolecular C—H···N hydrogen bond (Table 1). In the crystal structure, molecules are linked by intermolecular O–H···N and C—H···O hydrogen bonds into chains parallel to the *a* axis.

### Experimental

To a solution of *L*-phenylalaninol (15.1 g, 0.1 mol) in MeOH (50 ml) in an ice-bath, molar equivalents of dibenzoyl, 2-formyl pyridine and ammonium acetate were added. The mixture was kept stirring in the ice-bath until all the solids were dissolved before being heated to 60°C for 5 h. The mixture was then cooled to r.t. and the solvent was removed by evaporation. The residue was washed with $H_2O$ to obtain the crude product. Crystallization of the crude product in EtOH afforded colourless crystals of the title compound.

### Refinement

The H atoms associated to the hydroxy group and to the C29 methylene group were located in a difference Fourier map and refined freely. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93-0.98 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

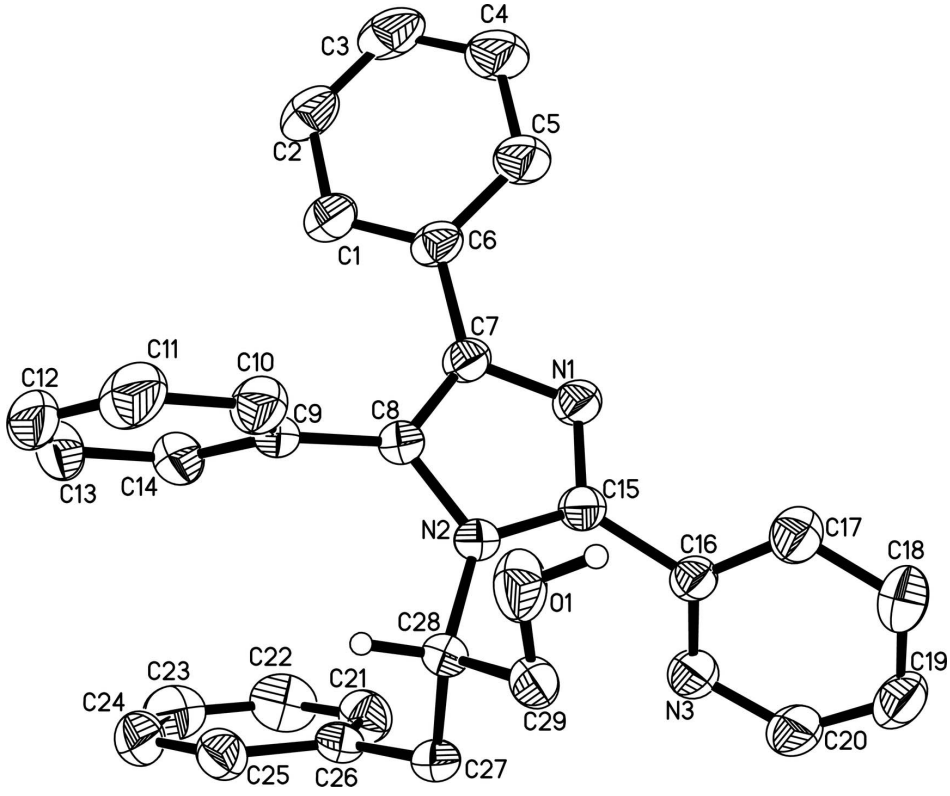


**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

### 2-[4,5-Diphenyl-2-(pyridin-2-yl)-1*H*-imidazol-1-yl]-3-phenylpropan-1-ol

*Crystal data*

$C_{29}H_{25}N_3O$
$M_r = 431.52$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 9.2695\ (4)$ Å
$b = 15.8818\ (6)$ Å
$c = 16.0498\ (6)$ Å
$V = 2362.79\ (16)$ Å$^3$
$Z = 4$
$F(000) = 912$
$D_x = 1.213$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 3448 reflections
$\theta = 3.9$–$70.3°$
$\mu = 0.58$ mm$^{-1}$
$T = 291$ K
Prismatic, colourless
0.38 × 0.28 × 0.25 mm

*Data collection*

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.809$, $T_{max} = 0.868$
9413 measured reflections
4442 independent reflections
3981 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 70.4°$, $\theta_{min} = 3.9°$
$h = -11 \rightarrow 6$
$k = -19 \rightarrow 19$
$l = -19 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.102$
$S = 1.04$
4442 reflections
311 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.1152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å$^{-3}$
$\Delta\rho_{min} = -0.13$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0043 (3)
Absolute structure: Flack (1983), 1871 Friedel pairs
Flack parameter: 0.2 (4)

*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.
**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 $F^2 > \sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.74800 (17) | 0.67325 (12) | 0.63461 (10) | 0.0746 (4) |
| H1 | 0.788 (3) | 0.6736 (19) | 0.5871 (18) | 0.094 (9)* |
| N1 | 0.38909 (18) | 0.81423 (9) | 0.51834 (9) | 0.0550 (4) |
| N2 | 0.45320 (16) | 0.73451 (8) | 0.62480 (8) | 0.0463 (3) |
| N3 | 0.3134 (2) | 0.60522 (11) | 0.49389 (10) | 0.0667 (5) |
| C1 | 0.3385 (3) | 1.00699 (12) | 0.64156 (14) | 0.0632 (5) |
| H1A | 0.3170 | 0.9829 | 0.6929 | 0.076* |
| C2 | 0.3175 (3) | 1.09285 (14) | 0.63001 (17) | 0.0765 (7) |
| H2 | 0.2801 | 1.1254 | 0.6731 | 0.092* |
| C3 | 0.3515 (4) | 1.12968 (14) | 0.55573 (18) | 0.0897 (9) |
| H3 | 0.3390 | 1.1873 | 0.5484 | 0.108* |
| C4 | 0.4043 (4) | 1.08104 (15) | 0.49205 (18) | 0.0922 (8) |
| H4 | 0.4270 | 1.1059 | 0.4413 | 0.111* |
| C5 | 0.4241 (3) | 0.99523 (14) | 0.50254 (15) | 0.0744 (6) |
| H5 | 0.4599 | 0.9629 | 0.4588 | 0.089* |
| C6 | 0.3908 (2) | 0.95713 (11) | 0.57826 (12) | 0.0559 (5) |
| C7 | 0.4089 (2) | 0.86522 (10) | 0.58664 (11) | 0.0507 (4) |
| C8 | 0.44924 (19) | 0.81699 (10) | 0.65331 (10) | 0.0462 (4) |
| C9 | 0.5020 (2) | 0.84066 (10) | 0.73772 (10) | 0.0499 (4) |
| C10 | 0.6491 (3) | 0.84668 (14) | 0.75092 (14) | 0.0680 (5) |
| H10 | 0.7133 | 0.8351 | 0.7079 | 0.082* |
| C11 | 0.7002 (4) | 0.87002 (17) | 0.82853 (18) | 0.0939 (9) |

| | | | | |
|---|---|---|---|---|
| H11 | 0.7990 | 0.8748 | 0.8372 | 0.113* |
| C12 | 0.6071 (5) | 0.88607 (16) | 0.89254 (16) | 0.1047 (13) |
| H12 | 0.6425 | 0.9013 | 0.9446 | 0.126* |
| C13 | 0.4622 (4) | 0.87974 (17) | 0.87992 (14) | 0.0975 (10) |
| H13 | 0.3989 | 0.8909 | 0.9235 | 0.117* |
| C14 | 0.4087 (3) | 0.85679 (14) | 0.80277 (13) | 0.0712 (6) |
| H14 | 0.3096 | 0.8522 | 0.7947 | 0.085* |
| C15 | 0.4153 (2) | 0.73696 (11) | 0.54294 (10) | 0.0496 (4) |
| C16 | 0.4123 (2) | 0.66518 (10) | 0.48335 (10) | 0.0503 (4) |
| C17 | 0.5080 (3) | 0.66655 (14) | 0.41749 (13) | 0.0661 (5) |
| H17 | 0.5735 | 0.7105 | 0.4115 | 0.079* |
| C18 | 0.5044 (3) | 0.60158 (16) | 0.36082 (15) | 0.0778 (6) |
| H18 | 0.5682 | 0.6007 | 0.3161 | 0.093* |
| C19 | 0.4059 (3) | 0.53848 (14) | 0.37106 (15) | 0.0769 (6) |
| H19 | 0.4017 | 0.4934 | 0.3342 | 0.092* |
| C20 | 0.3140 (3) | 0.54377 (14) | 0.43719 (14) | 0.0771 (7) |
| H20 | 0.2462 | 0.5011 | 0.4433 | 0.093* |
| C21 | 0.1277 (2) | 0.65894 (16) | 0.71789 (14) | 0.0702 (5) |
| H21 | 0.1068 | 0.6486 | 0.6621 | 0.084* |
| C22 | 0.0228 (3) | 0.69407 (19) | 0.7686 (2) | 0.0900 (8) |
| H22 | −0.0677 | 0.7066 | 0.7469 | 0.108* |
| C23 | 0.0523 (3) | 0.71040 (17) | 0.85053 (19) | 0.0858 (8) |
| H23 | −0.0175 | 0.7347 | 0.8845 | 0.103* |
| C24 | 0.1850 (3) | 0.69072 (16) | 0.88228 (15) | 0.0768 (6) |
| H24 | 0.2050 | 0.7012 | 0.9381 | 0.092* |
| C25 | 0.2892 (2) | 0.65539 (14) | 0.83191 (13) | 0.0620 (5) |
| H25 | 0.3791 | 0.6423 | 0.8543 | 0.074* |
| C26 | 0.2624 (2) | 0.63902 (11) | 0.74854 (11) | 0.0518 (4) |
| C27 | 0.3778 (2) | 0.60045 (11) | 0.69460 (11) | 0.0550 (4) |
| H27A | 0.3347 | 0.5818 | 0.6427 | 0.066* |
| H27B | 0.4167 | 0.5513 | 0.7226 | 0.066* |
| C28 | 0.5014 (2) | 0.66113 (10) | 0.67490 (10) | 0.0475 (4) |
| H28 | 0.5348 | 0.6836 | 0.7284 | 0.057* |
| C29 | 0.6303 (2) | 0.61828 (12) | 0.63495 (11) | 0.0552 (4) |
| H29A | 0.607 (2) | 0.5961 (13) | 0.5795 (12) | 0.054 (5)* |
| H29B | 0.656 (2) | 0.5676 (14) | 0.6711 (13) | 0.058 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0663 (9) | 0.0981 (12) | 0.0593 (8) | −0.0147 (9) | 0.0172 (7) | −0.0167 (8) |
| N1 | 0.0679 (9) | 0.0455 (7) | 0.0516 (8) | −0.0010 (7) | −0.0131 (7) | 0.0021 (6) |
| N2 | 0.0545 (8) | 0.0394 (6) | 0.0449 (7) | −0.0044 (6) | 0.0003 (6) | 0.0021 (5) |
| N3 | 0.0840 (12) | 0.0588 (9) | 0.0571 (9) | −0.0182 (9) | −0.0078 (8) | −0.0028 (8) |
| C1 | 0.0696 (13) | 0.0496 (9) | 0.0703 (12) | −0.0003 (9) | −0.0161 (11) | −0.0032 (9) |
| C2 | 0.0835 (15) | 0.0513 (11) | 0.0947 (17) | 0.0112 (11) | −0.0284 (14) | −0.0126 (11) |
| C3 | 0.115 (2) | 0.0438 (9) | 0.110 (2) | 0.0078 (12) | −0.0412 (17) | 0.0066 (12) |
| C4 | 0.131 (2) | 0.0600 (13) | 0.0858 (16) | −0.0023 (15) | −0.0165 (18) | 0.0223 (12) |
| C5 | 0.1002 (18) | 0.0520 (10) | 0.0711 (12) | 0.0030 (11) | −0.0102 (13) | 0.0109 (9) |
| C6 | 0.0619 (12) | 0.0431 (8) | 0.0626 (10) | −0.0013 (8) | −0.0200 (9) | 0.0003 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0562 (10) | 0.0428 (8) | 0.0530 (9) | −0.0027 (8) | −0.0081 (8) | −0.0006 (7) |
| C8 | 0.0498 (9) | 0.0419 (7) | 0.0470 (8) | −0.0029 (7) | 0.0014 (7) | 0.0001 (6) |
| C9 | 0.0668 (10) | 0.0383 (7) | 0.0446 (8) | −0.0040 (7) | −0.0009 (8) | 0.0027 (6) |
| C10 | 0.0750 (13) | 0.0635 (11) | 0.0654 (11) | −0.0066 (10) | −0.0133 (11) | −0.0033 (10) |
| C11 | 0.118 (2) | 0.0734 (14) | 0.0907 (18) | −0.0084 (15) | −0.0504 (17) | −0.0026 (14) |
| C12 | 0.199 (4) | 0.0574 (12) | 0.0574 (13) | −0.0037 (19) | −0.0422 (19) | −0.0018 (10) |
| C13 | 0.172 (3) | 0.0718 (15) | 0.0484 (11) | 0.0041 (18) | 0.0144 (16) | −0.0023 (10) |
| C14 | 0.0922 (16) | 0.0635 (11) | 0.0578 (11) | −0.0013 (11) | 0.0134 (11) | 0.0014 (9) |
| C15 | 0.0545 (10) | 0.0452 (8) | 0.0492 (8) | −0.0024 (8) | −0.0041 (8) | 0.0019 (7) |
| C16 | 0.0595 (10) | 0.0438 (8) | 0.0478 (8) | 0.0027 (8) | −0.0096 (8) | 0.0010 (7) |
| C17 | 0.0654 (12) | 0.0655 (11) | 0.0675 (11) | −0.0032 (10) | 0.0017 (10) | −0.0087 (9) |
| C18 | 0.0777 (14) | 0.0837 (15) | 0.0721 (13) | 0.0122 (13) | 0.0085 (12) | −0.0193 (12) |
| C19 | 0.1013 (18) | 0.0572 (11) | 0.0721 (13) | 0.0065 (12) | −0.0160 (14) | −0.0179 (10) |
| C20 | 0.1032 (19) | 0.0589 (11) | 0.0693 (13) | −0.0229 (13) | −0.0153 (13) | −0.0068 (10) |
| C21 | 0.0683 (13) | 0.0761 (13) | 0.0663 (12) | −0.0071 (11) | −0.0070 (10) | 0.0059 (10) |
| C22 | 0.0617 (14) | 0.0954 (18) | 0.113 (2) | 0.0056 (13) | 0.0016 (14) | 0.0151 (16) |
| C23 | 0.0765 (16) | 0.0768 (15) | 0.1042 (19) | 0.0024 (12) | 0.0317 (15) | 0.0014 (14) |
| C24 | 0.0943 (17) | 0.0745 (13) | 0.0616 (12) | −0.0117 (13) | 0.0199 (12) | −0.0041 (10) |
| C25 | 0.0652 (12) | 0.0650 (11) | 0.0557 (10) | −0.0059 (9) | 0.0038 (9) | 0.0049 (9) |
| C26 | 0.0590 (10) | 0.0444 (8) | 0.0521 (9) | −0.0102 (8) | 0.0057 (8) | 0.0076 (7) |
| C27 | 0.0706 (12) | 0.0403 (8) | 0.0542 (9) | −0.0067 (8) | 0.0078 (9) | 0.0018 (7) |
| C28 | 0.0596 (10) | 0.0407 (7) | 0.0423 (7) | 0.0000 (7) | 0.0018 (7) | 0.0049 (6) |
| C29 | 0.0674 (11) | 0.0531 (9) | 0.0452 (8) | 0.0070 (9) | 0.0046 (8) | 0.0036 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—H1 | 0.85 (3) | C13—H13 | 0.9300 |
| O1—C29 | 1.397 (3) | C13—C14 | 1.383 (4) |
| N1—C7 | 1.375 (2) | C14—H14 | 0.9300 |
| N1—C15 | 1.312 (2) | C15—C16 | 1.488 (2) |
| N2—C8 | 1.388 (2) | C16—C17 | 1.380 (3) |
| N2—C15 | 1.360 (2) | C17—H17 | 0.9300 |
| N2—C28 | 1.485 (2) | C17—C18 | 1.376 (3) |
| N3—C16 | 1.333 (3) | C18—H18 | 0.9300 |
| N3—C20 | 1.334 (3) | C18—C19 | 1.366 (4) |
| C1—H1A | 0.9300 | C19—H19 | 0.9300 |
| C1—C2 | 1.390 (3) | C19—C20 | 1.364 (4) |
| C1—C6 | 1.376 (3) | C20—H20 | 0.9300 |
| C2—H2 | 0.9300 | C21—H21 | 0.9300 |
| C2—C3 | 1.365 (4) | C21—C22 | 1.385 (4) |
| C3—H3 | 0.9300 | C21—C26 | 1.379 (3) |
| C3—C4 | 1.371 (4) | C22—H22 | 0.9300 |
| C4—H4 | 0.9300 | C22—C23 | 1.368 (4) |
| C4—C5 | 1.385 (3) | C23—H23 | 0.9300 |
| C5—H5 | 0.9300 | C23—C24 | 1.368 (4) |
| C5—C6 | 1.392 (3) | C24—H24 | 0.9300 |
| C6—C7 | 1.476 (2) | C24—C25 | 1.379 (3) |
| C7—C8 | 1.368 (2) | C25—H25 | 0.9300 |
| C8—C9 | 1.488 (2) | C25—C26 | 1.386 (3) |
| C9—C10 | 1.384 (3) | C26—C27 | 1.507 (3) |

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| C9—C14 | 1.380 (3) | C27—H27A | 0.9700 |
| C10—H10 | 0.9300 | C27—H27B | 0.9700 |
| C10—C11 | 1.383 (3) | C27—C28 | 1.530 (2) |
| C11—H11 | 0.9300 | C28—H28 | 0.9800 |
| C11—C12 | 1.366 (5) | C28—C29 | 1.517 (3) |
| C12—H12 | 0.9300 | C29—H29A | 0.98 (2) |
| C12—C13 | 1.361 (5) | C29—H29B | 1.02 (2) |

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| C29—O1—H1 | 110 (2) | N3—C16—C15 | 118.61 (17) |
| C15—N1—C7 | 106.63 (14) | N3—C16—C17 | 123.39 (18) |
| C8—N2—C28 | 124.76 (14) | C17—C16—C15 | 117.91 (17) |
| C15—N2—C8 | 106.54 (14) | C16—C17—H17 | 120.7 |
| C15—N2—C28 | 128.55 (14) | C18—C17—C16 | 118.6 (2) |
| C16—N3—C20 | 115.7 (2) | C18—C17—H17 | 120.7 |
| C2—C1—H1A | 119.5 | C17—C18—H18 | 120.4 |
| C6—C1—H1A | 119.5 | C19—C18—C17 | 119.1 (2) |
| C6—C1—C2 | 121.0 (2) | C19—C18—H18 | 120.4 |
| C1—C2—H2 | 119.9 | C18—C19—H19 | 121.1 |
| C3—C2—C1 | 120.3 (2) | C20—C19—C18 | 117.8 (2) |
| C3—C2—H2 | 119.9 | C20—C19—H19 | 121.1 |
| C2—C3—H3 | 120.3 | N3—C20—C19 | 125.3 (2) |
| C2—C3—C4 | 119.5 (2) | N3—C20—H20 | 117.3 |
| C4—C3—H3 | 120.3 | C19—C20—H20 | 117.3 |
| C3—C4—H4 | 119.6 | C22—C21—H21 | 119.4 |
| C3—C4—C5 | 120.7 (3) | C26—C21—H21 | 119.4 |
| C5—C4—H4 | 119.6 | C26—C21—C22 | 121.2 (2) |
| C4—C5—H5 | 119.9 | C21—C22—H22 | 120.0 |
| C4—C5—C6 | 120.3 (2) | C23—C22—C21 | 120.1 (3) |
| C6—C5—H5 | 119.9 | C23—C22—H22 | 120.0 |
| C1—C6—C5 | 118.20 (19) | C22—C23—H23 | 120.2 |
| C1—C6—C7 | 122.82 (19) | C24—C23—C22 | 119.6 (3) |
| C5—C6—C7 | 118.96 (19) | C24—C23—H23 | 120.2 |
| N1—C7—C6 | 119.65 (16) | C23—C24—H24 | 119.8 |
| C8—C7—N1 | 109.29 (15) | C23—C24—C25 | 120.3 (2) |
| C8—C7—C6 | 131.02 (16) | C25—C24—H24 | 119.8 |
| N2—C8—C9 | 121.99 (15) | C24—C25—H25 | 119.4 |
| C7—C8—N2 | 106.12 (14) | C24—C25—C26 | 121.1 (2) |
| C7—C8—C9 | 131.32 (15) | C26—C25—H25 | 119.4 |
| C10—C9—C8 | 118.72 (18) | C21—C26—C25 | 117.7 (2) |
| C14—C9—C8 | 122.0 (2) | C21—C26—C27 | 122.11 (18) |
| C14—C9—C10 | 119.3 (2) | C25—C26—C27 | 120.24 (19) |
| C9—C10—H10 | 120.2 | C26—C27—H27A | 108.9 |
| C11—C10—C9 | 119.6 (3) | C26—C27—H27B | 108.9 |
| C11—C10—H10 | 120.2 | C26—C27—C28 | 113.23 (14) |
| C10—C11—H11 | 119.6 | H27A—C27—H27B | 107.7 |
| C12—C11—C10 | 120.7 (3) | C28—C27—H27A | 108.9 |
| C12—C11—H11 | 119.6 | C28—C27—H27B | 108.9 |
| C11—C12—H12 | 120.1 | N2—C28—C27 | 112.40 (15) |
| C13—C12—C11 | 119.8 (2) | N2—C28—H28 | 106.5 |

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| C13—C12—H12 | 120.1 | N2—C28—C29 | 111.11 (13) |
| C12—C13—H13 | 119.8 | C27—C28—H28 | 106.5 |
| C12—C13—C14 | 120.4 (3) | C29—C28—C27 | 113.22 (15) |
| C14—C13—H13 | 119.8 | C29—C28—H28 | 106.5 |
| C9—C14—C13 | 120.1 (3) | O1—C29—C28 | 109.65 (16) |
| C9—C14—H14 | 119.9 | O1—C29—H29A | 113.2 (12) |
| C13—C14—H14 | 119.9 | O1—C29—H29B | 108.3 (13) |
| N1—C15—N2 | 111.42 (15) | C28—C29—H29A | 111.7 (12) |
| N1—C15—C16 | 121.31 (15) | C28—C29—H29B | 107.3 (12) |
| N2—C15—C16 | 127.12 (15) | H29A—C29—H29B | 106.5 (16) |

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| N1—C7—C8—N2 | −0.3 (2) | C10—C9—C14—C13 | 0.8 (3) |
| N1—C7—C8—C9 | 170.93 (19) | C10—C11—C12—C13 | −0.5 (4) |
| N1—C15—C16—N3 | −116.1 (2) | C11—C12—C13—C14 | 0.3 (4) |
| N1—C15—C16—C17 | 60.7 (3) | C12—C13—C14—C9 | −0.5 (4) |
| N2—C8—C9—C10 | 77.2 (2) | C14—C9—C10—C11 | −1.0 (3) |
| N2—C8—C9—C14 | −102.9 (2) | C15—N1—C7—C6 | 178.44 (19) |
| N2—C15—C16—N3 | 68.7 (3) | C15—N1—C7—C8 | 0.6 (2) |
| N2—C15—C16—C17 | −114.5 (2) | C15—N2—C8—C7 | 0.0 (2) |
| N2—C28—C29—O1 | 64.47 (19) | C15—N2—C8—C9 | −172.28 (17) |
| N3—C16—C17—C18 | −1.9 (3) | C15—N2—C28—C27 | −72.9 (2) |
| C1—C2—C3—C4 | 1.1 (4) | C15—N2—C28—C29 | 55.2 (2) |
| C1—C6—C7—N1 | 147.0 (2) | C15—C16—C17—C18 | −178.6 (2) |
| C1—C6—C7—C8 | −35.7 (3) | C16—N3—C20—C19 | −0.2 (4) |
| C2—C1—C6—C5 | 0.9 (3) | C16—C17—C18—C19 | 0.6 (4) |
| C2—C1—C6—C7 | −177.3 (2) | C17—C18—C19—C20 | 0.8 (4) |
| C2—C3—C4—C5 | −0.4 (5) | C18—C19—C20—N3 | −1.0 (4) |
| C3—C4—C5—C6 | −0.1 (5) | C20—N3—C16—C15 | 178.34 (19) |
| C4—C5—C6—C1 | −0.2 (4) | C20—N3—C16—C17 | 1.7 (3) |
| C4—C5—C6—C7 | 178.2 (2) | C21—C22—C23—C24 | −0.9 (4) |
| C5—C6—C7—N1 | −31.3 (3) | C21—C26—C27—C28 | 108.7 (2) |
| C5—C6—C7—C8 | 146.0 (2) | C22—C21—C26—C25 | 0.0 (3) |
| C6—C1—C2—C3 | −1.4 (4) | C22—C21—C26—C27 | 179.8 (2) |
| C6—C7—C8—N2 | −177.9 (2) | C22—C23—C24—C25 | 0.6 (4) |
| C6—C7—C8—C9 | −6.6 (4) | C23—C24—C25—C26 | 0.0 (4) |
| C7—N1—C15—N2 | −0.6 (2) | C24—C25—C26—C21 | −0.3 (3) |
| C7—N1—C15—C16 | −176.46 (17) | C24—C25—C26—C27 | 179.95 (18) |
| C7—C8—C9—C10 | −92.9 (3) | C25—C26—C27—C28 | −71.5 (2) |
| C7—C8—C9—C14 | 87.0 (3) | C26—C21—C22—C23 | 0.6 (4) |
| C8—N2—C15—N1 | 0.4 (2) | C26—C27—C28—N2 | −64.04 (19) |
| C8—N2—C15—C16 | 175.96 (18) | C26—C27—C28—C29 | 169.04 (15) |
| C8—N2—C28—C27 | 112.38 (18) | C27—C28—C29—O1 | −167.93 (15) |
| C8—N2—C28—C29 | −119.57 (18) | C28—N2—C8—C7 | 175.71 (16) |
| C8—C9—C10—C11 | 178.9 (2) | C28—N2—C8—C9 | 3.4 (3) |
| C8—C9—C14—C13 | −179.1 (2) | C28—N2—C15—N1 | −175.13 (17) |
| C9—C10—C11—C12 | 0.9 (4) | C28—N2—C15—C16 | 0.4 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C27—H27*A*···N3 | 0.97 | 2.42 | 3.277 (2) | 146 |
| C22—H22···O1$^{i}$ | 0.93 | 2.54 | 3.350 (3) | 146 |
| O1—H1···N1$^{ii}$ | 0.85 (3) | 1.94 (3) | 2.789 (2) | 174 (3) |

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