organic compounds

5-Phenyl-2-(4-pyridyl)pyrimidine

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The title compound, $C_{15}H_{11}N_3$, crystallizes with two independent molecules in the asymmetric unit. The dihedral angles between the phenyl and pyridine rings in each molecule are 53.48 (5) and 50.80 (5)°. In the crystal structure, weak intermolecular C—H···N hydrogen bonds connect molecules into one-dimensional chains. In addition, the crystal structure is stabilized by weak C—H···π(arene) interactions.

Related literature

For related literature, see: Fang et al. (2002, 2007); Medlycott & Hanan (2005, 2006); Spek (2003).
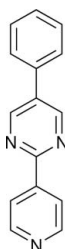
Experimental

Crystal data

$C_{15}H_{11}N_3$	$\gamma = 75.788$ (3)°
$M_r = 233.27$	$V = 1109.54$ (10) Å^3
Triclinic, $P\bar{1}$	$Z = 4$
$a = 9.2813$ (5) Å	Cu $K\alpha$ radiation
$b = 9.3609$ (5) Å	$\mu = 0.68$ mm^{-1}
$c = 13.9001$ (7) Å	$T = 100$ (2) K
$\alpha = 71.462$ (2)°	$0.40 \times 0.38 \times 0.08$ mm
$\beta = 86.957$ (2)°	

Data collection

Bruker SMART 6000 diffractometer	15167 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3967 independent reflections
	3226 reflections with $I > 2\sigma(I)$
$T_{min} = 0.734$, $T_{max} = 0.947$	$R_{int} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	325 parameters
$wR(F^2) = 0.139$	H-atom parameters constrained
$S = 1.00$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
3967 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···N5^i	0.95	2.55	3.3818 (18)	147
C9—H9···N6^{ii}	0.95	2.56	3.4027 (18)	148
C22—H22···N2^i	0.95	2.54	3.3784 (18)	147
C24—H24···N3^{ii}	0.95	2.56	3.4049 (19)	149
C1—H1···Cg3^{iii}	0.95	2.91	3.5925 (15)	129
C4—H4···Cg3	0.95	2.72	3.4163 (15)	130
C12—H12···Cg1^i	0.95	2.89	3.5844 (15)	131
C15—H15···Cg1^{iv}	0.95	2.92	3.5202 (15)	122
C17—H17···Cg6^v	0.95	2.84	3.5561 (16)	133
C20—H20···Cg6^{ii}	0.95	2.85	3.5251 (15)	129
C26—H26···Cg5	0.95	2.86	3.5242 (15)	128
C29—H29···Cg5^{vi}	0.95	2.77	3.4451 (15)	129

Symmetry codes: (i) $-x, -y + 2, -z + 2$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $x - 1, y, z$; (iv) $-x, -y + 1, -z + 2$; (v) $-x + 1, -y + 2, -z + 2$; (vi) $x + 1, y, z$. Cg1 is the centroid of the N1/C1–C5 ring, Cg3 is the centroid of the N4/C16–C20 ring, Cg5 is the centroid of the C10–C15 ring and Cg6 is the centroid of the C25–C30 ring.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: UdMX (local program).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2593).

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Fang, Y.-Q., Taylor, N. J., Laverdière, F., Hanan, G. S., Loiseau, F., Nastasi, F., Campagna, S., Nierengarten, H., Leize-Wagner, E. & Van Dorsselaer, A. (2007). Inorg. Chem. **46**, 2854–2863.
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supplementary materials

5-Phenyl-2-(4-pyridyl)pyrimidine

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Comment

Ruthenium polypyridyl complexes have long attracted attention due to their exceptional photophysical properties which makes them suitable as chromophores in light-harvesting devices (Medlycott & Hanan, 2005, 2006). Recently, we have reported new pyrimidine-substituted terpyridine ligands and their Ru(II) polypyridyl complexes (Fang *et al.*, 2002, 2007). Introduction of the pyrimidine motif on a terpyridine unit leads to planarization of the system through hydrogen bonds, thus extending pi-delocalization in the acceptor ligand of the metal-to-ligand charge transfer (MLCT) emitting excited-states, which improves the photophysical properties of the complexes. The title compound $C_{15}H_{11}N_3$ (3) [see Fig. 3] was designed for the enhanced π-acceptor character of pyridyl-type ligands for coordination and supramolecular chemistry.

The title compound crystallizes with two molecules per asymmetric unit. The assignment of the nitrogen atoms was confirmed by comparing the observed and expected torsion angles and bond lengths. Ligand (3) is less planar than the terpyridyl analogue (Fang *et al.*, 2007) despite weak intramolecular C—H⋯lone pair (N) interactions. All non-bonded N⋯H distances are shorter than 2.75 Å [N2⋯H2 = 2.57 Å, N3⋯H4 = 2.57 Å, N5⋯H17 = 2.62 Å, N6⋯H19 = 2.51 Å]. The dihedral angles between the phenyl and pyridine rings in each molecule are 53.48 (5)° and 50.80 (5)°. These deviations from planarity, in part, may be influenced by weak intermolecular C—H⋯N hydrogen bonds connecting molecules into one-dimensional chains and in addition, by the crystal structure being stabilized by weak C—H⋯π stacking interactions between "head-to-tail" molecules.

Experimental

4-Pyridylamidine hydrochloride (1) (10,0 g, 63.5 mmol), 2-phenyl-1,3-bis(dimethylamino)trimethinium hexafluorophosphate (2) (1 eq, 22.1 g, 63.5 mmol) and NaOMe (1.2 eq, 4.13 g, 76.5 mmol) were dissolved in anhydrous MeOH (500 ml). The resulting yellow solution was refluxed for 15 h under N_2. The white solid was isolated by filtration and dried under vacuum to give white shiny micro-crystals (11.0 g, 74%) of pure title compound (3). These crystals were suitable for X-ray diffraction measurements, m.p. 477.8–478.5 K. Anal Calcd for $C_{15}H_{11}N_3$ (233.3): C, 77.23; H, 4.75; N, 18.01. Found: C, 77.04; H, 4.69; N, 17.86.

Refinement

H atoms were generated geometrically (C—H = 0.95 Å) and were included in the refinement in the riding model approximation; their temperature factors were set to 1.2 times those of the equivalent isotropic temperature factors of the parent site. A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 2003).

supplementary materials

Figures
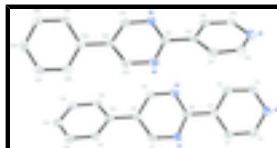
Fig. 1. The asymmetric unit with thermal ellipsoids shown at 50% probability levels. H atoms have been omitted.
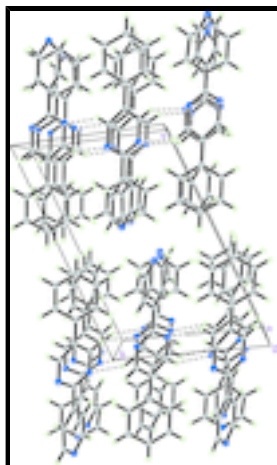
Fig. 2. Part of the crystal structure of (3). Hydrogen bonds are shown as dashed lines. Ellipsoids are shown at the 30% probabilty level.
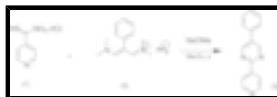
Fig. 3. The reaction scheme for the title compound.

5-Phenyl-2-(4-pyridyl)pyrimidine

Crystal data

$C_{15}H_{11}N_3$	$Z = 4$
$M_r = 233.27$	$F(000) = 488$
Triclinic, $P\bar{1}$	$D_x = 1.396$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 9.2813$ (5) Å	Cell parameters from 5655 reflections
$b = 9.3609$ (5) Å	$\theta = 3.4$–68.9°
$c = 13.9001$ (7) Å	$\mu = 0.68$ mm^{-1}
$\alpha = 71.462$ (2)°	$T = 100$ K
$\beta = 86.957$ (2)°	Block, colourless
$\gamma = 75.788$ (3)°	$0.40 \times 0.38 \times 0.08$ mm
$V = 1109.54$ (10) Å^3	

Data collection

Bruker SMART 6000 diffractometer	3967 independent reflections
Radiation source: Rotating anode	3226 reflections with $I > 2\sigma(I)$
Montel 200 optics	$R_{int} = 0.046$
Detector resolution: 5.5 pixels mm^{-1}	$\theta_{max} = 68.9°$, $\theta_{min} = 3.4°$

ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$k = -11 \rightarrow 11$
$T_{min} = 0.734$, $T_{max} = 0.947$	$l = -16 \rightarrow 16$
15167 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.139$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0925P)^2 + 0.1892P]$ where $P = (F_o^2 + 2F_c^2)/3$
3967 reflections	$(\Delta/\sigma)_{max} = 0.001$
325 parameters	$\Delta\rho_{max} = 0.27$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.30$ e Å^{-3}

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	$U_{iso}*/U_{eq}$
N1	−0.09769 (12)	0.44347 (13)	1.42209 (9)	0.0235 (3)
N2	−0.12326 (12)	0.79515 (13)	1.05916 (8)	0.0215 (3)
N3	0.10382 (12)	0.60327 (13)	1.06789 (9)	0.0230 (3)
C28	0.60351 (14)	1.04795 (15)	0.59991 (10)	0.0230 (3)
H28	0.6235	1.0980	0.5313	0.028*
C24	0.59612 (14)	0.67217 (15)	0.96148 (10)	0.0211 (3)
H24	0.6697	0.6196	0.9262	0.025*
C22	0.40977 (14)	0.89133 (15)	0.96659 (10)	0.0210 (3)
H22	0.3519	0.9935	0.9349	0.025*
C1	−0.20867 (14)	0.54005 (15)	1.35782 (10)	0.0222 (3)
H1	−0.3061	0.5581	1.3835	0.027*
C2	−0.18962 (14)	0.61497 (15)	1.25624 (10)	0.0206 (3)
H2	−0.2717	0.6841	1.2144	0.025*

C3	−0.04783 (14)	0.58719 (14)	1.21624 (10)	0.0188 (3)
C4	0.06828 (14)	0.48702 (15)	1.28198 (10)	0.0204 (3)
H4	0.1664	0.4647	1.2580	0.025*
C5	0.03846 (14)	0.42042 (15)	1.38280 (10)	0.0218 (3)
H5	0.1193	0.3543	1.4270	0.026*
C6	−0.02146 (13)	0.66572 (15)	1.10832 (10)	0.0190 (3)
C7	−0.09684 (14)	0.86669 (15)	0.96277 (10)	0.0207 (3)
H7	−0.1671	0.9585	0.9265	0.025*
C8	0.02937 (13)	0.81303 (14)	0.91253 (10)	0.0191 (3)
C9	0.12654 (14)	0.67759 (15)	0.97125 (10)	0.0224 (3)
H9	0.2138	0.6359	0.9407	0.027*
C10	0.05403 (13)	0.89220 (15)	0.80502 (10)	0.0192 (3)
C11	0.00409 (13)	1.05394 (15)	0.76275 (10)	0.0203 (3)
H11	−0.0429	1.1139	0.8045	0.024*
C12	0.02259 (14)	1.12719 (15)	0.66058 (10)	0.0217 (3)
H12	−0.0111	1.2368	0.6330	0.026*
C13	0.09030 (14)	1.04032 (16)	0.59868 (10)	0.0223 (3)
H13	0.1021	1.0903	0.5287	0.027*
C14	0.14063 (14)	0.88000 (15)	0.63960 (10)	0.0227 (3)
H14	0.1872	0.8206	0.5974	0.027*
C15	0.12309 (13)	0.80658 (15)	0.74159 (10)	0.0202 (3)
H15	0.1582	0.6971	0.7689	0.024*
C29	0.71673 (14)	0.94102 (15)	0.66453 (10)	0.0221 (3)
H29	0.8144	0.9178	0.6400	0.027*
C30	0.68821 (13)	0.86809 (15)	0.76430 (10)	0.0197 (3)
H30	0.7664	0.7944	0.8077	0.024*
C25	0.54460 (14)	0.90173 (15)	0.80227 (10)	0.0186 (3)
C26	0.43120 (14)	1.00916 (15)	0.73613 (10)	0.0203 (3)
H26	0.3332	1.0326	0.7601	0.024*
C27	0.46033 (15)	1.08163 (15)	0.63604 (10)	0.0230 (3)
H27	0.3825	1.1545	0.5919	0.028*
C23	0.51637 (13)	0.82266 (15)	0.90904 (10)	0.0184 (3)
N6	0.57446 (11)	0.59835 (13)	1.05838 (8)	0.0210 (3)
C21	0.46901 (13)	0.67626 (15)	1.10567 (10)	0.0187 (3)
N5	0.38525 (12)	0.82082 (12)	1.06340 (8)	0.0211 (3)
C18	0.44441 (13)	0.59364 (15)	1.21314 (10)	0.0186 (3)
C19	0.49348 (13)	0.43229 (15)	1.25172 (10)	0.0203 (3)
H19	0.5441	0.3745	1.2097	0.024*
C20	0.46761 (14)	0.35763 (15)	1.35169 (10)	0.0215 (3)
H20	0.4998	0.2476	1.3760	0.026*
N4	0.39970 (12)	0.43088 (13)	1.41673 (8)	0.0238 (3)
C16	0.35492 (14)	0.58659 (16)	1.37925 (10)	0.0231 (3)
H16	0.3079	0.6415	1.4238	0.028*
C17	0.37312 (13)	0.67179 (16)	1.27954 (10)	0.0207 (3)
H17	0.3377	0.7816	1.2568	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0246 (6)	0.0248 (6)	0.0228 (6)	−0.0064 (5)	−0.0001 (5)	−0.0092 (5)
N2	0.0197 (5)	0.0236 (6)	0.0209 (6)	−0.0007 (5)	−0.0027 (4)	−0.0095 (5)
N3	0.0199 (5)	0.0226 (6)	0.0238 (6)	−0.0003 (5)	0.0001 (5)	−0.0071 (5)
C28	0.0266 (7)	0.0257 (7)	0.0181 (7)	−0.0088 (6)	0.0001 (5)	−0.0070 (6)
C24	0.0192 (6)	0.0235 (7)	0.0211 (7)	−0.0017 (5)	−0.0004 (5)	−0.0104 (6)
C22	0.0198 (6)	0.0187 (6)	0.0229 (7)	−0.0011 (5)	−0.0013 (5)	−0.0068 (5)
C1	0.0192 (6)	0.0252 (7)	0.0250 (7)	−0.0050 (5)	0.0014 (5)	−0.0119 (6)
C2	0.0174 (6)	0.0218 (7)	0.0243 (7)	−0.0032 (5)	−0.0030 (5)	−0.0102 (6)
C3	0.0191 (6)	0.0176 (6)	0.0215 (7)	−0.0033 (5)	−0.0019 (5)	−0.0090 (5)
C4	0.0173 (6)	0.0208 (6)	0.0254 (7)	−0.0033 (5)	−0.0016 (5)	−0.0108 (6)
C5	0.0205 (6)	0.0209 (6)	0.0234 (7)	−0.0029 (5)	−0.0046 (5)	−0.0070 (6)
C6	0.0165 (6)	0.0191 (6)	0.0225 (7)	−0.0019 (5)	−0.0035 (5)	−0.0094 (6)
C7	0.0199 (6)	0.0213 (7)	0.0197 (7)	−0.0001 (5)	−0.0047 (5)	−0.0078 (5)
C8	0.0182 (6)	0.0194 (7)	0.0212 (7)	−0.0025 (5)	−0.0035 (5)	−0.0094 (6)
C9	0.0180 (6)	0.0250 (7)	0.0225 (7)	−0.0012 (5)	0.0010 (5)	−0.0080 (6)
C10	0.0135 (6)	0.0229 (7)	0.0225 (7)	−0.0037 (5)	−0.0025 (5)	−0.0090 (6)
C11	0.0171 (6)	0.0225 (7)	0.0230 (7)	−0.0028 (5)	−0.0029 (5)	−0.0106 (6)
C12	0.0194 (6)	0.0208 (6)	0.0247 (7)	−0.0041 (5)	−0.0049 (5)	−0.0064 (6)
C13	0.0211 (6)	0.0283 (7)	0.0191 (7)	−0.0085 (6)	−0.0010 (5)	−0.0075 (6)
C14	0.0187 (6)	0.0285 (7)	0.0257 (7)	−0.0066 (5)	0.0013 (5)	−0.0145 (6)
C15	0.0160 (6)	0.0193 (6)	0.0256 (7)	−0.0026 (5)	−0.0017 (5)	−0.0085 (6)
C29	0.0200 (6)	0.0279 (7)	0.0228 (7)	−0.0077 (6)	0.0017 (5)	−0.0128 (6)
C30	0.0167 (6)	0.0221 (7)	0.0206 (7)	−0.0016 (5)	−0.0044 (5)	−0.0089 (5)
C25	0.0182 (6)	0.0188 (6)	0.0213 (7)	−0.0040 (5)	−0.0016 (5)	−0.0096 (5)
C26	0.0166 (6)	0.0211 (6)	0.0242 (7)	−0.0030 (5)	−0.0008 (5)	−0.0093 (6)
C27	0.0224 (7)	0.0215 (7)	0.0239 (7)	−0.0032 (5)	−0.0061 (5)	−0.0059 (6)
C23	0.0143 (6)	0.0211 (7)	0.0211 (7)	−0.0030 (5)	−0.0025 (5)	−0.0092 (6)
N6	0.0197 (5)	0.0231 (6)	0.0197 (6)	−0.0008 (5)	−0.0017 (4)	−0.0090 (5)
C21	0.0154 (6)	0.0209 (7)	0.0214 (7)	−0.0029 (5)	−0.0031 (5)	−0.0094 (6)
N5	0.0195 (5)	0.0203 (6)	0.0214 (6)	−0.0014 (5)	0.0000 (4)	−0.0063 (5)
C18	0.0135 (6)	0.0232 (7)	0.0202 (7)	−0.0038 (5)	−0.0024 (5)	−0.0081 (6)
C19	0.0170 (6)	0.0229 (7)	0.0230 (7)	−0.0031 (5)	−0.0034 (5)	−0.0104 (6)
C20	0.0181 (6)	0.0217 (7)	0.0231 (7)	−0.0030 (5)	−0.0051 (5)	−0.0054 (6)
N4	0.0208 (6)	0.0288 (6)	0.0214 (6)	−0.0051 (5)	−0.0024 (5)	−0.0076 (5)
C16	0.0203 (6)	0.0288 (7)	0.0223 (7)	−0.0043 (6)	−0.0002 (5)	−0.0119 (6)
C17	0.0173 (6)	0.0228 (7)	0.0229 (7)	−0.0026 (5)	−0.0022 (5)	−0.0097 (6)

Geometric parameters (Å, °)

N1—C1	1.3429 (18)	C11—C12	1.3890 (18)
N1—C5	1.3451 (17)	C11—H11	0.95
N2—C7	1.3338 (17)	C12—C13	1.3904 (18)
N2—C6	1.3445 (17)	C12—H12	0.95
N3—C9	1.3344 (17)	C13—C14	1.3911 (19)
N3—C6	1.3474 (16)	C13—H13	0.95

C28—C29	1.3874 (19)	C14—C15	1.3854 (18)
C28—C27	1.3935 (19)	C14—H14	0.95
C28—H28	0.95	C15—H15	0.95
C24—N6	1.3341 (17)	C29—C30	1.3810 (18)
C24—C23	1.3987 (19)	C29—H29	0.95
C24—H24	0.95	C30—C25	1.4068 (18)
C22—N5	1.3321 (17)	C30—H30	0.95
C22—C23	1.4010 (18)	C25—C26	1.3998 (19)
C22—H22	0.95	C25—C23	1.4746 (18)
C1—C2	1.3861 (18)	C26—C27	1.3853 (18)
C1—H1	0.95	C26—H26	0.95
C2—C3	1.3982 (18)	C27—H27	0.95
C2—H2	0.95	N6—C21	1.3446 (16)
C3—C4	1.3924 (19)	C21—N5	1.3442 (17)
C3—C6	1.4829 (18)	C21—C18	1.4825 (18)
C4—C5	1.3847 (18)	C18—C19	1.3962 (19)
C4—H4	0.95	C18—C17	1.3970 (18)
C5—H5	0.95	C19—C20	1.3808 (18)
C7—C8	1.3998 (18)	C19—H19	0.95
C7—H7	0.95	C20—N4	1.3440 (17)
C8—C9	1.3949 (19)	C20—H20	0.95
C8—C10	1.4757 (18)	N4—C16	1.3458 (18)
C9—H9	0.95	C16—C17	1.3871 (19)
C10—C15	1.4027 (18)	C16—H16	0.95
C10—C11	1.4039 (19)	C17—H17	0.95
C1—N1—C5	116.27 (12)	C12—C13—C14	119.78 (13)
C7—N2—C6	116.84 (11)	C12—C13—H13	120.1
C9—N3—C6	116.34 (11)	C14—C13—H13	120.1
C29—C28—C27	119.71 (12)	C15—C14—C13	120.31 (12)
C29—C28—H28	120.1	C15—C14—H14	119.8
C27—C28—H28	120.1	C13—C14—H14	119.8
N6—C24—C23	123.58 (11)	C14—C15—C10	120.70 (12)
N6—C24—H24	118.2	C14—C15—H15	119.6
C23—C24—H24	118.2	C10—C15—H15	119.6
N5—C22—C23	123.44 (12)	C30—C29—C28	120.36 (12)
N5—C22—H22	118.3	C30—C29—H29	119.8
C23—C22—H22	118.3	C28—C29—H29	119.8
N1—C1—C2	123.93 (12)	C29—C30—C25	120.69 (12)
N1—C1—H1	118	C29—C30—H30	119.7
C2—C1—H1	118	C25—C30—H30	119.7
C1—C2—C3	119.00 (12)	C26—C25—C30	118.38 (12)
C1—C2—H2	120.5	C26—C25—C23	121.73 (11)
C3—C2—H2	120.5	C30—C25—C23	119.88 (11)
C4—C3—C2	117.68 (12)	C27—C26—C25	120.69 (12)
C4—C3—C6	121.26 (11)	C27—C26—H26	119.7
C2—C3—C6	121.03 (12)	C25—C26—H26	119.7
C5—C4—C3	118.96 (12)	C26—C27—C28	120.18 (12)
C5—C4—H4	120.5	C26—C27—H27	119.9
C3—C4—H4	120.5	C28—C27—H27	119.9

N1—C5—C4	124.14 (12)	C24—C23—C22	114.48 (12)
N1—C5—H5	117.9	C24—C23—C25	122.19 (11)
C4—C5—H5	117.9	C22—C23—C25	123.33 (12)
N2—C6—N3	125.23 (12)	C24—N6—C21	116.46 (11)
N2—C6—C3	117.34 (11)	N5—C21—N6	125.40 (12)
N3—C6—C3	117.42 (11)	N5—C21—C18	118.22 (11)
N2—C7—C8	123.18 (12)	N6—C21—C18	116.37 (11)
N2—C7—H7	118.4	C22—N5—C21	116.63 (11)
C8—C7—H7	118.4	C19—C18—C17	117.45 (12)
C9—C8—C7	114.70 (12)	C19—C18—C21	120.29 (11)
C9—C8—C10	123.20 (11)	C17—C18—C21	122.26 (12)
C7—C8—C10	122.08 (12)	C20—C19—C18	119.28 (12)
N3—C9—C8	123.71 (11)	C20—C19—H19	120.4
N3—C9—H9	118.1	C18—C19—H19	120.4
C8—C9—H9	118.1	N4—C20—C19	124.09 (12)
C15—C10—C11	118.38 (12)	N4—C20—H20	118
C15—C10—C8	120.59 (12)	C19—C20—H20	118
C11—C10—C8	120.99 (11)	C20—N4—C16	116.18 (12)
C12—C11—C10	120.74 (12)	N4—C16—C17	124.03 (12)
C12—C11—H11	119.6	N4—C16—H16	118
C10—C11—H11	119.6	C17—C16—H16	118
C11—C12—C13	120.08 (12)	C16—C17—C18	118.96 (12)
C11—C12—H12	120	C16—C17—H17	120.5
C13—C12—H12	120	C18—C17—H17	120.5
C5—N1—C1—C2	−0.23 (18)	C27—C28—C29—C30	−0.06 (19)
N1—C1—C2—C3	1.52 (19)	C28—C29—C30—C25	−0.50 (18)
C1—C2—C3—C4	−1.28 (18)	C29—C30—C25—C26	0.86 (18)
C1—C2—C3—C6	−179.38 (11)	C29—C30—C25—C23	−179.99 (11)
C2—C3—C4—C5	−0.09 (18)	C30—C25—C26—C27	−0.67 (18)
C6—C3—C4—C5	178.00 (11)	C23—C25—C26—C27	−179.80 (11)
C1—N1—C5—C4	−1.28 (19)	C25—C26—C27—C28	0.13 (18)
C3—C4—C5—N1	1.46 (19)	C29—C28—C27—C26	0.25 (19)
C7—N2—C6—N3	−0.15 (18)	N6—C24—C23—C22	−0.22 (18)
C7—N2—C6—C3	178.6 (1)	N6—C24—C23—C25	179.12 (11)
C9—N3—C6—N2	−0.02 (19)	N5—C22—C23—C24	0.14 (18)
C9—N3—C6—C3	−178.77 (11)	N5—C22—C23—C25	−179.20 (11)
C4—C3—C6—N2	−158.60 (12)	C26—C25—C23—C24	148.58 (13)
C2—C3—C6—N2	19.42 (17)	C30—C25—C23—C24	−30.54 (17)
C4—C3—C6—N3	20.25 (17)	C26—C25—C23—C22	−32.13 (18)
C2—C3—C6—N3	−161.73 (12)	C30—C25—C23—C22	148.75 (13)
C6—N2—C7—C8	0.11 (18)	C23—C24—N6—C21	0.22 (18)
N2—C7—C8—C9	0.08 (18)	C24—N6—C21—N5	−0.14 (18)
N2—C7—C8—C10	178.41 (11)	C24—N6—C21—C18	179.6 (1)
C6—N3—C9—C8	0.23 (19)	C23—C22—N5—C21	−0.07 (18)
C7—C8—C9—N3	−0.26 (19)	N6—C21—N5—C22	0.07 (19)
C10—C8—C9—N3	−178.57 (11)	C18—C21—N5—C22	−179.67 (11)
C9—C8—C10—C15	33.47 (18)	N5—C21—C18—C19	160.88 (12)
C7—C8—C10—C15	−144.72 (13)	N6—C21—C18—C19	−18.89 (17)
C9—C8—C10—C11	−148.99 (13)	N5—C21—C18—C17	−19.43 (18)

C7—C8—C10—C11	32.82 (18)	N6—C21—C18—C17	160.81 (12)
C15—C10—C11—C12	0.05 (18)	C17—C18—C19—C20	1.14 (18)
C8—C10—C11—C12	−177.54 (11)	C21—C18—C19—C20	−179.15 (10)
C10—C11—C12—C13	0.43 (18)	C18—C19—C20—N4	−1.45 (19)
C11—C12—C13—C14	−0.57 (19)	C19—C20—N4—C16	0.40 (18)
C12—C13—C14—C15	0.24 (19)	C20—N4—C16—C17	0.95 (19)
C13—C14—C15—C10	0.25 (18)	N4—C16—C17—C18	−1.19 (19)
C11—C10—C15—C14	−0.39 (18)	C19—C18—C17—C16	0.08 (18)
C8—C10—C15—C14	177.20 (11)	C21—C18—C17—C16	−179.62 (11)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···N5[i]	0.95	2.55	3.3818 (18)	147
C9—H9···N6[ii]	0.95	2.56	3.4027 (18)	148
C22—H22···N2[i]	0.95	2.54	3.3784 (18)	147
C24—H24···N3[ii]	0.95	2.56	3.4049 (19)	149
C1—H1···Cg3[iii]	0.95	2.91	3.5925 (15)	129.
C4—H4···Cg3	0.95	2.72	3.4163 (15)	130.
C12—H12···Cg1[i]	0.95	2.89	3.5844 (15)	131.
C15—H15···Cg1[iv]	0.95	2.92	3.5202 (15)	122.
C17—H17···Cg6[v]	0.95	2.84	3.5561 (16)	133.
C20—H20···Cg6[ii]	0.95	2.85	3.5251 (15)	129.
C26—H26···Cg5	0.95	2.86	3.5242 (15)	128.
C29—H29···Cg5[vi]	0.95	2.77	3.4451 (15)	129.

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

Fig. 1

Fig. 2

Fig. 3