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N—H···N hydrogen bonding in 4,6-diphenyl-2-pyrimidinylamine isolated from the plant *Justicia secunda* (Acanthaceae)

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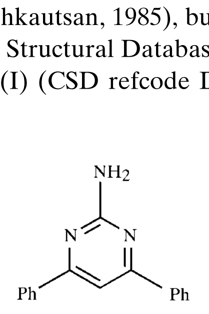
The title compound, $C_{16}H_{13}N_3$, isolated from *Justicia secunda* (Acanthaceae), comprises two molecules (which differ slightly in conformation) in the asymmetric unit of space group $P\overline{1}$. Intermolecular N_{amino}—H···N_{pyrm} interactions (N_{pyrm} is a pyrimidine ring N atom) involve only one of the two donor amino H atoms and pyrimidine N atoms per molecule, forming dimeric units *via* $R_2^2(8)$ rings, with N···N distances of 3.058 (2) and 3.106 (3) Å, and N—H···N angles of 172.7 (18) and 175.8 (17)°. The dimers are linked by C—H···π(arene) contacts, with an H···centroid distance of 2.77 Å and a C—H···centroid angle of 141°.

Comment

The title compound, 4,6-diphenyl-2-pyrimidinylamine, (I), was isolated as a natural product from the plant *Justicia secunda* (Acanthaceae) collected in Trinidad, West Indies. The parent structure, *viz.* 4,6-diphenyl-1,2-dihydropyrimidine, has been reported (Weis & Vishkautsan, 1985), but the coordinates are not in the Cambridge Structural Database (CSD; Allen, 2002) for comparison with (I) (CSD refcode DEZMEA for parent compound).



(I)

Compound (I) crystallizes in space group $P\overline{1}$ (No. 2) with two independent molecules, *A* and *B*, in the asymmetric unit, which differ slightly in conformation (Fig. 1). Bond lengths and angles are largely unexceptional and in accord with anticipated values (Orpen *et al.*, 1994); selected dimensions are given in Table 1. The central C—N bond lengths range from 1.340 (2) to 1.346 (2) Å, while the aromatic C—C distances are in the range 1.381 (3)–1.387 (3) Å. Torsion-angle differences are evident from analysis of the N1—C4—C21—C26 angles, which are −29.8 (3) and 36.5 (3)° in molecules *A* and *B*, respectively (Table 1). Even more dramatic is the difference in dihedral angles between the C11–C16 and C21–C26 planes, which are 52.15 (7) and 31.79 (7)° in molecules *A* and *B*, respectively. The weighted (unit weight) r.m.s. fit for the superposition of the non-H atoms in both molecules is 0.65 Å (0.55 Å) (Spek, 2003).

Molecules *A* and *B* associate in pairs through N_{amino}—H···N_{pyrm} intermolecular interactions (N_{pyrm} is a pyrimidine ring N atom), which only involve two of the four amino donor H atoms and N pyrimidine acceptors per *A*/*B* pair. The N···N distances are 3.058 (2) and 3.106 (3) Å, and the N—H···N angles are 172.7 (18) and 175.8 (17)° (Table 2), thus forming a hydrogen-bonded ring with an $R_2^2(8)$ graph set similar to that observed in centrosymmetric carboxylic acid pairs. A C—H···π(arene) contact from C12*A*—H12*A* to the C21*A*–C26*A* ring links the dimeric units into a dimer of dimers, which is further augmented *via* a contact from C26*A*—H26*A* group to the N1*A*/N2*A*/C1*A*–C4*A* ring into a one-dimensional stack (Fig. 2 and Table 2). These are the only contacts of note in the structure of (I), apart from the N—H···N hydrogen bonding.

Examination of the structure of (I) for interactions involving N2*A*/N2*B* reveals that, along the *b* direction, atom H24*A* (a potential donor) is 2.99 Å from N2*A*^{i}, with a C24*A*—H24*A*···N2*A*^{i} angle of 163° [symmetry code: (i) *x*, 1 + *y*, *z*]. Likewise, the closest N···H intermolecular distance involving atom N2*B* is N2*B*···H24*B*^{i} of 3.08 Å, with an N2*B*···H24*B*^{i}—C24*B*^{i} angle of 155°. Neither of these interactions constitutes a hydrogen bond.

Inspection of Fig. 2 shows the dimeric units in a two-dimensional cross-section through the crystal structure parallel to the [101] plane. In the crystal structure, a more efficient packing could involve dimer formation about inversion centres, which would necessitate rotation of the phenyl rings to align and fulfil symmetry requirements, *e.g.* the phenyl rings have interplanar angles of 52.12 (7) and 31.79 (7)° in molecules *A* and *B*, respectively. The reason why this does not arise is due to the initial hydrogen-bonded dimer formation. Utilization of only half of the N—H···N donor/acceptors per *A*/*B* hydrogen-bonded dimer prevents the N2*A*/N2*B* pair from forming hydrogen bonds, as potential (C)N—H···N donor/acceptor pairs cannot approach one another and because of the concurrent formation of unfavourable H···H contacts. Interactions in (I) are therefore limited to the two N—H···N interactions per *A*/*B* pair.

Ab initio calculations on (I) gave results similar to those observed in molecules *A* and *B*. Calculations were undertaken at the $6\text{-}31^{+}G(d)$ level in the search for a local minimum for comparison with molecules *A* and *B*, using *GAUSSIAN*03 (Frisch *et al.*, 2003). The N—C—C—C torsion angles are 27.55°, similar to the value of −29.8 (3)° found in molecule *A*.

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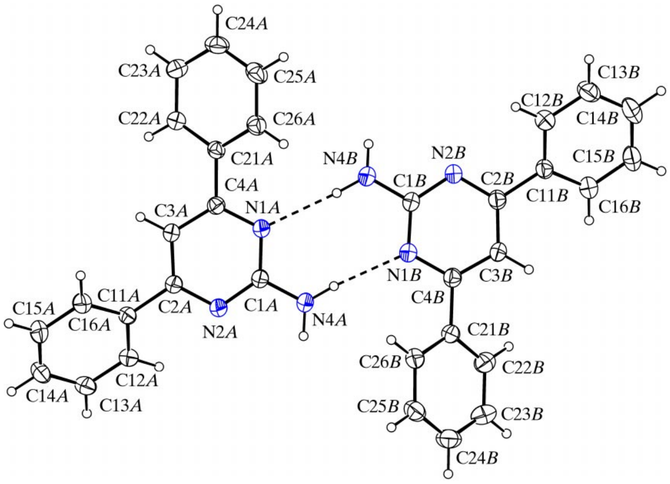

Figure 1
A view of the two independent molecules in (I) as a hydrogen-bonded dimer, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

The $H_2N—C$ distance is 1.362 Å and the N—C—N angle is 116.79° [range 116.15 (17)–117.05 (17)° in molecule *A*]. Overall, the calculated results resemble those of molecule *A*. However, no attempt was made to find the global minimum in the system.

Crystal structures with more than one molecule present in the asymmetric unit are not uncommon (Steiner, 2000; Gallagher *et al.*, 1998). Recently, Görbitz (2002, 2003) has reported on dipeptide derivatives, *e.g.* two forms of L-valyl-L-phenylalanine trihydrate ($P2_1$, $Z = 16$, $Z' = 8$; $P2_12_12_1$, $Z = 4$, $Z' = 1$) and L-methionyl-L-alanine ($P6_1$, $Z = 42$, $Z' = 7$), which provide rare examples of systems with $Z' = 8$ and 7 molecules in their respective asymmetric units, in contrast with $Z' = 2$, which is not uncommon. Analysis of the CSD (February 2004, version 5.25; Allen, 2002) reveals a total of 65 935 crystal structures in space group $P\overline{1}$ (No. 2) (and equivalents with no restrictions), 7625 with $Z' > 1$, some 11.6% of the total, and 6775 with $Z' = 2$. No attempt was made to examine incorrect space groups.

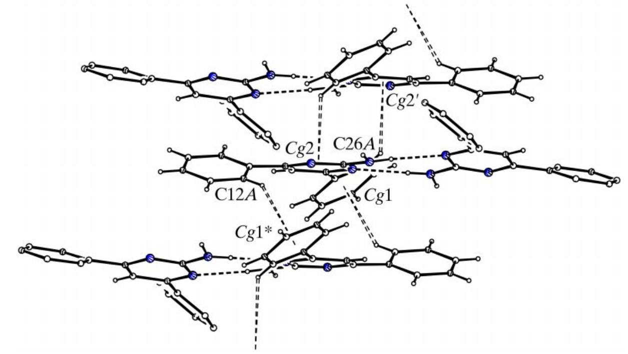

Figure 2
A view of the dimeric units in (I) linked by C—H···π(arene) interactions. Atoms are depicted as small spheres of arbitrary sizes. The ten phenyl-ring H atoms in molecule *B* have been omitted for clarity. The centroid labels are as defined in Table 2, and the centroids labelled with an asterisk (*) or a prime (′) are at symmetry positions (i) and (ii), respectively, given in Table 2.

Experimental

The plant *Justicia secunda* (Acanthaceae) was collected in Trinidad, West Indies, and dried at 308–313 K. A large quantity (1 kg) of this dried powdered plant (except root and flower/fruit) was placed in a large separating funnel and soaked in acetone overnight. The acetone layer was collected and the process repeated until the acetone layer became faintly green in colour. The combined acetone extracts were evaporated and the dry mass extracted with benzene. The benzene-soluble fraction was dried, dissolved in the minimum amount of dry warm $CHCl_3$ and spread over activated silica gel in a sintered glass Buchner funnel. It was then eluted with 50 ml portions of benzene and then a $CHCl_3$–benzene mixture (1:4) under a slight vacuum. The fraction obtained from $CHCl_3$–benzene (1:4) was collected and the solvent removed. It was then subjected to column chromatography with light petroleum (b.p. 313–333 K) and benzene. After concentration, the benzene fraction yielded gummy crystals upon refrigeration. These crystals were further purified by preparative chromatography to afford the pure title compound, (I), as well shaped crystals from $CHCl_3$.

Crystal data

$C_{16}H_{13}N_3$
$M_r = 247.29$
Triclinic, $P\overline{1}$
$a = 7.8263$ (9) Å
$b = 10.8009$ (9) Å
$c = 15.7878$ (12) Å
$\alpha = 83.457$ (5)°
$\beta = 77.039$ (7)°
$\gamma = 82.326$ (7)°
$V = 1284.0$ (2) Å^3

$Z = 4$
$D_x = 1.279$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 74 reflections
$\theta = 5.4$–17.9°
$\mu = 0.08$ mm^{-1}
$T = 294$ (1) K
Plate, colourless
0.50 × 0.30 × 0.08 mm

Data collection

Siemens *P*4 diffractometer
$\omega/2\theta$ scans
5607 measured reflections
4529 independent reflections
2987 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\rm max} = 25.0°$

$h = -9 \rightarrow 1$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$
4 standard reflections every 296 reflections intensity decay: 1%

Table 1
Selected geometric parameters (Å, °).

N1*A*—C1*A*	1.345 (2)	N1*B*—C1*B*	1.346 (2)
N1*A*—C4*A*	1.346 (2)	N1*B*—C4*B*	1.343 (2)
N2*A*—C1*A*	1.343 (2)	N2*B*—C1*B*	1.343 (2)
N2*A*—C2*A*	1.340 (2)	N2*B*—C2*B*	1.340 (2)
N4*A*—C1*A*	1.357 (2)	N4*B*—C1*B*	1.347 (2)
C2*A*—C3*A*	1.385 (2)	C2*B*—C3*B*	1.381 (3)
C2*A*—C11*A*	1.488 (2)	C2*B*—C11*B*	1.488 (3)
C3*A*—C4*A*	1.384 (2)	C3*B*—C4*B*	1.387 (3)
C4*A*—C21*A*	1.481 (2)	C4*B*—C21*B*	1.484 (3)
N1*A*—C1*A*—N2*A*	126.76 (17)	N1*B*—C1*B*—N2*B*	126.72 (17)
N1*A*—C1*A*—N4*A*	117.05 (17)	N1*B*—C1*B*—N4*B*	116.73 (18)
N2*A*—C1*A*—N4*A*	116.15 (17)	N2*B*—C1*B*—N4*B*	116.55 (18)
N1*A*—C4*A*—C21*A*—C26*A*	−29.8 (3)	N1*B*—C4*B*—C21*B*—C26*B*	−36.5 (3)
C3*A*—C4*A*—C21*A*—C26*A*	151.83 (19)	C3*B*—C4*B*—C21*B*—C26*B*	142.9 (2)
C3*A*—C2*A*—C11*A*—C12*A*	149.4 (2)	C3*B*—C2*B*—C11*B*—C12*B*	−152.6 (2)

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 1.01$
4529 reflections
359 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.13P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 2
Hydrogen-bonding and contact geometry (Å, °) for compound (I).

*Cg*1 and *Cg*2 represent the centroids of the rings C21*A*–C26*A* and N1*A*/N2*A*/C1*A*–C4*A*, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N4*A*—H1*A*···N1*B*	0.89 (2)	2.17 (2)	3.058 (2)	172.7 (18)
N4*B*—H2*B*···N1*A*	0.91 (2)	2.20 (2)	3.106 (3)	175.8 (17)
C12*A*—H12*A*···*Cg*1$^{\rm i}$	0.93	2.77	3.538 (2)	141
C26*A*—H26*A*···*Cg*2$^{\rm ii}$	0.93	2.78	3.393 (2)	124

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

Compound (I) crystallized in the triclinic system, the systematic absences permitting space group $P1$ or $P\overline{1}$; $P\overline{1}$ was assumed and confirmed by the analysis. All H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.93 Å, while the four amino H atoms were refined with isotropic displacement parameters, giving N—H distances in the range 0.89 (2)–0.91 (2) Å.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *NRCVAX*96 (Gabe *et al.*, 1989), *SHELXL*97 and *PREP*8 (Ferguson, 1998).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1292). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *NRCVAX96* (Gabe *et al.*, 1989), *SHELXL97* and PREP8 (Ferguson, 1998).

4,6-diphenyl-2-pyrimidinylamine

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c = 15.7878 (12) Å
α = 83.457 (5)°
β = 77.039 (7)°
γ = 82.326 (7)°
V = 1284.0 (2) Å^3

Z = 4
F(000) = 520
D_x = 1.279 Mg m^{-3}
Melting point: 408 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 74 reflections
θ = 5.4–17.9°
μ = 0.08 mm^{-1}
T = 294 K
Plate, colourless
0.50 × 0.30 × 0.08 × not measured (radius) mm

Data collection

Siemens P4
diffractometer
Radiation source: X-ray tube
Graphite monochromator
$\omega/2\theta$ scans
5607 measured reflections
4529 independent reflections
2987 reflections with $I > 2\sigma(I)$

R_{int} = 0.019
$\theta_{\max}$ = 25.0°, $\theta_{\min}$ = 1.9°
$h = -9 \rightarrow 1$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$
4 standard reflections every 296 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.119
S = 1.01
4529 reflections

359 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
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.13P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Geometry. Gaussian '03 reference =====================

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, *M*. A. Robb, J. *R*. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. *M*. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, *M*. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, *M*. Hada, *M*. Ehara, K. Toyota, *R*. Fukuda, J. Hasegawa, *M*. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, *M*. Klene, *X*. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, *R*. Gomperts, *R*. E. Stratmann, O. Yazyev, A. J. Austin, *R*. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, *M*. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, *R*. *L*. Martin, D. J. Fox, T. Keith, *M*. A. Al-Laham, C. Y. Peng, A. Nanayakkara, *M*. Challacombe, P. *M*. W. Gill, B. Johnson, W. Chen, *M*. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

Torsional angles #==============

Dihedral angle NCCC

−29.81 (26) N1A–C4A–C21A–C26A −36.46 (27) N1B–C4B–C21B–C26B 154.15 (18) N2A–C2A–C11A–C16A −152.50 (19) N2B–C2B–C11B–C16B

Dihedral angle CCCC

106.98 (22) C12A–C11A–C21A–C22A −170.55 (24) C12B–C11B–C21B–C22B 1.34 (32) C14A–C2A–C4A–C24A −1.40 (34) C14B–C2B–C4B–C24B

Mean plane data ex-*SHELXL97* for molecule (I) ##

Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

$-5.8182(0.0047)x + 6.0658(0.0079)y - 2.5280(0.0137)z = 2.8570(0.0128)$

* 0.0067 (0.0013) C11A * −0.0072 (0.0014) C12A * 0.0012 (0.0015) C13A * 0.0053 (0.0016) C14A * −0.0057 (0.0016) C15A * −0.0003 (0.0015) C16A

Rms deviation of fitted atoms = 0.0051

$7.2778(0.0022)x - 1.3368(0.0077)y + 7.0895(0.0113)z = 4.0232(0.0104)$

Angle to previous plane (with approximate e.s.d.) = 29.31 (8)

* 0.0120 (0.0013) C1A * −0.0045 (0.0013) C2A * 0.0136 (0.0013) C3A * −0.0108 (0.0013) C4A * −0.0020 (0.0012) N1A * −0.0082 (0.0012) N2A 0.0009 (0.0029) N4A

Rms deviation of fitted atoms = 0.0095

$5.4509(0.0048)x + 0.0533(0.0089)y + 13.2611(0.0074)z = 8.3696(0.0127)$

Angle to previous plane (with approximate e.s.d.) = 30.48 (8)

* −0.0048 (0.0013) C21A * 0.0072 (0.0014) C22A * −0.0026 (0.0016) C23A * −0.0045 (0.0015) C24A * 0.0068 (0.0015) C25A * −0.0021 (0.0014) C26A

Rms deviation of fitted atoms = 0.0050

$-5.8182(0.0047)x + 6.0658(0.0079)y - 2.5280(0.0137)z = 2.8570(0.0128)$

Angle to previous plane (with approximate e.s.d.) = 52.15 (7)

* 0.0067 (0.0013) C11A * −0.0072 (0.0014) C12A * 0.0012 (0.0015) C13A * 0.0053 (0.0016) C14A * −0.0057 (0.0016) C15A * −0.0003 (0.0015) C16A

Rms deviation of fitted atoms = 0.0051

$-6.9426(0.0035)x + 3.6543(0.0097)y - 2.9128(0.0142)z = 2.8663(0.0190)$

Angle to previous plane (with approximate e.s.d.) = 14.50 (11)

* −0.0005 (0.0014) C11B * 0.0078 (0.0015) C12B * −0.0089 (0.0017) C13B * 0.0028 (0.0017) C14B * 0.0045 (0.0016) C15B * −0.0056 (0.0015) C16B

Rms deviation of fitted atoms = 0.0058

$7.5633(0.0019)x + 0.8967(0.0086)y + 7.2350(0.0118)z = 6.2720(0.0176)$

Angle to previous plane (with approximate e.s.d.) = 27.74 (6)

* −0.0114 (0.0014) C1B * 0.0099 (0.0014) C2B * −0.0051 (0.0014) C3B * −0.0071 (0.0013) C4B * 0.0153 (0.0013) N1B * −0.0015 (0.0013) N2B −0.0378 (0.0033) N4B

Rms deviation of fitted atoms = 0.0095

$-7.1932(0.0030)x - 0.2947(0.0097)y + 2.7303(0.0144)z = 5.5969(0.0173)$

Angle to previous plane (with approximate e.s.d.) = 37.24 (5)

* −0.0060 (0.0014) C21B * −0.0018 (0.0016) C22B * 0.0059 (0.0017) C23B * −0.0022 (0.0017) C24B * −0.0056 (0.0016) C25B * 0.0097 (0.0015) C26B

Rms deviation of fitted atoms = 0.0058

$-6.9426(0.0035)x + 3.6543(0.0097)y - 2.9128(0.0142)z = 2.8663(0.0190)$

Angle to previous plane (with approximate e.s.d.) = 31.79 (7)

* −0.0005 (0.0014) C11B * 0.0078 (0.0015) C12B * −0.0089 (0.0017) C13B * 0.0028 (0.0017) C14B * 0.0045 (0.0016) C15B * −0.0056 (0.0015) C16B

Rms deviation of fitted atoms = 0.0058

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

	x	y	z	U_{iso}*/U_{eq}
N1A	0.2906 (2)	0.98395 (14)	0.45438 (9)	0.0400 (4)
N2A	0.1831 (2)	0.79337 (13)	0.52793 (10)	0.0414 (4)
N4A	0.3263 (3)	0.80359 (18)	0.38421 (12)	0.0534 (5)
C1A	0.2662 (2)	0.86235 (17)	0.45848 (12)	0.0398 (5)
C2A	0.1229 (2)	0.85133 (16)	0.60125 (11)	0.0379 (4)
C3A	0.1455 (3)	0.97573 (17)	0.60400 (12)	0.0431 (5)
C4A	0.2277 (2)	1.04082 (16)	0.52846 (12)	0.0380 (4)
C11A	0.0241 (2)	0.77766 (16)	0.67766 (12)	0.0409 (5)
C12A	−0.0673 (3)	0.68216 (17)	0.66437 (13)	0.0457 (5)
C13A	−0.1672 (3)	0.61669 (19)	0.73382 (14)	0.0562 (6)
C14A	−0.1751 (3)	0.6447 (2)	0.81763 (15)	0.0627 (6)
C15A	−0.0830 (3)	0.7372 (2)	0.83208 (14)	0.0619 (6)
C16A	0.0159 (3)	0.80401 (19)	0.76258 (13)	0.0534 (5)
C21A	0.2457 (2)	1.17614 (16)	0.52505 (11)	0.0377 (4)
C22A	0.1199 (3)	1.25391 (17)	0.57738 (12)	0.0468 (5)
C23A	0.1299 (3)	1.38105 (19)	0.57199 (14)	0.0562 (6)
C24A	0.2672 (3)	1.4328 (2)	0.51521 (15)	0.0595 (6)
C25A	0.3950 (3)	1.3568 (2)	0.46384 (14)	0.0569 (6)
C26A	0.3841 (3)	1.22946 (18)	0.46815 (12)	0.0464 (5)
N4B	0.4727 (3)	1.10820 (19)	0.27553 (13)	0.0658 (6)
N1B	0.5567 (2)	0.91786 (14)	0.21871 (10)	0.0446 (4)
N2B	0.6145 (2)	1.11152 (14)	0.13196 (10)	0.0487 (4)
C1B	0.5502 (3)	1.04366 (18)	0.20622 (12)	0.0458 (5)
C2B	0.6895 (3)	1.04656 (17)	0.06315 (12)	0.0426 (5)
C3B	0.6976 (3)	0.91746 (17)	0.06856 (12)	0.0464 (5)
C4B	0.6286 (2)	0.85520 (17)	0.14819 (12)	0.0422 (5)
C11B	0.7655 (3)	1.12079 (17)	−0.01874 (12)	0.0443 (5)
C12B	0.8234 (3)	1.23583 (19)	−0.01535 (14)	0.0543 (6)
C13B	0.8942 (3)	1.3053 (2)	−0.09111 (16)	0.0643 (6)
C14B	0.9032 (3)	1.2623 (2)	−0.17068 (16)	0.0689 (7)
C15B	0.8456 (3)	1.1497 (2)	−0.17527 (14)	0.0641 (6)
C16B	0.7778 (3)	1.0784 (2)	−0.09973 (13)	0.0533 (5)
C21B	0.6333 (3)	0.71662 (17)	0.15886 (12)	0.0444 (5)
C22B	0.6101 (3)	0.65153 (19)	0.09227 (14)	0.0573 (6)
C23B	0.6179 (3)	0.5226 (2)	0.10172 (17)	0.0677 (7)
C24B	0.6505 (3)	0.4568 (2)	0.17753 (17)	0.0679 (7)
C25B	0.6736 (3)	0.5198 (2)	0.24393 (15)	0.0617 (6)
C26B	0.6631 (3)	0.64968 (18)	0.23587 (13)	0.0517 (5)
H1A	0.397 (3)	0.8411 (18)	0.3389 (13)	0.052 (6)*
H2A	0.326 (3)	0.721 (2)	0.3912 (15)	0.076 (8)*
H1B	0.448 (3)	1.190 (2)	0.2646 (14)	0.067 (7)*
H2B	0.418 (3)	1.0687 (18)	0.3265 (14)	0.054 (6)*
H3A	0.1063	1.0147	0.6555	0.052*
H12A	−0.0610	0.6622	0.6079	0.055*
H13A	−0.2290	0.5538	0.7241	0.067*

H14A	−0.2429	0.6009	0.8646	0.075*
H15A	−0.0873	0.7550	0.8888	0.074*
H16A	0.0772	0.8669	0.7728	0.064*
H22A	0.0273	1.2196	0.6167	0.056*
H23A	0.0436	1.4319	0.6069	0.067*
H24A	0.2739	1.5186	0.5114	0.071*
H25A	0.4891	1.3915	0.4260	0.068*
H26A	0.4702	1.1792	0.4326	0.056*
H3B	0.7481	0.8734	0.0201	0.056*
H12B	0.8145	1.2664	0.0384	0.065*
H13B	0.9356	1.3812	−0.0882	0.077*
H14B	0.9487	1.3100	−0.2216	0.083*
H15B	0.8520	1.1209	−0.2294	0.077*
H16B	0.7403	1.0014	−0.1033	0.064*
H22B	0.5890	0.6953	0.0407	0.069*
H23B	0.6011	0.4799	0.0568	0.081*
H24B	0.6568	0.3698	0.1836	0.081*
H25B	0.6965	0.4752	0.2949	0.074*
H26B	0.6759	0.6919	0.2818	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1A	0.0424 (9)	0.0397 (9)	0.0362 (9)	−0.0074 (7)	−0.0027 (7)	−0.0043 (7)
N2A	0.0437 (9)	0.0400 (9)	0.0388 (9)	−0.0081 (7)	−0.0023 (8)	−0.0052 (7)
N4A	0.0684 (13)	0.0465 (11)	0.0400 (11)	−0.0141 (10)	0.0076 (9)	−0.0107 (9)
C1A	0.0409 (11)	0.0408 (11)	0.0364 (10)	−0.0054 (9)	−0.0042 (9)	−0.0057 (9)
C2A	0.0378 (11)	0.0381 (10)	0.0368 (10)	−0.0038 (8)	−0.0057 (9)	−0.0046 (8)
C3A	0.0526 (12)	0.0400 (11)	0.0341 (10)	−0.0068 (9)	−0.0016 (9)	−0.0058 (8)
C4A	0.0380 (11)	0.0379 (10)	0.0382 (10)	−0.0045 (8)	−0.0076 (9)	−0.0042 (8)
C11A	0.0430 (11)	0.0360 (10)	0.0397 (11)	−0.0026 (9)	−0.0034 (9)	0.0002 (8)
C12A	0.0505 (12)	0.0379 (11)	0.0462 (11)	−0.0046 (9)	−0.0062 (10)	−0.0021 (9)
C13A	0.0618 (14)	0.0419 (11)	0.0608 (14)	−0.0119 (10)	−0.0033 (11)	0.0009 (10)
C14A	0.0702 (16)	0.0513 (13)	0.0532 (14)	−0.0074 (12)	0.0075 (12)	0.0109 (11)
C15A	0.0799 (17)	0.0623 (14)	0.0371 (12)	−0.0054 (13)	−0.0026 (11)	−0.0003 (10)
C16A	0.0687 (15)	0.0500 (12)	0.0408 (12)	−0.0103 (11)	−0.0090 (11)	−0.0028 (9)
C21A	0.0432 (11)	0.0381 (10)	0.0335 (10)	−0.0091 (9)	−0.0102 (9)	−0.0011 (8)
C22A	0.0551 (13)	0.0404 (11)	0.0428 (11)	−0.0079 (10)	−0.0047 (10)	−0.0038 (9)
C23A	0.0710 (15)	0.0426 (12)	0.0547 (13)	−0.0037 (11)	−0.0115 (12)	−0.0094 (10)
C24A	0.0851 (18)	0.0393 (12)	0.0617 (14)	−0.0187 (12)	−0.0265 (13)	−0.0001 (11)
C25A	0.0640 (15)	0.0577 (14)	0.0533 (13)	−0.0290 (12)	−0.0132 (11)	0.0041 (11)
C26A	0.0482 (12)	0.0492 (12)	0.0439 (11)	−0.0135 (10)	−0.0095 (10)	−0.0033 (9)
N1B	0.0515 (10)	0.0420 (9)	0.0372 (9)	−0.0037 (8)	−0.0034 (8)	−0.0043 (7)
N2B	0.0606 (11)	0.0427 (9)	0.0376 (9)	−0.0063 (8)	0.0011 (8)	−0.0038 (8)
N4B	0.1016 (17)	0.0440 (12)	0.0395 (11)	−0.0028 (11)	0.0087 (11)	−0.0059 (9)
C1B	0.0541 (13)	0.0433 (11)	0.0361 (11)	−0.0027 (10)	−0.0017 (10)	−0.0065 (9)
C2B	0.0419 (11)	0.0448 (11)	0.0385 (11)	−0.0033 (9)	−0.0046 (9)	−0.0022 (9)
C3B	0.0543 (13)	0.0429 (11)	0.0362 (11)	0.0000 (10)	0.0007 (9)	−0.0063 (9)

C4B	0.0408 (11)	0.0445 (11)	0.0396 (11)	−0.0029 (9)	−0.0061 (9)	−0.0040 (9)
C11B	0.0437 (12)	0.0442 (11)	0.0393 (11)	−0.0006 (9)	−0.0007 (9)	−0.0005 (9)
C12B	0.0607 (14)	0.0488 (12)	0.0497 (13)	−0.0059 (11)	−0.0057 (11)	−0.0005 (10)
C13B	0.0643 (15)	0.0529 (13)	0.0692 (16)	−0.0151 (12)	−0.0027 (13)	0.0082 (12)
C14B	0.0619 (16)	0.0781 (17)	0.0542 (15)	−0.0091 (13)	0.0020 (12)	0.0199 (13)
C15B	0.0683 (16)	0.0774 (16)	0.0403 (12)	−0.0095 (13)	−0.0007 (11)	0.0014 (11)
C16B	0.0566 (13)	0.0573 (13)	0.0427 (12)	−0.0087 (11)	−0.0035 (10)	−0.0019 (10)
C21B	0.0434 (12)	0.0394 (11)	0.0456 (12)	−0.0026 (9)	−0.0008 (9)	−0.0035 (9)
C22B	0.0690 (15)	0.0501 (13)	0.0531 (13)	−0.0037 (11)	−0.0132 (12)	−0.0085 (10)
C23B	0.0787 (17)	0.0479 (13)	0.0796 (17)	−0.0068 (12)	−0.0177 (14)	−0.0172 (12)
C24B	0.0706 (17)	0.0415 (12)	0.0856 (18)	−0.0064 (12)	−0.0057 (14)	−0.0020 (13)
C25B	0.0654 (15)	0.0502 (13)	0.0601 (14)	−0.0036 (11)	−0.0021 (12)	0.0094 (11)
C26B	0.0546 (13)	0.0482 (12)	0.0464 (12)	−0.0045 (10)	−0.0005 (10)	−0.0017 (10)

Geometric parameters (Å, º)

N1A—C1A	1.345 (2)	N1B—C1B	1.346 (2)
N1A—C4A	1.346 (2)	N1B—C4B	1.343 (2)
N2A—C1A	1.343 (2)	N2B—C1B	1.343 (2)
N2A—C2A	1.340 (2)	N2B—C2B	1.340 (2)
N4A—C1A	1.357 (2)	N4B—C1B	1.347 (2)
C2A—C3A	1.385 (2)	C2B—C3B	1.381 (3)
C2A—C11A	1.488 (2)	C2B—C11B	1.488 (3)
C3A—C4A	1.384 (2)	C3B—C4B	1.387 (3)
C4A—C21A	1.481 (2)	C4B—C21B	1.484 (3)
C11A—C16A	1.388 (3)	C11B—C16B	1.386 (3)
C11A—C12A	1.390 (3)	C11B—C12B	1.389 (3)
C12A—C13A	1.378 (3)	C12B—C13B	1.382 (3)
C13A—C14A	1.377 (3)	C13B—C14B	1.372 (3)
C14A—C15A	1.374 (3)	C14B—C15B	1.368 (3)
C15A—C16A	1.382 (3)	C15B—C16B	1.383 (3)
C21A—C26A	1.387 (3)	C21B—C22B	1.386 (3)
C21A—C22A	1.389 (2)	C21B—C26B	1.392 (3)
C22A—C23A	1.378 (3)	C22B—C23B	1.378 (3)
C23A—C24A	1.373 (3)	C23B—C24B	1.377 (3)
C24A—C25A	1.378 (3)	C24B—C25B	1.369 (3)
C25A—C26A	1.383 (3)	C25B—C26B	1.387 (3)
N4A—H1A	0.89 (2)	N4B—H1B	0.89 (2)
N4A—H2A	0.89 (2)	N4B—H2B	0.91 (2)
C3A—H3A	0.9300	C3B—H3B	0.9300
C12A—H12A	0.9300	C12B—H12B	0.9300
C13A—H13A	0.9300	C13B—H13B	0.9300
C14A—H14A	0.9300	C14B—H14B	0.9300
C15A—H15A	0.9300	C15B—H15B	0.9300
C16A—H16A	0.9300	C16B—H16B	0.9300
C22A—H22A	0.9300	C22B—H22B	0.9300
C23A—H23A	0.9300	C23B—H23B	0.9300
C24A—H24A	0.9300	C24B—H24B	0.9300

C25A—H25A	0.9300	C25B—H25B	0.9300
C26A—H26A	0.9300	C26B—H26B	0.9300

C1A—N1A—C4A	116.02 (15)	C1B—N1B—C4B	115.96 (16)
C1A—N2A—C2A	116.30 (15)	C1B—N2B—C2B	116.09 (16)
N1A—C1A—N2A	126.76 (17)	N1B—C1B—N2B	126.72 (17)
N1A—C1A—N4A	117.05 (17)	N1B—C1B—N4B	116.73 (18)
N2A—C1A—N4A	116.15 (17)	N2B—C1B—N4B	116.55 (18)
N2A—C2A—C3A	121.13 (17)	N2B—C2B—C3B	121.59 (17)
N2A—C2A—C11A	116.88 (16)	N2B—C2B—C11B	116.43 (17)
C3A—C2A—C11A	121.94 (17)	C3B—C2B—C11B	121.98 (18)
C2A—C3A—C4A	118.63 (17)	C2B—C3B—C4B	118.26 (18)
N1A—C4A—C3A	121.11 (16)	N1B—C4B—C3B	121.32 (17)
N1A—C4A—C21A	117.32 (16)	N1B—C4B—C21B	117.49 (16)
C3A—C4A—C21A	121.56 (17)	C3B—C4B—C21B	121.19 (17)
C12A—C11A—C2A	119.64 (17)	C12B—C11B—C2B	120.26 (18)
C16A—C11A—C2A	121.73 (18)	C16B—C11B—C2B	121.24 (18)
C12A—C11A—C16A	118.59 (18)	C16B—C11B—C12B	118.49 (18)
C11A—C12A—C13A	120.85 (19)	C11B—C12B—C13B	120.6 (2)
C12A—C13A—C14A	119.8 (2)	C12B—C13B—C14B	119.9 (2)
C13A—C14A—C15A	120.1 (2)	C13B—C14B—C15B	120.2 (2)
C14A—C15A—C16A	120.3 (2)	C14B—C15B—C16B	120.2 (2)
C15A—C16A—C11A	120.3 (2)	C15B—C16B—C11B	120.5 (2)
C22A—C21A—C4A	120.32 (17)	C22B—C21B—C4B	120.76 (18)
C26A—C21A—C4A	121.40 (17)	C26B—C21B—C4B	120.34 (18)
C22A—C21A—C26A	118.25 (17)	C22B—C21B—C26B	118.89 (18)
C21A—C22A—C23A	121.08 (19)	C21B—C22B—C23B	120.6 (2)
C22A—C23A—C24A	120.1 (2)	C22B—C23B—C24B	120.1 (2)
C23A—C24A—C25A	119.64 (19)	C23B—C24B—C25B	119.9 (2)
C24A—C25A—C26A	120.4 (2)	C24B—C25B—C26B	120.6 (2)
C25A—C26A—C21A	120.4 (2)	C25B—C26B—C21B	119.8 (2)
C2A—C3A—H3A	120.7	C2B—C3B—H3B	120.9
C4A—C3A—H3A	120.7	C4B—C3B—H3B	120.9
C13A—C12A—H12A	119.6	C13B—C12B—H12B	119.7
C11A—C12A—H12A	119.6	C11B—C12B—H12B	119.7
C14A—C13A—H13A	120.1	C14B—C13B—H13B	120.0
C12A—C13A—H13A	120.1	C12B—C13B—H13B	120.0
C15A—C14A—H14A	119.9	C15B—C14B—H14B	119.9
C13A—C14A—H14A	119.9	C13B—C14B—H14B	119.9
C14A—C15A—H15A	119.9	C14B—C15B—H15B	119.9
C16A—C15A—H15A	119.9	C16B—C15B—H15B	119.9
C15A—C16A—H16A	119.8	C15B—C16B—H16B	119.7
C11A—C16A—H16A	119.8	C11B—C16B—H16B	119.7
C23A—C22A—H22A	119.5	C23B—C22B—H22B	119.7
C21A—C22A—H22A	119.5	C21B—C22B—H22B	119.7
C24A—C23A—H23A	119.9	C24B—C23B—H23B	119.9
C22A—C23A—H23A	119.9	C22B—C23B—H23B	119.9
C23A—C24A—H24A	120.2	C23B—C24B—H24B	120.1

C25A—C24A—H24A	120.2	C25B—C24B—H24B	120.1
C24A—C25A—H25A	119.8	C24B—C25B—H25B	119.7
C26A—C25A—H25A	119.8	C26B—C25B—H25B	119.7
C25A—C26A—H26A	119.8	C25B—C26B—H26B	120.1
C21A—C26A—H26A	119.8	C21B—C26B—H26B	120.1
C1A—N4A—H1A	119.5 (13)	C1B—N4B—H1B	116.3 (14)
C1A—N4A—H2A	114.8 (15)	C1B—N4B—H2B	121.1 (12)
H1A—N4A—H2A	122 (2)	H1B—N4B—H2B	119.8 (19)

N1A—C4A—C21A—C26A	−29.8 (3)	N1B—C4B—C21B—C26B	−36.5 (3)
C3A—C4A—C21A—C26A	151.83 (19)	C3B—C4B—C21B—C26B	142.9 (2)
C3A—C2A—C11A—C12A	149.4 (2)	C3B—C2B—C11B—C12B	−152.6 (2)
C2A—N2A—C1A—N1A	−2.0 (3)	C2B—N2B—C1B—N1B	1.4 (3)
C2A—N2A—C1A—N4A	−179.66 (17)	C2B—N2B—C1B—N4B	−179.29 (19)
C4A—N1A—C1A—N2A	1.4 (3)	C4B—N1B—C1B—N2B	−3.0 (3)
C4A—N1A—C1A—N4A	179.04 (17)	C4B—N1B—C1B—N4B	177.69 (19)
C1A—N2A—C2A—C3A	0.3 (3)	C1B—N2B—C2B—C3B	0.8 (3)
C1A—N2A—C2A—C11A	177.57 (17)	C1B—N2B—C2B—C11B	−178.38 (18)
N2A—C2A—C3A—C4A	1.8 (3)	N2B—C2B—C3B—C4B	−1.2 (3)
C11A—C2A—C3A—C4A	−175.34 (17)	C11B—C2B—C3B—C4B	177.94 (18)
C1A—N1A—C4A—C3A	0.9 (3)	C1B—N1B—C4B—C3B	2.4 (3)
C1A—N1A—C4A—C21A	−177.45 (16)	C1B—N1B—C4B—C21B	−178.26 (17)
C2A—C3A—C4A—N1A	−2.5 (3)	C2B—C3B—C4B—N1B	−0.5 (3)
C2A—C3A—C4A—C21A	175.85 (17)	C2B—C3B—C4B—C21B	−179.81 (18)
N2A—C2A—C11A—C16A	154.15 (18)	N2B—C2B—C11B—C16B	−152.50 (19)
C3A—C2A—C11A—C16A	−28.6 (3)	C3B—C2B—C11B—C16B	28.3 (3)
N2A—C2A—C11A—C12A	−27.9 (3)	N2B—C2B—C11B—C12B	26.5 (3)
C16A—C11A—C12A—C13A	1.4 (3)	C16B—C11B—C12B—C13B	−1.0 (3)
C2A—C11A—C12A—C13A	−176.68 (18)	C2B—C11B—C12B—C13B	180.0 (2)
C11A—C12A—C13A—C14A	−0.9 (3)	C11B—C12B—C13B—C14B	1.8 (3)
C12A—C13A—C14A—C15A	−0.3 (3)	C12B—C13B—C14B—C15B	−1.3 (4)
C13A—C14A—C15A—C16A	1.0 (3)	C13B—C14B—C15B—C16B	0.0 (4)
C14A—C15A—C16A—C11A	−0.5 (3)	C14B—C15B—C16B—C11B	0.8 (3)
C12A—C11A—C16A—C15A	−0.7 (3)	C12B—C11B—C16B—C15B	−0.3 (3)
C2A—C11A—C16A—C15A	177.30 (19)	C2B—C11B—C16B—C15B	178.7 (2)
N1A—C4A—C21A—C22A	148.11 (18)	N1B—C4B—C21B—C22B	144.24 (19)
C3A—C4A—C21A—C22A	−30.3 (3)	C3B—C4B—C21B—C22B	−36.4 (3)
C26A—C21A—C22A—C23A	1.2 (3)	C26B—C21B—C22B—C23B	−0.6 (3)
C4A—C21A—C22A—C23A	−176.82 (19)	C4B—C21B—C22B—C23B	178.7 (2)
C21A—C22A—C23A—C24A	−1.0 (3)	C21B—C22B—C23B—C24B	−0.6 (4)
C22A—C23A—C24A—C25A	−0.2 (3)	C22B—C23B—C24B—C25B	0.6 (4)
C23A—C24A—C25A—C26A	1.1 (3)	C23B—C24B—C25B—C26B	0.5 (4)
C24A—C25A—C26A—C21A	−0.9 (3)	C24B—C25B—C26B—C21B	−1.6 (3)
C22A—C21A—C26A—C25A	−0.3 (3)	C22B—C21B—C26B—C25B	1.7 (3)
C4A—C21A—C26A—C25A	177.71 (18)	C4B—C21B—C26B—C25B	−177.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H1*A*···N1*B*	0.89 (2)	2.17 (2)	3.058 (2)	172.7 (18)
N4*B*—H2*B*···N1*A*	0.91 (2)	2.20 (2)	3.106 (3)	175.8 (17)
C12*A*—H12*A*···*Cg*1^{i}	0.93	2.77	3.538 (2)	141
C26*A*—H26*A*···*Cg2*^{ii}	0.93	2.78	3.393 (2)	124

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