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2,2,3,3'-Tetraphenyl-7,7'-biquinoxaline

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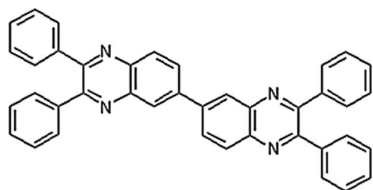
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.091; data-to-parameter ratio = 9.7.

In the crystal structure of the title compound, $\text{C}_{40}\text{H}_{26}\text{N}_4$, molecules reside on crystallographic centers of inversion and are linked *via* $\text{C}-\text{H}\cdots\text{N}$ interactions about inversion centers into one-dimensional chains: longer $\text{C}-\text{H}\cdots\pi(\text{arene})$ interactions complete the intermolecular interactions.

Related literature

For the synthesis of quinoxalines, see: Kowalski *et al.* (2006); Kou *et al.* (2006); Baek & Tan (2006). For applications of quinoxalines see: Mollegaard *et al.* (2000); Aldakov *et al.* (2005); Kaiwar *et al.* (1997); Anzenbacher *et al.* (2000). For related literature, see: Brown *et al.* (2004); Bruno *et al.* (2002); Gibson *et al.* (2006); Page *et al.* (1998); Pascal & Ho (1993); Salvatore *et al.* (2006); Simpson & Gordon (1995); Willett *et al.* (2001); Wozniak *et al.* (1993); Wu *et al.* (2002).



Experimental

Crystal data

$\text{C}_{40}\text{H}_{26}\text{N}_4$ $\gamma = 91.7510$ (10) $^\circ$
 $M_r = 562.65$ $V = 704.19$ (3) Å³
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 5.70240$ (10) Å $\text{Cu K}\alpha$ radiation
 $b = 9.9534$ (2) Å $\mu = 0.61$ mm⁻¹
 $c = 12.9785$ (3) Å $T = 100$ (2) K
 $\alpha = 105.3520$ (10) $^\circ$ $0.19 \times 0.12 \times 0.06$ mm
 $\beta = 96.6170$ (10) $^\circ$

Data collection

Bruker SMART APEXII CCD 12179 measured reflections
 diffractometer 2429 independent reflections
 Absorption correction: numerical 2156 reflections with $I > 2\sigma(I)$
 (SADABS; Sheldrick, 2004) $R_{\text{int}} = 0.033$
 $T_{\text{min}} = 0.893$, $T_{\text{max}} = 0.964$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$ 251 parameters
 $wR(F^2) = 0.091$ All H-atom parameters refined
 $S = 1.06$ $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 2429 reflections $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C2}-\text{H2}\cdots\text{C18}^i$	0.977 (15)	2.722 (15)	3.5521 (16)	143.1 (12)
$\text{C7}-\text{H7}\cdots\text{N2}^{ii}$	0.979 (15)	2.593 (16)	3.3635 (15)	135.6 (11)
$\text{C10}-\text{H10}\cdots\text{C3}^{iii}$	0.974 (13)	2.935 (12)	3.2994 (15)	103.4 (8)
$\text{C10}-\text{H10}\cdots\text{C6}^{iii}$	0.974 (13)	2.974 (13)	3.1801 (15)	93.1 (8)
$\text{C11}-\text{H11}\cdots\text{N1}^{iii}$	0.963 (15)	2.893 (14)	3.3233 (14)	108.3 (10)
$\text{C12}-\text{H12}\cdots\text{C18}^{iv}$	0.975 (15)	2.959 (15)	3.6146 (16)	125.6 (10)
$\text{C13}-\text{H13}\cdots\text{C18}^{iv}$	0.999 (15)	2.978 (15)	3.6141 (16)	122.5 (10)
$\text{C16}-\text{H16}\cdots\text{N2}^{ii}$	0.978 (14)	2.815 (14)	3.7256 (14)	155.2 (11)
$\text{C17}-\text{H17}\cdots\text{C1}^v$	0.969 (13)	2.993 (14)	3.7019 (16)	131.0 (9)
$\text{C17}-\text{H17}\cdots\text{C8}^v$	0.969 (13)	2.860 (14)	3.6338 (15)	137.5 (9)
$\text{C18}-\text{H18}\cdots\text{N1}^{vi}$	0.975 (14)	2.808 (14)	3.6217 (14)	141.5 (10)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: XSELL (Bruker, 2004); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2021).

References

- Aldakov, D., Palacios, M. A. & Anzenbacher, P. Jr (2005). *Chem. Mater.* **17**, 5238–5241.
 Anzenbacher, P. Jr, Try, A. C., Miyaji, H., Jursikova, K., Lynch, V. M., Marquez, M. & Sessler, J. L. (2000). *J. Am. Chem. Soc.* **122**, 10268–10272.
 Baek, J.-B. & Tan, L.-S. (2006). *Macromolecules*, **39**, 2794–2803.
 Brown, D. J., Taylor, E. C. & Wipf, P. (2004). *The Chemistry of Heterocyclic Compounds*, Vol. 61, *Quinoxalines*, Suppl. II, pp. 100–105. New York: Wiley.
 Bruker (2004). APEX2 (Version 2.0), SAINT-Plus (Version 7.12A) and XSELL (Version 6.3.1). Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* **B58**, 389–397.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Gibson, R. J. P., Kass, J. P., Zambrano, C. H., Fronczek, F. R. & Dueno, E. E. (2006). *Acta Cryst.* **E62**, o2947–o2948.
 Kaiwar, S. P., Vodacek, A., Blough, N. V. & Pilato, R. S. (1997). *J. Am. Chem. Soc.* **119**, 3311–3316.
 Kou, B.-B., Zhang, F., Yang, T.-M. & Liu, G. (2006). *J. Comb. Chem.* **8**, 841–847.

- Kowalski, J. A., Leonard, S. F. & Lee, G. E. Jr (2006). *J. Comb. Chem.* **8**, 774–779.
- Mollegaard, N. E., Bailly, C., Waring, M. J. & Nielsen, P. E. (2000). *Biochemistry*, **39**, 9502–9507.
- Page, S. E., Gordon, K. C. & Burrell, A. K. (1998). *Inorg. Chem.* **37**, 4452–4459.
- Pascal, R. A. Jr & Ho, D. M. (1993). *J. Am. Chem. Soc.* **115**, 8507–8508.
- Salvatore, R. N., Kass, J. P., Gibson, R. J. P., Zambrano, C. H., Pike, R. D. & Dueno, E. E. (2006). *Acta Cryst.* **E62**, o4547–o4548.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
- Simpson, T. J. & Gordon, K. C. (1995). *Inorg. Chem.* **34**, 6323–6329.
- Willett, R. D., Jentler, R. J. & Twamley, B. (2001). *Inorg. Chem.* **40**, 6502–6505.
- Wozniak, K., Krygowski, T. M., Grech, E., Kolodziejski, W. & Klinowski, J. (1993). *J. Phys. Chem.* **97**, 1862–1867.
- Wu, C. D., Lu, C.-Z., Zhuang, H.-H. & Huang, J.-S. (2002). *Inorg. Chem.* **41**, 5636–5637.

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2,2,3,3'-Tetraphenyl-7,7'-biquinoxaline

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S1. Comment

Quinoxalines and their derivatives have received considerable attention in the past several years due to their electronic properties (Page *et al.*, 1998; Simpson & Gordon, 1995), H-bonding ability (Pascal *et al.*, 1993; Wozniak *et al.*, 1993), and their capacity to coordinate to metals forming interesting three-dimensional structures (Wu *et al.*, 2002; Willett *et al.*, 2001). During our investigations, we have prepared a number of substituted quinoxalines and phenazines, some of which coordinate to metal salts forming novel structures (Dueno, *et al.*, unpublished). Our current work involves the synthesis of new nitrogen heterocycles (Gibson, *et al.*, 2006; Salvatore, *et al.*, 2006) which may lead to novel three dimensional structures upon coordination to metal salts. Here, we report the crystal structure of 2,2',3,3'-Tetraphenyl-7,7'-biquinoxaline (I), (Figure 1).

The structure of (I) has bond distances and angles that are unexceptional, as all fall within ranges found in the literature for similar nitrogen heterocycles (Brown *et al.*, 2004). The one molecule present in the asymmetric unit cell lies on an inversion center, so that half the molecule is related to its counterpart by symmetry (symmetry code, $-x, -y, -z$). As expected, the steric bulk of the phenyl substituents prevents them from being coplanar with the quinoxaline rings: the dihedral angle N2—C5—C15—C20 (phenyl ring 1) is 59.80 (11)°, and the dihedral angle N1—C4—C9—C10 (phenyl ring 2) is 25.98 (11)°. An interesting feature worth mentioning is that the two rings that make up the quinoxaline unit are not perfectly planar, for the angle between the N containing ring and the carbon-only ring is 3.50 (11)° (based on a least squares mean planes of N1—C4—C5—N2—C6—C3 and C1—C2—C3—C6—C7—C8). It is conceivable that this deviation from a planar structure is due to Van der Waals repulsion interactions between the aromatic substituents. Another interesting aspect of this molecule is that the packing diagram shows short contact interactions between phenyl substituents on one molecule and the quinoxaline ring of an adjacent molecule. Intermolecular distances range from 3.181 (2) Å (C10—C6) to 3.376 (2) Å (C11—C4), which suggests some degree of $\sigma(\text{CH})\cdots\pi$ interaction (Figure 2).

S2. Experimental

A 50 ml round-bottomed flask was charged with biphenyl-3,3',4,4'-tetramine (214 mg, 1 mmol), benzil (420 mg, 2 mmol), iodine (51 mg, 0.2 mmol), and acetonitrile (15 ml). The reaction was monitored by thin-layer chromatography until complete consumption of the starting materials (15 min). The resulting amber solution was concentrated to dryness under reduced pressure. The dark-brown crude product was then subjected to flash column chromatography using silica gel (eluent: 9:1 hexane–EtOAc) in order to remove residual iodine. The pale-yellow solution was evaporated to dryness under reduced pressure to give (I) (yield 0.413 mg, 74%), as a white powder (m.p. 573 K). This powder was then crystallized from a minimal amount of toluene, and afforded (I) as pale-yellow cubes.

S3. Refinement

H atoms were placed in idealized positions ($C-H = 0.96 - 1.00 \text{ \AA}$) and allowed to ride on their parent atoms with $U_{iso}(H) = 1.2 U_{eq}(C)$.

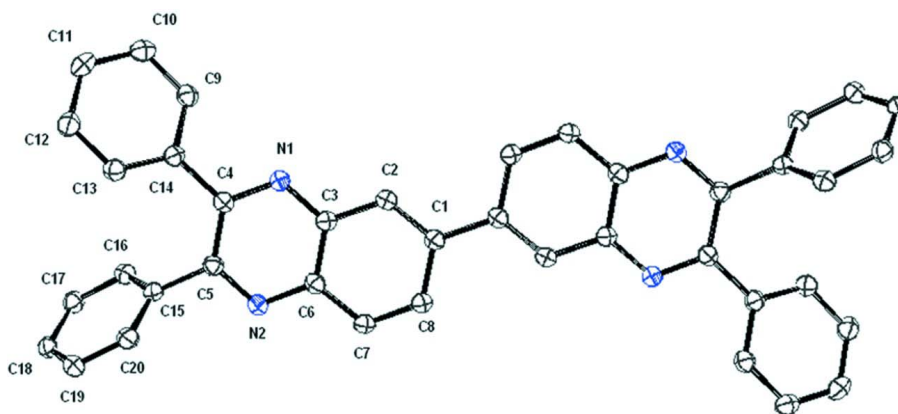


Figure 1

ORTEP (Farrugia, 1997) drawing of (I). Displacement ellipsoids have been drawn at the 50% probability level. Unlabeled atoms are related to labeled atoms by symmetry (code $-x, -y, -z$). H atoms have been omitted for clarity.

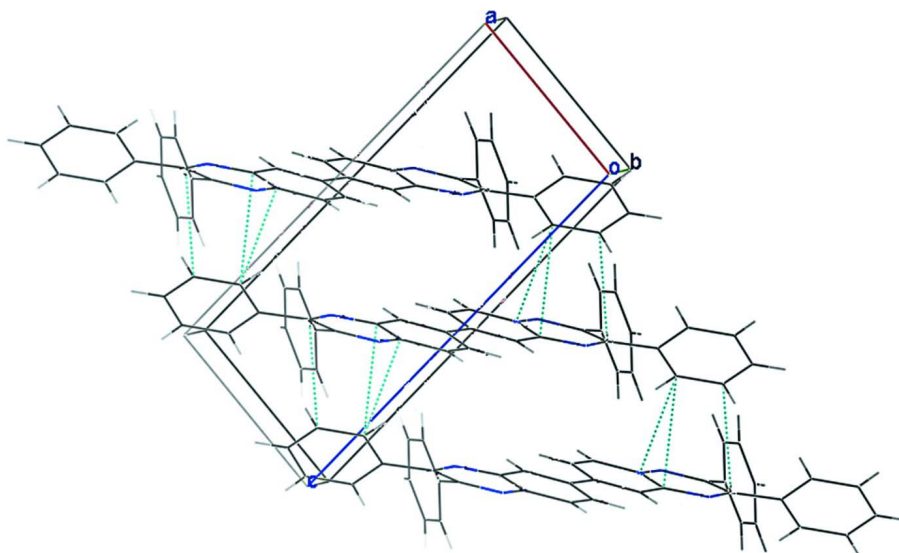


Figure 2

Mercury (Bruno *et al.*, 2002) packing diagram of (I) along the b axis showing short contact interactions.

2,2,3,3'-Tetraphenyl-7,7'-biquinoxaline

Crystal data

$C_{40}H_{26}N_4$

$M_r = 562.65$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.7024 (1) \text{ \AA}$

$b = 9.9534 (2) \text{ \AA}$

$c = 12.9785 (3) \text{ \AA}$

$\alpha = 105.352 (1)^\circ$

$\beta = 96.617 (1)^\circ$

$\gamma = 91.751 (1)^\circ$

$V = 704.19 (3) \text{ \AA}^3$

$Z = 1$

$F(000) = 294$

$D_x = 1.327 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$

Cell parameters from 585 reflections

$\theta = 3.6\text{--}67.0^\circ$
 $\mu = 0.61\text{ mm}^{-1}$
 $T = 100\text{ K}$

Block, colourless
 $0.19 \times 0.12 \times 0.06\text{ mm}$

Data collection

Bruker SMART APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω and ψ scans
 Absorption correction: numerical
 (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.893$, $T_{\max} = 0.964$

12179 measured reflections
 2429 independent reflections
 2156 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 67.0^\circ$, $\theta_{\min} = 3.6^\circ$
 $h = -6 \rightarrow 6$
 $k = -11 \rightarrow 11$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.091$
 $S = 1.06$
 2429 reflections
 251 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
 All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.1323P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.18\text{ e \AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.51854 (16)	0.85128 (10)	0.69940 (8)	0.0221 (2)
N2	0.23046 (17)	0.60236 (10)	0.64109 (8)	0.0224 (2)
C1	0.03603 (19)	0.94087 (11)	0.52202 (9)	0.0209 (3)
C2	0.2496 (2)	0.94755 (12)	0.58600 (9)	0.0226 (3)
C3	0.31629 (19)	0.83612 (11)	0.62942 (9)	0.0211 (3)
C4	0.57593 (19)	0.74558 (12)	0.73939 (9)	0.0212 (3)
C5	0.43238 (19)	0.61520 (12)	0.70434 (9)	0.0211 (3)
C6	0.1661 (2)	0.71321 (12)	0.60385 (9)	0.0217 (3)
C7	-0.0511 (2)	0.70597 (12)	0.53726 (9)	0.0231 (3)
C8	-0.1142 (2)	0.81609 (12)	0.49890 (9)	0.0225 (3)
C9	0.79004 (19)	0.77207 (11)	0.82117 (9)	0.0219 (3)
C10	0.9637 (2)	0.87320 (12)	0.81830 (10)	0.0239 (3)
C11	1.1675 (2)	0.90121 (13)	0.89186 (10)	0.0269 (3)

C12	1.2013 (2)	0.82934 (13)	0.97005 (10)	0.0288 (3)
C13	1.0272 (2)	0.73173 (13)	0.97578 (10)	0.0281 (3)
C14	0.8232 (2)	0.70364 (12)	0.90232 (10)	0.0252 (3)
C15	0.49998 (19)	0.48375 (11)	0.73197 (9)	0.0215 (3)
C16	0.7014 (2)	0.41920 (12)	0.69865 (9)	0.0240 (3)
C17	0.7507 (2)	0.29096 (12)	0.71734 (10)	0.0248 (3)
C18	0.6025 (2)	0.22840 (12)	0.77110 (9)	0.0244 (3)
C19	0.4035 (2)	0.29355 (13)	0.80581 (10)	0.0268 (3)
C20	0.3503 (2)	0.42037 (12)	0.78536 (10)	0.0247 (3)
H2	0.361 (3)	1.0290 (16)	0.6039 (12)	0.035 (4)*
H7	-0.153 (3)	0.6200 (16)	0.5199 (12)	0.035 (4)*
H8	-0.267 (2)	0.8096 (13)	0.4535 (11)	0.021 (3)*
H10	0.938 (2)	0.9233 (14)	0.7633 (11)	0.026 (3)*
H11	1.287 (3)	0.9694 (15)	0.8870 (12)	0.033 (4)*
H12	1.344 (3)	0.8484 (16)	1.0224 (12)	0.036 (4)*
H13	1.048 (2)	0.6786 (16)	1.0312 (13)	0.037 (4)*
H14	0.698 (3)	0.6366 (16)	0.9090 (12)	0.033 (4)*
H16	0.807 (2)	0.4646 (15)	0.6621 (12)	0.029 (3)*
H17	0.888 (2)	0.2451 (14)	0.6924 (11)	0.023 (3)*
H18	0.640 (2)	0.1387 (15)	0.7834 (11)	0.028 (3)*
H19	0.296 (2)	0.2499 (15)	0.8440 (12)	0.033 (4)*
H20	0.210 (3)	0.4660 (15)	0.8084 (12)	0.032 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0212 (5)	0.0209 (5)	0.0245 (5)	0.0010 (4)	0.0015 (4)	0.0073 (4)
N2	0.0241 (5)	0.0195 (5)	0.0240 (5)	0.0010 (4)	0.0019 (4)	0.0070 (4)
C1	0.0227 (6)	0.0196 (6)	0.0205 (6)	0.0010 (5)	0.0037 (4)	0.0052 (4)
C2	0.0228 (6)	0.0193 (6)	0.0258 (6)	-0.0015 (5)	0.0015 (4)	0.0073 (5)
C3	0.0204 (6)	0.0208 (6)	0.0216 (6)	0.0006 (5)	0.0027 (4)	0.0049 (4)
C4	0.0219 (6)	0.0196 (5)	0.0231 (6)	0.0019 (4)	0.0047 (4)	0.0067 (4)
C5	0.0204 (5)	0.0208 (6)	0.0224 (6)	0.0010 (4)	0.0035 (4)	0.0060 (4)
C6	0.0243 (6)	0.0189 (5)	0.0217 (6)	0.0012 (5)	0.0038 (4)	0.0051 (4)
C7	0.0238 (6)	0.0199 (6)	0.0244 (6)	-0.0024 (5)	0.0005 (4)	0.0053 (4)
C8	0.0224 (6)	0.0217 (6)	0.0227 (6)	-0.0013 (5)	0.0003 (4)	0.0058 (4)
C9	0.0207 (6)	0.0187 (5)	0.0249 (6)	0.0033 (4)	0.0025 (4)	0.0034 (4)
C10	0.0247 (6)	0.0207 (6)	0.0260 (6)	0.0034 (5)	0.0037 (5)	0.0057 (5)
C11	0.0227 (6)	0.0256 (6)	0.0302 (7)	-0.0002 (5)	0.0041 (5)	0.0036 (5)
C12	0.0224 (6)	0.0343 (7)	0.0261 (6)	0.0014 (5)	-0.0025 (5)	0.0042 (5)
C13	0.0279 (6)	0.0295 (6)	0.0270 (6)	0.0038 (5)	0.0002 (5)	0.0087 (5)
C14	0.0248 (6)	0.0235 (6)	0.0262 (6)	0.0008 (5)	0.0015 (5)	0.0058 (5)
C15	0.0218 (6)	0.0185 (5)	0.0225 (6)	-0.0011 (4)	-0.0023 (4)	0.0050 (4)
C16	0.0240 (6)	0.0229 (6)	0.0258 (6)	0.0002 (5)	0.0034 (5)	0.0077 (5)
C17	0.0238 (6)	0.0225 (6)	0.0264 (6)	0.0041 (5)	0.0008 (5)	0.0045 (5)
C18	0.0285 (6)	0.0180 (5)	0.0253 (6)	0.0009 (5)	-0.0048 (5)	0.0069 (4)
C19	0.0260 (6)	0.0259 (6)	0.0310 (7)	-0.0011 (5)	0.0017 (5)	0.0131 (5)
C20	0.0206 (6)	0.0248 (6)	0.0296 (6)	0.0023 (5)	0.0030 (5)	0.0089 (5)

Geometric parameters (Å, °)

N1—C4	1.3245 (15)	C10—H10	0.974 (14)
N1—C3	1.3613 (14)	C11—C12	1.3880 (18)
N2—C5	1.3166 (15)	C11—H11	0.966 (15)
N2—C6	1.3609 (15)	C12—C13	1.3899 (18)
C1—C2	1.3819 (16)	C12—H12	0.978 (15)
C1—C8	1.4301 (16)	C13—C14	1.3870 (17)
C1—C1 ⁱ	1.488 (2)	C13—H13	0.998 (15)
C2—C3	1.4141 (16)	C14—H14	0.988 (15)
C2—H2	0.976 (15)	C15—C16	1.3898 (17)
C3—C6	1.4129 (16)	C15—C20	1.3936 (16)
C4—C5	1.4484 (16)	C16—C17	1.3918 (16)
C4—C9	1.4900 (15)	C16—H16	0.976 (14)
C5—C15	1.4955 (15)	C17—C18	1.3865 (17)
C6—C7	1.4143 (16)	C17—H17	0.962 (14)
C7—C8	1.3604 (16)	C18—C19	1.3852 (18)
C7—H7	0.977 (15)	C18—H18	0.973 (14)
C8—H8	0.986 (13)	C19—C20	1.3922 (16)
C9—C14	1.3967 (17)	C19—H19	0.990 (15)
C9—C10	1.4010 (16)	C20—H20	0.971 (15)
C10—C11	1.3868 (17)		
C4—N1—C3	118.29 (10)	C9—C10—H10	118.5 (8)
C5—N2—C6	117.97 (10)	C12—C11—C10	120.12 (11)
C2—C1—C8	117.90 (10)	C12—C11—H11	120.4 (8)
C2—C1—C1 ⁱ	121.33 (13)	C10—C11—H11	119.4 (8)
C8—C1—C1 ⁱ	120.76 (12)	C11—C12—C13	119.59 (11)
C1—C2—C3	121.34 (11)	C11—C12—H12	120.8 (9)
C1—C2—H2	122.0 (8)	C13—C12—H12	119.6 (9)
C3—C2—H2	116.6 (9)	C14—C13—C12	120.35 (11)
N1—C3—C6	120.83 (10)	C14—C13—H13	118.8 (9)
N1—C3—C2	119.57 (10)	C12—C13—H13	120.9 (9)
C6—C3—C2	119.52 (10)	C13—C14—C9	120.67 (11)
N1—C4—C5	120.22 (10)	C13—C14—H14	119.5 (8)
N1—C4—C9	115.70 (10)	C9—C14—H14	119.8 (8)
C5—C4—C9	124.07 (10)	C16—C15—C20	119.65 (10)
N2—C5—C4	121.55 (10)	C16—C15—C5	120.82 (10)
N2—C5—C15	114.09 (10)	C20—C15—C5	119.38 (10)
C4—C5—C15	124.33 (10)	C15—C16—C17	119.93 (11)
N2—C6—C3	120.68 (10)	C15—C16—H16	119.3 (8)
N2—C6—C7	120.32 (10)	C17—C16—H16	120.8 (8)
C3—C6—C7	118.99 (10)	C18—C17—C16	120.38 (11)
C8—C7—C6	120.36 (11)	C18—C17—H17	119.8 (8)
C8—C7—H7	121.6 (9)	C16—C17—H17	119.8 (8)
C6—C7—H7	118.1 (9)	C19—C18—C17	119.78 (11)
C7—C8—C1	121.85 (11)	C19—C18—H18	121.0 (8)
C7—C8—H8	119.2 (7)	C17—C18—H18	119.2 (8)

C1—C8—H8	119.0 (7)	C18—C19—C20	120.18 (11)
C14—C9—C10	118.36 (11)	C18—C19—H19	120.6 (8)
C14—C9—C4	123.20 (10)	C20—C19—H19	119.2 (8)
C10—C9—C4	118.42 (10)	C15—C20—C19	120.05 (11)
C11—C10—C9	120.85 (11)	C15—C20—H20	119.3 (8)
C11—C10—H10	120.7 (8)	C19—C20—H20	120.7 (8)
C8—C1—C2—C3	-1.34 (17)	N1—C4—C9—C14	152.27 (11)
C1 ⁱ —C1—C2—C3	178.88 (12)	C5—C4—C9—C14	-26.95 (17)
C4—N1—C3—C6	2.79 (16)	N1—C4—C9—C10	-25.98 (15)
C4—N1—C3—C2	179.56 (10)	C5—C4—C9—C10	154.81 (11)
C1—C2—C3—N1	-174.44 (10)	C14—C9—C10—C11	2.26 (17)
C1—C2—C3—C6	2.37 (17)	C4—C9—C10—C11	-179.41 (10)
C3—N1—C4—C5	3.29 (16)	C9—C10—C11—C12	-0.35 (18)
C3—N1—C4—C9	-175.95 (9)	C10—C11—C12—C13	-1.57 (19)
C6—N2—C5—C4	3.88 (16)	C11—C12—C13—C14	1.55 (19)
C6—N2—C5—C15	-174.05 (9)	C12—C13—C14—C9	0.41 (18)
N1—C4—C5—N2	-6.97 (17)	C10—C9—C14—C13	-2.28 (17)
C9—C4—C5—N2	172.21 (10)	C4—C9—C14—C13	179.47 (10)
N1—C4—C5—C15	170.75 (10)	N2—C5—C15—C16	115.78 (12)
C9—C4—C5—C15	-10.07 (17)	C4—C5—C15—C16	-62.09 (15)
C5—N2—C6—C3	2.27 (16)	N2—C5—C15—C20	-59.79 (14)
C5—N2—C6—C7	-178.84 (10)	C4—C5—C15—C20	122.33 (12)
N1—C3—C6—N2	-5.86 (17)	C20—C15—C16—C17	0.92 (17)
C2—C3—C6—N2	177.37 (10)	C5—C15—C16—C17	-174.64 (10)
N1—C3—C6—C7	175.23 (10)	C15—C16—C17—C18	-1.36 (18)
C2—C3—C6—C7	-1.54 (16)	C16—C17—C18—C19	0.39 (17)
N2—C6—C7—C8	-179.17 (10)	C17—C18—C19—C20	1.01 (18)
C3—C6—C7—C8	-0.26 (17)	C16—C15—C20—C19	0.46 (18)
C6—C7—C8—C1	1.31 (18)	C5—C15—C20—C19	176.09 (10)
C2—C1—C8—C7	-0.51 (17)	C18—C19—C20—C15	-1.44 (18)
C1 ⁱ —C1—C8—C7	179.27 (13)		

Symmetry code: (i) $-x, -y+2, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 \cdots C18 ⁱⁱ	0.977 (15)	2.722 (15)	3.5521 (16)	143.1 (12)
C7—H7 \cdots N2 ⁱⁱⁱ	0.979 (15)	2.593 (16)	3.3635 (15)	135.6 (11)
C10—H10 \cdots C3 ^{iv}	0.974 (13)	2.935 (12)	3.2994 (15)	103.4 (8)
C10—H10 \cdots C6 ^{iv}	0.974 (13)	2.974 (13)	3.1801 (15)	93.1 (8)
C11—H11 \cdots N1 ^{iv}	0.963 (15)	2.893 (14)	3.3233 (14)	108.3 (10)
C12—H12 \cdots C18 ^v	0.975 (15)	2.959 (15)	3.6146 (16)	125.6 (10)
C13—H13 \cdots C18 ^v	0.999 (15)	2.978 (15)	3.6141 (16)	122.5 (10)
C16—H16 \cdots N2 ^{iv}	0.978 (14)	2.815 (14)	3.7256 (14)	155.2 (11)
C17—H17 \cdots C1 ^{vi}	0.969 (13)	2.993 (14)	3.7019 (16)	131.0 (9)

C17—H17···C8 ^{vi}	0.969 (13)	2.860 (14)	3.6338 (15)	137.5 (9)
C18—H18···N1 ^{vii}	0.975 (14)	2.808 (14)	3.6217 (14)	141.5 (10)

Symmetry codes: (ii) $x, y+1, z$; (iii) $-x, -y+1, -z+1$; (iv) $x+1, y, z$; (v) $-x+2, -y+1, -z+2$; (vi) $-x+1, -y+1, -z+1$; (vii) $x, y-1, z$.