

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N,N-Bis(pyridin-2-ylmethyl)cyclohexanamine

Matthew P. Akerman,* Mathias Chipangura, Allen Mambanda and Deogratius Jaganyi

School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X01, Scottsville 3209, Pietermaritzburg, South Africa
Correspondence e-mail: akermanm@ukzn.ac.za

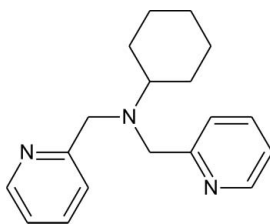
Received 6 June 2012; accepted 18 June 2012

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.038; wR factor = 0.085; data-to-parameter ratio = 11.2.

The pyridine rings of the title compound, $\text{C}_{18}\text{H}_{23}\text{N}_3$, are in a nearly perpendicular orientation relative to the plane defined by the three amino-bonded C atoms, making dihedral angles of $87.4(1)^\circ$ and $84.2(1)^\circ$. One of the pyridine N atoms acts as an hydrogen-bond acceptor for two pyridine C—H groups. By means of these intermolecular hydrogen bonds, the molecules form a two-dimensional network parallel to the *ab* plane.

Related literature

For a kinetic and mechanistic study of the platinum(II) chelate of the title compound, see: Mambanda & Jaganyi (2012). For the synthesis of the title compound, see: Sato *et al.* (1992); Toftlund & Yde-Andersen (1981); Anderegg & Wenk (1967). For the crystal structure of the related compound *N,N*-bis(2-pyridylmethyl)-*tert*-butylamine, see: Mambanda *et al.* (2009). For the crystal structures of the hexadentate analogues, see: Mambanda *et al.* (2007). For dinuclear platinum(II) complexes structurally related to the complex of the title compound, see: Hofmann & van Eldik (2003); Erteurk *et al.* (2007, 2008). For dinuclear metal complexes containing bis(tridentate) chelates structurally related to the title compound, see: Fujihara *et al.* (2004); Gunatilleke & Norman (2003); Fujii *et al.* (2003). For manganese-oxo complexes of *N,N*-bis(2-pyridylmethyl)ethylamine and *N,N*-bis(2-pyridylmethyl)-*tert*-butylamine, see: Pal *et al.* (1992) and Mok *et al.* (1997), respectively.



Experimental

Crystal data

$\text{C}_{18}\text{H}_{23}\text{N}_3$
 $M_r = 281.39$
Monoclinic, *Cc*
 $a = 6.2272(2)$ Å
 $b = 18.1729(7)$ Å
 $c = 14.3213(5)$ Å
 $\beta = 102.118(4)^\circ$
 $V = 1584.57(10)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 120$ K
 $0.60 \times 0.50 \times 0.30$ mm

Data collection

Oxford Diffraction Xcalibur 2 CCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.959$, $T_{\max} = 0.979$
7854 measured reflections
2521 independent reflections
2134 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.085$
 $S = 0.98$
2134 reflections
190 parameters
2 restraints
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.15$ e Å⁻³
 $\Delta\rho_{\min} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| C4—H4...N2 ⁱ | 0.95 | 2.55 | 3.475(2) | 166(1) |
| C11—H11...N2 ⁱⁱ | 0.95 | 2.64 | 3.511(2) | 153(1) |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors gratefully acknowledge financial support from the University of KwaZulu-Natal and the National Research Foundation (NRF, Pretoria). We thank Mr C. Grimmer for the NMR analysis of the samples.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2063).

References

- Anderegg, G. & Wenk, F. (1967). *Helv. Chim. Acta*, **50**, 2330–2332.
Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
Erteurk, H., Hofmann, A., Puchta, R. & van Eldik, R. (2007). *Dalton Trans.* pp. 2295–2301.
Erteurk, H., Maigut, J., Puchta, R. & van Eldik, R. (2008). *Dalton Trans.* pp. 2759–2766.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fujihara, T., Saito, M. & Nagasawa, A. (2004). *Acta Cryst.* **E60**, o262–o263.
Fujii, T., Naito, A., Yamaguchi, S., Wada, A., Funahashi, Y., Jitsukawa, K., Nagatomo, S., Kitagawa, T. & Masuda, H. (2003). *Chem. Commun.* **21**, 2700–2701.
Gunatilleke, S. S. & Norman, R. E. (2003). *Acta Cryst.* **E59**, o269–o271.
Hofmann, A. & van Eldik, R. (2003). *Dalton Trans.* pp. 2979–2985.
Mambanda, A. & Jaganyi, D. (2012). *Dalton Trans.* **41**, 908–920.

- Mambanda, A., Jaganyi, D. & Munro, O. Q. (2007). *Acta Cryst.* **C63**, o676–o680.
- Mambanda, A., Jaganyi, D. & Stewart, K. (2009). *Acta Cryst.* **E65**, o402.
- Mok, H. J., Davis, J. A., Pal, S., Mandal, S. K. & Armstrong, W. H. (1997). *Inorg. Chim. Acta*, **263**, 385–394.
- Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
- Pal, S., Chan, M. K. & Armstrong, W. H. (1992). *J. Am. Chem. Soc.* **114**, 6398–6404.
- Sato, M., Mori, Y. & Iida, T. (1992). *Synthesis*, **6**, 539–540.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Toftlund, H. & Yde-Andersen, S. (1981). *Acta Chem. Scand. Ser. A*, **35**, 575–581.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2012). E68, o2194–o2195 [doi:10.1107/S1600536812027572]

N,N*-Bis(pyridin-2-ylmethyl)cyclohexanamine*Matthew P. Akerman, Mathias Chipangura, Allen Mambanda and Deogratius Jaganyi****Comment**

The search for chelating ligands for the coordination of platinum(II) ions has led us to investigate bis-*N*-functionalized cyclohexylamine as a potential tridentate *N*-donor ligand.

The pyridine rings are in a near perpendicular orientation relative to the three-atom mean plane defined by the *N*-bonded carbon atoms making angles of 87.4 (1)° and 84.2 (1)° to the plane, for the rings containing N2 and N3, respectively. The near perpendicular orientation of the pyridyl rings allows for hydrogen bonding, stabilizing the lattice.

There are non-classical hydrogen bonds between the pyridine nitrogen atom, N2, and the pyridine hydrogen atoms, H4 and H11 of two separate, adjacent molecules. N2 acts as an acceptor for both hydrogen bonds. These bonds lead to the formation of an infinite two-dimensional hydrogen-bonded network. This network is co-planar with the *ab* plane. The network consists of one-dimensional chains with adjacent molecules linked by the N2⋯H4 hydrogen bond. These one-dimensional chains are then cross-linked by the N2⋯H11 hydrogen bond, thus forming an infinite, two-dimensional network. Although hydrogen bond length does not necessarily correlate linearly to bond strength, due to packing constraints in the lattice, these bonds are considerably shorter than the sum of their van der Waals radii and are thus likely to be moderate to high in strength. This also seems likely as the D—H⋯A bond angle of both bonds, 165.7 (1)° and 153.1 (1)° for N2⋯H4—C4 and N2⋯H11—C11 respectively, do not show a marked deviation from ideality. The hydrogen bond lengths and angles are summarized in Table 1.

Experimental

The tridentate ligand is formed by reacting two molar equivalents of 2-picoyl chloride hydrochloride under basic aqueous conditions with one molar equivalent of cyclohexylamine, following an improved method of Sato *et al.*, (1992) previously reported by Toftlund & Yde-Andersen (1981) as well as Anderegg & Wenk (1967). Colourless crystals were obtained by slow evaporation of an ethanol solution of the ligand over a period of several days. Yield: 1.276 g (44%).

Refinement

The positions of all C-bonded hydrogen atoms were calculated using the standard riding model of *SHELXL97* (Sheldrick, 2008) with C—H(aromatic) distances of 0.95 Å and $U_{\text{iso}} = 1.2 U_{\text{eq}}$, C—H(methylene) distances of 0.99 Å and $U_{\text{iso}} = 1.2 U_{\text{eq}}$ and a C—H(methine) distance of 1.00 Å and $U_{\text{iso}} = 1.2 U_{\text{eq}}$. In the absence of significant anomalous scattering, Friedel pairs were merged.

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED* (Oxford Diffraction, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

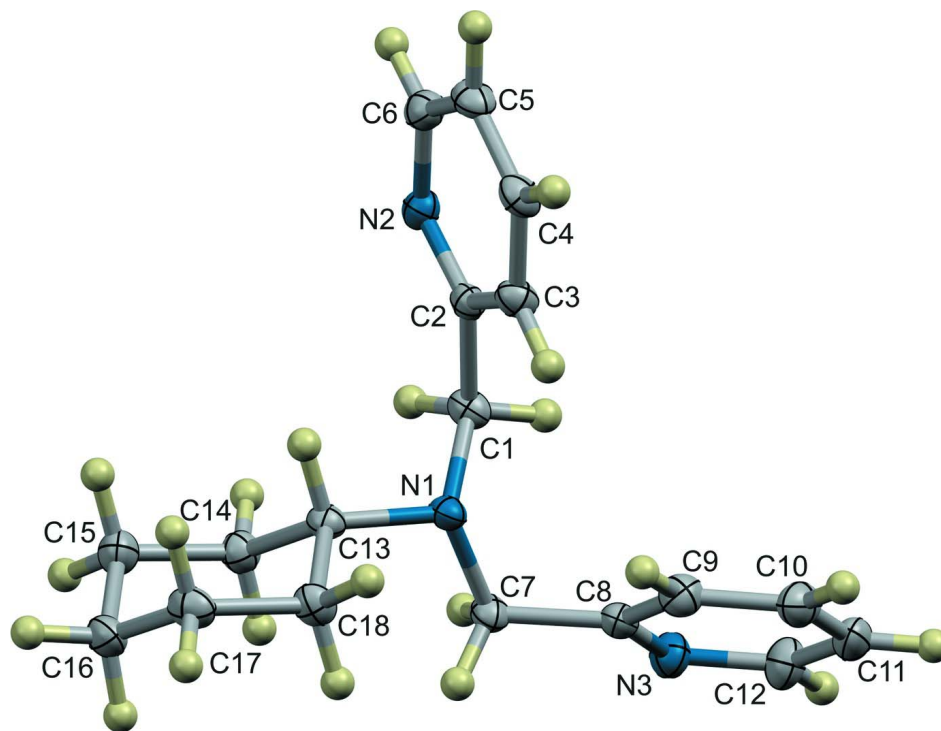
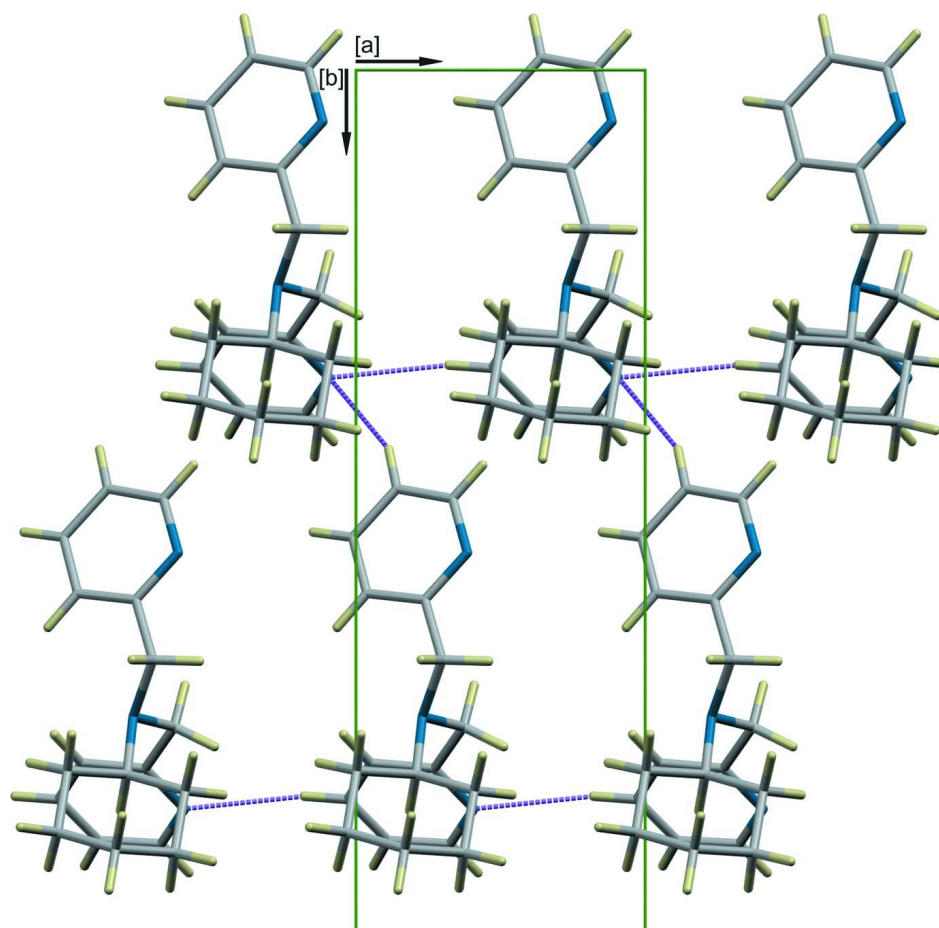


Figure 1

Thermal ellipsoid plot of (1), rendered at 50% probability. Hydrogen atoms are shown as spheres of arbitrary radius.

**Figure 2**

Two-dimensional hydrogen-bonded network of 1 viewed along the *c*-axis. Hydrogen bonds are represented by dashed purple lines.

N,N-Bis(pyridin-2-ylmethyl)cyclohexanamine

Crystal data

$C_{18}H_{23}N_3$

$M_r = 281.39$

Monoclinic, *Cc*

Hall symbol: C -2yc

$a = 6.2272 (2) \text{ \AA}$

$b = 18.1729 (7) \text{ \AA}$

$c = 14.3213 (5) \text{ \AA}$

$\beta = 102.118 (4)^\circ$

$V = 1584.57 (10) \text{ \AA}^3$

$Z = 4$

$F(000) = 608$

$D_x = 1.180 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2134 reflections

$\theta = 3.5\text{--}32.1^\circ$

$\mu = 0.07 \text{ mm}^{-1}$

$T = 120 \text{ K}$

Planar, colourless

$0.60 \times 0.50 \times 0.30 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur 2 CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans at fixed θ angles

Absorption correction: multi-scan
(Blessing, 1995)

$T_{\min} = 0.959$, $T_{\max} = 0.979$

7854 measured reflections

2521 independent reflections

2134 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\text{max}} = 32.1^\circ$, $\theta_{\text{min}} = 3.5^\circ$

$h = -9 \rightarrow 6$
 $k = -26 \rightarrow 25$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.085$
 $S = 0.98$
 2134 reflections
 190 parameters
 2 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.053P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.15 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. Yield: 1.3432 g (40%), colourless block crystals. ^1H NMR (400 MHz, CDCl_3) δ (p.p.m.): 8.58 (d, 2H); 8.50–7.60 (m, 4H); 7.05 (t, 2H); 3.39 (s, 4H); 2.55 (m, 1H); 1.90 (d, 2H); 1.8 (m, 2H); 1.60 (d, 2H); 1.35 (m, 2H); 1.19 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ / p.p.m.: 27.0; 29; 57.0; 60.5; 122.0; 123.0; 136.0; 148.0; 161. IR (KBr, 4000–400 cm^{-1}): 2958–2854 (alkyl C—H stretch); 1589 C=N (pyridyl). MS—ES⁺, m/e: 282.2069, ($M+1$)⁺. Anal. Calc. for $\text{C}_{18}\text{H}_{23}\text{N}_3$: C, 76.81; H, 8.24; N, 14.93; Found: C, 76.8; H, 8.18; N, 14.89.

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

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

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|--------------|--------------|----------------------------------|
| C1 | 0.8715 (2) | 0.26180 (9) | 0.20552 (11) | 0.0220 (3) |
| H1A | 1.0103 | 0.2846 | 0.1967 | 0.026* |
| H1B | 0.9082 | 0.2135 | 0.2369 | 0.026* |
| C2 | 0.7709 (2) | 0.31007 (8) | 0.27025 (10) | 0.0186 (3) |
| C3 | 0.5510 (2) | 0.30374 (9) | 0.27499 (11) | 0.0235 (3) |
| H3 | 0.4570 | 0.2709 | 0.2338 | 0.028* |
| C4 | 0.4709 (3) | 0.34586 (10) | 0.34038 (12) | 0.0258 (3) |
| H4 | 0.3215 | 0.3420 | 0.3451 | 0.031* |
| C5 | 0.6111 (3) | 0.39369 (10) | 0.39884 (12) | 0.0265 (3) |
| H5 | 0.5610 | 0.4230 | 0.4449 | 0.032* |
| C6 | 0.8260 (3) | 0.39748 (9) | 0.38825 (12) | 0.0253 (3) |
| H6 | 0.9221 | 0.4308 | 0.4278 | 0.030* |
| C7 | 0.7975 (3) | 0.18410 (9) | 0.06711 (11) | 0.0219 (3) |
| H7A | 0.9583 | 0.1856 | 0.0719 | 0.026* |
| H7B | 0.7258 | 0.1839 | -0.0015 | 0.026* |
| C8 | 0.7384 (3) | 0.11434 (8) | 0.11310 (11) | 0.0215 (3) |
| C9 | 0.5374 (3) | 0.10687 (10) | 0.14035 (12) | 0.0270 (3) |
| H9 | 0.4348 | 0.1463 | 0.1310 | 0.032* |

| | | | | |
|------|------------|---------------|---------------|------------|
| C10 | 0.4884 (3) | 0.04184 (10) | 0.18101 (13) | 0.0310 (4) |
| H10 | 0.3523 | 0.0358 | 0.2002 | 0.037* |
| C11 | 0.6412 (3) | -0.01444 (10) | 0.19330 (13) | 0.0313 (4) |
| H11 | 0.6137 | -0.0598 | 0.2216 | 0.038* |
| C12 | 0.8340 (3) | -0.00279 (10) | 0.16339 (14) | 0.0321 (4) |
| H12 | 0.9380 | -0.0417 | 0.1713 | 0.039* |
| C13 | 0.7079 (2) | 0.31684 (8) | 0.05181 (11) | 0.0196 (3) |
| H13 | 0.6855 | 0.3590 | 0.0936 | 0.024* |
| C14 | 0.9088 (3) | 0.33578 (9) | 0.01086 (12) | 0.0240 (3) |
| H14A | 1.0392 | 0.3406 | 0.0636 | 0.029* |
| H14B | 0.9370 | 0.2955 | -0.0315 | 0.029* |
| C15 | 0.8733 (3) | 0.40755 (10) | -0.04551 (13) | 0.0304 (4) |
| H15A | 1.0034 | 0.4179 | -0.0730 | 0.036* |
| H15B | 0.8567 | 0.4485 | -0.0020 | 0.036* |
| C16 | 0.6690 (3) | 0.40310 (10) | -0.12573 (12) | 0.0295 (4) |
| H16A | 0.6455 | 0.4510 | -0.1593 | 0.035* |
| H16B | 0.6910 | 0.3652 | -0.1725 | 0.035* |
| C17 | 0.4681 (3) | 0.38384 (10) | -0.08605 (12) | 0.0285 (4) |
| H17A | 0.3395 | 0.3782 | -0.1395 | 0.034* |
| H17B | 0.4367 | 0.4245 | -0.0449 | 0.034* |
| C18 | 0.5024 (3) | 0.31257 (10) | -0.02789 (12) | 0.0250 (3) |
| H18A | 0.3726 | 0.3034 | 0.0003 | 0.030* |
| H18B | 0.5165 | 0.2709 | -0.0707 | 0.030* |
| N1 | 0.7294 (2) | 0.24994 (7) | 0.11224 (9) | 0.0197 (3) |
| N2 | 0.9074 (2) | 0.35684 (7) | 0.32526 (10) | 0.0219 (3) |
| N3 | 0.8852 (2) | 0.05990 (8) | 0.12380 (11) | 0.0268 (3) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|------------|-------------|-------------|------------|-------------|
| C1 | 0.0195 (7) | 0.0269 (8) | 0.0196 (7) | 0.0041 (6) | 0.0039 (5) | 0.0007 (6) |
| C2 | 0.0202 (7) | 0.0190 (7) | 0.0164 (6) | 0.0021 (5) | 0.0033 (5) | 0.0032 (5) |
| C3 | 0.0205 (7) | 0.0296 (8) | 0.0199 (7) | -0.0015 (6) | 0.0031 (6) | -0.0010 (6) |
| C4 | 0.0231 (7) | 0.0326 (9) | 0.0235 (7) | 0.0012 (6) | 0.0089 (6) | 0.0022 (7) |
| C5 | 0.0319 (8) | 0.0269 (8) | 0.0231 (7) | 0.0061 (7) | 0.0114 (6) | -0.0004 (6) |
| C6 | 0.0289 (8) | 0.0217 (8) | 0.0249 (7) | 0.0004 (6) | 0.0043 (6) | -0.0015 (6) |
| C7 | 0.0248 (7) | 0.0214 (7) | 0.0212 (7) | 0.0019 (6) | 0.0090 (6) | 0.0002 (6) |
| C8 | 0.0253 (7) | 0.0221 (7) | 0.0173 (6) | -0.0018 (6) | 0.0049 (6) | -0.0011 (6) |
| C9 | 0.0246 (8) | 0.0273 (8) | 0.0302 (8) | -0.0003 (6) | 0.0081 (7) | -0.0021 (7) |
| C10 | 0.0311 (8) | 0.0324 (9) | 0.0317 (9) | -0.0092 (7) | 0.0114 (7) | -0.0034 (7) |
| C11 | 0.0393 (10) | 0.0259 (8) | 0.0277 (8) | -0.0097 (7) | 0.0048 (7) | 0.0014 (7) |
| C12 | 0.0336 (9) | 0.0242 (9) | 0.0384 (10) | 0.0013 (7) | 0.0072 (8) | 0.0044 (8) |
| C13 | 0.0198 (7) | 0.0208 (7) | 0.0187 (6) | 0.0015 (6) | 0.0049 (5) | -0.0010 (6) |
| C14 | 0.0224 (7) | 0.0251 (8) | 0.0248 (7) | -0.0013 (6) | 0.0058 (6) | 0.0008 (6) |
| C15 | 0.0363 (9) | 0.0266 (9) | 0.0282 (8) | -0.0056 (7) | 0.0065 (7) | 0.0020 (7) |
| C16 | 0.0395 (10) | 0.0269 (8) | 0.0211 (7) | 0.0012 (7) | 0.0041 (7) | 0.0029 (6) |
| C17 | 0.0291 (8) | 0.0307 (8) | 0.0234 (7) | 0.0062 (7) | 0.0002 (6) | 0.0014 (7) |
| C18 | 0.0205 (7) | 0.0295 (8) | 0.0238 (7) | 0.0003 (6) | 0.0016 (6) | 0.0027 (6) |
| N1 | 0.0226 (6) | 0.0211 (6) | 0.0157 (6) | 0.0025 (5) | 0.0048 (5) | -0.0003 (5) |
| N2 | 0.0215 (6) | 0.0202 (6) | 0.0238 (6) | 0.0006 (5) | 0.0040 (5) | 0.0008 (5) |

N3 0.0282 (7) 0.0224 (7) 0.0308 (7) 0.0022 (6) 0.0080 (6) 0.0018 (6)

Geometric parameters (Å, °)

| | | | |
|------------|-------------|---------------|-------------|
| C1—N1 | 1.4554 (19) | C10—H10 | 0.9500 |
| C1—C2 | 1.505 (2) | C11—C12 | 1.373 (3) |
| C1—H1A | 0.9900 | C11—H11 | 0.9500 |
| C1—H1B | 0.9900 | C12—N3 | 1.341 (2) |
| C2—N2 | 1.3359 (19) | C12—H12 | 0.9500 |
| C2—C3 | 1.390 (2) | C13—N1 | 1.4821 (19) |
| C3—C4 | 1.381 (2) | C13—C18 | 1.528 (2) |
| C3—H3 | 0.9500 | C13—C14 | 1.528 (2) |
| C4—C5 | 1.383 (2) | C13—H13 | 1.0000 |
| C4—H4 | 0.9500 | C14—C15 | 1.526 (2) |
| C5—C6 | 1.380 (2) | C14—H14A | 0.9900 |
| C5—H5 | 0.9500 | C14—H14B | 0.9900 |
| C6—N2 | 1.345 (2) | C15—C16 | 1.527 (2) |
| C6—H6 | 0.9500 | C15—H15A | 0.9900 |
| C7—N1 | 1.4642 (19) | C15—H15B | 0.9900 |
| C7—C8 | 1.509 (2) | C16—C17 | 1.520 (3) |
| C7—H7A | 0.9900 | C16—H16A | 0.9900 |
| C7—H7B | 0.9900 | C16—H16B | 0.9900 |
| C8—N3 | 1.334 (2) | C17—C18 | 1.530 (2) |
| C8—C9 | 1.394 (2) | C17—H17A | 0.9900 |
| C9—C10 | 1.380 (2) | C17—H17B | 0.9900 |
| C9—H9 | 0.9500 | C18—H18A | 0.9900 |
| C10—C11 | 1.383 (3) | C18—H18B | 0.9900 |
| | | | |
| N1—C1—C2 | 113.59 (12) | N1—C13—C18 | 110.69 (13) |
| N1—C1—H1A | 108.8 | N1—C13—C14 | 115.35 (12) |
| C2—C1—H1A | 108.8 | C18—C13—C14 | 110.47 (13) |
| N1—C1—H1B | 108.8 | N1—C13—H13 | 106.6 |
| C2—C1—H1B | 108.8 | C18—C13—H13 | 106.6 |
| H1A—C1—H1B | 107.7 | C14—C13—H13 | 106.6 |
| N2—C2—C3 | 122.37 (14) | C15—C14—C13 | 110.87 (14) |
| N2—C2—C1 | 116.00 (13) | C15—C14—H14A | 109.5 |
| C3—C2—C1 | 121.58 (14) | C13—C14—H14A | 109.5 |
| C4—C3—C2 | 119.13 (15) | C15—C14—H14B | 109.5 |
| C4—C3—H3 | 120.4 | C13—C14—H14B | 109.5 |
| C2—C3—H3 | 120.4 | H14A—C14—H14B | 108.1 |
| C3—C4—C5 | 119.17 (15) | C14—C15—C16 | 110.99 (14) |
| C3—C4—H4 | 120.4 | C14—C15—H15A | 109.4 |
| C5—C4—H4 | 120.4 | C16—C15—H15A | 109.4 |
| C6—C5—C4 | 117.92 (15) | C14—C15—H15B | 109.4 |
| C6—C5—H5 | 121.0 | C16—C15—H15B | 109.4 |
| C4—C5—H5 | 121.0 | H15A—C15—H15B | 108.0 |
| N2—C6—C5 | 123.87 (16) | C17—C16—C15 | 110.62 (14) |
| N2—C6—H6 | 118.1 | C17—C16—H16A | 109.5 |
| C5—C6—H6 | 118.1 | C15—C16—H16A | 109.5 |
| N1—C7—C8 | 111.97 (12) | C17—C16—H16B | 109.5 |

| | | | |
|-----------------|--------------|-----------------|--------------|
| N1—C7—H7A | 109.2 | C15—C16—H16B | 109.5 |
| C8—C7—H7A | 109.2 | H16A—C16—H16B | 108.1 |
| N1—C7—H7B | 109.2 | C16—C17—C18 | 111.50 (14) |
| C8—C7—H7B | 109.2 | C16—C17—H17A | 109.3 |
| H7A—C7—H7B | 107.9 | C18—C17—H17A | 109.3 |
| N3—C8—C9 | 122.00 (15) | C16—C17—H17B | 109.3 |
| N3—C8—C7 | 116.69 (14) | C18—C17—H17B | 109.3 |
| C9—C8—C7 | 121.29 (14) | H17A—C17—H17B | 108.0 |
| C10—C9—C8 | 119.52 (16) | C13—C18—C17 | 111.29 (14) |
| C10—C9—H9 | 120.2 | C13—C18—H18A | 109.4 |
| C8—C9—H9 | 120.2 | C17—C18—H18A | 109.4 |
| C9—C10—C11 | 118.68 (17) | C13—C18—H18B | 109.4 |
| C9—C10—H10 | 120.7 | C17—C18—H18B | 109.4 |
| C11—C10—H10 | 120.7 | H18A—C18—H18B | 108.0 |
| C12—C11—C10 | 118.01 (16) | C1—N1—C7 | 110.47 (12) |
| C12—C11—H11 | 121.0 | C1—N1—C13 | 112.17 (12) |
| C10—C11—H11 | 121.0 | C7—N1—C13 | 114.30 (12) |
| N3—C12—C11 | 124.36 (17) | C2—N2—C6 | 117.52 (14) |
| N3—C12—H12 | 117.8 | C8—N3—C12 | 117.42 (15) |
| C11—C12—H12 | 117.8 | | |
| | | | |
| N1—C1—C2—N2 | -142.02 (14) | C15—C16—C17—C18 | -55.53 (19) |
| N1—C1—C2—C3 | 40.6 (2) | N1—C13—C18—C17 | 175.48 (13) |
| N2—C2—C3—C4 | -1.6 (2) | C14—C13—C18—C17 | -55.51 (17) |
| C1—C2—C3—C4 | 175.56 (14) | C16—C17—C18—C13 | 55.43 (18) |
| C2—C3—C4—C5 | 0.6 (2) | C2—C1—N1—C7 | -159.59 (13) |
| C3—C4—C5—C6 | 0.6 (2) | C2—C1—N1—C13 | 71.62 (17) |
| C4—C5—C6—N2 | -0.8 (3) | C8—C7—N1—C1 | 73.28 (16) |
| N1—C7—C8—N3 | -140.81 (14) | C8—C7—N1—C13 | -159.09 (13) |
| N1—C7—C8—C9 | 40.9 (2) | C18—C13—N1—C1 | -159.74 (12) |
| N3—C8—C9—C10 | 1.0 (2) | C14—C13—N1—C1 | 73.93 (15) |
| C7—C8—C9—C10 | 179.14 (15) | C18—C13—N1—C7 | 73.51 (16) |
| C8—C9—C10—C11 | -0.2 (3) | C14—C13—N1—C7 | -52.83 (17) |
| C9—C10—C11—C12 | -0.6 (3) | C3—C2—N2—C6 | 1.4 (2) |
| C10—C11—C12—N3 | 0.7 (3) | C1—C2—N2—C6 | -175.90 (14) |
| N1—C13—C14—C15 | -176.97 (13) | C5—C6—N2—C2 | -0.2 (2) |
| C18—C13—C14—C15 | 56.58 (17) | C9—C8—N3—C12 | -0.9 (2) |
| C13—C14—C15—C16 | -57.35 (18) | C7—C8—N3—C12 | -179.15 (15) |
| C14—C15—C16—C17 | 56.55 (19) | C11—C12—N3—C8 | 0.1 (3) |

Hydrogen-bond geometry (Å, °)

| <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> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C4—H4 \cdots N2 ⁱ | 0.95 | 2.55 | 3.475 (2) | 166 (1) |
| C11—H11 \cdots N2 ⁱⁱ | 0.95 | 2.64 | 3.511 (2) | 153 (1) |

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