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# A third polymorph of *N*,*N*′-bis(pyridin-2-yl)benzene-1,4-diamine

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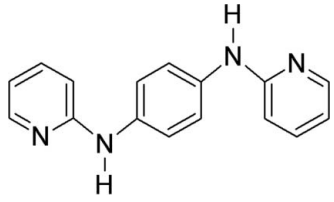
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.035; $wR$ factor = 0.094; data-to-parameter ratio = 13.2.

A third polymorph of the title compound, $C_{16}H_{14}N_4$, has been obtained. The molecule adopts a non-planar conformation with an *E* configuration at the two partially double *exo* C⋯N bonds of the 2-pyridylamine units. Like in the triclinic form [Bensemann *et al.* (2002). *New J. Chem.* **26**, 448–456], the recognition process between 2-pyridylamine units takes place through formation of a cyclic $R_2^2(8)$ hydrogen-bond motif, leading to the creation of tapes parallel to [001].

## Related literature

For the structures of the orthorhombic and triclinic polymorphs of *N*,*N*′-di(pyridin-2-yl)benzene-1,4-diamine, see: Bensemann *et al.* (2002).



## Experimental

### Crystal data

$C_{16}H_{14}N_4$
$M_r$ = 262.31
Monoclinic, $P2_1/c$
$a$ = 7.2534 (2) Å
$b$ = 20.8270 (6) Å
$c$ = 9.0681 (3) Å
$\beta$ = 106.746 (4)°
$V$ = 1311.79 (7) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.65 mm$^{-1}$
$T$ = 295 K
0.2 × 0.2 × 0.05 mm

### Data collection

Oxford Diffraction SuperNova diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.799, $T_{max}$ = 1.000
10413 measured reflections
2398 independent reflections
2221 reflections with $I > 2/s(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
$S$ = 1.07
2398 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N7—H7*N*⋯N16$^{i}$ | 0.90 | 2.25 | 3.1423 (13) | 175 |
| N14—H14*N*⋯N2$^{ii}$ | 0.90 | 2.12 | 3.0141 (14) | 175 |

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2657).

## References

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# supporting information

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## A third polymorph of *N*,*N*′-bis(pyridin-2-yl)benzene-1,4-diamine

**Barbara Wicher and Maria Gdaniec**

### S1. Comment

The compounds bearing two 2-pyridylamine groups separated by linkers can adopt either *E,E*, *Z,Z* or *E,Z* forms depending on the configuration of the partially double *exo* C⋯N bond of the 2-pyridylamine unit. In crystals the molecules in the *E, E* form tend to build one-dimensional networks *via* $R^2_2(8)$ synthons generated between self-complementary 2-pyridylamine groups. In turn, the *Z,Z* form generates the C(4) catemer motif that can lead to the formation of one-, two- and three-dimensional frameworks (Bensemann *et al.*, 2002). These compounds are known to exhibit conformational polymorphism and for *N*,*N*′-di(pyridin-2-yl)benzene-1,4-diamine two polymorphic forms were identified. In the orthorhombic form (Pbca, $Z'$=0.5), obtained by crystallization from acetonitrile, the molecules are nonplanar and adopt the *Z,Z* form. Hydrogen bonds between 2-pyridylamine groups generate catemeric motifs that assemble molecules into a two-dimensional framework. In the triclinic $P\bar{1}$ polymorph, obtained by crystallization from methanol, there are two symmetry independent molecules, each in the *E,E* form and located around inversion center. These molecules form tapes *via* strongly nonplanar $R^2_2(8)$ motif generated by N—H···N hydrogen bonds (Bensemann *et al.*, 2002).

Recently, during an attempt to cocrystallize *N*,*N*′-di(pyridin-2-yl)benzene-1,4-diamine with pyrazine from 2-butanone, a new monoclinic polymorph of *N*,*N*′-di(pyridin-2-yl)benzene-1,4-diamine was obtained. When crystallization was repeated from 2-butanone without addition of pyrazine the triclinic polymorph was formed.

In the new monoclinic polymorph the molecules adopt the *E,E* form and are assembled into tapes *via* strongly non-planar $R^2_2(8)$ hydrogen-bond motif. The overall shape of the tapes and their crystal packing are different from the arrangement found in the triclinic polymorph. As shown in Fig. 2a, the hydrogen-bonded tapes extended along [0 0 1] are grouped into pairs, with no specific interactions occurring between the two tapes, and these pairs of tapes are further arranged in a herring-bone manner (Fig. 2b).

The three polymorphs of *N*,*N*′-di(pyridin-2-yl)benzene-1,4-diamine have identical or very similar melting points: 478–479 K for the orthorhombic and triclinic polymorphs and 479 K for the monoclinic form. The calculated crystal densities are also similar: 1.335, 1.314 and 1.328 g cm$^{-3}$ for orthorhombic, triclinic and monoclinic forms, respectively.

### S2. Experimental

*N*,*N*′-Di(pyridin-2-yl)benzene-1,4-diamine was prepared according to the published procedure (Bensemann *et al.*, 2002). *N*,*N*′-Di(pyridin-2-yl)benzene-1,4-diamine (0.03 g, 0.11 mmol) and pyrazine (0.01 g, 0.11 mmol) were dissolved in 5 ml of 2-butanone and placed in a glass vial. After a few days colourless, plate-shaped crystals with a melting point of 479 K were obtained.

### S3. Refinement

H atoms of the N—H groups were located in difference electron-density maps. N—H bond lengths were standardized to 0.90 Å and $U_{iso}$(H) values were constrained to 1.2$U_{eq}$(N). All other H atoms were initially identified in difference maps but were placed at calculated positions with C—H = 0.93 Å, and were refined as riding on their carrier atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C).

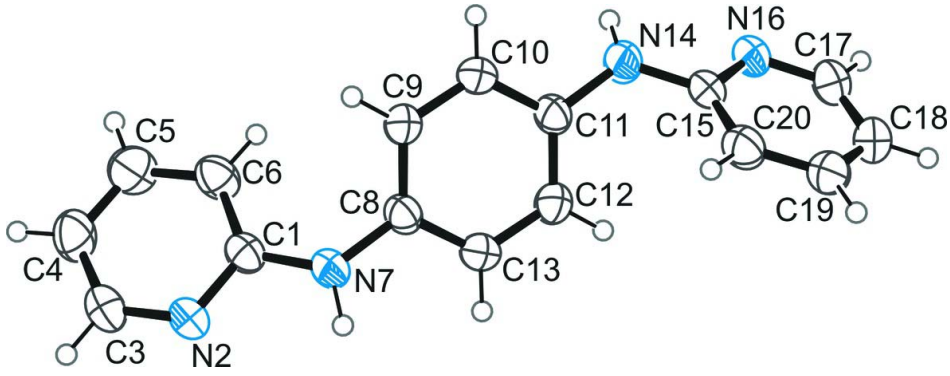


**Figure 1**

The asymmetric unit of the title compound with displacement ellipsoids shown at the 50% probability level.

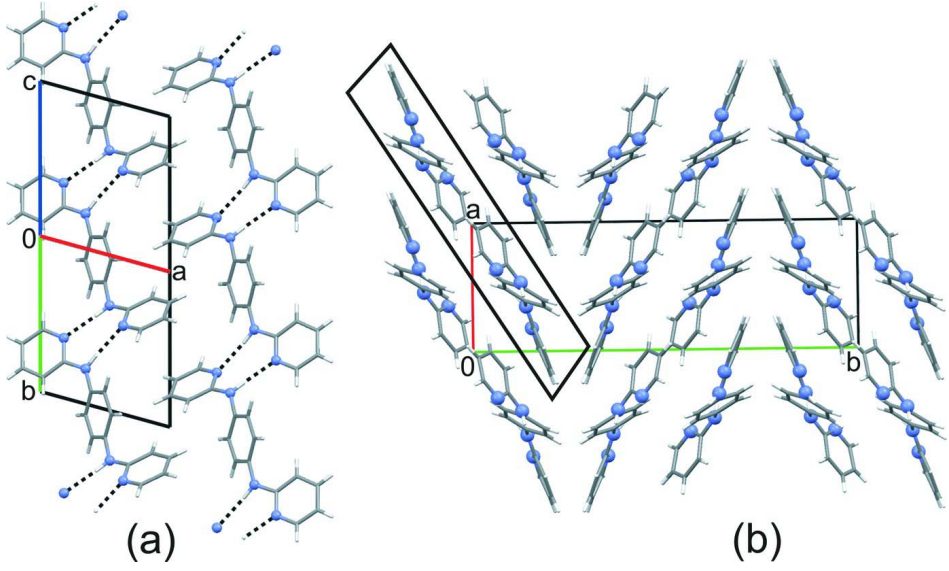


**Figure 2**

Crystal packing in the monoclinic polymorph of the title compound: (*a*) a pair of hydrogen bonded tapes extended along [0 0 1] and (*b*) herring-bone packing of the pairs of tapes (one pair is show with a black rhomboid). Hydrogen bonds are shown with dashed lines.

### *N*,*N*′-bis(pyridin-2-yl)benzene-1,4-diamine

*Crystal data*

$C_{16}H_{14}N_4$
$M_r$ = 262.31
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a$ = 7.2534 (2) Å
$b$ = 20.8270 (6) Å
$c$ = 9.0681 (3) Å
$\beta$ = 106.746 (4)°

$V$ = 1311.79 (7) Å$^3$
$Z$ = 4
$F$(000) = 552
$D_x$ = 1.328 Mg m$^{-3}$
Melting point: 479 K
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å

Cell parameters from 6262 reflections
$\theta$ = 2.1–75.8°
$\mu$ = 0.65 mm$^{-1}$
$T$ = 295 K
Plate, colourless
0.2 × 0.2 × 0.05 mm

*Data collection*

Oxford Diffraction SuperNova diffractometer
Radiation source: Nova Cu X-ray Source
Mirror monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.799, $T_{max}$ = 1.000

10413 measured reflections
2398 independent reflections
2221 reflections with $I > 2/s(I)$
$R_{int}$ = 0.019
$\theta_{max}$ = 68.2°, $\theta_{min}$ = 6.4°
$h$ = −8→8
$k$ = −25→25
$l$ = −10→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
$S$ = 1.07
2398 reflections
181 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.2155P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N2 | 0.18091 (14) | 0.15267 (5) | 0.53715 (10) | 0.0434 (2) |
| N7 | 0.34929 (14) | 0.13813 (5) | 0.36249 (10) | 0.0453 (2) |
| H7N | 0.4266 | 0.1142 | 0.4380 | 0.054* |
| N14 | 0.53458 (15) | 0.12536 (5) | −0.19925 (11) | 0.0521 (3) |
| H14N | 0.4314 | 0.1319 | −0.2811 | 0.063* |
| N16 | 0.63876 (14) | 0.06275 (5) | −0.36845 (10) | 0.0458 (2) |
| C1 | 0.18087 (15) | 0.15794 (5) | 0.38962 (12) | 0.0382 (2) |
| C3 | 0.02222 (18) | 0.17053 (6) | 0.57328 (14) | 0.0500 (3) |
| H3 | 0.0216 | 0.1663 | 0.6752 | 0.060* |
| C4 | −0.13952 (18) | 0.19473 (7) | 0.46964 (16) | 0.0572 (3) |

| | | | | |
|---|---|---|---|---|
| H4 | −0.2462 | 0.2071 | 0.5000 | 0.069* |
| C5 | −0.13771 (18) | 0.19995 (7) | 0.31846 (16) | 0.0581 (3) |
| H5 | −0.2449 | 0.2161 | 0.2448 | 0.070* |
| C6 | 0.02097 (17) | 0.18144 (6) | 0.27640 (13) | 0.0486 (3) |
| H6 | 0.0224 | 0.1844 | 0.1744 | 0.058* |
| C8 | 0.39192 (15) | 0.13618 (5) | 0.22059 (12) | 0.0387 (3) |
| C9 | 0.34861 (17) | 0.18587 (5) | 0.11355 (13) | 0.0435 (3) |
| H9 | 0.2842 | 0.2220 | 0.1332 | 0.052* |
| C10 | 0.40017 (17) | 0.18215 (6) | −0.02162 (12) | 0.0445 (3) |
| H10 | 0.3685 | 0.2157 | −0.0920 | 0.053* |
| C11 | 0.49825 (15) | 0.12933 (5) | −0.05437 (12) | 0.0406 (3) |
| C12 | 0.54745 (16) | 0.08080 (5) | 0.05517 (13) | 0.0425 (3) |
| H12 | 0.6177 | 0.0457 | 0.0380 | 0.051* |
| C13 | 0.49368 (16) | 0.08396 (5) | 0.18909 (13) | 0.0419 (3) |
| H13 | 0.5262 | 0.0505 | 0.2597 | 0.050* |
| C15 | 0.67958 (16) | 0.08914 (5) | −0.22815 (12) | 0.0418 (3) |
| C17 | 0.7754 (2) | 0.02598 (6) | −0.39897 (15) | 0.0539 (3) |
| H17 | 0.7477 | 0.0068 | −0.4955 | 0.065* |
| C18 | 0.9526 (2) | 0.01483 (7) | −0.29741 (16) | 0.0603 (4) |
| H18 | 1.0408 | −0.0122 | −0.3228 | 0.072* |
| C19 | 0.99619 (18) | 0.04509 (7) | −0.15578 (15) | 0.0574 (3) |
| H19 | 1.1173 | 0.0402 | −0.0855 | 0.069* |
| C20 | 0.85928 (17) | 0.08235 (7) | −0.11991 (14) | 0.0506 (3) |
| H20 | 0.8858 | 0.1028 | −0.0249 | 0.061* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N2 | 0.0485 (5) | 0.0489 (5) | 0.0360 (5) | 0.0011 (4) | 0.0174 (4) | 0.0017 (4) |
| N7 | 0.0482 (5) | 0.0582 (6) | 0.0316 (5) | 0.0106 (4) | 0.0148 (4) | 0.0050 (4) |
| N14 | 0.0529 (6) | 0.0744 (7) | 0.0294 (5) | 0.0220 (5) | 0.0123 (4) | 0.0021 (4) |
| N16 | 0.0504 (6) | 0.0555 (6) | 0.0349 (5) | 0.0066 (4) | 0.0177 (4) | 0.0011 (4) |
| C1 | 0.0431 (6) | 0.0385 (5) | 0.0343 (5) | −0.0050 (4) | 0.0132 (4) | −0.0027 (4) |
| C3 | 0.0539 (7) | 0.0573 (7) | 0.0456 (6) | −0.0034 (5) | 0.0253 (5) | −0.0006 (5) |
| C4 | 0.0427 (6) | 0.0708 (9) | 0.0636 (8) | −0.0016 (6) | 0.0242 (6) | −0.0007 (6) |
| C5 | 0.0386 (6) | 0.0760 (9) | 0.0563 (8) | −0.0020 (6) | 0.0081 (5) | 0.0052 (6) |
| C6 | 0.0438 (6) | 0.0638 (7) | 0.0365 (6) | −0.0053 (5) | 0.0090 (5) | −0.0002 (5) |
| C8 | 0.0403 (6) | 0.0454 (6) | 0.0313 (5) | 0.0006 (4) | 0.0117 (4) | −0.0013 (4) |
| C9 | 0.0497 (6) | 0.0445 (6) | 0.0392 (6) | 0.0108 (5) | 0.0174 (5) | 0.0014 (5) |
| C10 | 0.0505 (6) | 0.0488 (6) | 0.0352 (6) | 0.0122 (5) | 0.0139 (5) | 0.0080 (5) |
| C11 | 0.0409 (6) | 0.0511 (6) | 0.0302 (5) | 0.0054 (5) | 0.0108 (4) | −0.0014 (4) |
| C12 | 0.0465 (6) | 0.0415 (6) | 0.0411 (6) | 0.0078 (5) | 0.0150 (5) | −0.0023 (4) |
| C13 | 0.0474 (6) | 0.0413 (6) | 0.0377 (6) | 0.0046 (5) | 0.0134 (5) | 0.0051 (4) |
| C15 | 0.0471 (6) | 0.0488 (6) | 0.0335 (5) | 0.0057 (5) | 0.0178 (5) | 0.0048 (4) |
| C17 | 0.0630 (8) | 0.0606 (7) | 0.0455 (7) | 0.0103 (6) | 0.0273 (6) | −0.0004 (5) |
| C18 | 0.0604 (8) | 0.0689 (8) | 0.0618 (8) | 0.0204 (6) | 0.0337 (7) | 0.0123 (7) |
| C19 | 0.0445 (7) | 0.0763 (9) | 0.0538 (7) | 0.0105 (6) | 0.0180 (6) | 0.0175 (6) |
| C20 | 0.0489 (7) | 0.0660 (8) | 0.0373 (6) | 0.0036 (5) | 0.0131 (5) | 0.0023 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N2—C3 | 1.3372 (15) | C8—C13 | 1.3895 (15) |
| N2—C1 | 1.3422 (13) | C8—C9 | 1.3916 (15) |
| N7—C1 | 1.3771 (14) | C9—C10 | 1.3829 (15) |
| N7—C8 | 1.4079 (13) | C9—H9 | 0.9300 |
| N7—H7N | 0.9001 | C10—C11 | 1.3879 (16) |
| N14—C15 | 1.3793 (14) | C10—H10 | 0.9300 |
| N14—C11 | 1.4148 (14) | C11—C12 | 1.3898 (16) |
| N14—H14N | 0.9000 | C12—C13 | 1.3799 (15) |
| N16—C15 | 1.3385 (14) | C12—H12 | 0.9300 |
| N16—C17 | 1.3427 (15) | C13—H13 | 0.9300 |
| C1—C6 | 1.3974 (16) | C15—C20 | 1.3947 (16) |
| C3—C4 | 1.3706 (19) | C17—C18 | 1.3682 (19) |
| C3—H3 | 0.9300 | C17—H17 | 0.9300 |
| C4—C5 | 1.3790 (18) | C18—C19 | 1.383 (2) |
| C4—H4 | 0.9300 | C18—H18 | 0.9300 |
| C5—C6 | 1.3681 (18) | C19—C20 | 1.3713 (18) |
| C5—H5 | 0.9300 | C19—H19 | 0.9300 |
| C6—H6 | 0.9300 | C20—H20 | 0.9300 |
| | | | |
| C3—N2—C1 | 117.93 (10) | C8—C9—H9 | 119.6 |
| C1—N7—C8 | 127.71 (9) | C9—C10—C11 | 121.35 (10) |
| C1—N7—H7N | 114.8 | C9—C10—H10 | 119.3 |
| C8—N7—H7N | 115.3 | C11—C10—H10 | 119.3 |
| C15—N14—C11 | 124.37 (9) | C10—C11—C12 | 117.74 (10) |
| C15—N14—H14N | 115.1 | C10—C11—N14 | 119.28 (10) |
| C11—N14—H14N | 115.1 | C12—C11—N14 | 122.89 (10) |
| C15—N16—C17 | 117.13 (10) | C13—C12—C11 | 120.99 (10) |
| N2—C1—N7 | 114.09 (10) | C13—C12—H12 | 119.5 |
| N2—C1—C6 | 121.52 (10) | C11—C12—H12 | 119.5 |
| N7—C1—C6 | 124.39 (10) | C12—C13—C8 | 121.32 (10) |
| N2—C3—C4 | 124.16 (11) | C12—C13—H13 | 119.3 |
| N2—C3—H3 | 117.9 | C8—C13—H13 | 119.3 |
| C4—C3—H3 | 117.9 | N16—C15—N14 | 115.68 (10) |
| C3—C4—C5 | 117.34 (12) | N16—C15—C20 | 122.22 (10) |
| C3—C4—H4 | 121.3 | N14—C15—C20 | 122.07 (10) |
| C5—C4—H4 | 121.3 | N16—C17—C18 | 124.33 (12) |
| C6—C5—C4 | 120.31 (12) | N16—C17—H17 | 117.8 |
| C6—C5—H5 | 119.8 | C18—C17—H17 | 117.8 |
| C4—C5—H5 | 119.8 | C17—C18—C19 | 117.84 (12) |
| C5—C6—C1 | 118.73 (11) | C17—C18—H18 | 121.1 |
| C5—C6—H6 | 120.6 | C19—C18—H18 | 121.1 |
| C1—C6—H6 | 120.6 | C20—C19—C18 | 119.38 (12) |
| C13—C8—C9 | 117.73 (10) | C20—C19—H19 | 120.3 |
| C13—C8—N7 | 118.69 (10) | C18—C19—H19 | 120.3 |
| C9—C8—N7 | 123.44 (10) | C19—C20—C15 | 118.97 (12) |
| C10—C9—C8 | 120.81 (10) | C19—C20—H20 | 120.5 |

| | | | |
|---|---|---|---|
| C10—C9—H9 | 119.6 | C15—C20—H20 | 120.5 |
| | | | |
| C3—N2—C1—N7 | −179.60 (10) | C15—N14—C11—C10 | 157.24 (12) |
| C3—N2—C1—C6 | 0.15 (16) | C15—N14—C11—C12 | −26.30 (18) |
| C8—N7—C1—N2 | 178.25 (10) | C10—C11—C12—C13 | 2.54 (17) |
| C8—N7—C1—C6 | −1.49 (19) | N14—C11—C12—C13 | −173.97 (11) |
| C1—N2—C3—C4 | −0.97 (18) | C11—C12—C13—C8 | −1.25 (17) |
| N2—C3—C4—C5 | 0.9 (2) | C9—C8—C13—C12 | −1.05 (17) |
| C3—C4—C5—C6 | −0.1 (2) | N7—C8—C13—C12 | −176.94 (10) |
| C4—C5—C6—C1 | −0.7 (2) | C17—N16—C15—N14 | −178.51 (11) |
| N2—C1—C6—C5 | 0.65 (18) | C17—N16—C15—C20 | 3.62 (18) |
| N7—C1—C6—C5 | −179.63 (12) | C11—N14—C15—N16 | 145.45 (11) |
| C1—N7—C8—C13 | −139.63 (12) | C11—N14—C15—C20 | −36.68 (18) |
| C1—N7—C8—C9 | 44.73 (17) | C15—N16—C17—C18 | −1.0 (2) |
| C13—C8—C9—C10 | 2.02 (17) | N16—C17—C18—C19 | −2.2 (2) |
| N7—C8—C9—C10 | 177.69 (11) | C17—C18—C19—C20 | 2.9 (2) |
| C8—C9—C10—C11 | −0.71 (18) | C18—C19—C20—C15 | −0.5 (2) |
| C9—C10—C11—C12 | −1.57 (18) | N16—C15—C20—C19 | −2.90 (19) |
| C9—C10—C11—N14 | 175.07 (11) | N14—C15—C20—C19 | 179.36 (12) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N7—H7*N*···N16$^{i}$ | 0.90 | 2.25 | 3.1423 (13) | 175 |
| N14—H14*N*···N2$^{ii}$ | 0.90 | 2.12 | 3.0141 (14) | 175 |

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