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7-Chloro-5-(2-ethoxyphenyl)-1-methyl-3-propyl-2,6-dihydro-1*H*-pyrazolo[4,3-*d*]-pyrimidine

Ming-Qiu Zhou, Kai Zhu, Xiao-Ping Lv, Ping-Fang Han* and Ping Wei

College of Biotechnology and Pharmaceutical Engineering, Nanjing University of Technology, Ximofan Road No. 5 Nanjing, Nanjing 210009, People's Republic of China

Correspondence e-mail: hpf@njut.edu.cn

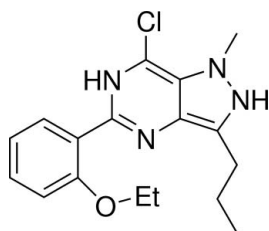
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.064; wR factor = 0.182; data-to-parameter ratio = 14.7.

In the title compound, $\text{C}_{17}\text{H}_{21}\text{ClN}_4\text{O}$, the benzene ring is oriented at dihedral angles of 1.59 (3) and 1.27 (3)° with respect to the pyrimidine and pyrazole rings, while the dihedral angle between the pyrimidine and pyrazole rings is 0.83 (3)°. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond results in the formation of a planar (r.m.s. deviation 0.004 Å) six-membered ring.

Related literature

For a related structure, see: Rajesh & Joshi (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{21}\text{ClN}_4\text{O}$
 $M_r = 332.83$

 Triclinic, $P\bar{1}$
 $a = 4.6700$ (9) Å

 $b = 11.647$ (2) Å
 $c = 16.064$ (3) Å
 $\alpha = 78.56$ (3)°
 $\beta = 86.75$ (3)°
 $\gamma = 79.81$ (3)°
 $V = 842.7$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 294$ K
 $0.30 \times 0.10 \times 0.10$ mm

Data collection

 Enraf–Nonius CAD-4
 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.932$, $T_{\max} = 0.977$
 3470 measured reflections

 3061 independent reflections
 2353 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 3 standard reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.182$
 $S = 1.00$
 3061 reflections

 208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.38$ e Å⁻³
 $\Delta\rho_{\min} = -0.52$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------------|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1A}\cdots\text{O1}$ | 0.86 | 1.91 | 2.616 (3) | 138 |

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2761).

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supplementary materials

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7-Chloro-5-(2-ethoxyphenyl)-1-methyl-3-propyl-2,6-dihydro-1*H*-pyrazolo[4,3-*d*]pyrimidine

M.-Q. Zhou, K. Zhu, X.-P. Lv, P.-F. Han and P. Wei

Comment

Some derivatives of 5-(2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound, (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C3-C8), B (N1/N2/C9-C12) and C (N3/N4/C10/C11/C13) are, of course, planar. The dihedral angles between them are A/B = 1.59 (3), A/C = 1.27 (3) and B/C = 0.83 (3) °. The intramolecular N-H...O hydrogen bond (Table 1) results in the formation of a planar six-membered ring D (O1/N1/C3/C8/C9/H1A), which is oriented with respect to the other rings at dihedral angles of A/D = 1.01 (3), B/D = 0.63 (3) and C/D = 0.83 (3) °. So, the rings are almost coplanar.

Experimental

For the preparation of the title compound, 5-(2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydro-7*H*-pyrazolo[4,3-*d*]pyrimidin-7-one (15.6 g) and phosphorus trichloride (13.7 g) were added into carbon tetrachloride (100 ml) at 345-350 K. The gross products were extracted with *n*-hexane, dried under vacuum, and then recrystallized in dichloromethane. Finally the title compound is obtained (yield; 1.5 g) (Rajesh *et al.*, 2007). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically with N-H = 0.86 Å (for NH) and C-H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Figures

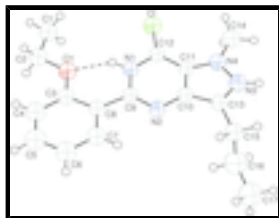


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Hydrogen bond is shown as dashed line.

7-Chloro-5-(2-ethoxyphenyl)-1-methyl-3-propyl-2,6-dihydro- 1H-pyrazolo[4,3-d]pyrimidine

Crystal data

| | |
|-------------------------------|---|
| $C_{17}H_{21}ClN_4O$ | $Z = 2$ |
| $M_r = 332.83$ | $F_{000} = 352$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.312 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 4.6700 (9) \text{ \AA}$ | Cell parameters from 25 reflections |
| $b = 11.647 (2) \text{ \AA}$ | $\theta = 9\text{--}13^\circ$ |
| $c = 16.064 (3) \text{ \AA}$ | $\mu = 0.24 \text{ mm}^{-1}$ |
| $\alpha = 78.56 (3)^\circ$ | $T = 294 \text{ K}$ |
| $\beta = 86.75 (3)^\circ$ | Block, yellow |
| $\gamma = 79.81 (3)^\circ$ | $0.30 \times 0.10 \times 0.10 \text{ mm}$ |
| $V = 842.7 (3) \text{ \AA}^3$ | |

Data collection

| | |
|---|------------------------------------|
| Enraf–Nonius CAD-4 diffractometer | $R_{\text{int}} = 0.033$ |
| Radiation source: fine-focus sealed tube | $\theta_{\text{max}} = 25.3^\circ$ |
| Monochromator: graphite | $\theta_{\text{min}} = 1.3^\circ$ |
| $T = 294 \text{ K}$ | $h = 0 \rightarrow 5$ |
| $\omega/2\theta$ scans | $k = -13 \rightarrow 13$ |
| Absorption correction: ψ scan (North <i>et al.</i> , 1968) | $l = -19 \rightarrow 19$ |
| $T_{\text{min}} = 0.932$, $T_{\text{max}} = 0.977$ | 3 standard reflections |
| 3470 measured reflections | every 120 min |
| 3061 independent reflections | intensity decay: 1% |
| 2353 reflections with $I > 2\sigma(I)$ | |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.064$ | H-atom parameters constrained |
| $wR(F^2) = 0.182$ | $w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.6P]$ |
| $S = 1.00$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3061 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 208 parameters | $\Delta\rho_{\text{max}} = 0.38 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.52 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|--------------|----------------------------------|
| Cl | 0.45734 (19) | 0.18716 (7) | 0.56202 (5) | 0.0581 (3) |
| O1 | 0.4864 (5) | 0.49028 (18) | 0.68108 (14) | 0.0528 (6) |
| N1 | 0.6871 (5) | 0.2658 (2) | 0.68131 (14) | 0.0420 (6) |
| H1A | 0.5753 | 0.3313 | 0.6613 | 0.050* |
| N2 | 1.0314 (5) | 0.1732 (2) | 0.78486 (14) | 0.0414 (6) |
| N3 | 1.1345 (6) | -0.1091 (2) | 0.72458 (16) | 0.0506 (7) |
| H3A | 1.2075 | -0.1828 | 0.7269 | 0.061* |
| N4 | 0.9354 (6) | -0.0435 (2) | 0.66884 (16) | 0.0466 (6) |
| C1 | 0.1508 (7) | 0.5709 (3) | 0.5722 (2) | 0.0605 (9) |
| H1B | 0.0284 | 0.6416 | 0.5443 | 0.091* |
| H1C | 0.0335 | 0.5119 | 0.5956 | 0.091* |
| H1D | 0.2893 | 0.5410 | 0.5319 | 0.091* |
| C2 | 0.3079 (7) | 0.5992 (3) | 0.6417 (2) | 0.0550 (8) |
| H2B | 0.4278 | 0.6587 | 0.6189 | 0.066* |
| H2C | 0.1703 | 0.6297 | 0.6829 | 0.066* |
| C3 | 0.6554 (7) | 0.4882 (3) | 0.74759 (19) | 0.0452 (7) |
| C4 | 0.6545 (8) | 0.5877 (3) | 0.7839 (2) | 0.0597 (9) |
| H4A | 0.5325 | 0.6587 | 0.7632 | 0.072* |
| C5 | 0.8344 (9) | 0.5806 (3) | 0.8503 (2) | 0.0671 (10) |
| H5A | 0.8325 | 0.6470 | 0.8744 | 0.081* |
| C6 | 1.0161 (9) | 0.4770 (3) | 0.8812 (2) | 0.0635 (9) |
| H6A | 1.1384 | 0.4735 | 0.9257 | 0.076* |
| C7 | 1.0177 (7) | 0.3782 (3) | 0.8465 (2) | 0.0528 (8) |
| H7A | 1.1418 | 0.3082 | 0.8683 | 0.063* |
| C8 | 0.8384 (6) | 0.3800 (3) | 0.77958 (18) | 0.0428 (7) |
| C9 | 0.8566 (6) | 0.2674 (2) | 0.74811 (17) | 0.0393 (6) |
| C10 | 1.0325 (6) | 0.0743 (2) | 0.75138 (17) | 0.0397 (6) |
| C11 | 0.8671 (6) | 0.0690 (2) | 0.68347 (17) | 0.0398 (6) |
| C12 | 0.6759 (6) | 0.1717 (2) | 0.64296 (17) | 0.0389 (6) |
| C13 | 1.1973 (6) | -0.0409 (3) | 0.77464 (19) | 0.0443 (7) |
| C14 | 0.8296 (8) | -0.0978 (3) | 0.6049 (2) | 0.0606 (9) |
| H14A | 0.9214 | -0.1795 | 0.6116 | 0.091* |
| H14B | 0.8752 | -0.0562 | 0.5493 | 0.091* |

supplementary materials

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|------|-------------|-------------|--------------|-------------|
| H14C | 0.6226 | -0.0934 | 0.6116 | 0.091* |
| C15 | 1.3994 (7) | -0.0863 (3) | 0.84708 (19) | 0.0502 (8) |
| H15A | 1.4993 | -0.0232 | 0.8551 | 0.060* |
| H15B | 1.5449 | -0.1506 | 0.8332 | 0.060* |
| C16 | 1.2456 (9) | -0.1304 (5) | 0.9283 (2) | 0.0868 (14) |
| H16A | 1.0974 | -0.0661 | 0.9409 | 0.104* |
| H16B | 1.1471 | -0.1936 | 0.9197 | 0.104* |
| C17 | 1.4345 (10) | -0.1757 (5) | 1.0040 (2) | 0.0865 (13) |
| H17A | 1.3173 | -0.2021 | 1.0527 | 0.130* |
| H17B | 1.5283 | -0.1132 | 1.0147 | 0.130* |
| H17C | 1.5793 | -0.2410 | 0.9932 | 0.130* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0624 (5) | 0.0586 (5) | 0.0533 (5) | -0.0064 (4) | -0.0254 (4) | -0.0076 (4) |
| O1 | 0.0595 (13) | 0.0387 (11) | 0.0578 (13) | 0.0041 (10) | -0.0213 (11) | -0.0087 (9) |
| N1 | 0.0438 (13) | 0.0384 (13) | 0.0421 (13) | -0.0020 (10) | -0.0136 (11) | -0.0050 (10) |
| N2 | 0.0417 (13) | 0.0432 (13) | 0.0385 (12) | -0.0065 (10) | -0.0090 (10) | -0.0040 (10) |
| N3 | 0.0554 (16) | 0.0390 (13) | 0.0539 (15) | 0.0040 (12) | -0.0135 (12) | -0.0079 (11) |
| N4 | 0.0530 (15) | 0.0395 (13) | 0.0472 (14) | -0.0013 (11) | -0.0119 (12) | -0.0106 (11) |
| C1 | 0.0518 (19) | 0.061 (2) | 0.063 (2) | 0.0071 (16) | -0.0128 (16) | -0.0078 (17) |
| C2 | 0.0521 (19) | 0.0433 (17) | 0.063 (2) | 0.0070 (14) | -0.0095 (16) | -0.0055 (15) |
| C3 | 0.0453 (16) | 0.0440 (16) | 0.0469 (17) | -0.0074 (13) | -0.0020 (13) | -0.0102 (13) |
| C4 | 0.065 (2) | 0.0452 (18) | 0.070 (2) | -0.0044 (16) | -0.0089 (18) | -0.0163 (16) |
| C5 | 0.081 (3) | 0.057 (2) | 0.072 (2) | -0.0113 (19) | -0.012 (2) | -0.0298 (18) |
| C6 | 0.074 (2) | 0.065 (2) | 0.057 (2) | -0.0163 (19) | -0.0199 (18) | -0.0194 (17) |
| C7 | 0.0583 (19) | 0.0499 (18) | 0.0516 (18) | -0.0076 (15) | -0.0168 (15) | -0.0102 (14) |
| C8 | 0.0430 (16) | 0.0428 (16) | 0.0432 (15) | -0.0088 (13) | -0.0052 (13) | -0.0068 (12) |
| C9 | 0.0376 (14) | 0.0407 (15) | 0.0383 (14) | -0.0069 (12) | -0.0037 (12) | -0.0037 (12) |
| C10 | 0.0399 (15) | 0.0404 (15) | 0.0374 (14) | -0.0049 (12) | -0.0043 (12) | -0.0044 (12) |
| C11 | 0.0409 (15) | 0.0400 (15) | 0.0379 (14) | -0.0066 (12) | -0.0045 (12) | -0.0048 (12) |
| C12 | 0.0376 (14) | 0.0413 (15) | 0.0377 (14) | -0.0097 (12) | -0.0031 (12) | -0.0040 (12) |
| C13 | 0.0419 (16) | 0.0431 (16) | 0.0441 (16) | -0.0004 (12) | -0.0055 (13) | -0.0042 (13) |
| C14 | 0.074 (2) | 0.0503 (19) | 0.061 (2) | -0.0034 (17) | -0.0181 (18) | -0.0203 (16) |
| C15 | 0.0476 (17) | 0.0463 (17) | 0.0524 (18) | 0.0036 (13) | -0.0128 (14) | -0.0060 (14) |
| C16 | 0.060 (2) | 0.135 (4) | 0.057 (2) | -0.028 (2) | -0.0162 (19) | 0.014 (2) |
| C17 | 0.081 (3) | 0.117 (4) | 0.055 (2) | -0.024 (3) | -0.015 (2) | 0.010 (2) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|---------|-----------|
| C1—C12 | 1.660 (3) | C5—C6 | 1.367 (5) |
| O1—C2 | 1.439 (4) | C5—H5A | 0.9300 |
| O1—C3 | 1.358 (4) | C6—C7 | 1.373 (5) |
| N1—C9 | 1.374 (3) | C6—H6A | 0.9300 |
| N1—C12 | 1.369 (4) | C7—C8 | 1.395 (4) |
| N1—H1A | 0.8600 | C7—H7A | 0.9300 |
| N2—C9 | 1.304 (4) | C8—C9 | 1.484 (4) |
| N2—C10 | 1.363 (4) | C10—C11 | 1.389 (4) |

| | | | |
|------------|-----------|---------------|-----------|
| N3—N4 | 1.350 (3) | C10—C13 | 1.414 (4) |
| N3—C13 | 1.315 (4) | C11—C12 | 1.425 (4) |
| N3—H3A | 0.8600 | C13—C15 | 1.493 (4) |
| N4—C11 | 1.356 (4) | C14—H14A | 0.9600 |
| N4—C14 | 1.458 (4) | C14—H14B | 0.9600 |
| C1—C2 | 1.489 (5) | C14—H14C | 0.9600 |
| C1—H1B | 0.9600 | C15—C16 | 1.497 (5) |
| C1—H1C | 0.9600 | C15—H15A | 0.9700 |
| C1—H1D | 0.9600 | C15—H15B | 0.9700 |
| C2—H2B | 0.9700 | C16—C17 | 1.496 (5) |
| C2—H2C | 0.9700 | C16—H16A | 0.9700 |
| C3—C4 | 1.396 (4) | C16—H16B | 0.9700 |
| C3—C8 | 1.412 (4) | C17—H17A | 0.9600 |
| C4—C5 | 1.375 (5) | C17—H17B | 0.9600 |
| C4—H4A | 0.9300 | C17—H17C | 0.9600 |
| C3—O1—C2 | 120.4 (2) | C3—C8—C9 | 125.6 (3) |
| C12—N1—C9 | 127.4 (2) | N2—C9—N1 | 122.1 (3) |
| C12—N1—H1A | 116.3 | N2—C9—C8 | 119.1 (3) |
| C9—N1—H1A | 116.3 | N1—C9—C8 | 118.8 (2) |
| C9—N2—C10 | 114.6 (2) | N2—C10—C11 | 125.1 (3) |
| C13—N3—N4 | 108.1 (2) | N2—C10—C13 | 129.4 (3) |
| C13—N3—H3A | 125.9 | C11—C10—C13 | 105.4 (3) |
| N4—N3—H3A | 125.9 | N4—C11—C10 | 106.8 (2) |
| N3—N4—C11 | 110.3 (2) | N4—C11—C12 | 132.7 (3) |
| N3—N4—C14 | 119.5 (2) | C10—C11—C12 | 120.5 (3) |
| C11—N4—C14 | 130.2 (3) | N1—C12—C11 | 110.1 (2) |
| C2—C1—H1B | 109.5 | N1—C12—C1 | 120.5 (2) |
| C2—C1—H1C | 109.5 | C11—C12—C1 | 129.4 (2) |
| H1B—C1—H1C | 109.5 | N3—C13—C10 | 109.3 (3) |
| C2—C1—H1D | 109.5 | N3—C13—C15 | 122.6 (3) |
| H1B—C1—H1D | 109.5 | C10—C13—C15 | 127.9 (3) |
| H1C—C1—H1D | 109.5 | N4—C14—H14A | 109.5 |
| O1—C2—C1 | 106.9 (3) | N4—C14—H14B | 109.5 |
| O1—C2—H2B | 110.3 | H14A—C14—H14B | 109.5 |
| C1—C2—H2B | 110.3 | N4—C14—H14C | 109.5 |
| O1—C2—H2C | 110.3 | H14A—C14—H14C | 109.5 |
| C1—C2—H2C | 110.3 | H14B—C14—H14C | 109.5 |
| H2B—C2—H2C | 108.6 | C13—C15—C16 | 112.7 (3) |
| O1—C3—C4 | 122.6 (3) | C13—C15—H15A | 109.1 |
| O1—C3—C8 | 117.3 (3) | C16—C15—H15A | 109.1 |
| C4—C3—C8 | 120.1 (3) | C13—C15—H15B | 109.1 |
| C5—C4—C3 | 119.9 (3) | C16—C15—H15B | 109.1 |
| C5—C4—H4A | 120.0 | H15A—C15—H15B | 107.8 |
| C3—C4—H4A | 120.0 | C17—C16—C15 | 115.6 (3) |
| C6—C5—C4 | 120.8 (3) | C17—C16—H16A | 108.4 |
| C6—C5—H5A | 119.6 | C15—C16—H16A | 108.4 |
| C4—C5—H5A | 119.6 | C17—C16—H16B | 108.4 |
| C5—C6—C7 | 119.9 (3) | C15—C16—H16B | 108.4 |
| C5—C6—H6A | 120.1 | H16A—C16—H16B | 107.5 |

supplementary materials

| | | | |
|----------------|------------|-----------------|------------|
| C7—C6—H6A | 120.1 | C16—C17—H17A | 109.5 |
| C6—C7—C8 | 121.8 (3) | C16—C17—H17B | 109.5 |
| C6—C7—H7A | 119.1 | H17A—C17—H17B | 109.5 |
| C8—C7—H7A | 119.1 | C16—C17—H17C | 109.5 |
| C7—C8—C3 | 117.5 (3) | H17A—C17—H17C | 109.5 |
| C7—C8—C9 | 116.9 (3) | H17B—C17—H17C | 109.5 |
| C3—O1—C2—C1 | -179.6 (3) | C6—C7—C8—C9 | -179.3 (3) |
| C2—O1—C3—C4 | 3.4 (5) | O1—C3—C8—C7 | 178.4 (3) |
| C2—O1—C3—C8 | -176.2 (3) | C4—C3—C8—C7 | -1.2 (5) |
| C12—N1—C9—N2 | -1.2 (5) | O1—C3—C8—C9 | -1.6 (5) |
| C12—N1—C9—C8 | 179.2 (3) | C4—C3—C8—C9 | 178.8 (3) |
| C9—N1—C12—C11 | 1.1 (4) | C7—C8—C9—N2 | 1.4 (4) |
| C9—N1—C12—C1 | -179.6 (2) | C3—C8—C9—N2 | -178.6 (3) |
| C10—N2—C9—N1 | 0.4 (4) | C7—C8—C9—N1 | -179.0 (3) |
| C10—N2—C9—C8 | 180.0 (2) | C3—C8—C9—N1 | 1.1 (4) |
| C9—N2—C10—C11 | 0.3 (4) | N2—C10—C11—N4 | 178.7 (3) |
| C9—N2—C10—C13 | 178.9 (3) | C13—C10—C11—N4 | -0.2 (3) |
| C13—N3—N4—C11 | -0.4 (3) | N2—C10—C11—C12 | -0.3 (4) |
| C13—N3—N4—C14 | 179.3 (3) | C13—C10—C11—C12 | -179.1 (3) |
| N4—N3—C13—C10 | 0.2 (3) | N4—C11—C12—N1 | -179.1 (3) |
| N4—N3—C13—C15 | 176.7 (3) | C10—C11—C12—N1 | -0.4 (4) |
| N3—N4—C11—C10 | 0.3 (3) | N4—C11—C12—C1 | 1.7 (5) |
| C14—N4—C11—C10 | -179.3 (3) | C10—C11—C12—C1 | -179.6 (2) |
| N3—N4—C11—C12 | 179.1 (3) | N2—C10—C13—N3 | -178.9 (3) |
| C14—N4—C11—C12 | -0.5 (6) | C11—C10—C13—N3 | -0.1 (3) |
| O1—C3—C4—C5 | -178.9 (3) | N2—C10—C13—C15 | 4.9 (5) |
| C8—C3—C4—C5 | 0.7 (5) | C11—C10—C13—C15 | -176.3 (3) |
| C3—C4—C5—C6 | 0.3 (6) | N3—C13—C15—C16 | -90.3 (4) |
| C4—C5—C6—C7 | -0.7 (6) | C10—C13—C15—C16 | 85.5 (4) |
| C5—C6—C7—C8 | 0.2 (6) | C13—C15—C16—C17 | -179.2 (4) |
| C6—C7—C8—C3 | 0.7 (5) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|-------|-------------|-------------|---------------|
| N1—H1A \cdots O1 | 0.86 | 1.91 | 2.616 (3) | 138 |

Fig. 1

