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# Crystal structure of pencycuron

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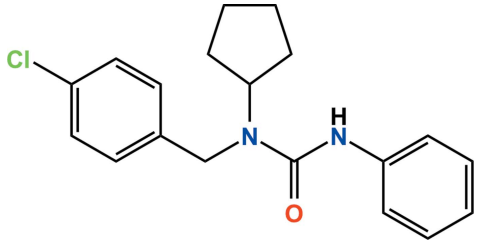
In the title compound [systematic name: 1-(4-chlorobenzyl)-1-cyclopentyl-3-phenylurea], $C_{19}H_{21}ClN_2O$, which is a urea fungicide, the cyclopentyl ring adopts an envelope conformation, with one of the methylene C atoms adjacent to the C atom bonding to the N atom as the flap. The dihedral angles between the mean planes of the central cyclopentyl ring (all atoms) and the chlorobenzyl and phenyl rings are 77.96 (6) and 57.77 (7)°, respectively. In the crystal, N—H···O hydrogen bonds link adjacent molecules, forming $C(4)$ chains propagating along the $b$-axis direction. The chains are linked by weak $\pi$–$\pi$ interactions between the chlorobenzene rings [centroid–centroid separation = 3.9942 (9) Å], resulting in two-dimensional networks extending parellel to the (110) plane.

**Keywords:** crystal structure; pencycuron; urea; fungicide; hydrogen bonding; $\pi$–$\pi$ interactions.

**CCDC reference**: 1409194

## 1. Related literature

For information on the fungicidal properties of the title compound, see: Pal *et al.* (2005). For a related crystal structure, see: Bjerglund *et al.* (2012).




## 2. Experimental

### 2.1. Crystal data

$C_{19}H_{21}ClN_2O$
$M_r$ = 328.83
Orthorhombic, *Pbca*
$a$ = 12.1585 (5) Å
$b$ = 8.6721 (4) Å
$c$ = 32.6152 (12) Å
$V$ = 3438.9 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 173 K
0.50 × 0.11 × 0.09 mm

### 2.2. Data collection

Bruker APEX-II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.894, $T_{max}$ = 0.980
27037 measured reflections
3374 independent reflections
2698 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
$S$ = 1.04
3374 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2*N*···O1$^{i}$ | 0.828 (19) | 2.081 (19) | 2.8838 (17) | 163.1 (17) |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick 2008).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7456).

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Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Pal, P., Chakrabarti, K., Chakraborty, A. & Chowdhury, A. (2005). *Pest. Manag. Sci.* **61**, 1220–1223.
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Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

# supporting information

*Acta Cryst.* (2015). E**71**, o532 [https://doi.org/10.1107/S2056989015012414]

## Crystal structure of pencycuron

**Gihaeng Kang, Jineun Kim, Eunjin Kwon and Tae Ho Kim**

### S1. Comment

Pencycuron, [systematic name: 1-(4-chlorobenzyl)-1-cyclopentyl-3-phenylurea], is a urea fungicide and it has been used for the control of diseases in various crops, including rice (Pal *et al.*, 2005). However, until now its crystal structure has not been reported. In the title compound (Fig. 1), the dihedral angles between the mean planes of the central cyclopentyl ring [r.m.s. deviation = 0.1693] and the chlorobenzyl and phenyl rings are 77.96 (6) and 57.778 (7)°, respectively. All bond lengths and bond angles are normal and comparable to those observed in the crystal structure of a similar compound (Bjerglund *et al.*, 2012).

In the crystal (Fig. 2), N—H···O hydrogen bonds link adjacent molecules, forming a one-dimensional chains along the *b* axis direction (Table. 1). The chains are linked by weak *π*–*π* interactions [*Cg*1···*Cg*1$^{ii}$, 3.9942 (9) Å], resulting in a two-dimensional networks parellel to the (110) plane (*Cg*1 is the centroid of the C1–C6 ring)[for symmetry codes: (ii), -*x*, -*y*, -*z*].

### S2. Experimental

The title compound was purchased from the Dr Ehrenstorfer GmbH Company. Slow evaporation of a solution in $CH_2Cl_2$ gave colourless needles.

### S3. Refinement

The N-bound H atom was located in a difference Fourier map and freely refined (N—H = 0.828 (19) Å). The C-bound H atoms were positioned geometrically and refined using a riding model with d(C—H) = 1.00 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for C$sp^3$—H, d(C—H) = 0.99 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for $CH_2$ groups, d(C—H) = 0.95 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for aromatic C—H.

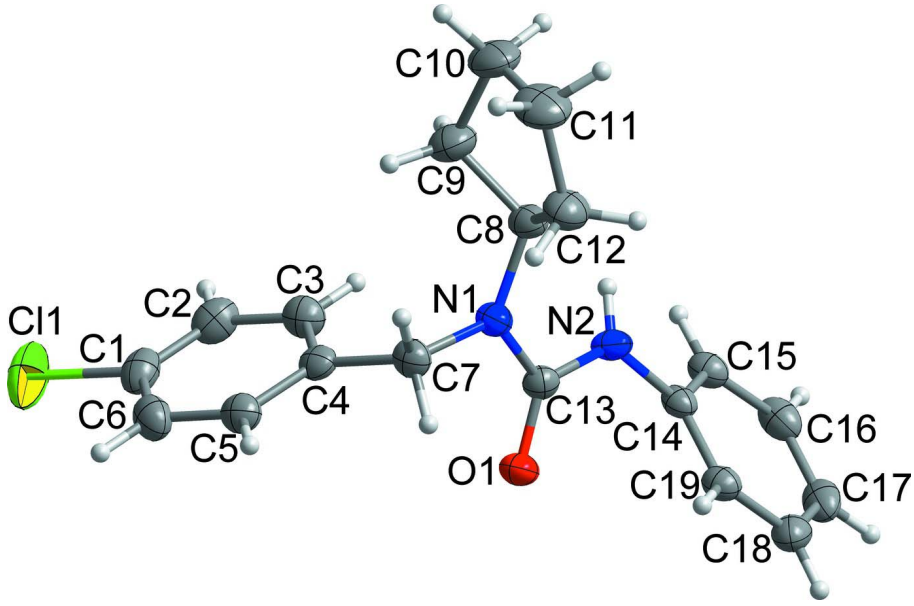


**Figure 1**

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

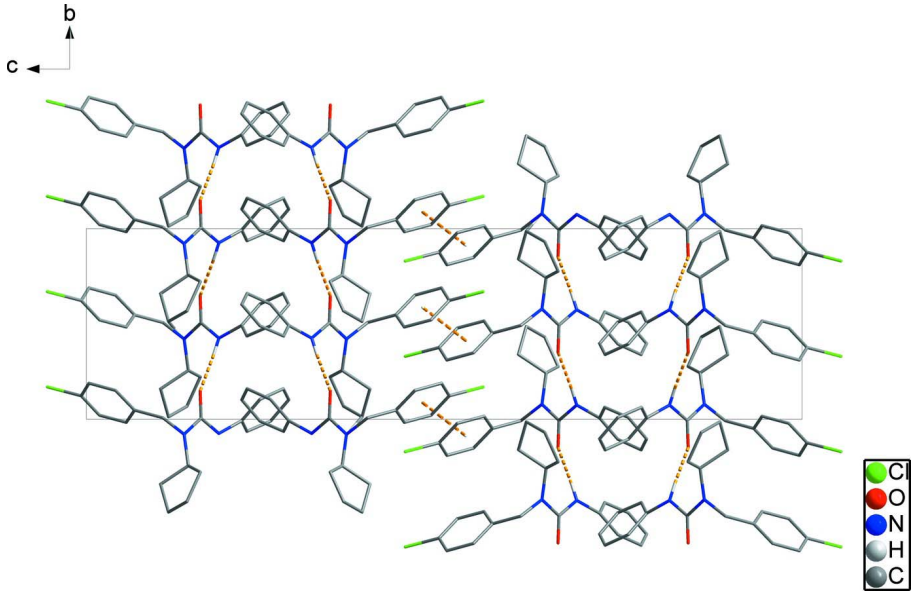


**Figure 2**

Crystal packing viewed along the *a* axis. The intermolecular N—H···O hydrogen bonds and weak $\pi$–$\pi$ interactions are shown as dashed lines.

### 1-(4-Chlorobenzyl)-1-cyclopentyl-3-phenylurea

*Crystal data*

$C_{19}H_{21}ClN_2O$
$M_r$ = 328.83
Orthorhombic, *Pbca*
*a* = 12.1585 (5) Å
*b* = 8.6721 (4) Å
*c* = 32.6152 (12) Å
*V* = 3438.9 (2) Å$^3$
*Z* = 8

$F(000) = 1392$
$D_x = 1.270$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6227 reflections
$\theta = 2.5$–$27.3°$
$\mu = 0.23$ mm$^{-1}$
$T = 173$ K
Needle, colourless
0.50 × 0.11 × 0.09 mm

*Data collection*

Bruker APEX-II CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.894$, $T_{max} = 0.980$
27037 measured reflections
3374 independent reflections
2698 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -14 \rightarrow 14$
$k = -6 \rightarrow 10$
$l = -40 \rightarrow 40$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.095$
$S = 1.04$
3374 reflections
212 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.2518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ 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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.23590 (4) | −0.16966 (8) | −0.05434 (2) | 0.06131 (19) |
| O1 | 0.15878 (8) | −0.14846 (11) | 0.15909 (3) | 0.0287 (2) |
| N1 | 0.08966 (10) | 0.07872 (15) | 0.13656 (4) | 0.0278 (3) |
| N2 | 0.23017 (10) | 0.07453 (16) | 0.18515 (4) | 0.0288 (3) |
| H2N | 0.2489 (14) | 0.162 (2) | 0.1777 (5) | 0.039 (5)* |
| C1 | 0.17668 (14) | −0.1232 (2) | −0.00710 (5) | 0.0384 (4) |
| C2 | 0.22919 (13) | −0.0213 (2) | 0.01841 (5) | 0.0397 (4) |
| H2 | 0.2975 | 0.0233 | 0.0106 | 0.048* |
| C3 | 0.18127 (12) | 0.0160 (2) | 0.05576 (5) | 0.0355 (4) |
| H3 | 0.2173 | 0.0863 | 0.0736 | 0.043* |
| C4 | 0.08150 (12) | −0.04807 (17) | 0.06739 (4) | 0.0277 (3) |
| C5 | 0.03091 (13) | −0.15110 (19) | 0.04097 (5) | 0.0327 (4) |
| H5 | −0.0373 | −0.1962 | 0.0486 | 0.039* |
| C6 | 0.07769 (14) | −0.1895 (2) | 0.00376 (5) | 0.0390 (4) |
| H6 | 0.0423 | −0.2604 | −0.0141 | 0.047* |
| C7 | 0.02356 (12) | −0.00774 (19) | 0.10708 (4) | 0.0298 (3) |
| H7A | −0.0428 | 0.0535 | 0.1005 | 0.036* |
| H7B | −0.0012 | −0.1045 | 0.1203 | 0.036* |

| | | | | |
|---|---|---|---|---|
| C8 | 0.06470 (12) | 0.24352 (18) | 0.14250 (5) | 0.0315 (4) |
| H8 | 0.1190 | 0.2854 | 0.1627 | 0.038* |
| C9 | 0.07296 (15) | 0.3403 (2) | 0.10377 (5) | 0.0436 (4) |
| H9A | 0.0381 | 0.2873 | 0.0802 | 0.052* |
| H9B | 0.1506 | 0.3629 | 0.0969 | 0.052* |
| C10 | 0.01105 (17) | 0.4869 (2) | 0.11481 (6) | 0.0532 (5) |
| H10A | −0.0149 | 0.5406 | 0.0898 | 0.064* |
| H10B | 0.0584 | 0.5579 | 0.1307 | 0.064* |
| C11 | −0.08580 (17) | 0.4315 (2) | 0.14061 (7) | 0.0565 (5) |
| H11A | −0.1520 | 0.4182 | 0.1233 | 0.068* |
| H11B | −0.1027 | 0.5070 | 0.1625 | 0.068* |
| C12 | −0.05145 (14) | 0.2774 (2) | 0.15928 (6) | 0.0421 (4) |
| H12A | −0.1033 | 0.1949 | 0.1511 | 0.050* |
| H12B | −0.0502 | 0.2841 | 0.1896 | 0.050* |
| C13 | 0.15966 (11) | −0.00577 (17) | 0.16037 (4) | 0.0249 (3) |
| C14 | 0.29239 (11) | 0.00718 (17) | 0.21711 (4) | 0.0255 (3) |
| C15 | 0.39770 (12) | 0.06323 (18) | 0.22439 (5) | 0.0300 (3) |
| H15 | 0.4283 | 0.1387 | 0.2066 | 0.036* |
| C16 | 0.45819 (13) | 0.0096 (2) | 0.25737 (5) | 0.0357 (4) |
| H16 | 0.5295 | 0.0500 | 0.2625 | 0.043* |
| C17 | 0.41528 (14) | −0.1025 (2) | 0.28280 (5) | 0.0381 (4) |
| H17 | 0.4569 | −0.1396 | 0.3054 | 0.046* |
| C18 | 0.31135 (14) | −0.16039 (19) | 0.27514 (5) | 0.0354 (4) |
| H18 | 0.2822 | −0.2390 | 0.2923 | 0.043* |
| C19 | 0.24920 (12) | −0.10478 (18) | 0.24270 (4) | 0.0293 (3) |
| H19 | 0.1772 | −0.1434 | 0.2381 | 0.035* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0543 (3) | 0.0950 (5) | 0.0346 (2) | 0.0261 (3) | 0.0028 (2) | −0.0022 (3) |
| O1 | 0.0304 (5) | 0.0214 (5) | 0.0343 (6) | −0.0008 (5) | −0.0029 (4) | −0.0001 (5) |
| N1 | 0.0293 (6) | 0.0238 (7) | 0.0303 (6) | 0.0018 (6) | −0.0084 (5) | −0.0012 (6) |
| N2 | 0.0295 (7) | 0.0207 (6) | 0.0361 (7) | −0.0033 (6) | −0.0097 (5) | 0.0054 (6) |
| C1 | 0.0388 (9) | 0.0465 (10) | 0.0298 (8) | 0.0157 (8) | −0.0022 (7) | 0.0049 (8) |
| C2 | 0.0300 (8) | 0.0476 (11) | 0.0414 (9) | 0.0029 (8) | 0.0011 (7) | 0.0082 (9) |
| C3 | 0.0303 (8) | 0.0365 (9) | 0.0396 (9) | −0.0018 (7) | −0.0046 (7) | −0.0005 (8) |
| C4 | 0.0274 (7) | 0.0269 (8) | 0.0290 (7) | 0.0030 (7) | −0.0073 (6) | 0.0041 (7) |
| C5 | 0.0300 (8) | 0.0331 (9) | 0.0350 (8) | −0.0003 (7) | −0.0070 (6) | 0.0014 (7) |
| C6 | 0.0408 (9) | 0.0412 (10) | 0.0352 (8) | 0.0044 (8) | −0.0113 (7) | −0.0056 (8) |
| C7 | 0.0254 (7) | 0.0316 (9) | 0.0324 (8) | −0.0024 (7) | −0.0056 (6) | −0.0017 (7) |
| C8 | 0.0354 (8) | 0.0245 (8) | 0.0345 (8) | 0.0026 (7) | −0.0091 (7) | 0.0022 (7) |
| C9 | 0.0495 (10) | 0.0358 (10) | 0.0454 (10) | 0.0022 (8) | −0.0033 (8) | 0.0120 (9) |
| C10 | 0.0705 (13) | 0.0338 (10) | 0.0552 (11) | 0.0087 (10) | −0.0153 (10) | 0.0118 (9) |
| C11 | 0.0532 (11) | 0.0433 (12) | 0.0730 (14) | 0.0190 (10) | −0.0099 (10) | 0.0020 (11) |
| C12 | 0.0459 (10) | 0.0343 (9) | 0.0459 (10) | 0.0084 (8) | 0.0025 (8) | −0.0006 (8) |
| C13 | 0.0231 (7) | 0.0246 (8) | 0.0269 (7) | −0.0011 (6) | 0.0017 (6) | 0.0016 (7) |
| C14 | 0.0265 (7) | 0.0211 (7) | 0.0290 (7) | 0.0047 (6) | −0.0049 (6) | −0.0033 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.0278 (8) | 0.0253 (8) | 0.0369 (8) | 0.0015 (6) | −0.0026 (6) | −0.0027 (7) |
| C16 | 0.0271 (7) | 0.0346 (9) | 0.0454 (9) | 0.0065 (7) | −0.0104 (7) | −0.0104 (8) |
| C17 | 0.0430 (9) | 0.0375 (10) | 0.0339 (8) | 0.0145 (8) | −0.0141 (7) | −0.0038 (8) |
| C18 | 0.0440 (9) | 0.0297 (9) | 0.0326 (8) | 0.0073 (8) | −0.0023 (7) | 0.0018 (7) |
| C19 | 0.0286 (7) | 0.0249 (8) | 0.0342 (8) | 0.0023 (7) | −0.0038 (6) | −0.0013 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.7478 (17) | C8—H8 | 1.0000 |
| O1—C13 | 1.2382 (17) | C9—C10 | 1.521 (3) |
| N1—C13 | 1.3654 (18) | C9—H9A | 0.9900 |
| N1—C7 | 1.4604 (18) | C9—H9B | 0.9900 |
| N1—C8 | 1.474 (2) | C10—C11 | 1.525 (3) |
| N2—C13 | 1.3686 (19) | C10—H10A | 0.9900 |
| N2—C14 | 1.4141 (18) | C10—H10B | 0.9900 |
| N2—H2N | 0.828 (19) | C11—C12 | 1.527 (3) |
| C1—C2 | 1.371 (2) | C11—H11A | 0.9900 |
| C1—C6 | 1.380 (2) | C11—H11B | 0.9900 |
| C2—C3 | 1.389 (2) | C12—H12A | 0.9900 |
| C2—H2 | 0.9500 | C12—H12B | 0.9900 |
| C3—C4 | 1.387 (2) | C14—C19 | 1.384 (2) |
| C3—H3 | 0.9500 | C14—C15 | 1.390 (2) |
| C4—C5 | 1.385 (2) | C15—C16 | 1.384 (2) |
| C4—C7 | 1.515 (2) | C15—H15 | 0.9500 |
| C5—C6 | 1.381 (2) | C16—C17 | 1.380 (2) |
| C5—H5 | 0.9500 | C16—H16 | 0.9500 |
| C6—H6 | 0.9500 | C17—C18 | 1.382 (2) |
| C7—H7A | 0.9900 | C17—H17 | 0.9500 |
| C7—H7B | 0.9900 | C18—C19 | 1.387 (2) |
| C8—C9 | 1.520 (2) | C18—H18 | 0.9500 |
| C8—C12 | 1.543 (2) | C19—H19 | 0.9500 |
| | | | |
| C13—N1—C7 | 116.23 (12) | H9A—C9—H9B | 109.0 |
| C13—N1—C8 | 125.02 (12) | C9—C10—C11 | 104.42 (15) |
| C7—N1—C8 | 118.11 (12) | C9—C10—H10A | 110.9 |
| C13—N2—C14 | 124.07 (13) | C11—C10—H10A | 110.9 |
| C13—N2—H2N | 117.8 (12) | C9—C10—H10B | 110.9 |
| C14—N2—H2N | 116.5 (12) | C11—C10—H10B | 110.9 |
| C2—C1—C6 | 121.24 (15) | H10A—C10—H10B | 108.9 |
| C2—C1—Cl1 | 119.44 (13) | C10—C11—C12 | 106.55 (15) |
| C6—C1—Cl1 | 119.32 (14) | C10—C11—H11A | 110.4 |
| C1—C2—C3 | 119.13 (15) | C12—C11—H11A | 110.4 |
| C1—C2—H2 | 120.4 | C10—C11—H11B | 110.4 |
| C3—C2—H2 | 120.4 | C12—C11—H11B | 110.4 |
| C4—C3—C2 | 120.91 (15) | H11A—C11—H11B | 108.6 |
| C4—C3—H3 | 119.5 | C11—C12—C8 | 105.99 (14) |
| C2—C3—H3 | 119.5 | C11—C12—H12A | 110.5 |
| C5—C4—C3 | 118.45 (14) | C8—C12—H12A | 110.5 |

| | | | |
|---|---|---|---|
| C5—C4—C7 | 118.30 (13) | C11—C12—H12B | 110.5 |
| C3—C4—C7 | 123.23 (14) | C8—C12—H12B | 110.5 |
| C6—C5—C4 | 121.28 (15) | H12A—C12—H12B | 108.7 |
| C6—C5—H5 | 119.4 | O1—C13—N1 | 120.78 (13) |
| C4—C5—H5 | 119.4 | O1—C13—N2 | 122.27 (13) |
| C1—C6—C5 | 118.98 (16) | N1—C13—N2 | 116.96 (13) |
| C1—C6—H6 | 120.5 | C19—C14—C15 | 119.46 (13) |
| C5—C6—H6 | 120.5 | C19—C14—N2 | 122.10 (13) |
| N1—C7—C4 | 115.17 (12) | C15—C14—N2 | 118.31 (14) |
| N1—C7—H7A | 108.5 | C16—C15—C14 | 120.32 (15) |
| C4—C7—H7A | 108.5 | C16—C15—H15 | 119.8 |
| N1—C7—H7B | 108.5 | C14—C15—H15 | 119.8 |
| C4—C7—H7B | 108.5 | C17—C16—C15 | 120.21 (15) |
| H7A—C7—H7B | 107.5 | C17—C16—H16 | 119.9 |
| N1—C8—C9 | 114.36 (13) | C15—C16—H16 | 119.9 |
| N1—C8—C12 | 114.81 (13) | C16—C17—C18 | 119.51 (15) |
| C9—C8—C12 | 104.49 (13) | C16—C17—H17 | 120.2 |
| N1—C8—H8 | 107.6 | C18—C17—H17 | 120.2 |
| C9—C8—H8 | 107.6 | C17—C18—C19 | 120.64 (16) |
| C12—C8—H8 | 107.6 | C17—C18—H18 | 119.7 |
| C8—C9—C10 | 103.43 (14) | C19—C18—H18 | 119.7 |
| C8—C9—H9A | 111.1 | C14—C19—C18 | 119.83 (14) |
| C10—C9—H9A | 111.1 | C14—C19—H19 | 120.1 |
| C8—C9—H9B | 111.1 | C18—C19—H19 | 120.1 |
| C10—C9—H9B | 111.1 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.2 (3) | C9—C10—C11—C12 | 24.7 (2) |
| Cl1—C1—C2—C3 | 179.54 (13) | C10—C11—C12—C8 | −1.9 (2) |
| C1—C2—C3—C4 | −0.2 (3) | N1—C8—C12—C11 | −147.64 (15) |
| C2—C3—C4—C5 | 0.4 (2) | C9—C8—C12—C11 | −21.56 (18) |
| C2—C3—C4—C7 | −177.90 (15) | C7—N1—C13—O1 | −6.1 (2) |
| C3—C4—C5—C6 | −0.3 (2) | C8—N1—C13—O1 | 164.53 (14) |
| C7—C4—C5—C6 | 178.12 (14) | C7—N1—C13—N2 | 173.51 (12) |
| C2—C1—C6—C5 | 0.4 (3) | C8—N1—C13—N2 | −15.8 (2) |
| Cl1—C1—C6—C5 | −179.41 (12) | C14—N2—C13—O1 | −13.1 (2) |
| C4—C5—C6—C1 | −0.1 (2) | C14—N2—C13—N1 | 167.32 (13) |
| C13—N1—C7—C4 | −81.80 (16) | C13—N2—C14—C19 | −40.2 (2) |
| C8—N1—C7—C4 | 106.87 (15) | C13—N2—C14—C15 | 144.02 (15) |
| C5—C4—C7—N1 | 169.45 (13) | C19—C14—C15—C16 | −1.1 (2) |
| C3—C4—C7—N1 | −12.2 (2) | N2—C14—C15—C16 | 174.79 (14) |
| C13—N1—C8—C9 | 131.17 (15) | C14—C15—C16—C17 | 1.4 (2) |
| C7—N1—C8—C9 | −58.34 (18) | C15—C16—C17—C18 | −0.2 (2) |
| C13—N1—C8—C12 | −108.04 (16) | C16—C17—C18—C19 | −1.3 (2) |
| C7—N1—C8—C12 | 62.45 (18) | C15—C14—C19—C18 | −0.3 (2) |
| N1—C8—C9—C10 | 163.14 (14) | N2—C14—C19—C18 | −176.06 (14) |
| C12—C8—C9—C10 | 36.79 (18) | C17—C18—C19—C14 | 1.5 (2) |
| C8—C9—C10—C11 | −38.08 (18) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*N*···O1$^{i}$ | 0.828 (19) | 2.081 (19) | 2.8838 (17) | 163.1 (17) |

Symmetry code: (i) −*x*+1/2, *y*+1/2, *z*.