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# 2,4-Dichloro-*N*-{[1-(2,4-dichlorobenzoyl)piperidin-4-yl]methyl}benzamide

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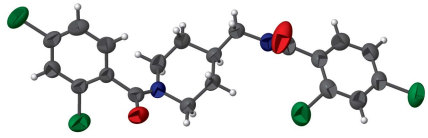
**Keywords:** crystal structure; piperidine; piperidone; benzamide; N—H···O hydrogen bonding.

**CCDC reference**: 1484074

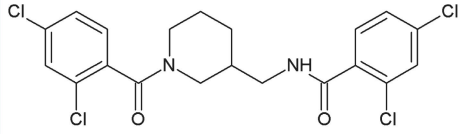
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{18}Cl_4N_2O_2$, the piperdine ring adopts a chair conformation. The dihedral angles between its mean plane and the two benzene rings are 45.5 (3) and 28.0 (3)°, while the benzene rings are inclined to one another by 54.5 (3)°. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming chains along the *a*-axis direction. Neighbouring chains are linked by C—H···$\pi$ interactions, forming double-stranded chains along [100].

**3D view**



**Chemical scheme**




## Structure description

Piperidones are an important group of heterocyclic compounds in the field of medicinal chemistry due to their biological activities which include cytotoxic and anticancer properties (Dimmock *et al.*, 2001). They are also reported to possess analgesic, anti-inflammatory, central nervous system (*CNS*), local anaesthetic, anticancer and anti-microbial activities (Perumal *et al.*, 2001). Piperidine derivatives have been observed to exhibit antimicrobial, anti-inflammatory, antiviral, antimalarial and general anesthetic activities (Aridoss *et al.*, 2009). Functionalized piperidines are familiar substructures found in biologically active natural products and synthetic pharmaceuticals (Michael, 2001; Pinder, 1992; Rubiralta *et al.*, 1991). Piperidines have also been found to exhibit blood-cholesterol-lowering activities (Nalanishi *et al.*, 1974). Herein, we report on the synthesis and crystal structure of the title piperidone derivative.

The molecular structure of the title compound is illustrated in Fig. 1. The bond distances and bond angles are close to those observed for similar structures (Revathi *et al.*, 2015; Prathebha *et al.*, 2015). The the piperdine ring (N1/C8–C12) adopts a chair conformation. The dihedral angles between its mean plane and the two benzene rings

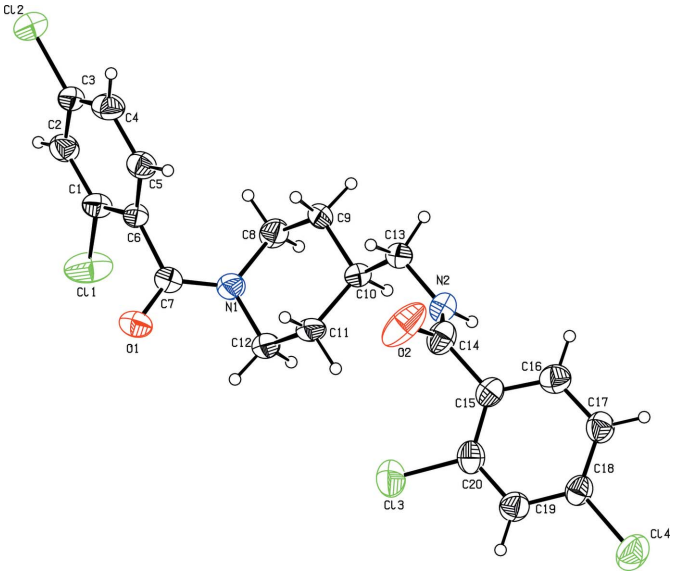



**Figure 1**
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

(C1–C6 and C15–C20) are 44.5 (3) and 28.0 (3)°, respectively, while the benzene rings are inclined to one another by 54.5 (3)°.

In the crystal, adjacent molecules are linked through N—H···O hydrogen bonds, forming chains along the *a*-axis direction (Table 1 and Fig. 2). Neighbouring chains are linked *via* C—H···$\pi$ interactions, forming double-stranded chains along [100]; see Table 1 and Fig. 3.

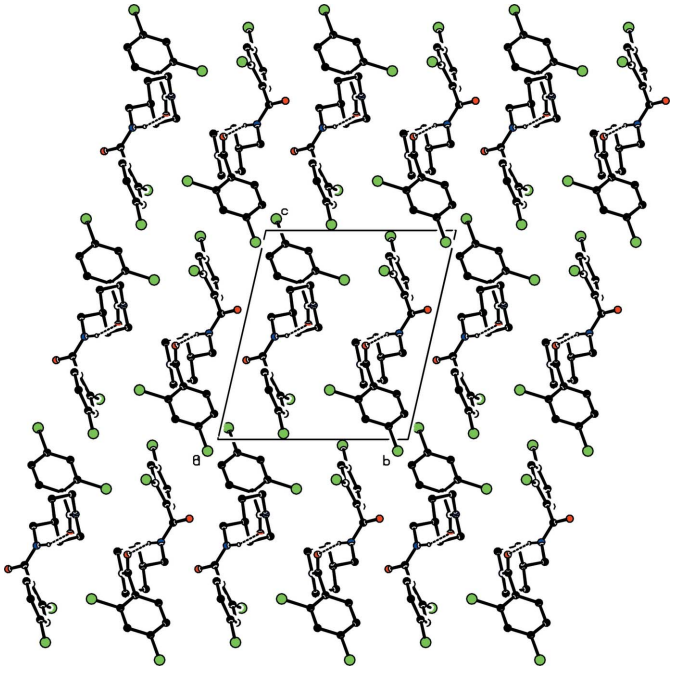



**Figure 2**
A view along the *a* axis of the crystal packing of the title compound, with hydrogen bonds shown as dashed lines (see Table 1). For clarity, the C-bound H atoms have been omitted.

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

*Cg*1 is the centroid of the C15–C20 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1$^{i}$ | 0.90 (6) | 1.94 (6) | 2.809 (8) | 163 (5) |
| C4—H4···*Cg*1 | 0.93 | 2.93 | 3.628 (8) | 132 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{20}H_{18}Cl_4N_2O_2$ |
| $M_r$ | 460.16 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 293 |
| *a*, *b*, *c* (Å) | 8.2338 (2), 10.9617 (2), 12.2646 (3) |
| $\alpha$, $\beta$, $\gamma$ (°) | 76.239 (1), 83.571 (1), 80.407 (1) |
| *V* (Å$^3$) | 1057.12 (4) |
| *Z* | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.58 |
| Crystal size (mm) | 0.30 × 0.20 × 0.20 |
| Data collection | |
| Diffractometer | Bruker Kappa APEXII CCD diffractometer |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2004) |
| $T_{min}$, $T_{max}$ | 0.870, 0.891 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 3729, 3729, 2242 |
| $R_{int}$ | 0.000 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.086, 0.186, 1.07 |
| No. of reflections | 3726 |
| No. of parameters | 258 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.37, −0.34 |

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

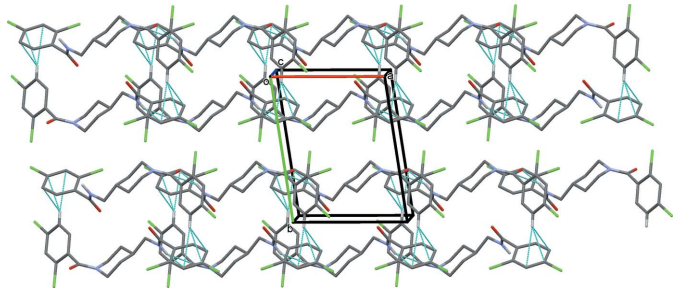



**Figure 3**
A view along the *c* axis of the crystal packing of the title compound, with hydrogen bonds and C—H···$\pi$ interactions shown as dashed lines (see Table 1). For clarity, H atoms not involved in these interactions have been omitted.

## Synthesis and crystallization

The title compound was synthesized following a published procedure (Revathi *et al.*, 2015). In a 250 ml round-bottomed flask, 120 ml of ethylmethylketone was added to 4-aminomethylpiperidine (0.02 mol) and stirred at room temperature. After 5 min, triethylamine (0.04 mol) was added and the mixture was stirred for 15 min. Then 2,4-dichloro benzoyl chloride (0.04 mol) was added and the reaction mixture was stirred at room temperature for 2 h. A white precipitate of triethylammonium chloride was formed, which was filtered and the filtrate was evaporated to give the crude title product. It was recrystallized twice from ethyl methyl ketone to give colourless block-like crystals of the title compound (yield: 82%).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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# full crystallographic data

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## 2,4-Dichloro-*N*-{[1-(2,4-dichlorobenzoyl)piperidin-4-yl]methyl}benzamide

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### 2,4-Dichloro-*N*-{[1-(2,4-dichlorobenzoyl)piperidin-4-yl]methyl}benzamide

*Crystal data*

$C_{20}H_{18}Cl_4N_2O_2$
$M_r$ = 460.16
Triclinic, $P\overline{1}$
$a$ = 8.2338 (2) Å
$b$ = 10.9617 (2) Å
$c$ = 12.2646 (3) Å
$\alpha$ = 76.239 (1)°
$\beta$ = 83.571 (1)°
$\gamma$ = 80.407 (1)°
$V$ = 1057.12 (4) Å$^3$
$Z$ = 2
$F(000)$ = 472
$D_x$ = 1.446 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2242 reflections
$\theta$ = 1.7–25.0°
$\mu$ = 0.58 mm$^{-1}$
$T$ = 293 K
Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and \ f scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min}$ = 0.870, $T_{max}$ = 0.891
3729 measured reflections
3729 independent reflections
2242 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.000
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.7°
$h$ = −9→9
$k$ = −12→13
$l$ = 0→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.186
$S$ = 1.07
3726 reflections
258 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 4.198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.1778 (8) | 0.3093 (6) | 0.8072 (5) | 0.0539 (16) |
| C2 | −0.2618 (8) | 0.2486 (7) | 0.9025 (5) | 0.0619 (18) |
| H2 | −0.3430 | 0.2935 | 0.9428 | 0.074* |
| C3 | −0.2213 (8) | 0.1181 (7) | 0.9365 (5) | 0.0622 (19) |
| C4 | −0.1047 (9) | 0.0510 (7) | 0.8774 (6) | 0.0659 (19) |
| H4 | −0.0819 | −0.0369 | 0.9006 | 0.079* |
| C5 | −0.0200 (8) | 0.1148 (6) | 0.7821 (5) | 0.0578 (17) |
| H5 | 0.0618 | 0.0697 | 0.7425 | 0.069* |
| C6 | −0.0572 (7) | 0.2457 (6) | 0.7458 (5) | 0.0454 (14) |
| C7 | 0.0273 (8) | 0.3122 (6) | 0.6384 (5) | 0.0493 (15) |
| C8 | 0.2759 (8) | 0.2995 (7) | 0.7375 (5) | 0.0634 (18) |
| H8A | 0.2080 | 0.2654 | 0.8040 | 0.076* |
| H8B | 0.3193 | 0.3711 | 0.7510 | 0.076* |
| C9 | 0.4171 (7) | 0.1987 (6) | 0.7159 (5) | 0.0564 (17) |
| H9A | 0.3731 | 0.1228 | 0.7133 | 0.068* |
| H9B | 0.4879 | 0.1773 | 0.7778 | 0.068* |
| C10 | 0.5195 (8) | 0.2414 (6) | 0.6063 (5) | 0.0517 (16) |
| H10 | 0.5754 | 0.3109 | 0.6138 | 0.062* |
| C11 | 0.4077 (8) | 0.2907 (7) | 0.5107 (5) | 0.0644 (19) |
| H11A | 0.3605 | 0.2208 | 0.4971 | 0.077* |
| H11B | 0.4726 | 0.3254 | 0.4428 | 0.077* |
| C12 | 0.2685 (8) | 0.3931 (7) | 0.5361 (6) | 0.068 (2) |
| H12A | 0.3141 | 0.4666 | 0.5434 | 0.082* |
| H12B | 0.1960 | 0.4193 | 0.4751 | 0.082* |
| C13 | 0.6490 (8) | 0.1333 (6) | 0.5858 (5) | 0.0601 (18) |
| H13A | 0.7081 | 0.0977 | 0.6530 | 0.072* |
| H13B | 0.5960 | 0.0672 | 0.5703 | 0.072* |
| C14 | 0.7855 (9) | 0.1351 (7) | 0.3983 (7) | 0.068 (2) |
| C15 | 0.9081 (8) | 0.1928 (6) | 0.3085 (6) | 0.0558 (16) |
| C16 | 1.0746 (9) | 0.1642 (6) | 0.3215 (6) | 0.0663 (19) |
| H16 | 1.1103 | 0.1139 | 0.3893 | 0.080* |
| C17 | 1.1912 (9) | 0.2076 (7) | 0.2368 (6) | 0.0652 (19) |
| H17 | 1.3034 | 0.1860 | 0.2471 | 0.078* |
| C18 | 1.1380 (8) | 0.2830 (6) | 0.1379 (6) | 0.0588 (17) |
| C19 | 0.9714 (9) | 0.3206 (7) | 0.1231 (6) | 0.0642 (18) |
| H19 | 0.9362 | 0.3746 | 0.0566 | 0.077* |
| C20 | 0.8589 (8) | 0.2759 (7) | 0.2094 (6) | 0.0631 (18) |
| N1 | 0.1756 (7) | 0.3417 (5) | 0.6411 (4) | 0.0586 (14) |
| N2 | 0.7647 (7) | 0.1751 (6) | 0.4921 (5) | 0.0603 (15) |
| O1 | −0.0451 (6) | 0.3363 (4) | 0.5513 (4) | 0.0681 (13) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.7133 (9) | 0.0541 (6) | 0.3794 (5) | 0.120 (3) |
| Cl1 | −0.2283 (3) | 0.47199 (19) | 0.76344 (18) | 0.1046 (9) |
| Cl2 | −0.3249 (3) | 0.0404 (3) | 1.05567 (19) | 0.1082 (9) |
| Cl3 | 0.6511 (3) | 0.3285 (3) | 0.1925 (2) | 0.1024 (8) |
| Cl4 | 1.2777 (3) | 0.3376 (2) | 0.02837 (18) | 0.0933 (7) |
| H2A | 0.822 (7) | 0.237 (5) | 0.497 (5) | 0.042 (17)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.064 (4) | 0.051 (4) | 0.043 (4) | −0.003 (3) | −0.005 (3) | −0.007 (3) |
| C2 | 0.061 (4) | 0.073 (5) | 0.047 (4) | 0.000 (4) | −0.004 (3) | −0.012 (3) |
| C3 | 0.057 (4) | 0.074 (5) | 0.050 (4) | −0.022 (4) | −0.013 (3) | 0.008 (4) |
| C4 | 0.086 (6) | 0.050 (4) | 0.061 (5) | −0.016 (4) | −0.016 (4) | −0.003 (4) |
| C5 | 0.066 (4) | 0.054 (4) | 0.055 (4) | −0.008 (3) | −0.012 (3) | −0.012 (3) |
| C6 | 0.047 (4) | 0.050 (4) | 0.040 (3) | −0.008 (3) | −0.004 (3) | −0.008 (3) |
| C7 | 0.056 (4) | 0.046 (4) | 0.045 (4) | −0.001 (3) | −0.005 (3) | −0.013 (3) |
| C8 | 0.065 (4) | 0.087 (5) | 0.044 (4) | −0.023 (4) | 0.000 (3) | −0.018 (4) |
| C9 | 0.048 (4) | 0.075 (5) | 0.043 (4) | −0.011 (3) | −0.012 (3) | −0.002 (3) |
| C10 | 0.053 (4) | 0.055 (4) | 0.044 (4) | −0.012 (3) | −0.003 (3) | −0.001 (3) |
| C11 | 0.063 (4) | 0.077 (5) | 0.040 (4) | −0.006 (4) | 0.002 (3) | 0.006 (3) |
| C12 | 0.054 (4) | 0.077 (5) | 0.059 (4) | −0.005 (4) | 0.001 (3) | 0.010 (4) |
| C13 | 0.051 (4) | 0.064 (4) | 0.056 (4) | −0.006 (3) | −0.004 (3) | 0.003 (3) |
| C14 | 0.060 (5) | 0.064 (5) | 0.082 (5) | −0.010 (4) | 0.010 (4) | −0.025 (4) |
| C15 | 0.059 (4) | 0.050 (4) | 0.062 (4) | −0.015 (3) | 0.004 (3) | −0.019 (3) |
| C16 | 0.074 (5) | 0.060 (4) | 0.064 (5) | −0.013 (4) | −0.005 (4) | −0.011 (4) |
| C17 | 0.055 (4) | 0.066 (5) | 0.072 (5) | −0.004 (4) | −0.001 (4) | −0.018 (4) |
| C18 | 0.056 (4) | 0.067 (4) | 0.057 (4) | −0.013 (3) | 0.005 (3) | −0.022 (4) |
| C19 | 0.066 (5) | 0.073 (5) | 0.056 (4) | −0.014 (4) | −0.002 (3) | −0.016 (4) |
| C20 | 0.055 (4) | 0.068 (5) | 0.072 (5) | −0.008 (4) | −0.003 (4) | −0.027 (4) |
| N1 | 0.055 (3) | 0.066 (4) | 0.049 (3) | −0.003 (3) | 0.002 (3) | −0.005 (3) |
| N2 | 0.053 (4) | 0.064 (4) | 0.064 (4) | −0.015 (3) | 0.002 (3) | −0.013 (3) |
| O1 | 0.082 (3) | 0.069 (3) | 0.051 (3) | −0.008 (3) | −0.016 (2) | −0.004 (2) |
| O2 | 0.154 (6) | 0.125 (5) | 0.110 (5) | −0.092 (5) | 0.054 (4) | −0.061 (4) |
| Cl1 | 0.157 (2) | 0.0591 (12) | 0.0783 (14) | 0.0125 (13) | 0.0236 (14) | −0.0114 (10) |
| Cl2 | 0.0897 (16) | 0.135 (2) | 0.0803 (15) | −0.0405 (14) | −0.0055 (12) | 0.0306 (14) |
| Cl3 | 0.0602 (12) | 0.143 (2) | 0.0965 (16) | −0.0136 (13) | −0.0045 (11) | −0.0129 (15) |
| Cl4 | 0.0793 (14) | 0.130 (2) | 0.0720 (13) | −0.0303 (13) | 0.0173 (11) | −0.0250 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.375 (9) | C11—C12 | 1.526 (9) |
| C1—C6 | 1.376 (8) | C11—H11A | 0.9700 |
| C1—Cl1 | 1.729 (6) | C11—H11B | 0.9700 |
| C2—C3 | 1.385 (9) | C12—N1 | 1.462 (8) |
| C2—H2 | 0.9300 | C12—H12A | 0.9700 |
| C3—C4 | 1.360 (9) | C12—H12B | 0.9700 |
| C3—Cl2 | 1.720 (7) | C13—N2 | 1.445 (8) |

| | | | |
|---|---|---|---|
| C4—C5 | 1.391 (9) | C13—H13A | 0.9700 |
| C4—H4 | 0.9300 | C13—H13B | 0.9700 |
| C5—C6 | 1.389 (8) | C14—O2 | 1.224 (8) |
| C5—H5 | 0.9300 | C14—N2 | 1.310 (9) |
| C6—C7 | 1.503 (8) | C14—C15 | 1.504 (9) |
| C7—O1 | 1.234 (7) | C15—C16 | 1.373 (9) |
| C7—N1 | 1.320 (8) | C15—C20 | 1.390 (9) |
| C8—N1 | 1.458 (8) | C16—C17 | 1.386 (9) |
| C8—C9 | 1.511 (9) | C16—H16 | 0.9300 |
| C8—H8A | 0.9700 | C17—C18 | 1.367 (9) |
| C8—H8B | 0.9700 | C17—H17 | 0.9300 |
| C9—C10 | 1.521 (8) | C18—C19 | 1.384 (9) |
| C9—H9A | 0.9700 | C18—Cl4 | 1.728 (7) |
| C9—H9B | 0.9700 | C19—C20 | 1.380 (9) |
| C10—C13 | 1.505 (8) | C19—H19 | 0.9300 |
| C10—C11 | 1.512 (8) | C20—Cl3 | 1.732 (7) |
| C10—H10 | 0.9800 | N2—H2A | 0.90 (6) |

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| C2—C1—C6 | 122.6 (6) | C10—C11—H11B | 109.2 |
| C2—C1—Cl1 | 118.1 (5) | C12—C11—H11B | 109.2 |
| C6—C1—Cl1 | 119.3 (5) | H11A—C11—H11B | 107.9 |
| C1—C2—C3 | 117.7 (6) | N1—C12—C11 | 108.9 (5) |
| C1—C2—H2 | 121.2 | N1—C12—H12A | 109.9 |
| C3—C2—H2 | 121.2 | C11—C12—H12A | 109.9 |
| C4—C3—C2 | 121.8 (6) | N1—C12—H12B | 109.9 |
| C4—C3—Cl2 | 119.8 (6) | C11—C12—H12B | 109.9 |
| C2—C3—Cl2 | 118.4 (6) | H12A—C12—H12B | 108.3 |
| C3—C4—C5 | 119.4 (6) | N2—C13—C10 | 111.2 (5) |
| C3—C4—H4 | 120.3 | N2—C13—H13A | 109.4 |
| C5—C4—H4 | 120.3 | C10—C13—H13A | 109.4 |
| C6—C5—C4 | 120.3 (6) | N2—C13—H13B | 109.4 |
| C6—C5—H5 | 119.9 | C10—C13—H13B | 109.4 |
| C4—C5—H5 | 119.9 | H13A—C13—H13B | 108.0 |
| C1—C6—C5 | 118.2 (6) | O2—C14—N2 | 124.6 (7) |
| C1—C6—C7 | 122.0 (5) | O2—C14—C15 | 118.3 (7) |
| C5—C6—C7 | 119.7 (5) | N2—C14—C15 | 117.1 (7) |
| O1—C7—N1 | 122.9 (6) | C16—C15—C20 | 117.2 (6) |
| O1—C7—C6 | 118.3 (6) | C16—C15—C14 | 120.8 (6) |
| N1—C7—C6 | 118.8 (5) | C20—C15—C14 | 122.0 (6) |
| N1—C8—C9 | 110.3 (5) | C15—C16—C17 | 122.2 (7) |
| N1—C8—H8A | 109.6 | C15—C16—H16 | 118.9 |
| C9—C8—H8A | 109.6 | C17—C16—H16 | 118.9 |
| N1—C8—H8B | 109.6 | C18—C17—C16 | 118.7 (7) |
| C9—C8—H8B | 109.6 | C18—C17—H17 | 120.7 |
| H8A—C8—H8B | 108.1 | C16—C17—H17 | 120.7 |
| C8—C9—C10 | 112.5 (5) | C17—C18—C19 | 121.3 (6) |
| C8—C9—H9A | 109.1 | C17—C18—Cl4 | 120.7 (5) |
| C10—C9—H9A | 109.1 | C19—C18—Cl4 | 117.9 (5) |

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| C8—C9—H9B | 109.1 | C20—C19—C18 | 118.3 (7) |
| C10—C9—H9B | 109.1 | C20—C19—H19 | 120.9 |
| H9A—C9—H9B | 107.8 | C18—C19—H19 | 120.9 |
| C13—C10—C11 | 112.4 (5) | C19—C20—C15 | 122.0 (6) |
| C13—C10—C9 | 109.5 (5) | C19—C20—Cl3 | 118.0 (6) |
| C11—C10—C9 | 109.8 (5) | C15—C20—Cl3 | 120.0 (5) |
| C13—C10—H10 | 108.3 | C7—N1—C8 | 124.9 (6) |
| C11—C10—H10 | 108.3 | C7—N1—C12 | 119.9 (6) |
| C9—C10—H10 | 108.3 | C8—N1—C12 | 113.5 (5) |
| C10—C11—C12 | 112.0 (6) | C14—N2—C13 | 124.7 (6) |
| C10—C11—H11A | 109.2 | C14—N2—H2A | 117 (4) |
| C12—C11—H11A | 109.2 | C13—N2—H2A | 118 (4) |

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| C6—C1—C2—C3 | 0.0 (10) | O2—C14—C15—C20 | 71.3 (10) |
| Cl1—C1—C2—C3 | 179.6 (5) | N2—C14—C15—C20 | −109.3 (8) |
| C1—C2—C3—C4 | −1.1 (10) | C20—C15—C16—C17 | −4.8 (10) |
| C1—C2—C3—Cl2 | 179.9 (5) | C14—C15—C16—C17 | 174.8 (7) |
| C2—C3—C4—C5 | 1.9 (11) | C15—C16—C17—C18 | 1.0 (11) |
| Cl2—C3—C4—C5 | −179.1 (5) | C16—C17—C18—C19 | 2.9 (10) |
| C3—C4—C5—C6 | −1.7 (10) | C16—C17—C18—Cl4 | −178.8 (5) |
| C2—C1—C6—C5 | 0.1 (10) | C17—C18—C19—C20 | −2.6 (10) |
| Cl1—C1—C6—C5 | −179.4 (5) | Cl4—C18—C19—C20 | 179.0 (5) |
| C2—C1—C6—C7 | 176.7 (6) | C18—C19—C20—C15 | −1.5 (11) |
| Cl1—C1—C6—C7 | −2.8 (9) | C18—C19—C20—Cl3 | 177.4 (5) |
| C4—C5—C6—C1 | 0.7 (9) | C16—C15—C20—C19 | 5.0 (10) |
| C4—C5—C6—C7 | −175.9 (6) | C14—C15—C20—C19 | −174.5 (7) |
| C1—C6—C7—O1 | −79.8 (8) | C16—C15—C20—Cl3 | −173.9 (5) |
| C5—C6—C7—O1 | 96.7 (7) | C14—C15—C20—Cl3 | 6.6 (9) |
| C1—C6—C7—N1 | 100.6 (7) | O1—C7—N1—C8 | −170.7 (6) |
| C5—C6—C7—N1 | −83.0 (8) | C6—C7—N1—C8 | 8.9 (9) |
| N1—C8—C9—C10 | 53.7 (7) | O1—C7—N1—C12 | −6.7 (9) |
| C8—C9—C10—C13 | −175.6 (5) | C6—C7—N1—C12 | 172.9 (5) |
| C8—C9—C10—C11 | −51.7 (7) | C9—C8—N1—C7 | 106.5 (7) |
| C13—C10—C11—C12 | 175.5 (6) | C9—C8—N1—C12 | −58.4 (7) |
| C9—C10—C11—C12 | 53.3 (8) | C11—C12—N1—C7 | −106.3 (7) |
| C10—C11—C12—N1 | −56.6 (8) | C11—C12—N1—C8 | 59.4 (8) |
| C11—C10—C13—N2 | 66.5 (7) | O2—C14—N2—C13 | −2.5 (13) |
| C9—C10—C13—N2 | −171.1 (5) | C15—C14—N2—C13 | 178.1 (6) |
| O2—C14—C15—C16 | −108.2 (9) | C10—C13—N2—C14 | −116.8 (7) |
| N2—C14—C15—C16 | 71.2 (9) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C15–C20 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1$^{i}$ | 0.90 (6) | 1.94 (6) | 2.809 (8) | 163 (5) |

| | | | | |
|---|---|---|---|---|
| C4—H4···*Cg*1 | 0.93 | 2.93 | 3.628 (8) | 132 |

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