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# *N*′-(3,5-Dichloro-2-hydroxybenzylidene)-4-nitrobenzohydrazide methanol solvate

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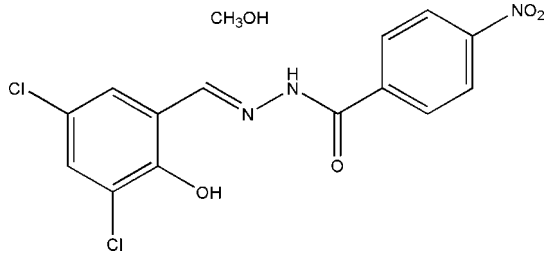
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.054; $wR$ factor = 0.124; data-to-parameter ratio = 14.9.

In the title compound, $C_{14}H_9Cl_2N_3O_4\cdot CH_4O$, the dihedral angle between the two benzene rings in the hydrazone molecule is 6.3 (3)°. An intramolecular N—H···O hydrogen bond stabilizes the molecular conformation. In the crystal, centrosymmetrically related molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds.

## Related literature

For general background to hydrazone compounds, see: Rasras *et al.* (2010); Fan *et al.* (2010); Ajani *et al.* (2010); Avaji *et al.* (2009). For the crystal structures of related hydrazone compounds, see: Khaledi *et al.* (2010); Han *et al.* (2010); Hussain *et al.* (2010); Ji & Lu (2010). For reference bond-length data, see: Allen *et al.* (1987).




## Experimental

### *Crystal data*

$C_{14}H_9Cl_2N_3O_4\cdot CH_4O$
$M_r$ = 386.18
Monoclinic, $P2_1/n$
$a$ = 7.415 (3) Å
$b$ = 13.408 (3) Å
$c$ = 16.674 (2) Å
$\beta$ = 99.716 (3)°
$V$ = 1634.0 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 298 K
0.15 × 0.13 × 0.10 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.938, $T_{max}$ = 0.958
8410 measured reflections
3467 independent reflections
2099 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.124
$S$ = 1.02
3467 reflections
232 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.92 | 2.633 (3) | 145 |
| N2—H2···O5 | 0.90 (1) | 1.91 (1) | 2.793 (3) | 167 (3) |
| O5—H5···O2$^{i}$ | 0.82 | 2.15 | 2.903 (3) | 153 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2485).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2562 [doi:10.1107/S1600536810036184]

# *N*′-(3,5-Dichloro-2-hydroxybenzylidene)-4-nitrobenzohydrazide methanol solvate

**Hai-Yun Zhu**

## S1. Comment

In recent years, considerable interest has been focused on the preparation and biological properties of hydrazone compounds (Rasras *et al.*, 2010; Fan *et al.*, 2010; Ajani *et al.*, 2010; Avaji *et al.*, 2009). The crystal structures of a number of hydrazone compounds have been reported (Khaledi *et al.*, 2010; Han *et al.*, 2010; Hussain *et al.*, 2010; Ji & Lu, 2010). The author reports in this paper the title new hydrazone compound.

The asymmetric unit of the title compound (Fig. 1) consists of a hydrazone molecule and a methanol molecule. The dihedral angle between the C1—C6 and C9—C14 benzene rings is 6.3 (3)°. There is an intramolecular O—H···N hydrogen bond (Table 1) stabilizing the conformation of the hydrazone molecule. All bond lengths are within normal values (Allen *et al.*, 1987), and are comparable with those in the similar hydrazone compounds as cited above. In the crystal structure (Fig. 2), centrosymmetrically related molecules are linked through intermolecular O—H···O and N—H···O hydrogen bonds (Table 1).

## S2. Experimental

3,5-Dichlorosalicylaldehyde (0.191 g, 1 mmol) and 4-nitrobenzohydrazide (0.181 g, 1 mmol) were dissolved in 30 ml absolute methanol. The mixture was stirred at reflux for 10 min, and cooled to room temperature. The clear yellow solution was left to slowly evaporate in air for a week, yielding yellow needle crystals of the title compound suitable for X-ray analysis.

## S3. Refinement

The H2 atom attached to N2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å, and with $U_{iso}$ fixed at 0.08 Å$^2$. The remaining H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.93–0.96 Å, O—H = 0.82 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(C, O) for methyl and hydroxy H atoms.

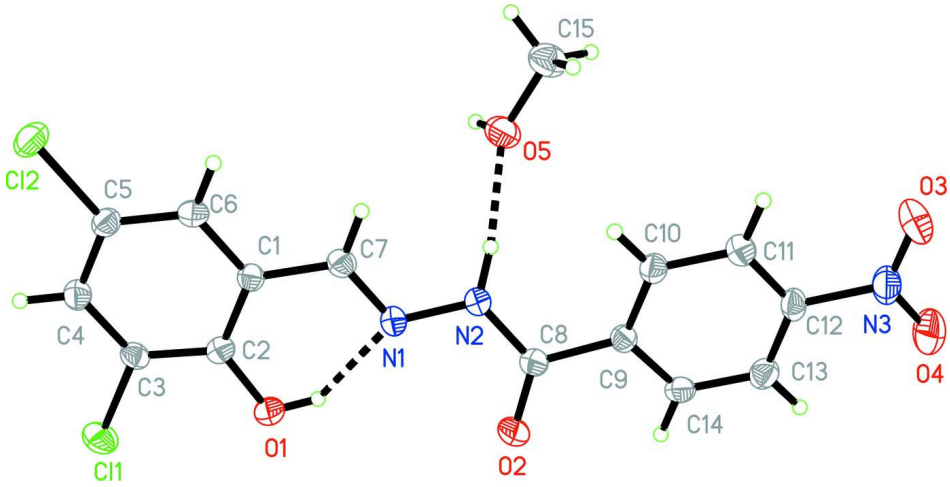


**Figure 1**

The molecular structure of the title compound with 30% probability displacement ellipsoids for non-hydrogen atoms. Hydrogen bonds are drawn as dashed lines.

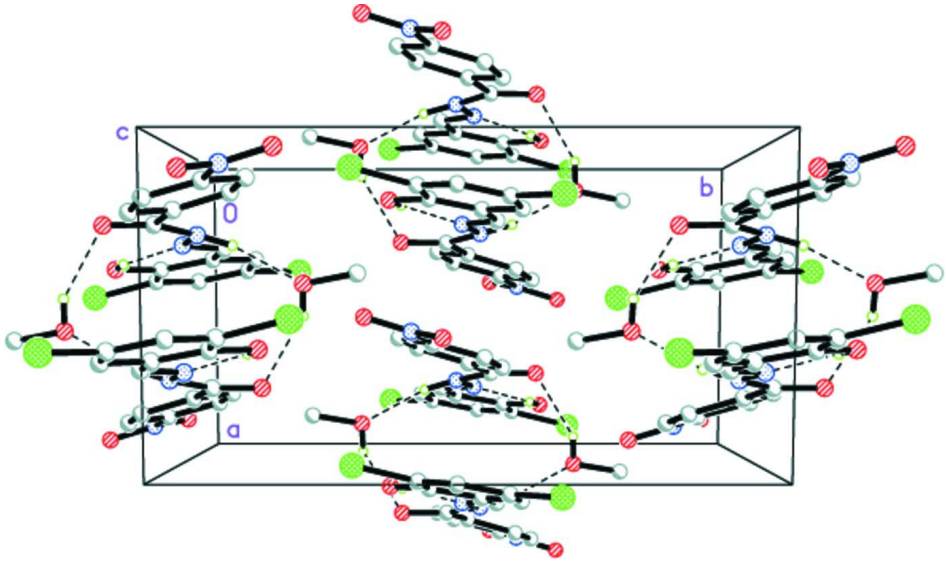


**Figure 2**

The molecular packing of the title compound viewed along the *c* axis. Hydrogen atoms not involved in hydrogen bonds (dashed lines) are omitted for clarity.

### *N*′-(3,5-Dichloro-2-hydroxybenzylidene)-4-nitrobenzohydrazide methanol solvate

*Crystal data*

$C_{14}H_9Cl_2N_3O_4·CH_4O$
$M_r$ = 386.18
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 7.415 (3) Å
$b$ = 13.408 (3) Å
$c$ = 16.674 (2) Å
$\beta$ = 99.716 (3)°
$V$ = 1634.0 (8) Å$^3$
$Z$ = 4
$F$(000) = 792
$D_x$ = 1.570 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1245 reflections
$\theta$ = 2.4–24.5°
$\mu$ = 0.43 mm$^{-1}$

$T$ = 298 K
Cut from needle, yellow

0.15 × 0.13 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.938, $T_{max}$ = 0.958

8410 measured reflections
3467 independent reflections
2099 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.5°
$h$ = −9→9
$k$ = −14→17
$l$ = −21→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.124
$S$ = 1.02
3467 reflections
232 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.0676P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.46614 (12) | −0.21402 (6) | 0.15195 (5) | 0.0565 (3) |
| Cl2 | 0.37115 (12) | 0.17025 (6) | 0.06479 (5) | 0.0538 (3) |
| N1 | 0.2955 (3) | −0.01141 (17) | 0.40697 (13) | 0.0378 (6) |
| N2 | 0.2663 (3) | 0.02375 (17) | 0.48171 (14) | 0.0388 (6) |
| N3 | 0.0804 (4) | 0.1043 (3) | 0.84113 (17) | 0.0567 (8) |
| O1 | 0.3717 (3) | −0.14918 (14) | 0.30523 (12) | 0.0481 (6) |
| H1 | 0.3572 | −0.1275 | 0.3497 | 0.072* |
| O2 | 0.2382 (3) | −0.13351 (15) | 0.52776 (12) | 0.0552 (6) |
| O3 | 0.0317 (4) | 0.1905 (2) | 0.84516 (15) | 0.0786 (8) |
| O4 | 0.1004 (4) | 0.0463 (2) | 0.89825 (15) | 0.0911 (9) |
| O5 | 0.4237 (3) | 0.21205 (16) | 0.51288 (15) | 0.0619 (7) |
| H5 | 0.5275 | 0.2100 | 0.5021 | 0.093* |
| C1 | 0.3366 (4) | 0.0260 (2) | 0.27209 (16) | 0.0329 (6) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.3712 (4) | −0.0733 (2) | 0.25280 (16) | 0.0356 (7) |
| C3 | 0.4095 (4) | −0.0933 (2) | 0.17535 (16) | 0.0349 (7) |
| C4 | 0.4077 (4) | −0.0197 (2) | 0.11735 (17) | 0.0410 (7) |
| H4 | 0.4311 | −0.0353 | 0.0657 | 0.049* |
| C5 | 0.3705 (4) | 0.0773 (2) | 0.13695 (16) | 0.0370 (7) |
| C6 | 0.3342 (4) | 0.1002 (2) | 0.21322 (16) | 0.0363 (7) |
| H6 | 0.3079 | 0.1656 | 0.2256 | 0.044* |
| C7 | 0.3046 (4) | 0.0552 (2) | 0.35267 (16) | 0.0373 (7) |
| H7 | 0.2908 | 0.1223 | 0.3647 | 0.045* |
| C8 | 0.2371 (4) | −0.0435 (2) | 0.53888 (17) | 0.0369 (7) |
| C9 | 0.1972 (4) | −0.0003 (2) | 0.61643 (16) | 0.0332 (7) |
| C10 | 0.1438 (4) | 0.0976 (2) | 0.62461 (17) | 0.0395 (7) |
| H10 | 0.1332 | 0.1406 | 0.5803 | 0.047* |
| C11 | 0.1061 (4) | 0.1320 (2) | 0.69819 (18) | 0.0440 (8) |
| H11 | 0.0710 | 0.1978 | 0.7040 | 0.053* |
| C12 | 0.1216 (4) | 0.0669 (2) | 0.76247 (17) | 0.0405 (7) |
| C13 | 0.1716 (4) | −0.0309 (2) | 0.75640 (17) | 0.0439 (8) |
| H13 | 0.1796 | −0.0737 | 0.8008 | 0.053* |
| C14 | 0.2096 (4) | −0.0643 (2) | 0.68295 (17) | 0.0400 (7) |
| H14 | 0.2439 | −0.1304 | 0.6777 | 0.048* |
| C15 | 0.3910 (5) | 0.3073 (2) | 0.5430 (2) | 0.0592 (9) |
| H15A | 0.4591 | 0.3147 | 0.5970 | 0.089* |
| H15B | 0.2628 | 0.3147 | 0.5444 | 0.089* |
| H15C | 0.4288 | 0.3574 | 0.5082 | 0.089* |
| H2 | 0.300 (5) | 0.0871 (11) | 0.494 (2) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0704 (6) | 0.0374 (5) | 0.0641 (6) | 0.0041 (4) | 0.0181 (4) | −0.0126 (4) |
| Cl2 | 0.0633 (6) | 0.0514 (5) | 0.0479 (5) | −0.0048 (4) | 0.0127 (4) | 0.0148 (4) |
| N1 | 0.0435 (15) | 0.0393 (14) | 0.0321 (13) | −0.0018 (12) | 0.0109 (11) | −0.0040 (11) |
| N2 | 0.0501 (16) | 0.0345 (14) | 0.0334 (13) | −0.0035 (13) | 0.0120 (11) | −0.0031 (11) |
| N3 | 0.0562 (19) | 0.072 (2) | 0.0457 (18) | −0.0123 (17) | 0.0203 (14) | −0.0134 (16) |
| O1 | 0.0704 (16) | 0.0325 (12) | 0.0429 (12) | −0.0015 (11) | 0.0138 (12) | 0.0040 (9) |
| O2 | 0.0864 (18) | 0.0301 (12) | 0.0527 (14) | −0.0008 (12) | 0.0223 (12) | −0.0067 (10) |
| O3 | 0.098 (2) | 0.076 (2) | 0.0684 (18) | 0.0053 (17) | 0.0328 (15) | −0.0264 (15) |
| O4 | 0.143 (3) | 0.093 (2) | 0.0445 (15) | −0.0060 (19) | 0.0359 (16) | −0.0005 (15) |
| O5 | 0.0673 (17) | 0.0488 (14) | 0.0767 (17) | −0.0132 (12) | 0.0326 (14) | −0.0180 (12) |
| C1 | 0.0328 (16) | 0.0336 (16) | 0.0335 (15) | −0.0002 (13) | 0.0089 (12) | −0.0015 (12) |
| C2 | 0.0350 (17) | 0.0346 (17) | 0.0375 (16) | −0.0021 (13) | 0.0065 (13) | 0.0027 (13) |
| C3 | 0.0342 (17) | 0.0311 (16) | 0.0406 (16) | 0.0007 (13) | 0.0094 (13) | −0.0066 (13) |
| C4 | 0.0444 (19) | 0.0441 (18) | 0.0354 (16) | −0.0056 (15) | 0.0095 (13) | −0.0027 (14) |
| C5 | 0.0375 (17) | 0.0383 (17) | 0.0357 (16) | −0.0036 (14) | 0.0081 (13) | 0.0039 (13) |
| C6 | 0.0371 (17) | 0.0290 (15) | 0.0423 (17) | 0.0011 (13) | 0.0056 (13) | 0.0008 (13) |
| C7 | 0.0401 (18) | 0.0323 (16) | 0.0406 (16) | 0.0026 (14) | 0.0099 (13) | −0.0024 (13) |
| C8 | 0.0384 (18) | 0.0350 (17) | 0.0378 (16) | −0.0028 (14) | 0.0078 (13) | −0.0025 (14) |
| C9 | 0.0307 (16) | 0.0351 (16) | 0.0344 (15) | −0.0016 (13) | 0.0075 (12) | −0.0028 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0459 (19) | 0.0368 (17) | 0.0387 (17) | 0.0034 (14) | 0.0157 (14) | 0.0019 (13) |
| C11 | 0.048 (2) | 0.0404 (18) | 0.0461 (18) | 0.0010 (15) | 0.0150 (15) | −0.0044 (15) |
| C12 | 0.0340 (17) | 0.054 (2) | 0.0356 (16) | −0.0081 (15) | 0.0132 (13) | −0.0094 (15) |
| C13 | 0.048 (2) | 0.047 (2) | 0.0368 (17) | −0.0054 (16) | 0.0068 (14) | 0.0039 (14) |
| C14 | 0.0417 (18) | 0.0332 (17) | 0.0458 (18) | −0.0059 (14) | 0.0094 (14) | −0.0009 (14) |
| C15 | 0.058 (2) | 0.047 (2) | 0.074 (2) | 0.0044 (17) | 0.0156 (18) | −0.0058 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.733 (3) | C4—C5 | 1.380 (4) |
| Cl2—C5 | 1.733 (3) | C4—H4 | 0.9300 |
| N1—C7 | 1.282 (3) | C5—C6 | 1.378 (4) |
| N1—N2 | 1.383 (3) | C6—H6 | 0.9300 |
| N2—C8 | 1.356 (4) | C7—H7 | 0.9300 |
| N2—H2 | 0.898 (10) | C8—C9 | 1.492 (4) |
| N3—O3 | 1.217 (4) | C9—C10 | 1.385 (4) |
| N3—O4 | 1.219 (3) | C9—C14 | 1.393 (4) |
| N3—C12 | 1.483 (4) | C10—C11 | 1.383 (4) |
| O1—C2 | 1.341 (3) | C10—H10 | 0.9300 |
| O1—H1 | 0.8200 | C11—C12 | 1.372 (4) |
| O2—C8 | 1.221 (3) | C11—H11 | 0.9300 |
| O5—C15 | 1.409 (3) | C12—C13 | 1.371 (4) |
| O5—H5 | 0.8200 | C13—C14 | 1.377 (4) |
| C1—C6 | 1.396 (4) | C13—H13 | 0.9300 |
| C1—C2 | 1.403 (4) | C14—H14 | 0.9300 |
| C1—C7 | 1.457 (4) | C15—H15A | 0.9600 |
| C2—C3 | 1.394 (4) | C15—H15B | 0.9600 |
| C3—C4 | 1.380 (4) | C15—H15C | 0.9600 |
| | | | |
| C7—N1—N2 | 115.7 (2) | C1—C7—H7 | 120.0 |
| C8—N2—N1 | 118.3 (2) | O2—C8—N2 | 123.0 (3) |
| C8—N2—H2 | 123 (2) | O2—C8—C9 | 121.5 (3) |
| N1—N2—H2 | 116 (2) | N2—C8—C9 | 115.4 (2) |
| O3—N3—O4 | 124.2 (3) | C10—C9—C14 | 119.1 (3) |
| O3—N3—C12 | 118.5 (3) | C10—C9—C8 | 123.7 (3) |
| O4—N3—C12 | 117.3 (3) | C14—C9—C8 | 117.1 (3) |
| C2—O1—H1 | 109.5 | C11—C10—C9 | 120.5 (3) |
| C15—O5—H5 | 109.5 | C11—C10—H10 | 119.8 |
| C6—C1—C2 | 119.7 (2) | C9—C10—H10 | 119.8 |
| C6—C1—C7 | 118.2 (3) | C12—C11—C10 | 118.6 (3) |
| C2—C1—C7 | 122.1 (3) | C12—C11—H11 | 120.7 |
| O1—C2—C3 | 118.6 (3) | C10—C11—H11 | 120.7 |
| O1—C2—C1 | 123.4 (3) | C13—C12—C11 | 122.6 (3) |
| C3—C2—C1 | 118.0 (2) | C13—C12—N3 | 119.2 (3) |
| C4—C3—C2 | 122.1 (3) | C11—C12—N3 | 118.2 (3) |
| C4—C3—Cl1 | 119.0 (2) | C12—C13—C14 | 118.4 (3) |
| C2—C3—Cl1 | 118.9 (2) | C12—C13—H13 | 120.8 |
| C5—C4—C3 | 119.1 (3) | C14—C13—H13 | 120.8 |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 120.4 | C13—C14—C9 | 120.8 (3) |
| C3—C4—H4 | 120.4 | C13—C14—H14 | 119.6 |
| C6—C5—C4 | 120.4 (3) | C9—C14—H14 | 119.6 |
| C6—C5—Cl2 | 120.3 (2) | O5—C15—H15A | 109.5 |
| C4—C5—Cl2 | 119.3 (2) | O5—C15—H15B | 109.5 |
| C5—C6—C1 | 120.6 (3) | H15A—C15—H15B | 109.5 |
| C5—C6—H6 | 119.7 | O5—C15—H15C | 109.5 |
| C1—C6—H6 | 119.7 | H15A—C15—H15C | 109.5 |
| N1—C7—C1 | 120.0 (3) | H15B—C15—H15C | 109.5 |
| N1—C7—H7 | 120.0 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.92 | 2.633 (3) | 145 |
| N2—H2···O5 | 0.90 (1) | 1.91 (1) | 2.793 (3) | 167 (3) |
| O5—H5···O2$^{i}$ | 0.82 | 2.15 | 2.903 (3) | 153 |

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