# organic compounds

## 2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone

**Yakini Brandy, Ray J. Butcher,\* Tolulope A. Adesiyun, Solomon Berhe and Oladapo Bakare**

Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA

Correspondence e-mail: rbutcher99@yahoo.com

The naphthoquinone ring is almost perpendicular [dihedral angle 71.02 (3)°] to the phenyl group of the title compound, $C_{17}H_9Cl_2NO_3$, while the dihedral angle between the amide group and the 4-chlorophenyl ring is 21.9 (2)°. The conformation of the N—H and C=O bonds are *anti* to each other. N—H···Cl hydrogen bonds link the molecules into chains in the *a*-axis direction. In addition, these chains are linked by weak intermolecular C—H···O interactions.

### Related literature

For similar structures see: Lien *et al.* (1997); Huang *et al.* (2005); Bakare *et al.* (2003); Copeland *et al.* (2007); Win *et al.* (2005); Rubin-Preminger *et al.* (2004). For related literature, see: Gowda, Kožíšek *et al.* (2008); Gowda, Tokarčík *et al.* (2008); van Oosten *et al.* (2008); Shen *et al.* (2008).
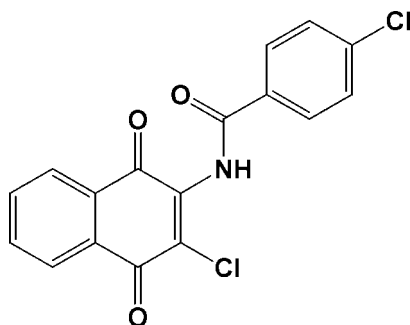


### Experimental

#### Crystal data

| | |
|---|---|
| $C_{17}H_9Cl_2NO_3$ | $b$ = 8.7237 (3) Å |
| $M_r$ = 346.15 | $c$ = 29.7957 (9) Å |
| Monoclinic, $P2_1/c$ | $\beta$ = 93.504 (3)° |
| $a$ = 5.6011 (2) Å | $V$ = 1453.16 (8) Å$^3$ |

| | |
|---|---|
| $Z$ = 4 | $T$ = 200 (2) K |
| Mo $K\alpha$ radiation | $0.49 \times 0.41 \times 0.12$ mm |
| $\mu$ = 0.46 mm$^{-1}$ | |

#### Data collection

| | |
|---|---|
| Oxford Diffraction Gemini R diffractometer | $T_{min}$ = 0.887, $T_{max}$ = 1.000 (expected range = 0.839–0.946) |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007) | 13882 measured reflections |
| | 4842 independent reflections |
| | 2832 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.035 |

#### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | 208 parameters |
| $wR(F^2)$ = 0.086 | H-atom parameters constrained |
| $S$ = 0.93 | $\Delta\rho_{max}$ = 0.29 e Å$^{-3}$ |
| 4842 reflections | $\Delta\rho_{min}$ = −0.36 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N—H0$A$···Cl1$^i$ | 0.88 | 2.89 | 3.6491 (12) | 145 |
| C14—H14$A$···O2$^{ii}$ | 0.95 | 2.40 | 3.2517 (19) | 149 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

### References

Bakare, O., Ashendel, C. L., Peng, H., Zalkow, L. H. & Burgess, E. M. (2003). *Bioorg. Med. Chem.* **11**, 3165–3170.

Copeland, R. L., Das, J. R., Bakare, O., Enwerem, N. M., Berhe, S., Hillaire, K., White, D., Beyene, D., Kassim, O. O. & Kanaan, Y. M. (2007). *Anticancer Res.* **27**, 1537–1546.

Gowda, B. T., Kožíšek, J., Tokarčík, M. & Fuess, H. (2008). *Acta Cryst.* E**64**, o987.

Gowda, B. T., Tokarčík, M., Kožíšek, J., Sowmya, B. P. & Fuess, H. (2008). *Acta Cryst.* E**64**, o950.

Huang, L., Chang, F., Lee, K., Wang, J., Teng, C. & Kuo, S. (2005). *Bioorg. Med. Chem.* **6**, 2261–2269.

Lien, J., Huang, L., Wang, J., Teng, C., Lee, K. & Kuo, S. (1997). *Bioorg. Med. Chem.* **5**, 2111–2120.

Oosten, E. M. van, Lough, A. J. & Vasdev, N. (2008). *Acta Cryst.* E**64**, o1005.

Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED* (including *SCALE3 ABSPACK*). Oxford Diffraction Ltd, Abingdon, England.

Rubin-Preminger, J. M., Win, T., Granot, Y. & Bittner, S. (2004). *Z. Kristallogr. New Cryst. Struct.* **219**, 323–324.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shen, Q., Yu, S.-Q., Hu, B.-B. & Lu, P. (2008). *Acta Cryst.* E**64**, o996.

Win, T., Yerushalmi, S. & Bittner, S. (2005). *Synthesis*, pp. 1631–1634.

# supporting information

## 2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone

### Yakini Brandy, Ray J. Butcher, Tolulope A. Adesiyun, Solomon Berhe and Oladapo Bakare

### S1. Comment

The amido and imido derivatives of 3-chloro-1,4-naphthoquinone are well known for their anti-inflammatory, antiplatelet, antiallergic and anticancer activities (Lien *et al.*, 1997; Huang *et al.*, 2005; Bakare *et al.*, 2003; Copeland *et al.*, 2007). The title compound, 2-chloro-3-(*p*-chlorobenzamido)-1,4-naphthoquinone was obtained as an intermediate in the synthesis of some oxazolo-1,4-naphthoquinone and imido-substituted-1,4-naphthoquinone analogs.

The naphthoquinone ring is almost perpendicular to the phenyl group of the title compound $C_{17}H_9Cl_2NO_3$, while the dihedral angle betwen the amide group and the 4-chlorophenyl ring is 21.9 (2)° (Fig. 1). The conformation of the N—H and C=O bonds are anti to each other (Gowda, Kožíšek *et al.*, 2008; Gowda, Tokarčík *et al.*, 2008). N—H···Cl hydrogen bonds link the molecules into chains in the *a* direction. In addition, these chains are linked by weak intermolecular Ar—H···O interactions (Fig. 2, Table 1).

### S2. Experimental

A mixture of 2-amino-3-chloro-1,4-naphthoquinone (213 mg, 1.03 mmol) and 4-chloro-benzoylchloride (2 ml) was refluxed for 2 1/2 h (powerstat setting at 70). The reaction mixture was cooled to room temperature. The precipitate was isolated by vacuum filtration and the yellow-grey solid was washed with diethyl ether. The crude was recrystallized from ethanol (20 ml) to obtain a yellow solid (67 mg, 18.8%). Crystals for *x*-ray study were obtained by recrystallization from methanol.
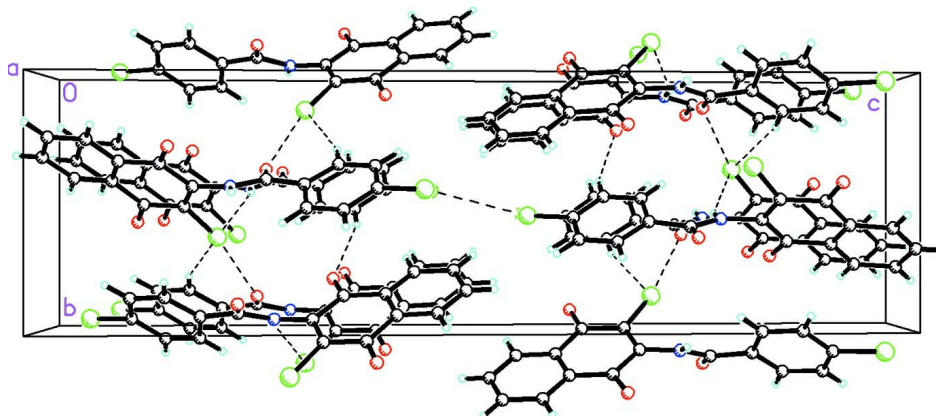
### S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.95 Å, N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}(C, N)$.
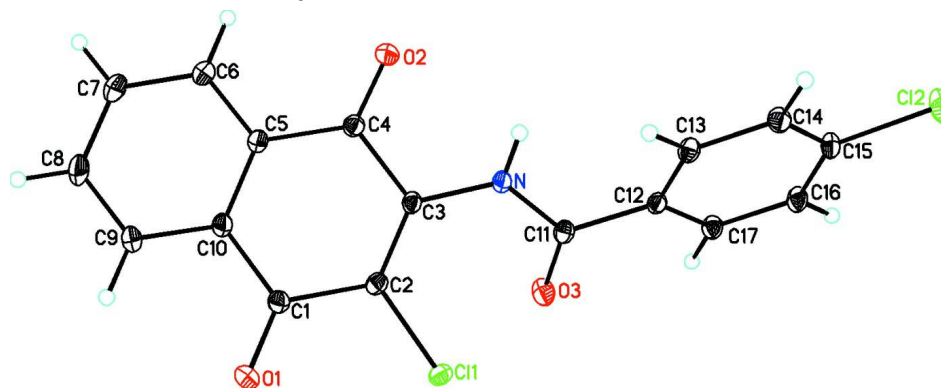
## Figure 1

View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 20% probability level.



## Figure 2

View of the packing viewed down the *a* axis. Dashed bonds show weak C—H···O interactions.

**2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone**

*Crystal data*

| | |
|---|---|
| $C_{17}H_9Cl_2NO_3$ | $F(000) = 704$ |
| $M_r = 346.15$ | $D_x = 1.582$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 4629 reflections |
| $a = 5.6011$ (2) Å | $\theta = 4.6$–$32.5°$ |
| $b = 8.7237$ (3) Å | $\mu = 0.46$ mm$^{-1}$ |
| $c = 29.7957$ (9) Å | $T = 200$ K |
| $\beta = 93.504$ (3)° | Plate, pale yellow |
| $V = 1453.16$ (8) Å$^3$ | $0.49 \times 0.41 \times 0.12$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R diffractometer | 13882 measured reflections |
| Radiation source: fine-focus sealed tube | 4842 independent reflections |
| Graphite monochromator | 2832 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.5081 pixels mm$^{-1}$ | $R_{int} = 0.035$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 32.6°$, $\theta_{min} = 4.6°$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007) | $h = -8 \rightarrow 8$ |
| | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.887$, $T_{max} = 1.000$ | $l = -44 \rightarrow 44$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | |
| $wR(F^2) = 0.086$ | |
| $S = 0.93$ | Hydrogen site location: inferred from neighbouring sites |
| 4842 reflections | H-atom parameters constrained |
| 208 parameters | |
| 0 restraints | |

$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$  
   where $P = (F_o^2 + 2F_c^2)/3$  
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.29$ e Å⁻³  
$\Delta\rho_{min} = -0.36$ e Å⁻³

*Special details*

**Experimental**. (CrysAlis RED; Oxford Diffraction, 2007) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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 (Å²)*

|       | *x*          | *y*          | *z*          | $U_{iso}*/U_{eq}$ |
|-------|--------------|--------------|--------------|-------------------|
| Cl1   | 0.42210 (6)  | 0.13331 (4)  | 0.298854 (11)| 0.02796 (10)      |
| Cl2   | −0.42944 (7) | −0.05032 (6) | 0.057164 (13)| 0.04852 (14)      |
| O1    | 0.54644 (18) | 0.07511 (14) | 0.39281 (4)  | 0.0401 (3)        |
| O2    | −0.26101 (17)| −0.20745 (14)| 0.33569 (3)  | 0.0378 (3)        |
| O3    | 0.31583 (17) | −0.12832 (14)| 0.24103 (3)  | 0.0364 (3)        |
| N     | −0.02512 (19)| −0.06128 (15)| 0.27365 (4)  | 0.0273 (3)        |
| H0A   | −0.1786      | −0.0415      | 0.2689       | 0.033*            |
| C1    | 0.3653 (2)   | 0.00688 (18) | 0.38026 (5)  | 0.0275 (3)        |
| C2    | 0.2705 (2)   | 0.01309 (17) | 0.33244 (4)  | 0.0251 (3)        |
| C3    | 0.0712 (2)   | −0.06238 (17)| 0.31773 (4)  | 0.0240 (3)        |
| C4    | −0.0749 (2)  | −0.14777 (18)| 0.34975 (5)  | 0.0264 (3)        |
| C5    | 0.0144 (2)   | −0.15604 (18)| 0.39758 (5)  | 0.0272 (3)        |
| C6    | −0.1138 (3)  | −0.2369 (2)  | 0.42817 (5)  | 0.0391 (4)        |
| H6A   | −0.2591      | −0.2864      | 0.4186       | 0.047*            |
| C7    | −0.0289 (3)  | −0.2451 (3)  | 0.47288 (5)  | 0.0477 (5)        |
| H7A   | −0.1169      | −0.3002      | 0.4939       | 0.057*            |
| C8    | 0.1823 (3)   | −0.1737 (2)  | 0.48705 (5)  | 0.0477 (5)        |
| H8A   | 0.2390       | −0.1794      | 0.5177       | 0.057*            |
| C9    | 0.3111 (3)   | −0.0940 (2)  | 0.45660 (5)  | 0.0391 (4)        |
| H9A   | 0.4574       | −0.0459      | 0.4663       | 0.047*            |
| C10   | 0.2273 (2)   | −0.08383 (18)| 0.41170 (5)  | 0.0287 (3)        |
| C11   | 0.1070 (3)   | −0.08964 (17)| 0.23680 (5)  | 0.0263 (3)        |
| C12   | −0.0252 (2)  | −0.07098 (17)| 0.19218 (4)  | 0.0245 (3)        |
| C13   | −0.2316 (2)  | 0.01736 (18) | 0.18635 (5)  | 0.0277 (3)        |
| H13A  | −0.2882      | 0.0726       | 0.2110       | 0.033*            |
| C14   | −0.3550 (3)  | 0.02492 (19) | 0.14462 (5)  | 0.0315 (3)        |
| H14A  | −0.4966      | 0.0846       | 0.1406       | 0.038*            |
| C15   | −0.2697 (3)  | −0.05531 (19)| 0.10907 (5)  | 0.0307 (3)        |
| C16   | −0.0608 (3)  | −0.1395 (2)  | 0.11357 (5)  | 0.0319 (3)        |
| H16A  | −0.0020      | −0.1913      | 0.0885       | 0.038*            |

| | | | | |
|---|---|---|---|---|
| C17 | 0.0618 (3) | −0.14706 (19) | 0.15551 (5) | 0.0295 (3) |
| H17A | 0.2058 | −0.2045 | 0.1592 | 0.035* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.02827 (17) | 0.0286 (2) | 0.02758 (17) | −0.00541 (15) | 0.00608 (13) | 0.00212 (15) |
| Cl2 | 0.0514 (2) | 0.0680 (4) | 0.02503 (18) | 0.0176 (2) | −0.00744 (17) | −0.0029 (2) |
| O1 | 0.0364 (6) | 0.0500 (8) | 0.0334 (6) | −0.0141 (6) | −0.0034 (5) | −0.0042 (5) |
| O2 | 0.0321 (5) | 0.0490 (8) | 0.0318 (6) | −0.0152 (5) | −0.0010 (5) | 0.0023 (5) |
| O3 | 0.0328 (6) | 0.0476 (8) | 0.0288 (5) | 0.0120 (5) | 0.0007 (4) | −0.0072 (5) |
| N | 0.0240 (6) | 0.0383 (8) | 0.0196 (5) | 0.0012 (5) | 0.0019 (5) | 0.0013 (5) |
| C1 | 0.0266 (7) | 0.0307 (9) | 0.0253 (7) | −0.0004 (6) | 0.0021 (6) | −0.0031 (6) |
| C2 | 0.0272 (7) | 0.0247 (8) | 0.0239 (7) | 0.0006 (6) | 0.0058 (6) | −0.0012 (6) |
| C3 | 0.0252 (6) | 0.0278 (8) | 0.0192 (6) | 0.0026 (6) | 0.0028 (5) | −0.0013 (6) |
| C4 | 0.0278 (7) | 0.0268 (8) | 0.0248 (7) | −0.0014 (6) | 0.0030 (6) | −0.0008 (6) |
| C5 | 0.0294 (7) | 0.0302 (9) | 0.0220 (6) | 0.0000 (6) | 0.0023 (6) | 0.0005 (6) |
| C6 | 0.0374 (8) | 0.0517 (12) | 0.0286 (7) | −0.0087 (8) | 0.0041 (7) | 0.0049 (8) |
| C7 | 0.0502 (10) | 0.0654 (14) | 0.0282 (8) | −0.0078 (9) | 0.0083 (7) | 0.0117 (9) |
| C8 | 0.0532 (10) | 0.0680 (15) | 0.0214 (7) | 0.0003 (10) | −0.0008 (7) | 0.0049 (8) |
| C9 | 0.0374 (8) | 0.0562 (12) | 0.0232 (7) | −0.0047 (8) | −0.0026 (6) | −0.0018 (7) |
| C10 | 0.0296 (7) | 0.0348 (9) | 0.0218 (6) | 0.0004 (6) | 0.0023 (6) | −0.0028 (6) |
| C11 | 0.0306 (7) | 0.0258 (8) | 0.0228 (7) | 0.0018 (6) | 0.0033 (6) | −0.0012 (6) |
| C12 | 0.0275 (7) | 0.0260 (8) | 0.0201 (6) | −0.0020 (6) | 0.0034 (5) | 0.0002 (6) |
| C13 | 0.0321 (7) | 0.0282 (8) | 0.0233 (7) | 0.0034 (6) | 0.0060 (6) | −0.0017 (6) |
| C14 | 0.0293 (7) | 0.0361 (9) | 0.0291 (7) | 0.0071 (7) | 0.0022 (6) | 0.0014 (7) |
| C15 | 0.0359 (8) | 0.0359 (9) | 0.0202 (6) | 0.0015 (7) | −0.0008 (6) | 0.0018 (7) |
| C16 | 0.0347 (8) | 0.0400 (10) | 0.0215 (7) | 0.0064 (7) | 0.0051 (6) | −0.0032 (7) |
| C17 | 0.0292 (7) | 0.0348 (9) | 0.0246 (7) | 0.0052 (6) | 0.0035 (6) | −0.0009 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C2 | 1.7105 (15) | C7—C8 | 1.380 (2) |
| Cl2—C15 | 1.7394 (14) | C7—H7A | 0.9500 |
| O1—C1 | 1.2154 (17) | C8—C9 | 1.381 (2) |
| O2—C4 | 1.2166 (16) | C8—H8A | 0.9500 |
| O3—C11 | 1.2167 (16) | C9—C10 | 1.3932 (19) |
| N—C11 | 1.3834 (18) | C9—H9A | 0.9500 |
| N—C3 | 1.3890 (15) | C11—C12 | 1.4905 (19) |
| N—H0A | 0.8800 | C12—C17 | 1.392 (2) |
| C1—C10 | 1.480 (2) | C12—C13 | 1.392 (2) |
| C1—C2 | 1.4907 (18) | C13—C14 | 1.3867 (19) |
| C2—C3 | 1.3461 (19) | C13—H13A | 0.9500 |
| C3—C4 | 1.494 (2) | C14—C15 | 1.379 (2) |
| C4—C5 | 1.4829 (19) | C14—H14A | 0.9500 |
| C5—C6 | 1.387 (2) | C15—C16 | 1.381 (2) |
| C5—C10 | 1.391 (2) | C16—C17 | 1.3903 (19) |
| C6—C7 | 1.389 (2) | C16—H16A | 0.9500 |

| C6—H6A | 0.9500 | C17—H17A | 0.9500 |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C11—N—C3 | 123.62 (11) | C8—C9—C10 | 120.27 (15) |
| C11—N—H0A | 118.2 | C8—C9—H9A | 119.9 |
| C3—N—H0A | 118.2 | C10—C9—H9A | 119.9 |
| O1—C1—C10 | 121.71 (13) | C5—C10—C9 | 119.60 (14) |
| O1—C1—C2 | 121.20 (14) | C5—C10—C1 | 121.47 (12) |
| C10—C1—C2 | 117.08 (12) | C9—C10—C1 | 118.91 (13) |
| C3—C2—C1 | 122.21 (13) | O3—C11—N | 121.65 (12) |
| C3—C2—Cl1 | 122.74 (11) | O3—C11—C12 | 123.01 (13) |
| C1—C2—Cl1 | 114.90 (10) | N—C11—C12 | 115.34 (12) |
| C2—C3—N | 124.82 (13) | C17—C12—C13 | 119.63 (12) |
| C2—C3—C4 | 120.79 (12) | C17—C12—C11 | 118.00 (12) |
| N—C3—C4 | 114.27 (12) | C13—C12—C11 | 122.36 (12) |
| O2—C4—C5 | 122.80 (13) | C14—C13—C12 | 120.19 (13) |
| O2—C4—C3 | 119.01 (12) | C14—C13—H13A | 119.9 |
| C5—C4—C3 | 118.19 (12) | C12—C13—H13A | 119.9 |
| C6—C5—C10 | 120.03 (13) | C15—C14—C13 | 119.16 (13) |
| C6—C5—C4 | 119.89 (13) | C15—C14—H14A | 120.4 |
| C10—C5—C4 | 120.08 (13) | C13—C14—H14A | 120.4 |
| C5—C6—C7 | 119.71 (15) | C14—C15—C16 | 121.78 (13) |
| C5—C6—H6A | 120.1 | C14—C15—Cl2 | 119.11 (11) |
| C7—C6—H6A | 120.1 | C16—C15—Cl2 | 119.11 (11) |
| C8—C7—C6 | 120.49 (16) | C15—C16—C17 | 118.79 (14) |
| C8—C7—H7A | 119.8 | C15—C16—H16A | 120.6 |
| C6—C7—H7A | 119.8 | C17—C16—H16A | 120.6 |
| C7—C8—C9 | 119.89 (14) | C16—C17—C12 | 120.37 (13) |
| C7—C8—H8A | 120.1 | C16—C17—H17A | 119.8 |
| C9—C8—H8A | 120.1 | C12—C17—H17A | 119.8 |

| | | | |
|---|---|---|---|
| O1—C1—C2—C3 | 179.54 (14) | C6—C5—C10—C1 | −178.31 (15) |
| C10—C1—C2—C3 | −1.3 (2) | C4—C5—C10—C1 | 2.1 (2) |
| O1—C1—C2—Cl1 | −4.8 (2) | C8—C9—C10—C5 | −0.8 (3) |
| C10—C1—C2—Cl1 | 174.35 (11) | C8—C9—C10—C1 | 177.93 (16) |
| C1—C2—C3—N | −179.82 (14) | O1—C1—C10—C5 | 177.09 (15) |
| Cl1—C2—C3—N | 4.8 (2) | C2—C1—C10—C5 | −2.0 (2) |
| C1—C2—C3—C4 | 4.4 (2) | O1—C1—C10—C9 | −1.6 (2) |
| Cl1—C2—C3—C4 | −170.99 (11) | C2—C1—C10—C9 | 179.29 (14) |
| C11—N—C3—C2 | 49.6 (2) | C3—N—C11—O3 | 5.2 (2) |
| C11—N—C3—C4 | −134.37 (14) | C3—N—C11—C12 | −175.37 (13) |
| C2—C3—C4—O2 | 175.91 (14) | O3—C11—C12—C17 | 21.9 (2) |
| N—C3—C4—O2 | −0.3 (2) | N—C11—C12—C17 | −157.54 (14) |
| C2—C3—C4—C5 | −4.1 (2) | O3—C11—C12—C13 | −159.00 (15) |
| N—C3—C4—C5 | 179.64 (12) | N—C11—C12—C13 | 21.6 (2) |
| O2—C4—C5—C6 | 1.2 (2) | C17—C12—C13—C14 | 2.4 (2) |
| C3—C4—C5—C6 | −178.73 (15) | C11—C12—C13—C14 | −176.72 (14) |
| O2—C4—C5—C10 | −179.23 (15) | C12—C13—C14—C15 | −0.4 (2) |
| C3—C4—C5—C10 | 0.8 (2) | C13—C14—C15—C16 | −1.9 (2) |

| | | | |
|---|---|---|---|
| C10—C5—C6—C7 | 0.1 (3) | C13—C14—C15—Cl2 | 178.10 (12) |
| C4—C5—C6—C7 | 179.64 (16) | C14—C15—C16—C17 | 2.1 (2) |
| C5—C6—C7—C8 | −0.2 (3) | Cl2—C15—C16—C17 | −177.92 (13) |
| C6—C7—C8—C9 | −0.3 (3) | C15—C16—C17—C12 | 0.0 (2) |
| C7—C8—C9—C10 | 0.7 (3) | C13—C12—C17—C16 | −2.2 (2) |
| C6—C5—C10—C9 | 0.4 (2) | C11—C12—C17—C16 | 176.94 (14) |
| C4—C5—C10—C9 | −179.17 (15) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N—H0*A*···Cl1[i] | 0.88 | 2.89 | 3.6491 (12) | 145 |
| C14—H14*A*···O2[ii] | 0.95 | 2.40 | 3.2517 (19) | 149 |

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