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5-(2-Chlorophenyl)-3-(2*H*-chromen-3-yl)-1,2,4-oxadiazole

Nilofar Baral,[a] Sabita Nayak,[a] Satyanarayan Pal[b]* and Seetaram Mohapatra[a]

[a]Department of Chemistry, Ravenshaw University, Cuttack, Odisha, India, and [b]P.G. Department of Chemistry, Utkal University, Bhubaneswar, Odisha, India. *Correspondence e-mail: snpal75@gmail.com

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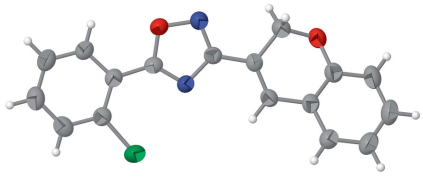
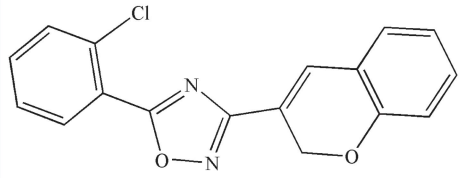
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{11}ClN_2O_2$, the central oxadiazole ring carries 2*H*-chromene and 2-chlorophenyl substituents at the 3- and 5-positions, respectively. C—H···O and C—H···Cl hydrogen bonds form two-dimensional sheets parallel to (212), with each individual molecule involved in six of these weak interactions. The sheets are stacked perpendicular to (212) by offset π–π stacking interactions.

3D view



Chemical scheme



Structure description

Oxadiazole derivatives have attracted considerable interest due to their unique chemical structures and wide variety of biological applications. These include use as antitumour (Maftei *et al.*, 2013), antifungal, antibacterial and anti-inflammatory agents (Rakesh *et al.*, 2009). Chromene (benzopyran) is also an important medicinal pharmacophore. It is an integral part of many natural alkaloids and flavonoids and is known to possess biological activities similar to the oxadiazoles, together with antivascular, antimicrobial and antioxidant properties (Gourdeau *et al.*, 2004). Another important feature is its lipophilic nature which helps it to pass readily through cell membranes. We are interested in the design and synthesis of chromene-based oxadiazole derivatives and studies of their biological activity, and we report here the structure of the chromene–oxadiazole derivative 5-(2-chlorophenyl)-3-(2*H*-chromen-3-yl)-1,2,4-oxadiazole.

A perspective view of the molecule is shown in Fig. 1. The molecule is not completely planar. The plane of the central oxadiazole ring is inclined at 1.2 (1)° to the plane of the 2-chlorophenyl ring and 12.24 (9)° to the best-fit plane of the chromene ring system. The C—Cl distance [1.7221 (17) Å] is consistent with the reported values (Hathwar *et al.*, 2010). The bond lengths and angles of the chromene and oxadiazole units are also similar to those reported in the literature (Devarajegowda *et al.*, 2015; Du & Zhao, 2004). In the crystal, weak intermolecular C—H···Cl and C—H···O interactions (Desiraju *et al.*,

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.62	3.389 (2)	140
C14—H14···Cl1^{ii}	0.93	2.94	3.625 (2)	132
C2—H2···O2^{iii}	0.93	2.67	3.550 (2)	158

Symmetry codes: (i) $-x+1, -y+3, -z+2$; (ii) $-x+2, -y+1, -z+2$; (iii) $x-1, y, z+1$.

Table 2
π–π interaction details (Å, °).

$Cg1$ and $Cg2$ are the centroids of the C7/N1/C8/N2/O2 and C11–C16 rings, respectively

Centroid (Cg)	Centroid (Cg)	Cg···Cg distance	Dihedral angle	Slippage distance
$Cg1$	$Cg2^{i}$	3.9370 (11)	14.57 (10)	1.69
$Cg2$	$Cg1^{i}$	3.9370 (11)	14.57 (10)	2.318

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

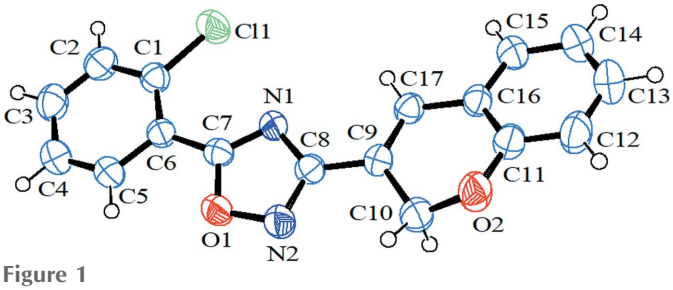


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

1999) are found. C14—H14···Cl1 hydrogen bonds form inversion dimers enclosing $R_2^2(24)$ rings, while a second inversion dimer forms through C5—H5···O1 contacts with an $R_2^2(10)$ ring motif (Bernstein *et al.*, 1995). A C2—H2···O2 interaction completes the hydrogen-bonding network, forming sheets of molecules parallel to (212), with each individual molecule in the sheet bound to four others through six nonclassical hydrogen-bonding interactions (Table 1 and Fig. 2). Adjacent sheets are linked by inversion related offset π–π stacking interactions (Table 2 and Fig. 3), forming a three-dimensional network.

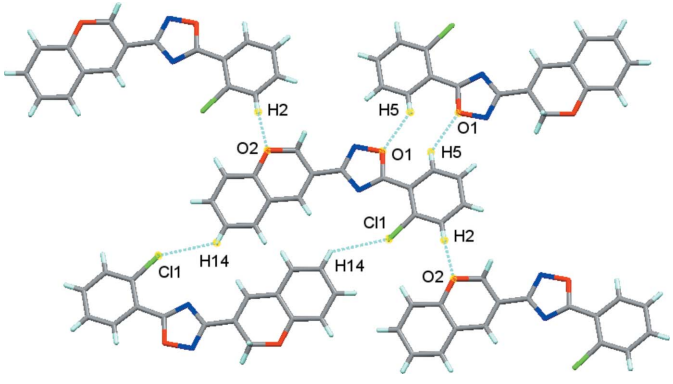


Figure 2
A view of two-dimensional sheet structure formed from C—H···O and C—H···Cl hydrogen bonds (cyan dotted lines).

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{11}ClN_2O_2$
M_r	310.73
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.7208 (4), 8.7703 (3), 9.6278 (4)
α, β, γ (°)	86.035 (3), 80.227 (3), 79.352 (2)
V (Å^3)	712.65 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	0.40 × 0.28 × 0.20
Data collection	
Diffractometer	Bruker APEXII
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11000, 3518, 2452
R_{int}	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.134, 1.11
No. of reflections	3518
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.26

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

Synthesis and crystallization

This compound was prepared by the treatment of *N*-hydroxy-2*H*-chromene-3-carboximidamide (1 equiv.) with 2-chlorobenzoic acid (0.8 equiv.) in the presence of ethylene dicarboimide (EDCI, 1.2 equiv) and *N*-hydroxybenzotriazole

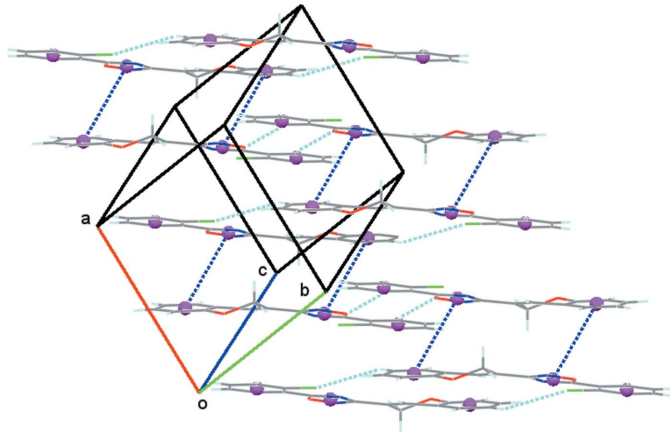


Figure 3
Packing of the title compound, showing the π–π interactions stacking adjacent molecular sheets (dark blue dotted lines show the π–π interactions and cyan dotted lines indicate hydrogen bonds).

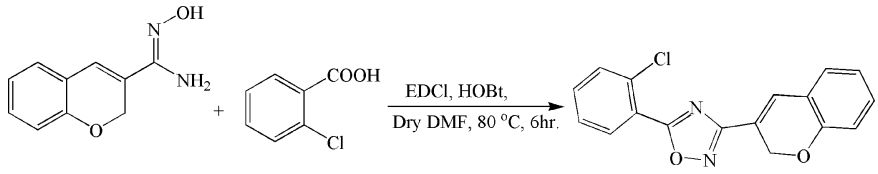


Figure 4
The synthetic scheme for the title compound.

(HOBt, 1.2 equiv.) in dry DMF at 353 K for 6 h (Fig. 4). The reaction mixture was extracted with water and ethyl acetate. The pure compound was isolated by column chromatography, eluting with 2–5% ethyl acetate/hexane. The solvents were evaporated and dried to give the title compound in 75% yield (m.p. 478 K). Colourless rectangular crystals were obtained by slow evaporation of a solution of the compound in a dichloromethane/hexane mixture. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (*d*, *J* = 8.0 Hz, 2H), 7.37–7.33 (*m*, 3H), 7.21–7.17 (*m*, 2H), 6.94 (*t*, *J* = 8.0 Hz, 1H), 6.89 (*d*, *J* = 8.0 Hz, 1H), 5.26 (*s*, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.9, 166.0, 154.7, 134.8, 131.9, 131.6, 131.1, 128.6, 128.5, 128.4, 127.2, 126.8, 121.9, 121.4, 119.2, 116.2, 64.2.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

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References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2014). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. & Steiner, T. (1999). In *The Weak Hydrogen Bond in Structural Chemistry and Biology*. New York: Oxford University Press Inc.
Devarajegowda, H. C., Suchetan, P. A., Sreenivasa, S., Srinivasa, H. T. & Palakshamurthy, B. S. (2015). *Acta Cryst.* E**71**, o374–o375.
Du, M. & Zhao, X.-J. (2004). *Acta Cryst.* C**60**, o54–o56.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gourdeau, H., Leblond, L., Hamelin, B., Desputeau, C., Dong, K., Kianicka, I., Custeau, D., Boudreau, C., Geerts, L., Cai, S. X., Drewe, J., Labrecque, D., Kasibhatla, S. & Tseng, B. (2004). *Mol. Cancer Ther.* **3**, 1375–1384.
Hathwar, V., Roopan, S. M., Subashini, R., Khan, F. N. & Guru Row, T. N. (2010). *J. Chem. Sci.* **122**, 677–685.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Maftei, C. V., Fodor, E., Jones, P. G., Franz, M. H., Kelter, G., Fiebig, H. & Neda, I. (2013). *Beilstein J. Org. Chem.* **9**, 2202–2215.
Rakesh, D. S., Sun, D., Lee, R. B., Tangallapally, R. P. & Lee, R. E. (2009). *Eur. J. Med. Chem.* **44**, 460–472.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2018). **3**, x180129 [https://doi.org/10.1107/S2414314618001293]

5-(2-Chlorophenyl)-3-(2*H*-chromen-3-yl)-1,2,4-oxadiazole

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Crystal data

$C_{17}H_{11}ClN_2O_2$
M_r = 310.73
Triclinic, $P\overline{1}$
a = 8.7208 (4) Å
b = 8.7703 (3) Å
c = 9.6278 (4) Å
α = 86.035 (3)°
β = 80.227 (3)°
γ = 79.352 (2)°
V = 712.65 (5) Å^3
Z = 2
$F(000)$ = 320
D_x = 1.448 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2986 reflections
θ = 2.4–26.6°
μ = 0.28 mm^{-1}
T = 296 K
Rectangular block, colourless
0.40 × 0.28 × 0.20 mm

Data collection

Bruker APEXII diffractometer
Radiation source: sealed tube
φ and ω scans
11000 measured reflections
3518 independent reflections
2452 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −11→11
k = −11→11
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.134
S = 1.11
3518 reflections
199 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.0537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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.

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.52115 (6)	0.91781 (6)	1.30274 (6)	0.0650 (2)

O1	0.61910 (15)	1.27500 (14)	0.95744 (13)	0.0529 (3)
O2	1.09361 (16)	0.89357 (16)	0.61902 (13)	0.0601 (4)
N1	0.69651 (16)	1.03574 (15)	1.03518 (15)	0.0418 (3)
N2	0.75145 (19)	1.21176 (18)	0.86047 (16)	0.0536 (4)
C3	0.2109 (2)	1.3029 (2)	1.3854 (2)	0.0597 (5)
H3	0.1264	1.3352	1.4559	0.072*
C4	0.2528 (2)	1.4042 (2)	1.2754 (2)	0.0602 (5)
H4	0.1969	1.5052	1.2720	0.072*
C5	0.3759 (2)	1.3563 (2)	1.1718 (2)	0.0527 (5)
H5	0.4019	1.4259	1.0981	0.063*
C6	0.4649 (2)	1.20576 (19)	1.17225 (18)	0.0409 (4)
C7	0.5951 (2)	1.16306 (19)	1.05849 (18)	0.0401 (4)
C8	0.7906 (2)	1.07079 (19)	0.91245 (17)	0.0410 (4)
C9	0.9241 (2)	0.9627 (2)	0.84305 (17)	0.0408 (4)
C17	0.9677 (2)	0.81924 (19)	0.89577 (18)	0.0421 (4)
H17	0.9143	0.7866	0.9814	0.051*
C16	1.09781 (19)	0.71486 (19)	0.81982 (18)	0.0426 (4)
C11	1.1551 (2)	0.7555 (2)	0.6807 (2)	0.0492 (4)
C12	1.2678 (3)	0.6539 (3)	0.5981 (2)	0.0649 (6)
H12	1.3036	0.6817	0.5048	0.078*
C13	1.3268 (3)	0.5112 (3)	0.6547 (3)	0.0706 (6)
H13	1.4018	0.4422	0.5987	0.085*
C15	1.1619 (2)	0.5702 (2)	0.8749 (2)	0.0526 (5)
H15	1.1270	0.5414	0.9680	0.063*
C14	1.2766 (3)	0.4691 (2)	0.7928 (2)	0.0634 (6)
H14	1.3194	0.3734	0.8306	0.076*
C10	1.0205 (2)	1.0176 (2)	0.7108 (2)	0.0544 (5)
H10A	0.9526	1.0945	0.6607	0.065*
H10B	1.1017	1.0674	0.7362	0.065*
C1	0.4216 (2)	1.1052 (2)	1.28580 (19)	0.0448 (4)
C2	0.2945 (2)	1.1539 (2)	1.3905 (2)	0.0550 (5)
H2	0.2658	1.0855	1.4643	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0698 (4)	0.0491 (3)	0.0657 (3)	0.0012 (2)	−0.0008 (3)	0.0144 (2)
O1	0.0564 (8)	0.0409 (7)	0.0530 (7)	0.0005 (6)	0.0021 (6)	0.0062 (6)
O2	0.0636 (9)	0.0618 (8)	0.0435 (7)	0.0030 (7)	0.0058 (6)	0.0027 (6)
N1	0.0400 (8)	0.0382 (7)	0.0443 (8)	−0.0025 (6)	−0.0040 (6)	0.0007 (6)
N2	0.0542 (10)	0.0472 (8)	0.0510 (9)	0.0000 (7)	0.0033 (7)	0.0038 (7)
C3	0.0527 (12)	0.0641 (13)	0.0588 (12)	−0.0051 (10)	0.0000 (10)	−0.0152 (10)
C4	0.0564 (12)	0.0483 (11)	0.0706 (14)	0.0004 (9)	−0.0031 (11)	−0.0086 (10)
C5	0.0533 (11)	0.0406 (10)	0.0595 (12)	−0.0028 (8)	−0.0022 (9)	−0.0016 (8)
C6	0.0390 (9)	0.0390 (9)	0.0457 (9)	−0.0064 (7)	−0.0090 (8)	−0.0040 (7)
C7	0.0424 (9)	0.0374 (8)	0.0418 (9)	−0.0083 (7)	−0.0102 (7)	0.0014 (7)
C8	0.0399 (9)	0.0423 (9)	0.0408 (9)	−0.0074 (7)	−0.0080 (7)	0.0018 (7)
C9	0.0382 (9)	0.0446 (9)	0.0387 (9)	−0.0061 (7)	−0.0045 (7)	−0.0033 (7)

C17	0.0415 (9)	0.0453 (9)	0.0383 (9)	−0.0077 (8)	−0.0034 (7)	−0.0001 (7)
C16	0.0365 (9)	0.0454 (9)	0.0455 (9)	−0.0065 (7)	−0.0045 (7)	−0.0055 (7)
C11	0.0433 (10)	0.0538 (11)	0.0479 (10)	−0.0055 (8)	−0.0036 (8)	−0.0017 (8)
C12	0.0573 (13)	0.0732 (14)	0.0548 (12)	−0.0021 (11)	0.0098 (10)	−0.0084 (10)
C13	0.0588 (13)	0.0673 (14)	0.0755 (15)	0.0068 (11)	0.0050 (12)	−0.0180 (12)
C15	0.0502 (11)	0.0470 (10)	0.0565 (11)	−0.0026 (8)	−0.0045 (9)	−0.0004 (8)
C14	0.0574 (13)	0.0497 (11)	0.0767 (15)	0.0034 (9)	−0.0046 (11)	−0.0071 (10)
C10	0.0570 (12)	0.0520 (11)	0.0474 (10)	−0.0034 (9)	0.0016 (9)	0.0047 (8)
C1	0.0434 (10)	0.0444 (9)	0.0468 (10)	−0.0065 (8)	−0.0095 (8)	−0.0021 (8)
C2	0.0557 (12)	0.0625 (12)	0.0458 (10)	−0.0125 (10)	−0.0030 (9)	−0.0012 (9)

Geometric parameters (Å, º)

Cl1—C1	1.7221 (17)	C9—C17	1.337 (2)
O1—C7	1.352 (2)	C9—C10	1.504 (3)
O1—N2	1.407 (2)	C17—C16	1.445 (2)
O2—C11	1.370 (2)	C17—H17	0.9300
O2—C10	1.434 (2)	C16—C11	1.394 (3)
N1—C7	1.297 (2)	C16—C15	1.396 (2)
N1—C8	1.370 (2)	C11—C12	1.379 (3)
N2—C8	1.308 (2)	C12—C13	1.375 (3)
C3—C2	1.375 (3)	C12—H12	0.9300
C3—C4	1.379 (3)	C13—C14	1.375 (3)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.360 (3)	C15—C14	1.383 (3)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.403 (2)	C14—H14	0.9300
C5—H5	0.9300	C10—H10A	0.9700
C6—C1	1.402 (3)	C10—H10B	0.9700
C6—C7	1.452 (2)	C1—C2	1.390 (3)
C8—C9	1.454 (2)	C2—H2	0.9300
C7—O1—N2	106.58 (12)	C11—C16—C17	118.38 (16)
C11—O2—C10	117.19 (14)	C15—C16—C17	123.41 (17)
C7—N1—C8	103.21 (14)	O2—C11—C12	117.82 (17)
C8—N2—O1	103.13 (13)	O2—C11—C16	120.90 (16)
C2—C3—C4	119.87 (19)	C12—C11—C16	121.14 (18)
C2—C3—H3	120.1	C13—C12—C11	119.4 (2)
C4—C3—H3	120.1	C13—C12—H12	120.3
C5—C4—C3	119.97 (18)	C11—C12—H12	120.3
C5—C4—H4	120.0	C14—C13—C12	121.0 (2)
C3—C4—H4	120.0	C14—C13—H13	119.5
C4—C5—C6	122.36 (19)	C12—C13—H13	119.5
C4—C5—H5	118.8	C14—C15—C16	120.9 (2)
C6—C5—H5	118.8	C14—C15—H15	119.6
C1—C6—C5	116.77 (17)	C16—C15—H15	119.6
C1—C6—C7	123.92 (15)	C13—C14—C15	119.4 (2)
C5—C6—C7	119.31 (16)	C13—C14—H14	120.3

N1—C7—O1	112.46 (15)	C15—C14—H14	120.3
N1—C7—C6	131.83 (16)	O2—C10—C9	112.57 (15)
O1—C7—C6	115.70 (14)	O2—C10—H10A	109.1
N2—C8—N1	114.61 (15)	C9—C10—H10A	109.1
N2—C8—C9	121.46 (16)	O2—C10—H10B	109.1
N1—C8—C9	123.93 (15)	C9—C10—H10B	109.1
C17—C9—C8	122.38 (16)	H10A—C10—H10B	107.8
C17—C9—C10	119.06 (16)	C2—C1—C6	120.70 (17)
C8—C9—C10	118.51 (15)	C2—C1—Cl1	117.01 (15)
C9—C17—C16	120.03 (16)	C6—C1—Cl1	122.29 (14)
C9—C17—H17	120.0	C3—C2—C1	120.32 (19)
C16—C17—H17	120.0	C3—C2—H2	119.8
C11—C16—C15	118.04 (17)	C1—C2—H2	119.8

C7—O1—N2—C8	0.60 (18)	C9—C17—C16—C15	172.52 (17)
C2—C3—C4—C5	0.4 (3)	C10—O2—C11—C12	−159.35 (17)
C3—C4—C5—C6	−0.5 (3)	C10—O2—C11—C16	24.9 (3)
C4—C5—C6—C1	−0.2 (3)	C15—C16—C11—O2	177.84 (16)
C4—C5—C6—C7	−179.70 (17)	C17—C16—C11—O2	2.3 (3)
C8—N1—C7—O1	0.53 (18)	C15—C16—C11—C12	2.2 (3)
C8—N1—C7—C6	−178.65 (17)	C17—C16—C11—C12	−173.26 (17)
N2—O1—C7—N1	−0.73 (19)	O2—C11—C12—C13	−176.98 (19)
N2—O1—C7—C6	178.58 (14)	C16—C11—C12—C13	−1.2 (3)
C1—C6—C7—N1	−1.2 (3)	C11—C12—C13—C14	−0.8 (4)
C5—C6—C7—N1	178.26 (17)	C11—C16—C15—C14	−1.3 (3)
C1—C6—C7—O1	179.69 (15)	C17—C16—C15—C14	173.99 (18)
C5—C6—C7—O1	−0.9 (2)	C12—C13—C14—C15	1.7 (4)
O1—N2—C8—N1	−0.3 (2)	C16—C15—C14—C13	−0.7 (3)
O1—N2—C8—C9	179.76 (15)	C11—O2—C10—C9	−40.1 (2)
C7—N1—C8—N2	−0.1 (2)	C17—C9—C10—O2	30.5 (2)
C7—N1—C8—C9	179.81 (16)	C8—C9—C10—O2	−152.22 (15)
N2—C8—C9—C17	178.75 (16)	C5—C6—C1—C2	1.1 (3)
N1—C8—C9—C17	−1.2 (3)	C7—C6—C1—C2	−179.50 (16)
N2—C8—C9—C10	1.6 (3)	C5—C6—C1—Cl1	−179.00 (13)
N1—C8—C9—C10	−178.30 (16)	C7—C6—C1—Cl1	0.4 (2)
C8—C9—C17—C16	177.80 (15)	C4—C3—C2—C1	0.4 (3)
C10—C9—C17—C16	−5.1 (3)	C6—C1—C2—C3	−1.2 (3)
C9—C17—C16—C11	−12.2 (3)	Cl1—C1—C2—C3	178.89 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.62	3.389 (2)	140
C14—H14···Cl1^{ii}	0.93	2.94	3.625 (2)	132
C2—H2···O2^{iii}	0.93	2.67	3.550 (2)	158

Symmetry codes: (i) −*x*+1, −*y*+3, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) *x*−1, *y*, *z*+1.