# organic compounds

# 6,8-Dichloro-N-methyl-3-nitro-4-nitro-methyl-4H-chromen-2-amine

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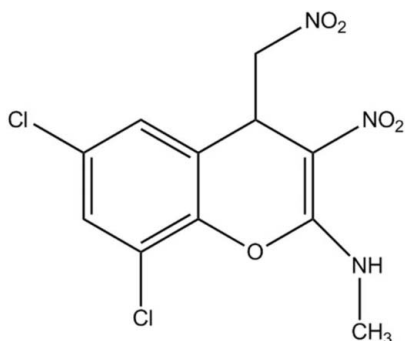Correspondence e-mail: krishstrucbio@gmail.com

In the title compound, $C_{11}H_9Cl_2N_3O_5$, the dihydropyran ring adopts a near-half-chair conformation. The benzene ring makes a torsion angle of 5.02 (5)° with the dihydropyran ring. Adjacent molecules are interlinked through intermolecular C—H···O, N—H···O and C—Cl···$\pi$ [3.4743 (9) Å] interactions. The intermolecular N—H···O hydrogen bond generates an $R_2^2(12)$ motif, which is observed to contribute to the crystal packing stability. Moreover, the molecular structure displays an $S(6)$ motif formed by intramolecular N—H···O hydrogen bonding.

## Related literature

For related structures, see: Gayathri *et al.* (2006); Bhaskaran *et al.* (2006). For the biological importance of 4H-chromene derivatives, see: Cai (2007, 2008); Cai *et al.* (2006); Gabor (1988); Brooks (1998); Valenti *et al.* (1993); Hyana & Saimoto (1987); Tang *et al.* (2007). For ring-puckering analysis, see: Cremer & Pople (1975).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{11}H_9Cl_2N_3O_5$ | $\gamma$ = 87.579 (6)° |
| $M_r$ = 334.11 | $V$ = 677.68 (9) Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z$ = 2 |
| $a$ = 8.7426 (7) Å | Mo $K\alpha$ radiation |
| $b$ = 9.2727 (7) Å | $\mu$ = 0.50 mm$^{-1}$ |
| $c$ = 9.3420 (7) Å | $T$ = 293 K |
| $\alpha$ = 70.017 (7)° | 0.4 × 0.35 × 0.2 mm |
| $\beta$ = 72.609 (7)° | |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur Eos diffractometer | 15150 measured reflections |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009) | 2385 independent reflections |
| | 2072 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.792, $T_{max}$ = 1.000 | $R_{int}$ = 0.034 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.032 | 191 parameters |
| $wR(F^2)$ = 0.110 | H-atom parameters constrained |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.34 e Å$^{-3}$ |
| 2385 reflections | $\Delta\rho_{min}$ = −0.30 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2 | 0.86 | 2.00 | 2.613 (2) | 128 |
| N1—H1···O2$^i$ | 0.86 | 2.12 | 2.881 (2) | 147 |
| C7—H7···O3$^{ii}$ | 0.98 | 2.50 | 3.1944 (19) | 128 |
| C11—H11$B$···O3$^{ii}$ | 0.97 | 2.54 | 3.103 (2) | 117 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2089).

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**supplementary materials**

## 6,8-Dichloro-*N*-methyl-3-nitro-4-nitromethyl-4*H*-chromen-2-amine

## J. Muthukumaran, A. Parthiban, M. Kannan, H. S. P. Rao and R. Krishna

### Comment

4*H*-Chromenes are biologically important compounds used as synthetic ligands for drug designing and discovery process. They exhibit numerous biological and pharmacological properties such as anti-viral, anti-fungal, anti-inflammatory, anti-diabetic, cardionthonic, anti-anaphylactic and anti-cancer activity (Cai, 2008; Cai, 2007; Cai *et al.*, 2006; Gabor *et al.*, 1988; Brooks, 1998; Valenti *et al.*, 1993; Hyana & Saimoto, 1987; Tang *et al.*, 2007). In view of the growing medicinal importance of 4*H*-chromene derivatives, a single-crystal X-ray diffraction study on the title compound was carried out and analyzed.

The title compound (Fig. 1) contains the 4*H*-chromene moiety with four different substituents [–Cl$_2$, –NO$_2$, –CH$_2$NO$_2$ and –NHCH$_3$]. The Cl1 group attached to C2 by an (+) anti-periplanar conformation with the torsion angle (Cl1/C2/C3/C4) of 178.76 (14) °, whereas another chlorine attached to C4 with the torsion angle (Cl2/C4/C3/C2) of -176.94 (14) °, which oriented in (-) anti-periplanar conformations. From the puckering analysis (Cremer & Pople, 1975), the fused dihydropyran ring (O1/C1/C6/C7/C8/C9) of 4*H*-chromene is very similar to half chair (H form) conformation with puckering parameters of Q = 0.1772 (17) Å, θ = 104.5 (5) ° and Φ = 11.6 (6) °. The molecular structure is stabilized by intramolecular N—H···O and C—H···O interactions. The intramolecular N1—H1···O2 interaction generates a graph-set motif *S* (6) (Fig. 2) with a *D*···*A* bond distance of 2.613 (2) Å. The crystal packing of the molecule (Fig. 3) is stabilized by intermolecular N1—H1···O2 (symmetry code: -*x* + 2, -*y* + 1, -*z* + 1), C7—H7···O3 (symmetry code: -*x* + 2, -*y* + 2, -*z*), C11—H11B···O3 (symmetry code:-*x* + 2, -*y* + 2, -*z*) and C—Cl··· π (symmetry code: 1 - *x*, 1 - *y*, -*z*) interactions (Fig. 4). The intermolecular N1—H1···O2 interaction generates a ring of graph-set $R^2_2$ (12) with the bond distance of 2.881 (2) Å (Fig. 5).

### Experimental

(*E*)-2,4-Dichloro-6-(2-nitrovinyl)phenol (100 mg, 0.427 mmol) was taken in a 25 ml round bottom flask in methanol (4 ml). To this solution, 1,8-diazabicyclo[5.4.0] undec-7-ene (DBU) (8 mg, 0.042 mmol) was added and stirred thoroughly for 10 minutes at room temperature. To this stirred solution, NMSM ((*E*) *N*-methyl-1-(methylthio)-2-nitroethenamine) was added and stirred for 10 h for completion (TLC, hexane: EtOAc, 3:2, $R_f$ of I = 0.3). The reaction mixture was then kept in a refrigerator for 2 h to afford racemic mixture of the product (I), white precipitate, which was filtered. Good crystals were obtained by recrystallization with a solution of dichloromethane: hexane (9:3 *v*/*v*).

### Refinement

All hydrogen atoms were placed in calculated positions, with N—H=0.86 and C—H=0.97 and included in the final cycles of refinement using a riding model with $U_{iso}$(H) = 1.2 $U_{eq}$(*C*).
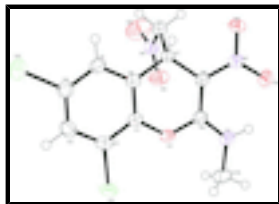
# supplementary materials

**Figures**

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.
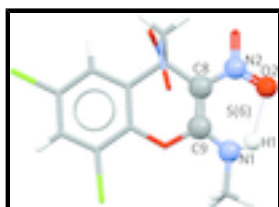
Fig. 2. A view of intramolecular motif $S$ (6) formed by N—H···O interaction in (I). The motif forming atoms are shown in ball and stick model and the Hydrogen bond are shown in blue dashed lines.
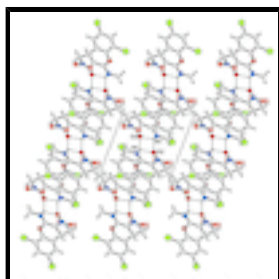
Fig. 3. The crystal packing of (I) viewed down the *XO*-axis, showing intermolecular hydrogen bonding interactions as dashed lines.
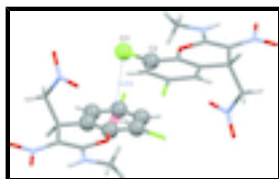
Fig. 4. The molecular interaction showing the weak C—Cl···pi interaction in (I). *Cg* is a centroid of C1—C6 ring in 4*H*-chromene moiety.
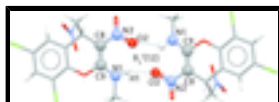
Fig. 5. A view of intermolecular ring motif $R_2^2$ (12) formed by N—H···O interaction in (I). The motif forming atoms are shown in ball and stick model and the hydrogen bond are shown in blue dashed lines.

## 6,8-dichloro-*N*-methyl-3-nitro-4-nitromethyl-4*H*-chromen-2-amine

*Crystal data*

| | |
|---|---|
| $C_{11}H_9Cl_2N_3O_5$ | $Z = 2$ |
| $M_r = 334.11$ | $F(000) = 340$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.637$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 485.65 K |
| $a = 8.7426$ (7) Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 9.2727$ (7) Å | Cell parameters from 8735 reflections |
| $c = 9.3420$ (7) Å | $\theta = 2.7–29.2°$ |
| $\alpha = 70.017$ (7)° | $\mu = 0.50$ mm$^{-1}$ |
| $\beta = 72.609$ (7)° | $T = 293$ K |
| $\gamma = 87.579$ (6)° | Block, colourless |
| $V = 677.68$ (9) Å$^3$ | 0.4 × 0.35 × 0.2 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Eos diffractometer | 2385 independent reflections |
| Radiation source: fine-focus sealed tube | 2072 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.034$ |
| Detector resolution: 15.9821 pixels mm$^{-1}$ | $\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$ |
| ω scans | $h = -10 \rightarrow 10$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009) | $k = -11 \rightarrow 11$ |
| $T_{min} = 0.792$, $T_{max} = 1.000$ | $l = -11 \rightarrow 11$ |
| 15150 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.110$ | H-atom parameters constrained |
| $S = 1.01$ | $w = 1/[\sigma^2(F_o^2) + (0.091P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2385 reflections | $(\Delta/\sigma)_{max} = 0.046$ |
| 191 parameters | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.30$ 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 | 0.66030 (6) | 0.29149 (5) | −0.00059 (6) | 0.04277 (19) |
| Cl2 | 0.68824 (8) | 0.83939 (6) | −0.46350 (6) | 0.0599 (2) |
| O1 | 0.77375 (15) | 0.46548 (12) | 0.15081 (14) | 0.0344 (3) |
| C6 | 0.79885 (19) | 0.71693 (18) | −0.05514 (19) | 0.0273 (4) |
| O3 | 1.02216 (15) | 0.86894 (13) | 0.20553 (15) | 0.0389 (3) |

| N2 | 0.98248 (17) | 0.72806 (15) | 0.25417 (16) | 0.0321 (3) |
| O2 | 1.01949 (18) | 0.63676 (15) | 0.37199 (16) | 0.0494 (4) |
| O4 | 0.55005 (17) | 0.69199 (16) | 0.26437 (17) | 0.0502 (4) |
| C1 | 0.7612 (2) | 0.55977 (18) | 0.00458 (19) | 0.0283 (4) |
| C5 | 0.7793 (2) | 0.80191 (19) | −0.20214 (19) | 0.0312 (4) |
| H5 | 0.8046 | 0.9075 | −0.2450 | 0.037* |
| C7 | 0.8539 (2) | 0.79260 (17) | 0.04217 (19) | 0.0275 (4) |
| H7 | 0.9526 | 0.8554 | −0.0288 | 0.033* |
| N1 | 0.8653 (2) | 0.40896 (17) | 0.35814 (18) | 0.0383 (4) |
| H1 | 0.9139 | 0.4331 | 0.4152 | 0.046* |
| C3 | 0.6865 (2) | 0.5726 (2) | −0.2272 (2) | 0.0365 (4) |
| H3 | 0.6498 | 0.5253 | −0.2850 | 0.044* |
| C8 | 0.8987 (2) | 0.67447 (18) | 0.17785 (19) | 0.0285 (4) |
| C2 | 0.7067 (2) | 0.48781 (19) | −0.0813 (2) | 0.0316 (4) |
| C9 | 0.8488 (2) | 0.51877 (19) | 0.23183 (19) | 0.0298 (4) |
| N3 | 0.56967 (19) | 0.83127 (18) | 0.19612 (18) | 0.0373 (4) |
| C11 | 0.7329 (2) | 0.90325 (17) | 0.0935 (2) | 0.0326 (4) |
| H11A | 0.7759 | 0.9524 | 0.1510 | 0.039* |
| H11B | 0.7223 | 0.9831 | −0.0017 | 0.039* |
| C4 | 0.7221 (2) | 0.7293 (2) | −0.2847 (2) | 0.0355 (4) |
| C10 | 0.8075 (3) | 0.2491 (2) | 0.4088 (3) | 0.0485 (5) |
| H10A | 0.8584 | 0.2078 | 0.3263 | 0.073* |
| H10B | 0.6932 | 0.2433 | 0.4287 | 0.073* |
| H10C | 0.8325 | 0.1909 | 0.5049 | 0.073* |
| O5 | 0.4625 (2) | 0.9172 (2) | 0.2075 (2) | 0.0744 (5) |

*Atomic displacement parameters ($Å^2$)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0508 (3) | 0.0246 (3) | 0.0566 (3) | −0.0001 (2) | −0.0175 (2) | −0.0172 (2) |
| Cl2 | 0.0942 (5) | 0.0534 (4) | 0.0365 (3) | 0.0011 (3) | −0.0335 (3) | −0.0086 (2) |
| O1 | 0.0450 (7) | 0.0202 (6) | 0.0367 (6) | −0.0035 (5) | −0.0182 (5) | −0.0025 (5) |
| C6 | 0.0271 (8) | 0.0246 (8) | 0.0290 (8) | 0.0025 (6) | −0.0077 (6) | −0.0084 (6) |
| O3 | 0.0469 (8) | 0.0250 (7) | 0.0444 (7) | −0.0074 (5) | −0.0186 (6) | −0.0064 (5) |
| N2 | 0.0362 (8) | 0.0250 (8) | 0.0314 (7) | −0.0018 (6) | −0.0139 (6) | −0.0018 (6) |
| O2 | 0.0678 (10) | 0.0365 (8) | 0.0478 (8) | −0.0027 (7) | −0.0388 (7) | −0.0004 (6) |
| O4 | 0.0407 (8) | 0.0409 (8) | 0.0602 (9) | −0.0049 (6) | −0.0082 (7) | −0.0117 (7) |
| C1 | 0.0295 (9) | 0.0229 (8) | 0.0299 (8) | 0.0040 (6) | −0.0083 (7) | −0.0068 (6) |
| C5 | 0.0348 (9) | 0.0245 (9) | 0.0293 (8) | 0.0015 (7) | −0.0071 (7) | −0.0053 (7) |
| C7 | 0.0308 (9) | 0.0186 (8) | 0.0295 (8) | −0.0006 (6) | −0.0096 (7) | −0.0030 (6) |
| N1 | 0.0483 (9) | 0.0252 (8) | 0.0387 (8) | −0.0021 (6) | −0.0221 (7) | 0.0006 (6) |
| C3 | 0.0392 (10) | 0.0387 (11) | 0.0383 (10) | 0.0041 (8) | −0.0126 (8) | −0.0208 (8) |
| C8 | 0.0309 (9) | 0.0229 (8) | 0.0307 (8) | 0.0002 (7) | −0.0130 (7) | −0.0044 (6) |
| C2 | 0.0309 (9) | 0.0238 (9) | 0.0401 (9) | 0.0028 (7) | −0.0077 (7) | −0.0136 (7) |
| C9 | 0.0296 (9) | 0.0248 (9) | 0.0322 (9) | 0.0021 (7) | −0.0109 (7) | −0.0050 (7) |
| N3 | 0.0405 (9) | 0.0388 (9) | 0.0378 (8) | 0.0085 (7) | −0.0150 (7) | −0.0177 (7) |
| C11 | 0.0397 (10) | 0.0210 (8) | 0.0383 (9) | 0.0022 (7) | −0.0163 (7) | −0.0078 (7) |
| C4 | 0.0409 (10) | 0.0369 (10) | 0.0277 (8) | 0.0045 (8) | −0.0101 (7) | −0.0106 (7) |

| | | | | | |
|---|---|---|---|---|---|
| C10 | 0.0579 (13) | 0.0245 (10) | 0.0514 (11) | −0.0055 (9) | −0.0192 (10) | 0.0047 (8) |
| O5 | 0.0539 (10) | 0.0656 (11) | 0.0901 (13) | 0.0263 (9) | −0.0061 (9) | −0.0262 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C2 | 1.7287 (16) | C7—H7 | 0.9800 |
| Cl2—C4 | 1.7391 (17) | N1—C9 | 1.311 (2) |
| O1—C9 | 1.352 (2) | N1—C10 | 1.455 (2) |
| O1—C1 | 1.3812 (19) | N1—H1 | 0.8600 |
| C6—C1 | 1.385 (2) | C3—C2 | 1.381 (2) |
| C6—C5 | 1.388 (2) | C3—C4 | 1.379 (2) |
| C6—C7 | 1.509 (2) | C3—H3 | 0.9300 |
| O3—N2 | 1.2537 (17) | C8—C9 | 1.398 (2) |
| N2—O2 | 1.2593 (18) | N3—O5 | 1.208 (2) |
| N2—C8 | 1.370 (2) | N3—C11 | 1.492 (2) |
| O4—N3 | 1.222 (2) | C11—H11A | 0.9700 |
| C1—C2 | 1.392 (2) | C11—H11B | 0.9700 |
| C5—C4 | 1.383 (2) | C10—H10A | 0.9600 |
| C5—H5 | 0.9300 | C10—H10B | 0.9600 |
| C7—C8 | 1.507 (2) | C10—H10C | 0.9600 |
| C7—C11 | 1.531 (2) | | |
| C9—O1—C1 | 120.56 (13) | N2—C8—C7 | 116.78 (13) |
| C1—C6—C5 | 118.53 (15) | C9—C8—C7 | 122.28 (14) |
| C1—C6—C7 | 119.89 (14) | C3—C2—C1 | 120.45 (15) |
| C5—C6—C7 | 121.54 (14) | C3—C2—Cl1 | 120.48 (13) |
| O3—N2—O2 | 120.24 (13) | C1—C2—Cl1 | 119.04 (13) |
| O3—N2—C8 | 119.38 (12) | N1—C9—O1 | 111.86 (15) |
| O2—N2—C8 | 120.38 (13) | N1—C9—C8 | 127.76 (16) |
| O1—C1—C6 | 123.02 (14) | O1—C9—C8 | 120.38 (14) |
| O1—C1—C2 | 116.01 (14) | O5—N3—O4 | 123.38 (17) |
| C6—C1—C2 | 120.97 (15) | O5—N3—C11 | 116.64 (16) |
| C4—C5—C6 | 119.86 (15) | O4—N3—C11 | 119.98 (14) |
| C4—C5—H5 | 120.1 | N3—C11—C7 | 115.17 (13) |
| C6—C5—H5 | 120.1 | N3—C11—H11A | 108.5 |
| C8—C7—C6 | 110.98 (13) | C7—C11—H11A | 108.5 |
| C8—C7—C11 | 114.16 (13) | N3—C11—H11B | 108.5 |
| C6—C7—C11 | 111.64 (13) | C7—C11—H11B | 108.5 |
| C8—C7—H7 | 106.5 | H11A—C11—H11B | 107.5 |
| C6—C7—H7 | 106.5 | C3—C4—C5 | 121.98 (15) |
| C11—C7—H7 | 106.5 | C3—C4—Cl2 | 118.91 (13) |
| C9—N1—C10 | 124.73 (17) | C5—C4—Cl2 | 119.08 (13) |
| C9—N1—H1 | 117.6 | N1—C10—H10A | 109.5 |
| C10—N1—H1 | 117.6 | N1—C10—H10B | 109.5 |
| C2—C3—C4 | 118.19 (15) | H10A—C10—H10B | 109.5 |
| C2—C3—H3 | 120.9 | N1—C10—H10C | 109.5 |
| C4—C3—H3 | 120.9 | H10A—C10—H10C | 109.5 |
| N2—C8—C9 | 120.80 (14) | H10B—C10—H10C | 109.5 |
| C9—O1—C1—C6 | −10.9 (2) | C4—C3—C2—Cl1 | 178.69 (13) |
| C9—O1—C1—C2 | 169.50 (14) | O1—C1—C2—C3 | 178.49 (15) |

| | | | |
|---|---|---|---|
| C5—C6—C1—O1 | −178.84 (15) | C6—C1—C2—C3 | −1.1 (2) |
| C7—C6—C1—O1 | −1.1 (2) | O1—C1—C2—Cl1 | 0.0 (2) |
| C5—C6—C1—C2 | 0.8 (2) | C6—C1—C2—Cl1 | −179.62 (13) |
| C7—C6—C1—C2 | 178.55 (15) | C10—N1—C9—O1 | −1.3 (3) |
| C1—C6—C5—C4 | 0.5 (2) | C10—N1—C9—C8 | 178.82 (18) |
| C7—C6—C5—C4 | −177.25 (15) | C1—O1—C9—N1 | −172.63 (14) |
| C1—C6—C7—C8 | 14.2 (2) | C1—O1—C9—C8 | 7.2 (2) |
| C5—C6—C7—C8 | −168.08 (15) | N2—C8—C9—N1 | 3.4 (3) |
| C1—C6—C7—C11 | −114.39 (16) | C7—C8—C9—N1 | −172.13 (17) |
| C5—C6—C7—C11 | 63.3 (2) | N2—C8—C9—O1 | −176.45 (15) |
| O3—N2—C8—C9 | −178.20 (15) | C7—C8—C9—O1 | 8.0 (2) |
| O2—N2—C8—C9 | 1.9 (2) | O5—N3—C11—C7 | −163.02 (15) |
| O3—N2—C8—C7 | −2.4 (2) | O4—N3—C11—C7 | 17.5 (2) |
| O2—N2—C8—C7 | 177.65 (15) | C8—C7—C11—N3 | −65.94 (19) |
| C6—C7—C8—N2 | 166.39 (14) | C6—C7—C11—N3 | 60.95 (17) |
| C11—C7—C8—N2 | −66.4 (2) | C2—C3—C4—C5 | 1.1 (3) |
| C6—C7—C8—C9 | −17.9 (2) | C2—C3—C4—Cl2 | −176.92 (14) |
| C11—C7—C8—C9 | 109.33 (17) | C6—C5—C4—C3 | −1.4 (3) |
| C4—C3—C2—C1 | 0.2 (3) | C6—C5—C4—Cl2 | 176.55 (13) |

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1—H1···O2 | 0.86 | 2.00 | 2.613 (2) | 128 |
| N1—H1···O2$^i$ | 0.86 | 2.12 | 2.881 (2) | 147. |
| C7—H7···O3$^{ii}$ | 0.98 | 2.50 | 3.1944 (19) | 128. |
| C11—H11B···O3$^{ii}$ | 0.97 | 2.54 | 3.103 (2) | 117. |

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

**Fig. 1**

**Fig. 2**

**Fig. 3**

**Fig. 4**

**Fig. 5**