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N-(3-Chlorophenyl)maleimide

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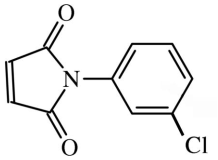
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.102; data-to-parameter ratio = 16.0.

The title compound, $C_{10}H_6ClNO_2$, has a dihedral angle of 46.46 (5)° between the benzene and maleimide rings. A short intermolecular halogen–oxygen contact is observed, with a Cl···O distance of 3.0966 (13) Å. Both CO groups are involved in two C—H···O interactions, which gives rise to sheets parallel to (100). In addition, these sheets exhibit a π–π stacking interaction between the benzene and maleimide rings [mean interplanar distance of 3.337 (3) Å].

Related literature

For related literature, see: Etter (1990); Howell & Zhang (2006); Metrangolo & Resnati (2001); Miller *et al.* (2000, 2001); Moreno-Fuquen *et al.* (2006); Sureshan *et al.* (2001).



Experimental

Crystal data

$C_{10}H_6ClNO_2$
M_r = 207.61
Monoclinic, $P2_1/n$
a = 7.3434 (3) Å
b = 11.9458 (5) Å
c = 10.3044 (4) Å
β = 101.121 (2)°
V = 886.96 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 291 (2) K
0.18 × 0.10 × 0.04 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: none
4426 measured reflections
2042 independent reflections
1680 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.101
S = 1.08
2042 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.25 e Å^{-3}
$\Delta\rho_{\min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2$^{\rm i}$	0.93	2.53	3.455 (2)	170
C8—H8···O2$^{\rm ii}$	0.93	2.71	3.513 (2)	146
C8—H8···O1$^{\rm iii}$	0.93	2.59	3.256 (2)	129
C2—H2···O1$^{\rm iv}$	0.93	2.72	3.308 (2)	122

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

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; 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); software used to prepare material for publication: *PARST95* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2114).

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supporting information

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N-(3-Chlorophenyl)maleimide

Rodolfo Moreno-Fuquen, Zulay Pardo-Botero and Javier Ellena

S1. Comment

Due to the interest created by the N-substituted maleimides in free radical polymerization process upon exposure to light (Howell & Zhang, 2006), the synthesis and study of the crystal structure of *N*-(*m*-chlorophenylmaleimide) (I) was undertaken. *N*-(*m*-nitrophenylmaleimide) (3NPMI) (Moreno-Fuquen *et al.*, 2006) and *N*-(*o*-chlorophenyl) maleimide (2ClPMI) (Miller *et al.*, 2001) systems can be taken as a reference systems to compare with the structural characteristics of (I). Perspective view of (I), showing the atomic numbering scheme, is given in Fig. 1. Photochemical properties of arylmaleimide systems have shown that they depend on the value of the dihedral angle between the benzene and imidic rings (Miller *et al.*, 2000). This angle is 56.2 (1)° and 52.9 (1)° for 3NPMI, 66.10 (4) ° for 2ClPMI, and 46.46 (5)° for (I). The molecules of (I) are linked into sheets by a combination of C—H···O hydrogen bonds (Nardelli, 1995) (Table 1). Indeed, the atoms C3^{i} in the molecule at (3/2 - *x*, 1/2 + *y*, 1/2 - *z*) and C8^{ii} in the molecule at (-1/2 + *x*, 1/2 - *y*, -1/2 + *z*) act as hydrogen-bond donors to maleimidic O2 atom in the molecule at (*x*, *y*, *z*), so generating by 2_1 screw axis a C(6) chain (Etter, 1990), which is running parallel to [010] direction (Fig. 2, supp. material). Within the asymmetric unit the atom C2 at (*x*, *y*, *z*) acts as hydrogen bond donor to maleimidic O1^{iii} in the molecule at (2 - *x*, -*y*, -*z*), so forming by translation a $R_2^2(14)$ centrosymmetric rings (Etter, 1990); in addition, atom C8 at (*x*, *y*, *z*) acts as a hydrogen bond donor to maleimidic O1^{ii} in the molecule at (2 - *x*, -*y*, 1 - *z*), so generating by translation a $R_2^2(8)$ centrosymmetric rings. Both rings are running along [001] direction (Fig.3, supp. material). In addition, (I) exhibits an aromatic $\pi\cdots\pi$ stacking interactions between benzene and maleimide rings with a mean interplanar distance of 3.337 (3) Å. The halogen-oxygen interaction is recognized as a strong driving force in formation of molecular crystals (Sureshan *et al.*, 2001). (I) shows a short Cl···O intermolecular contact, disposed about an inversion centre. The Cl1···O2, shows a distance of 3.0966 (13) Å, [O2 with symmetry 2 - *x*, 1 - *y*, -*z*] and this contact is shorter than the sum of their van der Waalś radii (3.27 Å, Metrangolo & Resnati, 2001). In (I), the angle of the oxygen O2 relative to the C6—Cl bond shows a slight deviation from linearity with a value of 174.31 (6)° and the angle of the chlorine atom relative to the C10—O2 bond shows a value of 136.96 (11)°, suggesting strong halogen bonding. This could also prevent a larger rotation between the planes of (I). The title system does not have enough influence on the processes of polymerization because the dihedral angle between their rings possess a low value with respect to other systems with substituents in the position *ortho* (Miller *et al.*, 2000).

S2. Experimental

Reagents and solvents for the synthesis were from Aldrich Chemical Co. and they were used without additional purification. Column chromatography was performed using silica gel H60 to purify the intermediates and final products. Thin layer chromatography (TLC) was used to confirm the structure of the individual compounds.

S3. Refinement

The space group P 2_1/n for (I) was uniquely assigned from the systematic absences. All H-atoms were located from difference maps and then treated as riding atoms [C—H= 0.93Å and U_{iso}(H)= 1.2U_{eq}(C)].

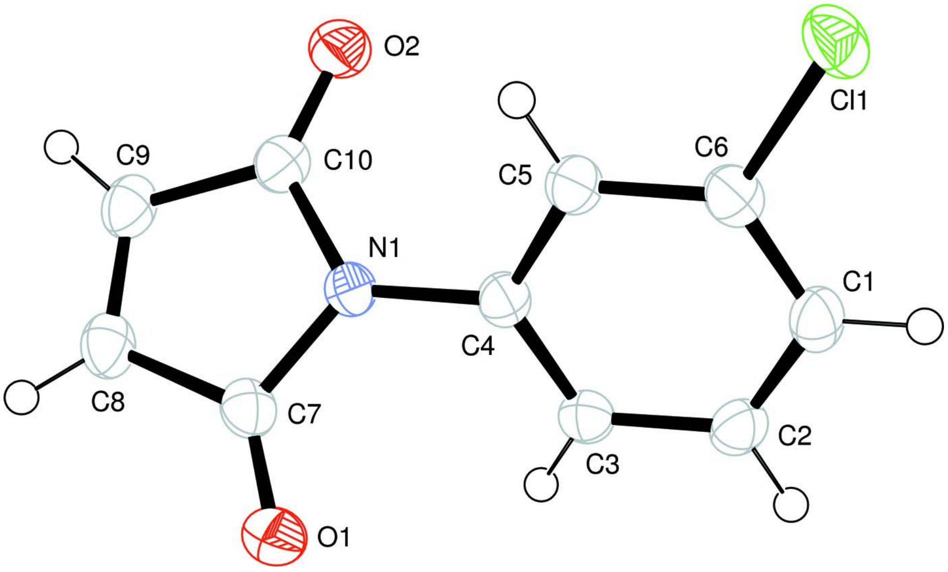

Figure 1

An *ORTEP-3* (Farrugia, 1997) plot of (I), with the atomic labelling scheme. The shapes of the ellipsoids correspond to 50% probability contours of atomic displacement.

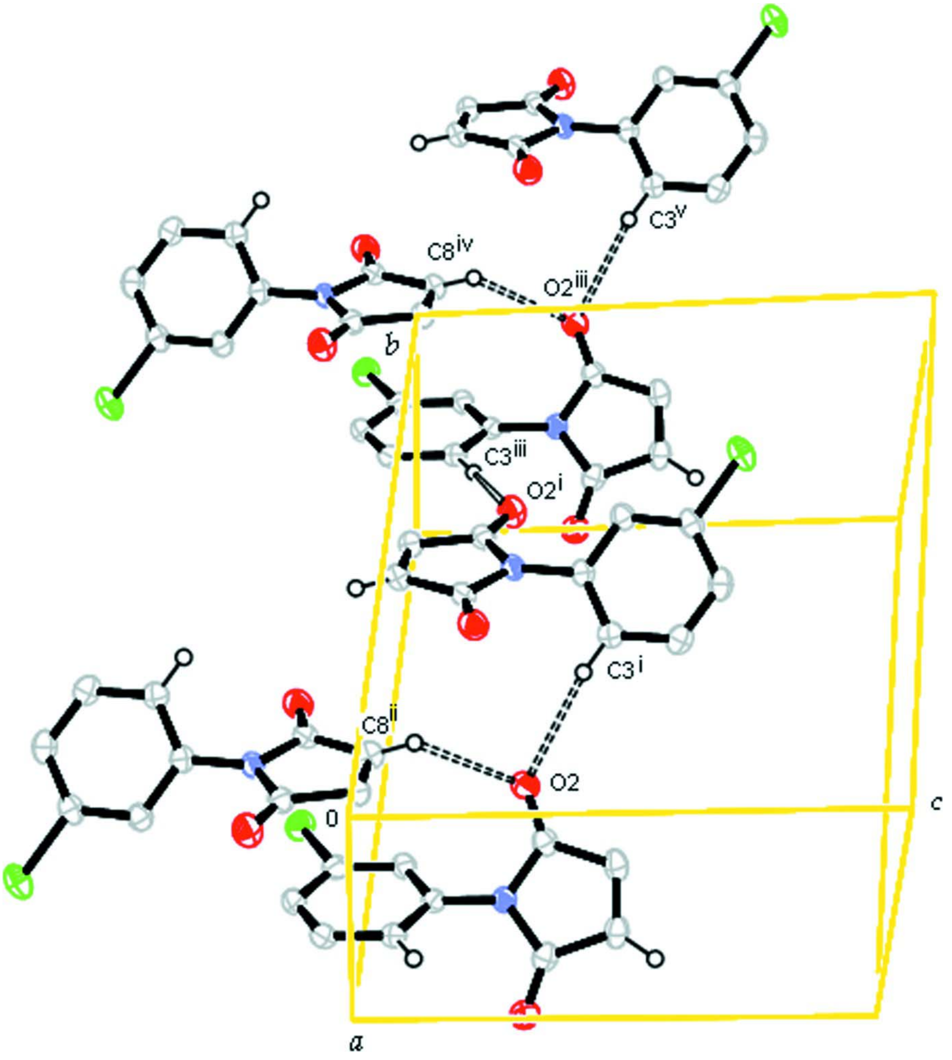

Figure 2

Part of the crystal structure of (I) showing the formation of the C(12) and C(13) chains along [010]. Symmetry codes: (i) 3/2 - *x*, 1/2 + *y*, 1/2 - *z*; (ii) -1/2 + *x*, 1/2 - *y*, -1/2 + *z*; (iii) *x*, 1 + *y*, *z*; (iv) -1/2 + *x*, 1/2 - *y*, -1/2 + *z*; (v) 3/2 - *x*, 3/2 + *y*, 1/2 - *z*. For the sake of clarity, the H atoms not involved in the motif shown have been omitted.

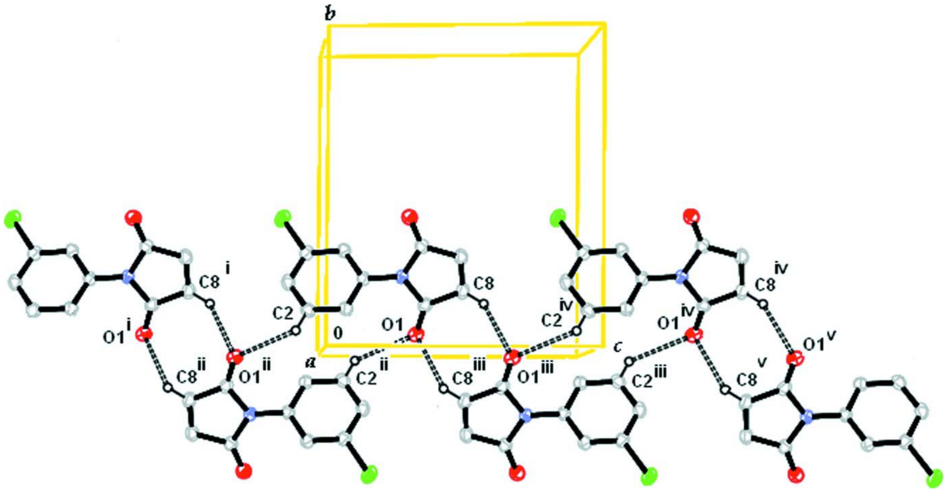

Figure 3

Part of the crystal structure of (I) showing the formation of a sheet of $R_2^2(8)$ and $R_2^2(14)$ centrosymmetric rings parallel to (100) generated by the C—H···O hydrogen bonds. Symmetry codes: (i) *x*, *y*, 1 - *z*; (ii) -*x*, -*y*, -*z*; (iii) -*x*, -*y*, 1 - *z*; (iv) *x*, *y*, 1 + *z*; (v) -*x*, -*y*, 2 - *z*. For the sake of clarity, the H atoms not involved in the motif have been omitted.

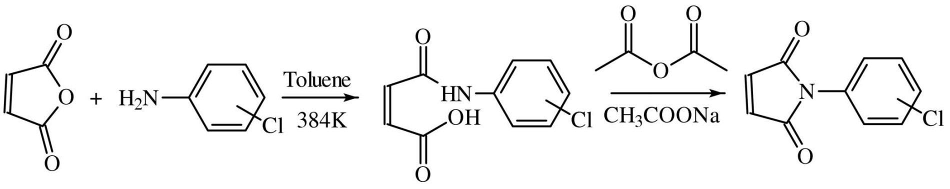

Figure 4

The formation of the title compound.

N-(3-Chlorophenyl)maleimide

Crystal data

$C_{10}H_6ClNO_2$
$M_r = 207.61$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.3434\ (3)$ Å
$b = 11.9458\ (5)$ Å
$c = 10.3044\ (4)$ Å
$\beta = 101.121\ (2)°$
$V = 886.96\ (6)$ Å^3
$Z = 4$

$F(000) = 424$
$D_x = 1.550$ Mg m^{-3}
Melting point: 364(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4426 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.40$ mm^{-1}
$T = 291$ K
Needle, colorless
0.18 × 0.10 × 0.04 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4426 measured reflections
2042 independent reflections

1680 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\rm max} = 27.5°$, $\theta_{\rm min} = 2.9°$
$h = -9 \rightarrow 8$
$k = -15 \rightarrow 15$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.101$
$S = 1.09$
2042 reflections
128 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.2501P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.031 (5)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Cl1	1.04083 (6)	0.39876 (4)	−0.16126 (4)	0.03549 (17)
O1	1.08785 (18)	0.03863 (10)	0.33200 (12)	0.0348 (3)
O2	0.83189 (18)	0.38885 (10)	0.29127 (12)	0.0348 (3)
N1	0.95758 (18)	0.21271 (11)	0.27188 (13)	0.0253 (3)
C1	0.8978 (2)	0.19208 (15)	−0.14130 (16)	0.0309 (4)
H1	0.8853	0.1877	−0.2327	0.037*
C2	0.8435 (2)	0.10389 (13)	−0.07035 (17)	0.0300 (4)
H2	0.7944	0.0396	−0.1148	0.036*
C3	0.8613 (2)	0.10986 (13)	0.06635 (16)	0.0267 (4)
H3	0.8224	0.0507	0.1131	0.032*
C4	0.9379 (2)	0.20552 (13)	0.13225 (15)	0.0245 (3)
C5	0.9937 (2)	0.29538 (13)	0.06274 (15)	0.0267 (4)
H5	1.0448	0.3594	0.1067	0.032*
C6	0.9710 (2)	0.28685 (14)	−0.07360 (16)	0.0285 (4)
C7	1.0295 (2)	0.12740 (14)	0.36145 (16)	0.0280 (4)
C8	1.0201 (2)	0.17113 (15)	0.49571 (16)	0.0321 (4)
H8	1.0594	0.1332	0.5750	0.038*
C9	0.9469 (2)	0.27274 (14)	0.48355 (16)	0.0320 (4)
H9	0.9263	0.3176	0.5530	0.038*
C10	0.9026 (2)	0.30376 (13)	0.34085 (16)	0.0276 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0406 (3)	0.0386 (3)	0.0306 (3)	0.00442 (17)	0.01531 (18)	0.01000 (17)
O1	0.0433 (7)	0.0275 (6)	0.0336 (7)	0.0019 (5)	0.0076 (5)	0.0034 (5)
O2	0.0438 (7)	0.0307 (7)	0.0318 (7)	0.0066 (5)	0.0122 (5)	0.0004 (5)

N1	0.0308 (7)	0.0245 (7)	0.0215 (7)	−0.0005 (5)	0.0071 (5)	0.0015 (5)
C1	0.0321 (8)	0.0380 (9)	0.0236 (8)	0.0098 (7)	0.0074 (6)	−0.0012 (7)
C2	0.0310 (8)	0.0294 (8)	0.0290 (8)	0.0061 (6)	0.0047 (7)	−0.0048 (6)
C3	0.0277 (8)	0.0254 (8)	0.0270 (8)	0.0030 (6)	0.0056 (6)	0.0007 (6)
C4	0.0245 (7)	0.0270 (8)	0.0228 (7)	0.0039 (6)	0.0063 (6)	0.0005 (6)
C5	0.0284 (8)	0.0280 (8)	0.0251 (8)	0.0015 (6)	0.0083 (6)	−0.0001 (6)
C6	0.0286 (8)	0.0314 (8)	0.0277 (8)	0.0064 (6)	0.0110 (6)	0.0043 (6)
C7	0.0295 (8)	0.0278 (8)	0.0265 (8)	−0.0057 (6)	0.0050 (6)	0.0039 (6)
C8	0.0376 (9)	0.0355 (9)	0.0237 (8)	−0.0080 (7)	0.0073 (7)	0.0024 (7)
C9	0.0389 (9)	0.0351 (9)	0.0240 (8)	−0.0076 (7)	0.0109 (7)	−0.0021 (7)
C10	0.0290 (8)	0.0285 (8)	0.0270 (8)	−0.0032 (6)	0.0093 (6)	−0.0012 (6)

Geometric parameters (Å, º)

Cl1—C6	1.7450 (17)	C3—C4	1.392 (2)
O1—C7	1.204 (2)	C3—H3	0.9300
O2—C10	1.209 (2)	C4—C5	1.395 (2)
N1—C10	1.401 (2)	C5—C6	1.386 (2)
N1—C7	1.408 (2)	C5—H5	0.9300
N1—C4	1.421 (2)	C7—C8	1.493 (2)
C1—C6	1.383 (2)	C8—C9	1.324 (3)
C1—C2	1.384 (2)	C8—H8	0.9300
C1—H1	0.9300	C9—C10	1.490 (2)
C2—C3	1.391 (2)	C9—H9	0.9300
C2—H2	0.9300		
C10—N1—C7	109.76 (13)	C4—C5—H5	120.9
C10—N1—C4	125.30 (13)	C1—C6—C5	122.04 (15)
C7—N1—C4	124.90 (13)	C1—C6—Cl1	119.38 (13)
C6—C1—C2	118.70 (15)	C5—C6—Cl1	118.57 (13)
C6—C1—H1	120.6	O1—C7—N1	125.39 (15)
C2—C1—H1	120.6	O1—C7—C8	128.61 (16)
C1—C2—C3	121.03 (15)	N1—C7—C8	106.00 (14)
C1—C2—H2	119.5	C9—C8—C7	108.89 (15)
C3—C2—H2	119.5	C9—C8—H8	125.6
C2—C3—C4	119.09 (15)	C7—C8—H8	125.6
C2—C3—H3	120.5	C8—C9—C10	109.20 (15)
C4—C3—H3	120.5	C8—C9—H9	125.4
C3—C4—C5	120.84 (15)	C10—C9—H9	125.4
C3—C4—N1	119.76 (14)	O2—C10—N1	125.51 (15)
C5—C4—N1	119.40 (14)	O2—C10—C9	128.34 (15)
C6—C5—C4	118.28 (15)	N1—C10—C9	106.14 (14)
C6—C5—H5	120.9		
C6—C1—C2—C3	0.2 (2)	C10—N1—C7—O1	179.89 (16)
C1—C2—C3—C4	−1.1 (2)	C4—N1—C7—O1	1.9 (3)
C2—C3—C4—C5	1.1 (2)	C10—N1—C7—C8	−0.97 (17)
C2—C3—C4—N1	−179.78 (14)	C4—N1—C7—C8	−178.92 (14)

C10—N1—C4—C3	−131.50 (16)	O1—C7—C8—C9	179.73 (17)
C7—N1—C4—C3	46.1 (2)	N1—C7—C8—C9	0.62 (18)
C10—N1—C4—C5	47.7 (2)	C7—C8—C9—C10	−0.05 (19)
C7—N1—C4—C5	−134.69 (16)	C7—N1—C10—O2	−178.35 (16)
C3—C4—C5—C6	−0.1 (2)	C4—N1—C10—O2	−0.4 (3)
N1—C4—C5—C6	−179.23 (14)	C7—N1—C10—C9	0.94 (17)
C2—C1—C6—C5	0.9 (2)	C4—N1—C10—C9	178.88 (14)
C2—C1—C6—Cl1	179.82 (12)	C8—C9—C10—O2	178.72 (17)
C4—C5—C6—C1	−0.9 (2)	C8—C9—C10—N1	−0.54 (19)
C4—C5—C6—Cl1	−179.88 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.93	2.53	3.455 (2)	170
C8—H8···O2^{ii}	0.93	2.71	3.513 (2)	146
C8—H8···O1^{iii}	0.93	2.59	3.256 (2)	129
C2—H2···O1^{iv}	0.93	2.72	3.308 (2)	122

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