Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-3-(2-Chloro-3-quinolyl)-1-phenyl-2,3-epoxypropan-1-one

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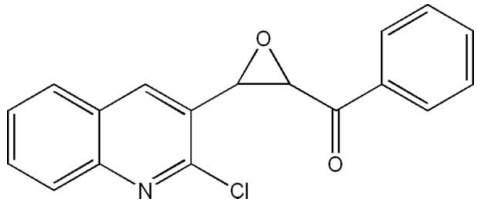
Received 24 July 2007; accepted 8 August 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.109; data-to-parameter ratio = 15.4.

In the title molecule, $C_{18}H_{12}ClNO_2$, a quinolyl moiety is linked to a functionalized epoxide system in a *trans* configuration. The epoxide ring forms dihedral angles of 62.27 (2) and 79.82 (2)° with the 2-chloropyridine ring of the 2-chloroquinolyl group and the phenyl ring, respectively. The mean plane of the atoms of the quinolyl ring system forms a dihedral angle of 35.03 (1)° with the phenyl ring. The crystal structure can be described as layers in which epoxide rings lie parallel to the (10$\bar{1}$) plane. The packing is stabilized by weak C—H···O and C—H···N intra- and intermolecular hydrogen bonds, resulting in the formation of a three-dimensional network.

Related literature

For related literature regarding synthetic procedures, see: Kidwai *et al.* (1996); Adam *et al.* (2001); De Vos *et al.* (1998). For applications, see: Ibrahim *et al.* (1991); Srivastava *et al.* (1991); Moiseer *et al.* (1988). For other related literature, see: Kedjadja *et al.* (2004); Lennette (1964); Maryanoff *et al.* (1994); Menasra *et al.* (2005); Moussaoui *et al.* (2002); Pearson & Ong (1981); Rezig *et al.* (2000); Rivers & Horsfall (1959); Sidwell & Hofmann (1971).



Experimental

Crystal data

$C_{18}H_{12}ClNO_2$
M_r = 309.74
Monoclinic, $P2_1/a$
a = 11.0782 (19) Å
b = 9.6177 (19) Å
c = 13.352 (3) Å
β = 96.511 (9)°
V = 1413.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 295 (2) K
0.15 × 0.11 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: none
9724 measured reflections
3164 independent reflections
2291 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.02
3164 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2	0.93	2.56	2.884 (3)	101
C11—H11···N1^{i}	0.98	2.56	3.510 (3)	164
C15—H15···O1^{ii}	0.93	2.58	3.494 (3)	170

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work is supported by Mentouri-Constantine University, Algeria.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2468).

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supplementary materials

Acta Cryst. (2007). E**63**, o3795-o3796 [**doi:10.1107/S1600536807039335**]

trans-3-(2-Chloro-3-quinolyl)-1-phenyl-2,3-epoxypropan-1-one

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Comment

Quinolines have been extensively investigated by organic chemsits due to their association with biological activities like antibacterial (Ibrahim *et al.*, 1991), antifungal (Moiseer *et al.*, 1988) and antifilarial (Srivastava *et al.*, 1991) activities. In addition, naturally occurring epoxides are associated with various industrial, mechanistic and biological activities (Pearson & Ong, 1981). New and less toxic antiviral agents are in great demand due to typical viral infections (Kidwai *et al.*, 1996). We thought it worthwhile to synthesize new quinoline substituted epoxides and screen them for their antiviral activity against EMC virus (Rivers & Horsfall, 1959). The antiviral activity of quinoline substituted epoxides were tested against Encephalomyocarditis Virus (EMCV) (Lennette, 1964) and cytotoxic assays of these compounds were also evaluated (Sidwell & Hofmann, 1971). As a result of their importance in synthesis, the preparation of epoxides has been of a considerable interest and many methods have been developed to date. An alternative and complementary approach utilizes aldehydes. The advantage of this approach is that potentially hazardous oxidizing agents are not required. Epoxides bearing electron-withdrawing groups are very important synthetic intermediates because of their rich and useful functionality (Adam *et al.*, 2001; De Vos *et al.*, 1998). These compounds have been most commonly synthesized by the Darzens reaction (Maryanoff *et al.*, 1994). This involves the initial addition of an α-halo enolate to a carbonyl compound, followed by ring-closure of the resulting alkoxide. In continuation of our research program directed towards the preparation of new quinoline derivatives (Menasra *et al.*, 2005; Moussaoui *et al.*, 2002; Rezig *et al.*, 2000; Kedjadja *et al.*, 2004), we present here our results concerning the epoxidation of 2-chloro-3-formylquinoline.

In this study, we have synthesized *trans*- 2,3-epoxy-3-(2'-chloroquinolyl)-1-phenylpropan-1-one and determined its crystal structure.

The molecular geometry and the atom-numbering scheme are shown in Fig. 1. The title molecule contains an epoxide group linked to a chloroquinolyl moiety and benzoyl group with 2, 3-*trans* configuration relationship.

The two rings of quinolyl group form a dihedral angle of 1.22 (1)° between them. The epoxide ring forms dihedral angles of 62.27 (2)° and 79.82 (2)° with the 2-chloropyridine ring of the 2-chloroquinolyl group and phenyl rings respectively. The mean plane of the atoms of the quinolyl ring fused rings system forms a dihedral angle of 35.03 (1)° with phenyl ring. The crystal structure can be described as layers in which the epoxide rings are parallel to (10–1) plane (Fig. 2).

The crystal packing is stabilized by C–H···O and C–H···N intra and intermolecular hydrogen bonds, resulting in the formation of three dimensional network (Fig. 3).

Experimental

To a solution of 2-chloro-3-formylquinoline (1 mmol) in toluene (15 mL) was added 1 mmol of 2-bromoacetophenone, and the mixture was cooled to 273 K. An aqueous solution of KOH 30% (2.5 ml) was added dropwise over a period of 2 minutes. This mixture was stired for 24 h at room temperature. The reaction was worked up by adding 15 ml of cold water

and 15 ml of saturated aqueous ammonium chloride. This solution was extracted twice with methylene chloride (25 ml) and the combined organic layers were washed twice with cold water (10 ml), saturated aqueous ammonium chloride (10 ml) and dried over $MgSO_4$ then concentrated *in vacuo*. The obtained residue was purified by a column chromatograpy (SiO_2, methylene chloride) to furnish the pure product.

Refinement

All H atoms were located in Fourier maps but introduced in calculated positions and treated as riding on their parent C atoms with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

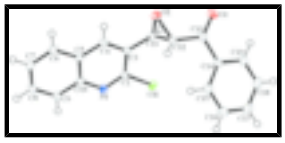

Fig. 1. The molecular structure of the title compound with the atomic labelling scheme. Displacement are drawn at the 50% probability level.

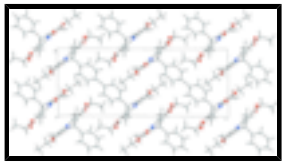

Fig. 2. The layered crystal packing of the title compound viewed down the *b* axis.

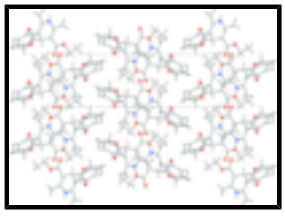

Fig. 3. The crystal packing, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

trans-3-(2-Chloro-3-quinolyl)-1-phenyl-2,3-epoxypropan-1-one

Crystal data

$C_{18}H_{12}ClNO_2$	F_{000} = 640
M_r = 309.74	D_x = 1.456 Mg m^{-3}
Monoclinic, $P2_1/a$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yab	Cell parameters from 1765 reflections
a = 11.0782 (19) Å	θ = 2.6–25.5º
b = 9.6177 (19) Å	μ = 0.28 mm^{-1}
c = 13.352 (3) Å	T = 295 (2) K
β = 96.511 (9)º	Needle, white
V = 1413.4 (5) Å^3	0.15 × 0.11 × 0.06 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.6º
T = 295(2) K	h = −14→13
CCD rotation images, thin slices, φ scans, and ω scans	k = −12→12
Absorption correction: none	l = −16→17
9724 measured reflections	Standard reflections: ?;
3164 independent reflections	every ? reflections
2291 reflections with $I > 2\sigma(I)$	intensity decay: ?
R_{int} = 0.055	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.3701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.109	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.02	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
3164 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
205 parameters	Extinction correction: SHELXL
Primary atom site location: structure-invariant direct methods	Extinction coefficient:
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.44660 (5)	0.15265 (5)	0.36554 (4)	0.0236 (2)
O1	0.04229 (14)	0.17899 (15)	0.13407 (12)	0.0278 (5)
O2	0.16982 (13)	0.41881 (14)	0.19793 (12)	0.0265 (5)
N1	0.56767 (15)	0.38265 (16)	0.39598 (13)	0.0185 (5)

C2	0.46357 (19)	0.33260 (18)	0.35826 (15)	0.0179 (6)
C3	0.36441 (18)	0.41018 (19)	0.30987 (15)	0.0176 (6)
C4	0.38174 (18)	0.55056 (19)	0.30233 (15)	0.0181 (6)
C5	0.49167 (18)	0.61229 (19)	0.34310 (15)	0.0170 (6)
C6	0.51367 (19)	0.7576 (2)	0.34001 (16)	0.0202 (6)
C7	0.6217 (2)	0.8103 (2)	0.38244 (16)	0.0224 (7)
C8	0.71302 (19)	0.7227 (2)	0.42894 (16)	0.0218 (7)
C9	0.69491 (18)	0.5820 (2)	0.43224 (16)	0.0200 (6)
C10	0.58343 (18)	0.52412 (19)	0.39002 (15)	0.0176 (6)
C11	0.24984 (18)	0.3409 (2)	0.26948 (16)	0.0200 (6)
C12	0.22971 (19)	0.3004 (2)	0.16239 (16)	0.0204 (7)
C13	0.15213 (19)	0.1740 (2)	0.13606 (16)	0.0204 (7)
C14	0.21784 (19)	0.0425 (2)	0.11805 (16)	0.0201 (6)
C15	0.34163 (19)	0.0396 (2)	0.10980 (16)	0.0243 (7)
C16	0.3989 (2)	−0.0854 (2)	0.09571 (18)	0.0284 (7)
C17	0.3340 (2)	−0.2086 (2)	0.09239 (16)	0.0266 (7)
C18	0.2115 (2)	−0.2074 (2)	0.10231 (18)	0.0315 (8)
C19	0.1532 (2)	−0.0821 (2)	0.11422 (18)	0.0280 (7)
H4	0.32027	0.60569	0.26996	0.0217*
H6	0.45435	0.81675	0.30903	0.0242*
H7	0.63515	0.90568	0.38061	0.0269*
H8	0.78615	0.76057	0.45762	0.0262*
H9	0.75609	0.52450	0.46231	0.0239*
H11	0.21102	0.28255	0.31677	0.0240*
H12	0.29615	0.31800	0.12147	0.0244*
H15	0.38607	0.12183	0.11377	0.0292*
H16	0.48134	−0.08671	0.08842	0.0340*
H17	0.37322	−0.29249	0.08344	0.0320*
H18	0.16824	−0.29038	0.10102	0.0378*
H19	0.07030	−0.08110	0.11969	0.0337*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0245 (3)	0.0128 (2)	0.0340 (3)	−0.0001 (2)	0.0056 (2)	0.0010 (2)
O1	0.0169 (9)	0.0316 (9)	0.0350 (10)	−0.0018 (6)	0.0039 (7)	−0.0073 (7)
O2	0.0214 (9)	0.0200 (7)	0.0366 (9)	0.0046 (6)	−0.0028 (7)	−0.0039 (6)
N1	0.0185 (9)	0.0161 (8)	0.0214 (9)	0.0000 (7)	0.0040 (7)	−0.0003 (6)
C2	0.0211 (12)	0.0125 (9)	0.0212 (11)	0.0009 (8)	0.0067 (9)	−0.0008 (7)
C3	0.0172 (11)	0.0165 (9)	0.0196 (10)	0.0001 (8)	0.0049 (8)	−0.0009 (8)
C4	0.0178 (11)	0.0174 (9)	0.0191 (10)	0.0025 (8)	0.0024 (9)	0.0005 (8)
C5	0.0164 (11)	0.0167 (9)	0.0184 (10)	0.0008 (8)	0.0045 (8)	−0.0003 (7)
C6	0.0211 (12)	0.0164 (9)	0.0234 (11)	0.0011 (8)	0.0041 (9)	0.0013 (8)
C7	0.0254 (13)	0.0148 (10)	0.0279 (12)	−0.0038 (8)	0.0070 (10)	−0.0005 (8)
C8	0.0175 (12)	0.0234 (11)	0.0246 (12)	−0.0038 (8)	0.0025 (9)	−0.0037 (8)
C9	0.0155 (11)	0.0217 (10)	0.0225 (11)	0.0008 (8)	0.0015 (9)	−0.0004 (8)
C10	0.0186 (11)	0.0166 (9)	0.0182 (10)	0.0004 (8)	0.0049 (8)	−0.0008 (8)
C11	0.0165 (11)	0.0168 (9)	0.0269 (12)	0.0009 (8)	0.0032 (9)	−0.0008 (8)

C12	0.0157 (12)	0.0192 (10)	0.0265 (12)	0.0001 (8)	0.0032 (9)	−0.0015 (8)
C13	0.0167 (12)	0.0237 (11)	0.0208 (11)	−0.0032 (8)	0.0017 (9)	−0.0013 (8)
C14	0.0175 (12)	0.0205 (10)	0.0223 (11)	−0.0021 (8)	0.0021 (9)	−0.0019 (8)
C15	0.0223 (13)	0.0213 (10)	0.0291 (12)	−0.0027 (8)	0.0019 (10)	0.0017 (9)
C16	0.0211 (12)	0.0295 (12)	0.0344 (13)	0.0041 (9)	0.0028 (10)	0.0028 (10)
C17	0.0344 (14)	0.0223 (10)	0.0229 (12)	0.0068 (9)	0.0020 (10)	−0.0010 (9)
C18	0.0370 (15)	0.0223 (11)	0.0349 (14)	−0.0085 (10)	0.0029 (11)	−0.0062 (9)
C19	0.0223 (12)	0.0291 (12)	0.0331 (13)	−0.0069 (9)	0.0048 (10)	−0.0069 (10)

Geometric parameters (Å, °)

Cl1—C2	1.7448 (18)	C14—C15	1.389 (3)
O1—C13	1.215 (3)	C14—C19	1.394 (3)
O2—C11	1.438 (3)	C15—C16	1.382 (3)
O2—C12	1.426 (2)	C16—C17	1.384 (3)
N1—C2	1.298 (3)	C17—C18	1.378 (3)
N1—C10	1.375 (2)	C18—C19	1.385 (3)
C2—C3	1.421 (3)	C4—H4	0.9300
C3—C4	1.369 (3)	C6—H6	0.9300
C3—C11	1.480 (3)	C7—H7	0.9300
C4—C5	1.408 (3)	C8—H8	0.9300
C5—C6	1.420 (3)	C9—H9	0.9300
C5—C10	1.414 (3)	C11—H11	0.9800
C6—C7	1.363 (3)	C12—H12	0.9800
C7—C8	1.406 (3)	C15—H15	0.9300
C8—C9	1.369 (3)	C16—H16	0.9300
C9—C10	1.412 (3)	C17—H17	0.9300
C11—C12	1.474 (3)	C18—H18	0.9300
C12—C13	1.507 (3)	C19—H19	0.9300
C13—C14	1.492 (3)		
Cl1···C15	3.646 (2)	C15···H12	2.7300
Cl1···C7^{i}	3.550 (2)	C16···H6^{ix}	3.0000
Cl1···C8^{i}	3.633 (2)	C17···H6^{ix}	3.0500
Cl1···H11	2.9000	C17···H4^{ix}	2.9900
Cl1···H9^{ii}	3.1100	C17···H12^{viii}	3.0600
Cl1···H11^{iii}	3.1300	C18···H4^{ix}	3.0100
O1···O2	2.787 (2)	C18···H12^{viii}	2.9900
O1···C2^{ii}	3.213 (3)	H4···O2	2.5600
O1···C3^{ii}	3.343 (3)	H4···C17^{x}	2.9900
O2···O1	2.787 (2)	H4···C18^{x}	3.0100
O1···H19	2.5300	H4···H6	2.5300
O1···H12^{ii}	2.7100	H4···C7^{v}	2.9100
O1···H15^{ii}	2.5800	H4···C8^{v}	3.0400
O2···H4	2.5600	H6···C16^{x}	3.0000
O2···H16^{ii}	2.9000	H6···C17^{x}	3.0500
N1···H8^{iv}	2.6700	H6···H4	2.5300

N1···H11^{iii}	2.5600	H7···H9^{xi}	2.5700
C2···C9^{i}	3.563 (3)	H7···C4^{vi}	3.0600
C2···O1^{iii}	3.213 (3)	H8···N1^{xi}	2.6700
C3···C9^{i}	3.579 (3)	H8···C4^{vi}	3.0400
C3···O1^{iii}	3.343 (3)	H9···H7^{iv}	2.5700
C4···C7^{v}	3.454 (3)	H9···Cl1^{iii}	3.1100
C4···C8^{v}	3.439 (3)	H11···Cl1	2.9000
C7···Cl1^{i}	3.550 (2)	H11···Cl1^{ii}	3.1300
C7···C4^{vi}	3.454 (3)	H11···N1^{ii}	2.5600
C8···Cl1^{i}	3.633 (2)	H11···C2^{ii}	3.0600
C8···C4^{vi}	3.439 (3)	H12···C15	2.7300
C9···C2^{i}	3.563 (3)	H12···H15	2.1400
C9···C3^{i}	3.579 (3)	H12···C17^{vii}	3.0600
C12···C17^{vii}	3.396 (3)	H12···C18^{vii}	2.9900
C13···C17^{vii}	3.273 (3)	H12···O1^{iii}	2.7100
C15···Cl1	3.646 (2)	H15···C12	2.5700
C17···C13^{viii}	3.273 (3)	H15···H12	2.1400
C17···C12^{viii}	3.396 (3)	H15···O1^{iii}	2.5800
C2···H11^{iii}	3.0600	H16···O2^{iii}	2.9000
C4···H7^{v}	3.0600	H16···H18^{xii}	2.3700
C4···H8^{v}	3.0400	H17···C13^{viii}	2.9300
C7···H4^{vi}	2.9100	H17···H19^{xii}	2.5000
C8···H4^{vi}	3.0400	H18···H16^{xiii}	2.3700
C12···H15	2.5700	H19···O1	2.5300
C13···H17^{vii}	2.9300	H19···H17^{xiii}	2.5000
C11—O2—C12	61.96 (13)	C14—C15—C16	120.07 (19)
C2—N1—C10	117.24 (17)	C15—C16—C17	120.3 (2)
Cl1—C2—N1	116.30 (15)	C16—C17—C18	120.22 (19)
Cl1—C2—C3	117.61 (15)	C17—C18—C19	119.69 (19)
N1—C2—C3	126.07 (17)	C14—C19—C18	120.5 (2)
C2—C3—C4	116.33 (18)	C3—C4—H4	120.00
C2—C3—C11	121.06 (16)	C5—C4—H4	120.00
C4—C3—C11	122.60 (18)	C5—C6—H6	120.00
C3—C4—C5	120.66 (18)	C7—C6—H6	120.00
C4—C5—C6	123.21 (18)	C6—C7—H7	119.00
C4—C5—C10	117.73 (17)	C8—C7—H7	120.00
C6—C5—C10	119.07 (18)	C7—C8—H8	120.00
C5—C6—C7	119.97 (19)	C9—C8—H8	120.00
C6—C7—C8	120.99 (18)	C8—C9—H9	120.00
C7—C8—C9	120.38 (19)	C10—C9—H9	120.00
C8—C9—C10	120.08 (18)	O2—C11—H11	116.00
N1—C10—C5	121.95 (18)	C3—C11—H11	116.00
N1—C10—C9	118.54 (17)	C12—C11—H11	116.00
C5—C10—C9	119.50 (17)	O2—C12—H12	117.00

O2—C11—C3	116.49 (16)	C11—C12—H12	117.00
O2—C11—C12	58.62 (13)	C13—C12—H12	117.00
C3—C11—C12	120.10 (18)	C14—C15—H15	120.00
O2—C12—C11	59.42 (13)	C16—C15—H15	120.00
O2—C12—C13	116.57 (17)	C15—C16—H16	120.00
C11—C12—C13	117.31 (18)	C17—C16—H16	120.00
O1—C13—C12	121.09 (18)	C16—C17—H17	120.00
O1—C13—C14	122.38 (18)	C18—C17—H17	120.00
C12—C13—C14	116.46 (18)	C17—C18—H18	120.00
C13—C14—C15	122.28 (18)	C19—C18—H18	120.00
C13—C14—C19	118.46 (19)	C14—C19—H19	120.00
C15—C14—C19	119.19 (18)	C18—C19—H19	120.00
C12—O2—C11—C3	110.6 (2)	C5—C6—C7—C8	0.5 (3)
C11—O2—C12—C13	107.5 (2)	C6—C7—C8—C9	0.1 (3)
C10—N1—C2—Cl1	179.30 (15)	C7—C8—C9—C10	−0.9 (3)
C10—N1—C2—C3	1.0 (3)	C8—C9—C10—N1	−179.05 (19)
C2—N1—C10—C5	−1.3 (3)	C8—C9—C10—C5	1.0 (3)
C2—N1—C10—C9	178.74 (19)	O2—C11—C12—C13	−106.2 (2)
Cl1—C2—C3—C4	−177.93 (15)	C3—C11—C12—O2	−104.50 (19)
Cl1—C2—C3—C11	1.5 (3)	C3—C11—C12—C13	149.27 (18)
N1—C2—C3—C4	0.4 (3)	O2—C12—C13—O1	8.4 (3)
N1—C2—C3—C11	179.8 (2)	O2—C12—C13—C14	−168.62 (18)
C2—C3—C4—C5	−1.5 (3)	C11—C12—C13—O1	75.9 (3)
C11—C3—C4—C5	179.12 (19)	C11—C12—C13—C14	−101.1 (2)
C2—C3—C11—O2	−162.68 (18)	O1—C13—C14—C15	173.1 (2)
C2—C3—C11—C12	−95.2 (2)	O1—C13—C14—C19	−10.0 (3)
C4—C3—C11—O2	16.7 (3)	C12—C13—C14—C15	−10.0 (3)
C4—C3—C11—C12	84.2 (3)	C12—C13—C14—C19	166.9 (2)
C3—C4—C5—C6	−178.3 (2)	C13—C14—C15—C16	178.3 (2)
C3—C4—C5—C10	1.2 (3)	C19—C14—C15—C16	1.4 (3)
C4—C5—C6—C7	179.0 (2)	C13—C14—C19—C18	−177.0 (2)
C10—C5—C6—C7	−0.4 (3)	C15—C14—C19—C18	0.0 (3)
C4—C5—C10—N1	0.3 (3)	C14—C15—C16—C17	−1.7 (3)
C4—C5—C10—C9	−179.75 (19)	C15—C16—C17—C18	0.5 (3)
C6—C5—C10—N1	179.68 (19)	C16—C17—C18—C19	0.9 (3)
C6—C5—C10—C9	−0.3 (3)	C17—C18—C19—C14	−1.2 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1/2, −*y*+1/2, *z*; (iii) *x*+1/2, −*y*+1/2, *z*; (iv) −*x*+3/2, *y*−1/2, −*z*+1; (v) *x*−1/2, −*y*+3/2, *z*; (vi) *x*+1/2, −*y*+3/2, *z*; (vii) −*x*+1/2, *y*+1/2, −*z*; (viii) −*x*+1/2, *y*−1/2, −*z*; (ix) *x*, *y*−1, *z*; (x) *x*, *y*+1, *z*; (xi) −*x*+3/2, *y*+1/2, −*z*+1; (xii) *x*+1/2, −*y*−1/2, *z*; (xiii) *x*−1/2, −*y*−1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2	0.9300	2.5600	2.884 (3)	101.00
C11—H11···N1^{ii}	0.9800	2.5600	3.510 (3)	164.00
C15—H15···O1^{iii}	0.9300	2.5800	3.494 (3)	170.00

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

Fig. 1

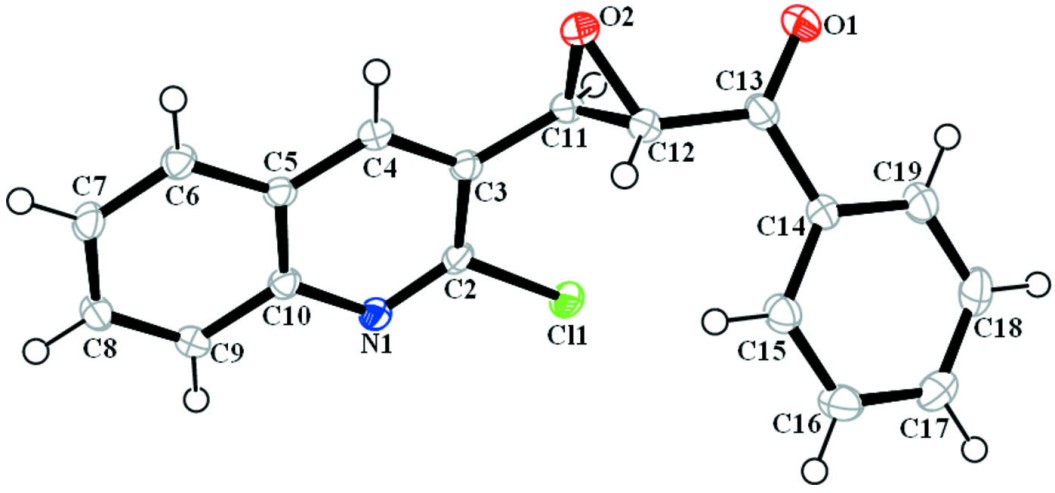
O2
O1
C13
C11
C12
C19
C5
C4
C3
C7
C6
C14
C2
C10
C18
C8
C9
N1
Cl1
C15
C16
C17

Fig. 2

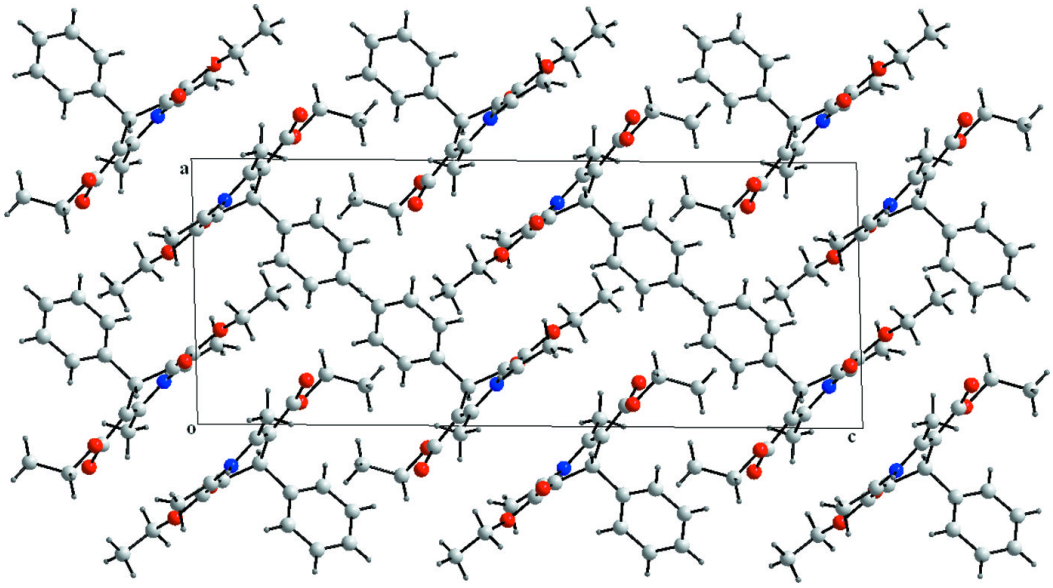

Fig. 3