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1,5-Bis(4-chlorophenyl)-3-(2-chloroquinolin-3-yl)pentane-1,5-dione: sheets of $R_4^4(26)$ rings built from C—H···N and C—H···O hydrogen bonds

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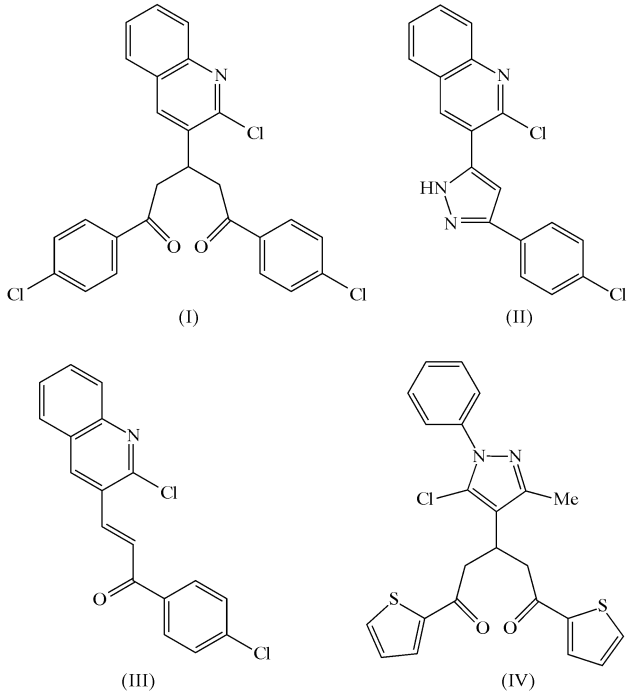
Molecules of the title compound, $C_{26}H_{18}Cl_3NO_2$, are linked into sheets of $R_4^4(26)$ rings by a combination of C—H···N and C—H···O hydrogen bonds.

Comment

With the aim of developing new classes of fused heterocyclic systems, we have prepared a range of novel chalcones appropriately functionalized for use as intermediates. The reactions used to prepare such chalcones involve methyl aryl ketones and aryl or heteroaryl aldehydes. We report here the structure of the title compound, (I) (Fig. 1), obtained in low yield as a by-product in the preparation of the pyrazolylquinoline (II) *via* the corresponding chalcone (III), formed by the reaction between 2-chloroquinoline-3-carbaldehyde and 4-chlorophenyl methyl ketone.

The bond distances within the quinoline portion of the molecule (Table 1) show evidence for significant bond fixation; the N31—C32 bond is thus significantly shorter than N31—C38*A*, while the C33—C34, C35—C36 and C37—C38 bonds are all significantly shorter than the other peripheral C—C bonds. The two independent 4-chlorobenzoylmethylene components adopt different conformations relative to the quinoline component so that the molecules have no internal symmetry and hence are chiral; however, the centrosymmetric space group *Pbca* accommodates equal numbers of the two enantiomorphic forms.

The molecules are linked into sheets by two hydrogen bonds, one each of the C—H···N and C—H···O types (Table 2), and the sheet formation is readily analysed in terms of two one-dimensional substructures. Quinolinyl atom C34 in the molecule at (x, y, z) acts as a hydrogen-bond donor to atom N31 in the molecule at $(-\frac{1}{2}+x, y, \frac{1}{2}-z)$, so forming a



C(5) (Bernstein *et al.*, 1995) chain running parallel to the [100] direction and generated by the *a*-glide plane at $z=\frac{1}{4}$ (Fig. 2). In addition, quinolinyl atom C37 in the molecule at (x, y, z) acts as a hydrogen-bond donor to atom O17 in the molecule at $(1-x, -\frac{1}{2}+y, \frac{1}{2}-z)$, so forming a *C*(11) chain running parallel to the [010] direction and generated by the 2_1 screw axis along $(\frac{1}{2}, y, \frac{1}{4})$ (Fig. 3).

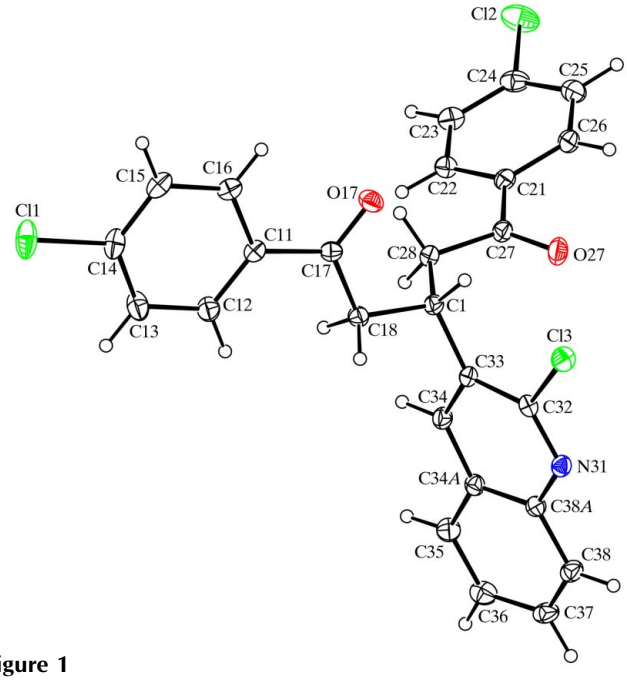


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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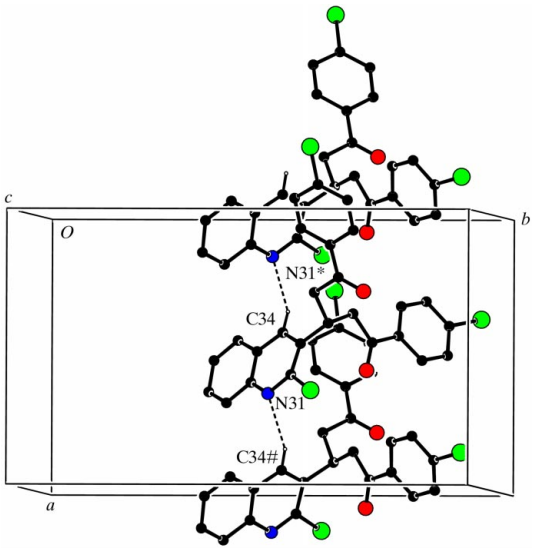

Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded $C(5)$ chain along [100]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(-\frac{1}{2}+x, y, \frac{1}{2}-z)$ and $(\frac{1}{2}+x, y, \frac{1}{2}-z)$, respectively.

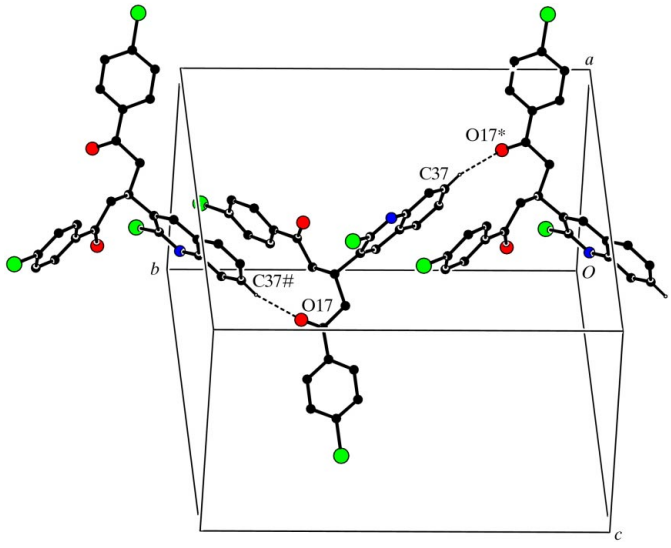

Figure 3
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded $C(11)$ chain along [010]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(1-x, -\frac{1}{2}+y, \frac{1}{2}-z)$ and $(1-x, \frac{1}{2}+y, \frac{1}{2}-z)$, respectively.

The combination of the [100] and [010] chains generates a (001) sheet in the form of a (4,4)-net (Batten & Robson, 1998) built from a single type of $R_4^4(26)$ ring, lying in the domain $-0.02 < z < 0.52$, and generated by the glide plane and screw axes at $z = \frac{1}{4}$ (Fig. 4). A second sheet, related to the first by inversion, lies in the domain $0.48 < z < 1.02$, and is generated by the glide plane and screw axes at $z = \frac{3}{4}$.

The only direction-specific interaction between adjacent sheets is a rather long C—H···O contact with aryl atom C15 as the donor (Table 2) but whose H···O distance is close to the van der Waals limit; this interaction is therefore probably of little or no structural significance.

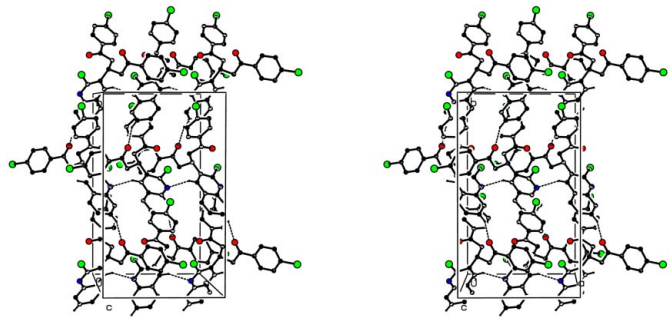

Figure 4
A stereoview of part of the crystal structure of (I), showing the formation of a (001) sheet built from $R_4^4(26)$ rings. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

The molecular constitution of (I) has some resemblance to that of the thienyl compound (IV), but the supramolecular arrangement is entirely different in (IV), where the molecules are linked into cyclic centrosymmetric dimers by paired C—H···π(thienyl) hydrogen bonds (Trilleras *et al.*, 2005).

Experimental

Hydrazine hydrate (0.70 g of a 55% aqueous solution, 12 mmol) was added dropwise to a solution of (*E*)-1-(4-chlorophenyl)-3-(2-chloroquinolin-3-yl)prop-2-en-1-one, (III) (2.3 g, 7 mmol), in methanol (40 ml), and the resulting mixture was then stirred at room temperature for 15 min. The solid product was collected by filtration and washed with cold methanol to give 2-chloro-3-[3-(4-chlorophenyl)-1*H*-pyrazol-5-yl]quinoline, (II) (2.2 g, 88% yield). Evaporation of the filtrate yielded crystals of (I) suitable for single-crystal X-ray diffraction (yield 10%, m.p. 505–506 K). MS (EI 70 eV), *m*/*z* (%) 481 (5, M^+), 328 (64, $[M - ClC_6H_4COCH_2]^+$), 292 (62), 139 (100).

Crystal data

$C_{26}H_{18}Cl_3NO_2$
$M_r = 482.76$
Orthorhombic, *Pbca*
$a = 11.2405$ (2) Å
$b = 18.8738$ (3) Å
$c = 21.0529$ (3) Å
$V = 4466.39$ (12) Å^3
$Z = 8$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5112 reflections
$\theta = 3.4$–$27.5°$
$\mu = 0.44$ mm^{-1}
$T = 120$ (2) K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.922$, $T_{max} = 0.938$
52455 measured reflections
5112 independent reflections
3921 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$
$h = -14 \rightarrow 14$
$k = -21 \rightarrow 24$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.116$
$S = 1.05$
5112 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 2.4672P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N31—C32	1.302 (2)	C35—C36	1.369 (3)
N31—C38*A*	1.368 (2)	C36—C37	1.402 (3)
C32—C33	1.422 (2)	C37—C38	1.369 (3)
C33—C34	1.370 (3)	C38—C38*A*	1.416 (3)
C34—C34*A*	1.414 (3)	C34*A*—C38*A*	1.409 (3)
C34*A*—C35	1.418 (3)	C32—Cl3	1.7463 (18)
C32—C33—C1—C18	−110.03 (19)	C32—C33—C1—C28	126.64 (18)
C33—C1—C18—C17	160.82 (15)	C33—C1—C28—C27	−67.55 (19)
C1—C18—C17—C11	171.11 (15)	C1—C28—C27—C21	−176.29 (15)
C18—C17—C11—C12	3.3 (3)	C28—C27—C21—C22	−16.4 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O17^{i}	0.95	2.59	3.502 (2)	160
C34—H34···N31^{ii}	0.95	2.39	3.244 (2)	150
C37—H37···O17^{iii}	0.95	2.45	3.330 (2)	155

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

The space group *Pbca* was uniquely assigned from the systematic absences. All H atoms were located from difference maps and then treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.99 (CH_2) and 1.00 Å (aliphatic CH), and with U_{iso}(H) values of $1.2U_{eq}$(C).

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. BI and HT thank COLCIENCIAS, UNIVALLE (Universidad del Valle, Colombia) and Universidad Nacional de Colombia for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1891). Services for accessing these data are described at the back of the journal.

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Trilleras, J., Quiroga, J., Cobo, J., Low, J. N. & Glidewell, C. (2005). *Acta Cryst.* E**61**, o1892–o1894.

supporting information

Acta Cryst. (2006). C**62**, o39–o41 [doi:10.1107/S0108270105039193]

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Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.2405\ (2)$ Å
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$V = 4466.39\ (12)$ Å^3
$Z = 8$
$F(000) = 1984$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
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$\theta = 3.4$–$27.5°$
$\mu = 0.44$ mm^{-1}
$T = 120$ K
Block, colourless
0.20 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Bruker-Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.922$, $T_{max} = 0.938$
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5112 independent reflections
3921 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -14 \rightarrow 14$
$k = -21 \rightarrow 24$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.116$
$S = 1.05$
5112 reflections
289 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

$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 2.4672P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.24463 (5)	0.60892 (4)	0.52239 (3)	0.05197 (19)
Cl2	0.36147 (7)	0.93210 (3)	0.02585 (3)	0.05640 (19)
Cl3	0.63263 (4)	0.59715 (3)	0.37707 (2)	0.03324 (13)
O17	0.27494 (12)	0.71370 (7)	0.40277 (7)	0.0345 (3)
O27	0.55516 (11)	0.70553 (8)	0.24637 (7)	0.0389 (3)
N31	0.64154 (13)	0.49686 (8)	0.29422 (7)	0.0261 (3)
C1	0.38694 (15)	0.62862 (9)	0.31345 (9)	0.0248 (4)
C11	0.10666 (16)	0.64331 (10)	0.42440 (8)	0.0254 (4)
C12	0.04763 (17)	0.57904 (11)	0.41819 (10)	0.0333 (4)
C13	−0.06099 (18)	0.56808 (13)	0.44833 (10)	0.0398 (5)
C14	−0.10900 (17)	0.62233 (12)	0.48422 (9)	0.0349 (5)
C15	−0.05275 (17)	0.68684 (11)	0.49112 (9)	0.0328 (4)
C16	0.05558 (17)	0.69703 (10)	0.46129 (8)	0.0281 (4)
C17	0.22362 (16)	0.65811 (9)	0.39326 (8)	0.0250 (4)
C18	0.27700 (16)	0.60194 (10)	0.35018 (9)	0.0262 (4)
C21	0.42731 (16)	0.76794 (10)	0.17734 (9)	0.0273 (4)
C22	0.31889 (17)	0.77041 (10)	0.14542 (9)	0.0308 (4)
C23	0.29949 (19)	0.81983 (11)	0.09786 (10)	0.0354 (4)
C24	0.3877 (2)	0.86827 (11)	0.08384 (10)	0.0362 (5)
C25	0.49545 (19)	0.86799 (11)	0.11552 (10)	0.0367 (5)
C26	0.51556 (17)	0.81716 (10)	0.16177 (9)	0.0317 (4)
C27	0.45339 (16)	0.71555 (10)	0.22867 (9)	0.0281 (4)
C28	0.34994 (15)	0.67711 (10)	0.25885 (9)	0.0257 (4)
C32	0.57374 (15)	0.54819 (10)	0.31410 (8)	0.0245 (4)
C33	0.45995 (15)	0.56650 (9)	0.28962 (8)	0.0237 (4)
C34	0.41842 (16)	0.52346 (10)	0.24216 (9)	0.0273 (4)
C34A	0.48628 (15)	0.46580 (10)	0.21923 (8)	0.0256 (4)
C35	0.44493 (17)	0.41947 (11)	0.17103 (9)	0.0324 (4)
C36	0.5168 (2)	0.36569 (11)	0.15028 (9)	0.0363 (5)
C37	0.63176 (18)	0.35695 (11)	0.17500 (10)	0.0340 (4)
C38	0.67301 (17)	0.40008 (10)	0.22242 (9)	0.0309 (4)
C38A	0.59988 (16)	0.45523 (9)	0.24592 (9)	0.0249 (4)
H1	0.4374	0.6567	0.3434	0.030*
H12	0.0816	0.5423	0.3932	0.040*
H13	−0.1014	0.5241	0.4443	0.048*
H15	−0.0877	0.7235	0.5158	0.039*
H16	0.0958	0.7410	0.4659	0.034*
H18A	0.2159	0.5862	0.3194	0.031*
H18B	0.3000	0.5604	0.3762	0.031*
H22	0.2577	0.7379	0.1563	0.037*
H23	0.2264	0.8204	0.0752	0.042*

H25	0.5548	0.9021	0.1057	0.044*
H26	0.5900	0.8157	0.1831	0.038*
H28A	0.3092	0.6485	0.2260	0.031*
H28B	0.2923	0.7125	0.2750	0.031*
H34	0.3424	0.5326	0.2242	0.033*
H35	0.3679	0.4257	0.1533	0.039*
H36	0.4885	0.3339	0.1187	0.044*
H37	0.6816	0.3206	0.1586	0.041*
H38	0.7503	0.3930	0.2395	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0292 (3)	0.0918 (5)	0.0349 (3)	−0.0112 (3)	0.0084 (2)	−0.0205 (3)
Cl2	0.0897 (5)	0.0385 (3)	0.0410 (3)	−0.0038 (3)	−0.0036 (3)	0.0106 (2)
Cl3	0.0315 (2)	0.0374 (3)	0.0308 (2)	−0.00001 (19)	−0.00860 (19)	−0.0048 (2)
O17	0.0409 (8)	0.0270 (7)	0.0357 (7)	−0.0066 (6)	0.0084 (6)	−0.0057 (6)
O27	0.0219 (7)	0.0454 (9)	0.0493 (9)	0.0002 (6)	0.0007 (6)	0.0106 (7)
N31	0.0236 (7)	0.0283 (8)	0.0263 (8)	0.0010 (6)	0.0026 (6)	0.0037 (6)
C1	0.0222 (8)	0.0248 (9)	0.0275 (9)	−0.0001 (7)	0.0012 (7)	−0.0046 (7)
C11	0.0263 (9)	0.0294 (10)	0.0205 (8)	0.0037 (7)	0.0003 (7)	0.0000 (7)
C12	0.0313 (10)	0.0364 (11)	0.0321 (10)	−0.0030 (8)	0.0044 (8)	−0.0086 (8)
C13	0.0332 (11)	0.0493 (13)	0.0369 (11)	−0.0126 (9)	0.0062 (9)	−0.0120 (10)
C14	0.0246 (9)	0.0575 (14)	0.0227 (9)	−0.0008 (9)	0.0004 (7)	−0.0055 (9)
C15	0.0332 (10)	0.0444 (12)	0.0207 (9)	0.0126 (9)	−0.0002 (7)	−0.0016 (8)
C16	0.0338 (10)	0.0296 (10)	0.0209 (9)	0.0064 (8)	−0.0004 (7)	0.0019 (7)
C17	0.0288 (9)	0.0234 (9)	0.0229 (9)	0.0013 (7)	−0.0003 (7)	0.0002 (7)
C18	0.0263 (9)	0.0250 (9)	0.0274 (9)	−0.0015 (7)	0.0028 (7)	−0.0025 (7)
C21	0.0276 (9)	0.0271 (10)	0.0273 (9)	0.0022 (7)	0.0073 (7)	−0.0038 (7)
C22	0.0307 (10)	0.0278 (10)	0.0339 (10)	−0.0003 (8)	0.0021 (8)	−0.0015 (8)
C23	0.0397 (11)	0.0328 (11)	0.0336 (10)	0.0041 (9)	−0.0026 (9)	−0.0017 (8)
C24	0.0527 (13)	0.0283 (10)	0.0276 (10)	0.0048 (9)	0.0068 (9)	−0.0011 (8)
C25	0.0436 (12)	0.0298 (11)	0.0367 (11)	−0.0038 (9)	0.0167 (9)	−0.0044 (9)
C26	0.0295 (9)	0.0321 (11)	0.0335 (10)	−0.0003 (8)	0.0105 (8)	−0.0043 (8)
C27	0.0236 (9)	0.0294 (10)	0.0313 (10)	0.0008 (7)	0.0033 (7)	−0.0040 (8)
C28	0.0211 (8)	0.0268 (9)	0.0290 (9)	0.0010 (7)	0.0015 (7)	−0.0009 (7)
C32	0.0231 (9)	0.0266 (9)	0.0238 (9)	−0.0049 (7)	0.0000 (7)	0.0012 (7)
C33	0.0201 (8)	0.0249 (9)	0.0261 (9)	0.0003 (7)	0.0036 (7)	−0.0007 (7)
C34	0.0223 (8)	0.0298 (10)	0.0300 (9)	−0.0004 (7)	−0.0011 (7)	−0.0036 (8)
C34A	0.0252 (9)	0.0269 (9)	0.0247 (9)	−0.0017 (7)	0.0045 (7)	−0.0004 (7)
C35	0.0340 (10)	0.0337 (11)	0.0294 (10)	−0.0011 (8)	0.0005 (8)	−0.0051 (8)
C36	0.0482 (12)	0.0325 (11)	0.0280 (10)	−0.0021 (9)	0.0071 (9)	−0.0049 (8)
C37	0.0418 (11)	0.0271 (10)	0.0331 (10)	0.0067 (8)	0.0132 (9)	0.0015 (8)
C38	0.0310 (9)	0.0302 (10)	0.0314 (10)	0.0056 (8)	0.0072 (8)	0.0046 (8)
C38A	0.0257 (9)	0.0243 (9)	0.0248 (9)	−0.0001 (7)	0.0055 (7)	0.0047 (7)

Geometric parameters (Å, º)

C1—C33	1.516 (2)	C24—C25	1.383 (3)
C1—C28	1.527 (3)	C24—Cl2	1.740 (2)
C1—C18	1.542 (2)	C25—C26	1.385 (3)
C1—H1	1.00	C25—H25	0.95
C11—C12	1.389 (3)	C26—H26	0.95
C11—C16	1.400 (2)	C27—O27	1.218 (2)
C11—C17	1.495 (2)	C27—C28	1.511 (2)
C12—C13	1.391 (3)	C28—H28A	0.99
C12—H12	0.95	C28—H28B	0.99
C13—C14	1.382 (3)	N31—C32	1.302 (2)
C13—H13	0.95	N31—C38A	1.368 (2)
C14—C15	1.380 (3)	C32—C33	1.422 (2)
C14—Cl1	1.742 (2)	C33—C34	1.370 (3)
C15—C16	1.384 (3)	C34—C34A	1.414 (3)
C15—H15	0.95	C34A—C35	1.418 (3)
C16—H16	0.95	C35—C36	1.369 (3)
C17—O17	1.214 (2)	C36—C37	1.402 (3)
C17—C18	1.519 (2)	C37—C38	1.369 (3)
C18—H18A	0.99	C38—C38A	1.416 (3)
C18—H18B	0.99	C34A—C38A	1.409 (3)
C21—C22	1.392 (3)	C32—Cl3	1.7463 (18)
C21—C26	1.398 (3)	C34—H34	0.95
C21—C27	1.494 (3)	C35—H35	0.95
C22—C23	1.386 (3)	C36—H36	0.95
C22—H22	0.95	C37—H37	0.95
C23—C24	1.381 (3)	C38—H38	0.95
C23—H23	0.95		

C33—C1—C28	111.21 (15)	C25—C24—Cl2	119.31 (17)
C33—C1—C18	110.30 (15)	C24—C25—C26	118.99 (19)
C28—C1—C18	110.79 (14)	C24—C25—H25	120.5
C33—C1—H1	108.1	C26—C25—H25	120.5
C28—C1—H1	108.1	C25—C26—C21	120.61 (19)
C18—C1—H1	108.1	C25—C26—H26	119.7
C12—C11—C16	119.25 (17)	C21—C26—H26	119.7
C12—C11—C17	122.82 (16)	O27—C27—C21	120.57 (17)
C16—C11—C17	117.93 (16)	O27—C27—C28	121.31 (17)
C11—C12—C13	120.42 (18)	C21—C27—C28	118.11 (15)
C11—C12—H12	119.8	C27—C28—C1	113.25 (14)
C13—C12—H12	119.8	C27—C28—H28A	108.9
C14—C13—C12	118.8 (2)	C1—C28—H28A	108.9
C14—C13—H13	120.6	C27—C28—H28B	108.9
C12—C13—H13	120.6	C1—C28—H28B	108.9
C15—C14—C13	122.17 (18)	H28A—C28—H28B	107.7
C15—C14—Cl1	118.74 (16)	C32—N31—C38A	117.79 (15)
C13—C14—Cl1	119.09 (17)	N31—C32—C33	126.24 (17)

C14—C15—C16	118.57 (18)	N31—C32—Cl3	114.58 (13)
C14—C15—H15	120.7	C33—C32—Cl3	119.18 (14)
C16—C15—H15	120.7	C34—C33—C32	115.27 (16)
C15—C16—C11	120.79 (18)	C34—C33—C1	121.02 (16)
C15—C16—H16	119.6	C32—C33—C1	123.71 (16)
C11—C16—H16	119.6	C33—C34—C34A	121.44 (17)
O17—C17—C11	120.47 (16)	C33—C34—H34	119.3
O17—C17—C18	120.93 (16)	C34A—C34—H34	119.3
C11—C17—C18	118.60 (15)	C38A—C34A—C34	117.50 (17)
C17—C18—C1	112.83 (15)	C38A—C34A—C35	119.68 (17)
C17—C18—H18A	109.0	C34—C34A—C35	122.82 (17)
C1—C18—H18A	109.0	C36—C35—C34A	119.47 (18)
C17—C18—H18B	109.0	C36—C35—H35	120.3
C1—C18—H18B	109.0	C34A—C35—H35	120.3
H18A—C18—H18B	107.8	C35—C36—C37	120.83 (19)
C22—C21—C26	119.05 (18)	C35—C36—H36	119.6
C22—C21—C27	122.89 (17)	C37—C36—H36	119.6
C26—C21—C27	118.05 (17)	C38—C37—C36	120.85 (18)
C23—C22—C21	120.60 (18)	C38—C37—H37	119.6
C23—C22—H22	119.7	C36—C37—H37	119.6
C21—C22—H22	119.7	C37—C38—C38A	119.69 (18)
C24—C23—C22	119.16 (19)	C37—C38—H38	120.2
C24—C23—H23	120.4	C38A—C38—H38	120.2
C22—C23—H23	120.4	N31—C38A—C34A	121.68 (16)
C23—C24—C25	121.56 (19)	N31—C38A—C38	118.91 (17)
C23—C24—Cl2	119.12 (17)	C34A—C38A—C38	119.41 (17)

C16—C11—C12—C13	−0.1 (3)	C27—C21—C26—C25	−178.58 (17)
C17—C11—C12—C13	179.87 (19)	C22—C21—C27—O27	165.11 (19)
C11—C12—C13—C14	0.3 (3)	C26—C21—C27—O27	−16.0 (3)
C12—C13—C14—C15	0.0 (3)	C26—C21—C27—C28	162.49 (16)
C12—C13—C14—Cl1	−179.73 (16)	O27—C27—C28—C1	2.2 (3)
C13—C14—C15—C16	−0.4 (3)	C18—C1—C28—C27	169.40 (15)
Cl1—C14—C15—C16	179.32 (14)	C38A—N31—C32—C33	−1.2 (3)
C14—C15—C16—C11	0.6 (3)	C38A—N31—C32—Cl3	178.55 (12)
C12—C11—C16—C15	−0.3 (3)	N31—C32—C33—C34	2.5 (3)
C17—C11—C16—C15	179.70 (16)	Cl3—C32—C33—C34	−177.30 (14)
C12—C11—C17—O17	−176.07 (18)	N31—C32—C33—C1	−177.86 (17)
C16—C11—C17—O17	3.9 (3)	Cl3—C32—C33—C1	2.4 (2)
C16—C11—C17—C18	−176.70 (16)	C28—C1—C33—C34	−53.7 (2)
O17—C17—C18—C1	−9.5 (2)	C18—C1—C33—C34	69.6 (2)
C32—C33—C1—C18	−110.03 (19)	C32—C33—C34—C34A	−0.9 (3)
C33—C1—C18—C17	160.82 (15)	C1—C33—C34—C34A	179.43 (16)
C1—C18—C17—C11	171.11 (15)	C33—C34—C34A—C38A	−1.6 (3)
C18—C17—C11—C12	3.3 (3)	C33—C34—C34A—C35	178.77 (18)
C32—C33—C1—C28	126.64 (18)	C38A—C34A—C35—C36	−1.1 (3)
C33—C1—C28—C27	−67.55 (19)	C34—C34A—C35—C36	178.56 (18)
C1—C28—C27—C21	−176.29 (15)	C34A—C35—C36—C37	−1.6 (3)

C28—C27—C21—C22	−16.4 (3)	C35—C36—C37—C38	2.8 (3)
C28—C1—C18—C17	−75.61 (19)	C36—C37—C38—C38A	−1.4 (3)
C26—C21—C22—C23	1.5 (3)	C32—N31—C38A—C34A	−1.6 (3)
C27—C21—C22—C23	−179.62 (18)	C32—N31—C38A—C38	178.55 (16)
C21—C22—C23—C24	−2.1 (3)	C34—C34A—C38A—N31	3.0 (3)
C22—C23—C24—C25	0.9 (3)	C35—C34A—C38A—N31	−177.39 (17)
C22—C23—C24—Cl2	−177.98 (15)	C34—C34A—C38A—C38	−177.21 (17)
C23—C24—C25—C26	0.9 (3)	C35—C34A—C38A—C38	2.4 (3)
Cl2—C24—C25—C26	179.80 (15)	C37—C38—C38A—N31	178.63 (17)
C24—C25—C26—C21	−1.6 (3)	C37—C38—C38A—C34A	−1.2 (3)
C22—C21—C26—C25	0.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O17^{i}	0.95	2.59	3.502 (2)	160
C34—H34···N31^{ii}	0.95	2.39	3.244 (2)	150
C37—H37···O17^{iii}	0.95	2.45	3.330 (2)	155

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