Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structures of five (2-chloroquinolin-3-yl)-methyl ethers: supramolecular assembly in one and two dimensions mediated by hydrogen bonding and π–π stacking

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Received 18 April 2015
Accepted 26 April 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; 2-chloroquinolines; molecular conformation; hydrogen bonding; π–π stacking interactions

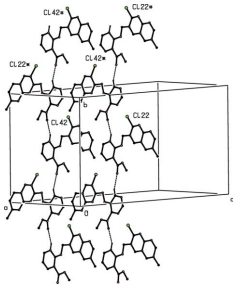
CCDC references: 1061944; 992268; 992267; 1061945; 1061946

Supporting information: this article has supporting information at journals.iucr.org/e

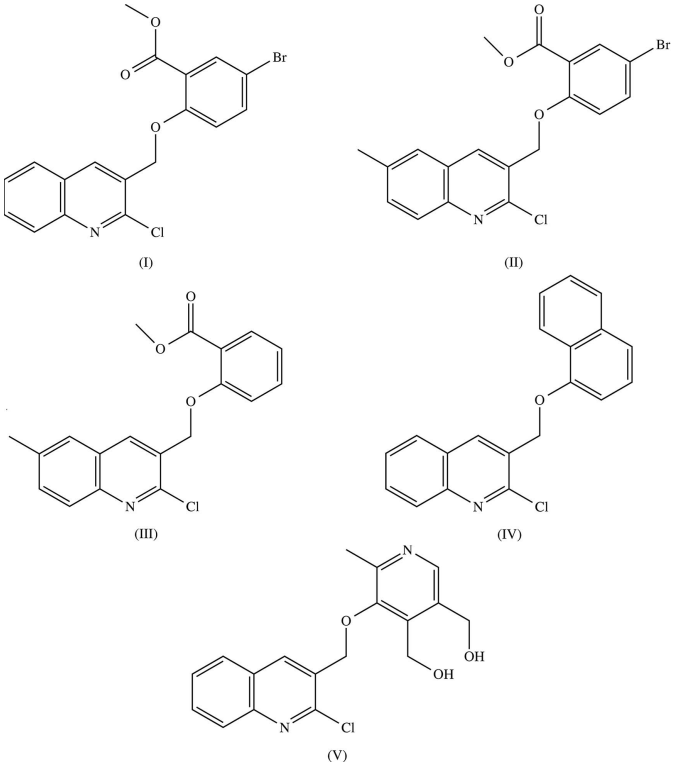
In the molecules of the title compounds, methyl 5-bromo-2-[(2-chloroquinolin-3-yl)methoxy]benzoate, $C_{18}H_{13}BrClNO_3$, (I), methyl 5-bromo-2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate, $C_{19}H_{15}BrClNO_3$, (II), methyl 2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate, $C_{19}H_{16}ClNO_3$, (III), which crystallizes with $Z' = 4$ in space group $P2_12_12_1$, and 2-chloro-3-[(naphthalen-1-yloxy)methyl]quinoline, $C_{20}H_{14}ClNO$, (IV), the non-H atoms are nearly coplanar, but in {5-[(2-chloroquinolin-3-yl)methoxy]-4-(hydroxymethyl)-6-methylpyridin-3-yl}methanol, $C_{18}H_{17}ClN_2O_3$, (V), the planes of the quinoline unit and of the unfused pyridine ring are almost parallel, although not coplanar. The molecules of (I) are linked by two independent π–π stacking interactions to form chains, but there are no hydrogen bonds present in the structure. In (II), the molecules are weakly linked into chains by a single type of π–π stacking interaction. In (III), three of the four independent molecules are linked by π–π stacking interactions but the other molecule does not participate in such interactions. Weak C—H···O hydrogen bonds link the molecules into three types of chains, two of which contain just one type of independent molecule while the third type of chain contains two types of molecule. The molecules of (IV) are linked into chains by a C—H···π(arene) hydrogen bond, but π–π stacking interactions are absent. In (V), there is an intramolecular O—H···O hydrogen bond, and molecules are linked into sheets by a combination of O—H···N hydrogen bonds and π–π stacking interactions.

1. Chemical context

The quinoline nucleus occurs in a number of natural compounds, such as the Cinchona alkaloids, and many of these are pharmacologically active substances displaying a broad range of biological activity. Quinoline itself has been found to possess antimalarial, anti-bacterial, antifungal, anthelminthic, cardiotonic, anticonvulsant, anti-inflammatory and analgesic activity (Marella *et al.*, 2013). The synthesis, reactions and biological applications of 2-chloroquinoline-3-carbaldehydes have been reviewed (Abdel-Wahab *et al.*, 2012), and the structure of a simple reduction product (2-chloroquinolin-3-yl)methanol, derived from the parent 2-chloroquinoline-3-carbaldehyde, has been reported (Hathwar *et al.*, 2010). The structures of two related esters, [(2-chloroquinolin-3-yl)methyl acetate and (2-chloro-6-methylquinolin-3-yl)methyl acetate], have also been reported recently along with a study of their radical-scavenging and antimicrobial activities



(Tabassum *et al.*, 2014). Here we report the structures of five related ethers, namely methyl 5-bromo-2-[(2-chloroquinolin-3-yl)methoxy]benzoate, (I) (Fig. 1), methyl 5-bromo-2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate, (II) (Fig. 2), methyl 2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate, (III) (Figs. 3–6), 2-chloro-3-[(naphthalen-1-yloxy)methyl]-quinoline (IV) (Fig. 7) and {5-[(2-chloroquinolin-3-yl)methoxy]-4-(hydroxymethyl)-6-methylpyridin-3-yl}methanol, (V) (Fig. 8). Compounds (I)–(V) are all of general type QCH_2OR, where Q represents a 2-chloroquinolin-3-yl unit, which carries a 6-methyl substituent in compounds (II) and (III), although not in compounds (I), (IV) and (V), and where R represents a methoxycarbonylphenyl unit in compounds (I)–(III), a 1-naphthyl unit in compound (IV), and a multiply-substituted pyridyl unit in compound (V). Compound (I)–(V) were all prepared by reaction of the corresponding chloromethyl compounds QCH_2Cl with the appropriate hydroxy compound ROH under basic conditions, with yields ranging from 86 to 97%.



2. Structural commentary

As noted above, the molecular constitutions of compounds (I)–(III) are very similar: those of compounds (I) and (II) differ only in the presence of a 6-methyl substituent in (II) which is absent from (I), while those of compounds (II) and (III) differ only in the presence of a bromo substituent in (II) which is absent from (III). Despite these close similarities, compounds (I)–(III) all crystallize in different space groups, $P2_1/n$ and Pbca, respectively, for (I) and (II), both with $Z' = 1$, and $P2_12_12_1$ with $Z' = 4$ for (III). A search for possible addi-

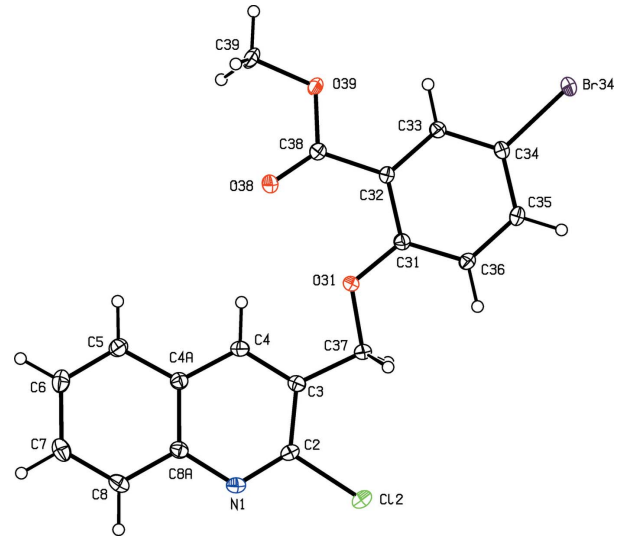


Figure 1
The molecular structure of compound (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

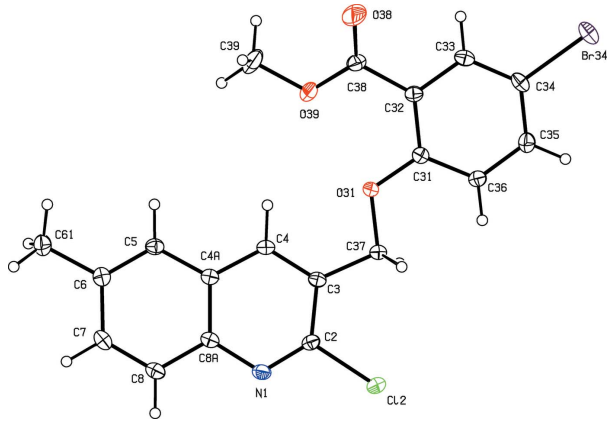


Figure 2
The molecular structure of compound (II) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

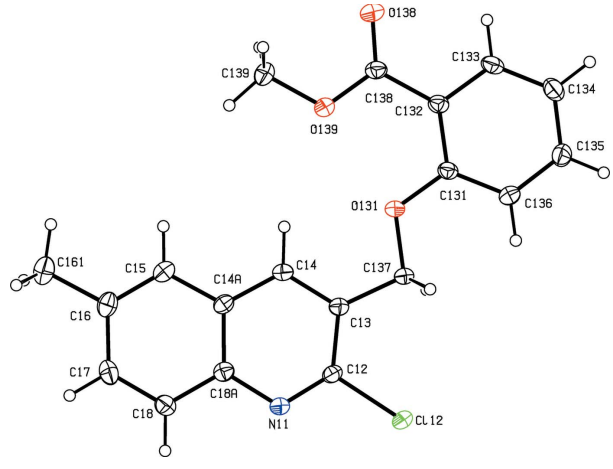


Figure 3
The structure of a type 1 molecule of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

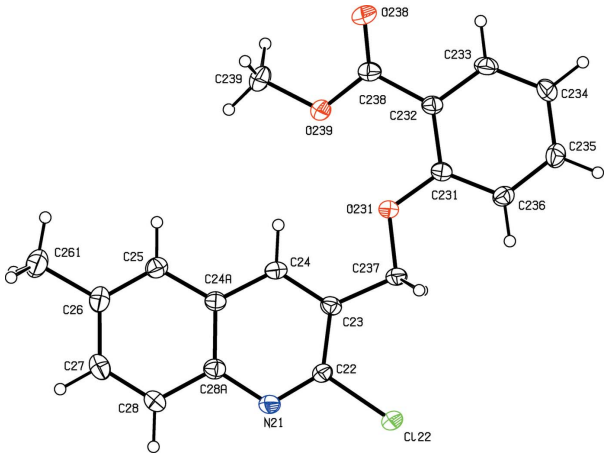


Figure 4
The structure of a type 2 molecule of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

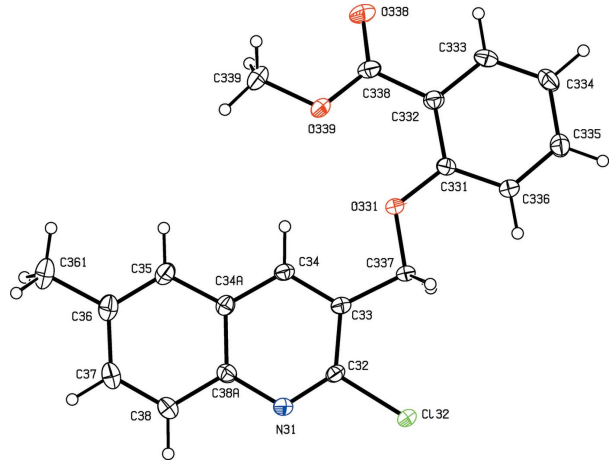


Figure 5
The structure of a type 3 molecule of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

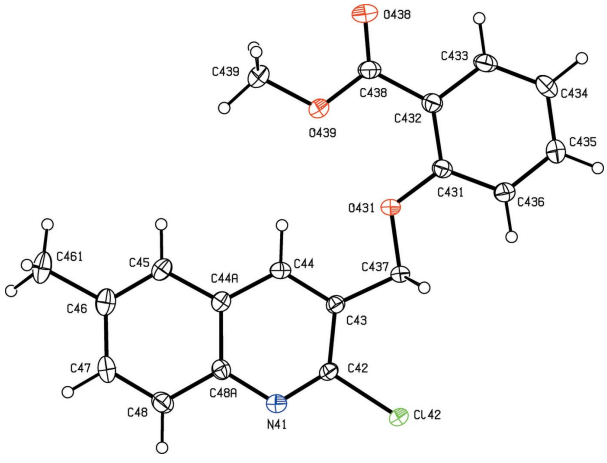


Figure 6
The structure of a type 4 molecule of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

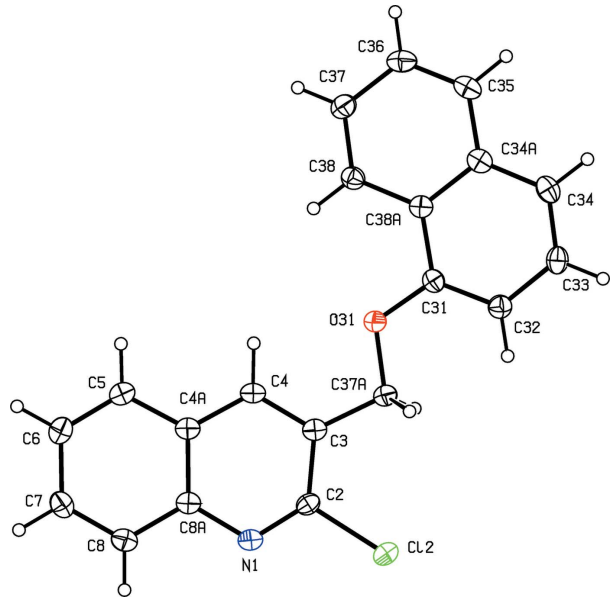


Figure 7
The molecular structure of compound (IV) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

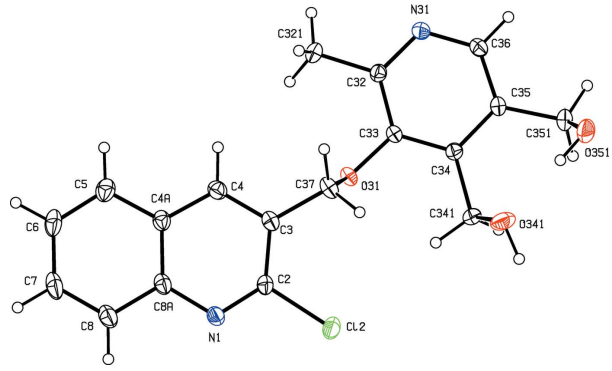


Figure 8
The molecular structure of compound (V) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

tional crystallographic symmetry in compound (III) found none: comparison of the atomic coordinates for the Cl atoms within the selected asymmetric unit shows that while the *x*-coordinates of atoms Cl12 and Cl32 differ by *ca* 0.5 and their *z*-coordinates are almost identical, the *y*-coordinates of these two atoms differ by *ca* 0.13; similarly the *x*-coordinates of atoms Cl22 and Cl42 again differ by *ca* 0.5 but now the *y*-coordinates are almost identical, while the *z*-coordinates differ by *ca* 0.18. Hence it is not possible to identify even pseudosymmetry here. For compound (III), it will be convenient to refer to the molecules containing atoms N11—N14 as molecules of types 1–4, respectively. Compounds (IV) and (V) both crystallize with $Z' = 1$, in space groups $P2_1$ and $P2_1/c$, respectively.

In compounds (I)–(III), the non-H atoms are almost co-planar, as shown by the relevant torsional and dihedral angles (Table 1). It is interesting to note that the orientation of the

Table 1
Selected torsional and dihedral angles (°) for compounds (I)–(III).

'Dihedral 1' represents the dihedral angle between the mean planes of the quinoline and phenyl rings. 'Dihedral 2' represents the dihedral angle between the mean planes of the phenyl ring and the carboxyl unit.

Parameter	(I)	(II)	(III)			
x	nil	nil	1	2	3	4
C*x*2—C*x*3—C*x*37—O*x*31	−174.63 (17)	−176.93 (18)	−179.4 (3)	179.8 (3)	178.4 (3)	−177.6 (3)
C*x*3—C*x*37—O*x*31—C*x*31	−175.71 (16)	−179.57 (17)	177.2 (3)	−175.9 (3)	−178.9 (3)	176.4 (3)
C*x*37—O*x*31—C*x*31—C*x*32	173.73 (17)	−172.62 (18)	−176.8 (3)	174.5 (3)	177.7 (3)	−174.4 (3)
C*x*31—C*x*32—C*x*38—O*x*38	4.1 (3)	159.5 (3)	−177.5 (4)	166.4 (4)	−168.7 (4)	178.9 (4)
C*x*31—C*x*32—C*x*38—O*x*39	−177.01 (17)	−20.7 (3)	2.8 (6)	−14.8 (5)	12.7 (5)	−0.7 (5)
C*x*32—C*x*38—O*x*39—C*x*39	−175.77 (17)	−176.4 (2)	179.2 (3)	−176.4 (3)	178.3 (4)	180.0 (3)
Dihedral 1	0.66 (6)	10.72 (8)	5.44 (2)	4.18 (2)	3.825 (13)	5.55 (3)
Dihedral 2	4.27 (8)	19.25 (15)	2.52 (3)	14.66 (7)	12.29 (8)	1.78 (6)

Table 2
Hydrogen bonds and short intermolecular contacts (Å, °) for compounds (II)–(V).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings C231–C236, C331–C336 and C31–C34,C34*A*,C38*A*, respectively.

Compound	*D*—H···*A*	*D*—H	H···A	*D*···*A*	*D*—H···*A*
(II)	C36—H36···O38^{i}	0.95	2.53	3.277 (3)	136
(III)	C28—H28···N41^{ii}	0.95	2.63	3.565 (5)	169
	C136—H136···O138^{iii}	0.95	2.50	3.261 (4)	137
	C236—H236···O438^{iv}	0.95	2.43	3.223 (4)	141
	C336—H336···O338^{v}	0.95	2.46	3.238 (4)	139
	C436—H436···O238^{iv}	0.95	2.51	3.254 (4)	136
	C337—H33*B*···*Cg*1	0.99	2.64	3.441 (4)	138
	C437—H43*A*···*Cg*2	0.99	2.64	3.446 (4)	138
(IV)	C37—H37*A*···*Cg*3^{vi}	0.99	2.74	3.552 (3)	139
(V)	O341—H341···N31^{vii}	0.91	1.81	2.7098 (19)	174
	O351—H351···O341	0.91	1.86	2.7209 (19)	158
	C4—H4···O351^{viii}	0.95	2.60	3.374 (2)	139

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

ester function in compound (I) differs from that in compounds (II) and (III) (Table 1 and Figs. 1–6): this difference may arise, at least in part, from the participation of the carbonyl O atom of the ester unit in short C—H···O interactions in all of the molecules of compounds (II) and (III) but not in compound (I) (Table 2). The non-H atoms in compound (IV) are also nearly coplanar, with a dihedral angle between the mean planes of the quinoline and naphthalene units of 7.39 (12)°. By contrast, while the quinoline and pyridine units in compound (V) are nearly parallel (Fig. 8), with a dihedral angle between their mean planes of only 3.10 (9)°, they are by no means coplanar, as indicated by the values of the torsional angles C2—C3—C37—O31, 92.08 (18), C3—C37—O31—C33, 165.21 (13) and C37—O31—C33—C32, −90.17 (17)°. This again may perhaps be ascribed in part to the strong hydrogen bonds present in the crystal structure of (V) (Table 2).

None of the molecules of compounds (I)–(V) exhibits any internal symmetry and hence all are conformationally chiral. For compounds (I), (II) and (V), the centrosymmetric space groups accommodate equal numbers of the two conformational enantiomers, but only one such enantiomer is present in each crystal of compound (IV): the absolute configuration of the enantiomer present in the crystal selected for data collection was established by means of the Flack *x* parameter (Flack, 1983), although this has no chemical significance. For compound (III), the value of the Flack *x* parameter gives evidence of partial inversion twinning.

3. Supramolecular interactions

The supramolecular assembly in compounds (I)–(V) is determined by a variety of direction-specific intermolecular interactions, including both π–π stacking interactions and hydrogen bonds of C—H···N, C—H···O and C—H···π types, as well as O—H···N hydrogen bonds in compound (V) only. In compound (III), there are two fairly short intermolecular C—H···N contacts involving C—H bonds from methyl groups bonded to the quinoline nucleus: not only are such bonds of low acidity, but these methyl groups are likely to be undergoing very rapid rotation about the adjacent C—C bonds

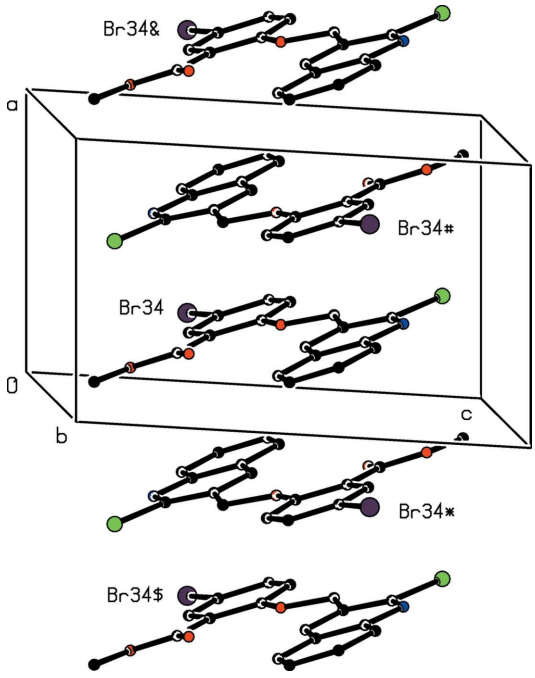


Figure 9
Part of the crystal structure of compound (I) showing the formation of a π-stacked chain along [100]. For the sake of clarity, H atoms have been omitted. Atoms marked with an asterisk (*), a hash (#), a dollar sign ($) or an ampersand (&) are at the symmetry positions $(-x, -y+1, -z+1)$, $(-x+1, -y+1, -z+1)$, $(x-1, y, z)$ and $(x+1, y, z)$, respectively.

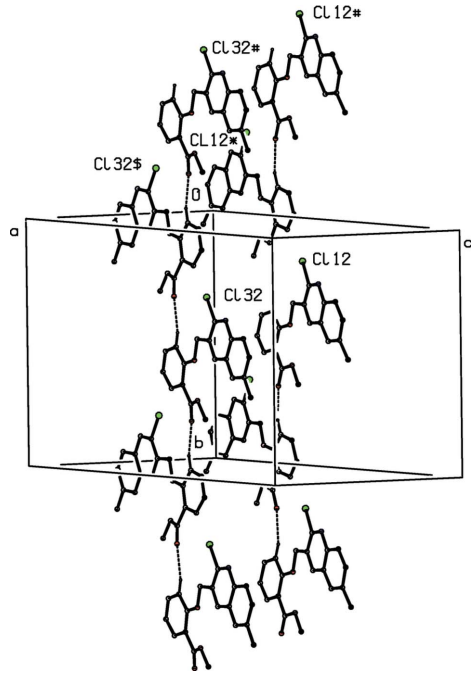


Figure 10
Part of the crystal structure of compound (III) showing the formation of two independent chains running parallel to the [010] direction and formed separately by the molecules of types 1 and 3. For the sake of clarity, H atoms not involved in the motifs shown have been omitted. Atoms marked with an asterisk (*), a hash (#) or a dollar sign ($) are at the symmetry positions $(-x, y-\frac{1}{2}, -z+\frac{1}{2})$, $(x, y-1, z)$ and $(-x+1, y-\frac{1}{2}, -z++\frac{1}{2})$, respectively.

(Riddell & Rogerson, 1996, 1997). When a group having local C_3 symmetry, such as a methyl group, is directly bonded to a group having approximate local C_2 symmetry, such as an aryl ring, the rotational barrier between these two groups is extremely low, of the order of J mol^{-1} rather than the usual kJ mol^{-1} (Naylor & Wilson, 1957; Tannenbaum *et al.*, 1956). Accordingly, these contacts in (III) are not regarded as having any structural significance. Likewise, the C—H···O contact in (V) involving the methyl group bonded to the unfused pyridine ring is not regarded as significant.

There are no hydrogen bonds of any kind in the crystal structure of compound (I), but molecules are linked into chains by π–π stacking interactions. The fused aryl ring of the molecule at (x, y, z) and the brominated ring of the molecule at $(-x+1, -y+1, -z+1)$ make a dihedral angle of 1.04°; the ring centroid separation is 3.6168 (10) Å, and the shortest perpendicular distance from the centroid of one ring to the plane of the other is 3.4132 (6) Å, with a ring-centroid offset of *ca* 1.20 Å. For the heterocyclic ring at (x, y, z) and the brominated aryl ring at $(-x, 1-y, 1-z)$, the corresponding values are 1.52 (9)°, 3.7454 (11) Å, 3.4357 (8) Å and *ca* 1.49 Å. The combination of these two stacking interactions links the molecules of (I) into a chain running parallel to the [100] direction (Fig. 9). Two chains of this type pass through each unit cell but there are no direction-specific interactions between adjacent chains.

The only short C—H···O contact in the structure of compound (II) has a C—H···O angle of only 136° (Table 2), and so it is unlikely to be of major structural significance (Wood *et al.*, 2009). However, there is a weak π–π stacking interaction between molecules related by a 2_1 screw axis. The pyridyl ring at (x, y, z) and the brominated aryl ring at $(-x+\frac{1}{2}, y+\frac{1}{2}, z)$ make a dihedral angle of 3.87 (10)°: the shortest perpendicular distance from the centroid of one ring to the plane of the other is 3.3816 (9) Å, but the ring-centroid separation is 3.882 (12), resulting in a ring-centroid offset of *ca* 1.78 Å. Thus there is only a very modest overlap of these rings and a consequently weak stacking interaction: if this interaction is, in fact, regarded as significant, it links the molecules into a π-stacked chain running parallel to [010].

Within the selected asymmetric unit for compound (III), three of the four independent molecules, those of types 2, 3 and 4 (*cf.* Figs. 3–6), are linked by two π–π stacking interactions, but the type 1 molecule does not participate in any such interaction. One of these stacking interactions involves the pyridyl ring of the type 2 molecule and the fused aryl ring of the type 3 molecule, while the other involves the pyridyl ring of the type 3 molecule and the fused aryl ring of the type 4 molecule. The dihedral angles between the ring planes within these two interactions are 3.11 (18) and 0.96 (7)°, respectively, the ring-centroid separations are 3.553 (2) Å and 3.544 (2) Å, and the shortest perpendicular distances from the centroid of one ring in each interaction to the plane of the other ring are 3.4014 (15) and 3.3820 (15) Å, corresponding to ring-centroid offsets of *ca* 1.03 and *ca* 1.06 Å, respectively. The only short C—H···N contact within the crystal structure of compound

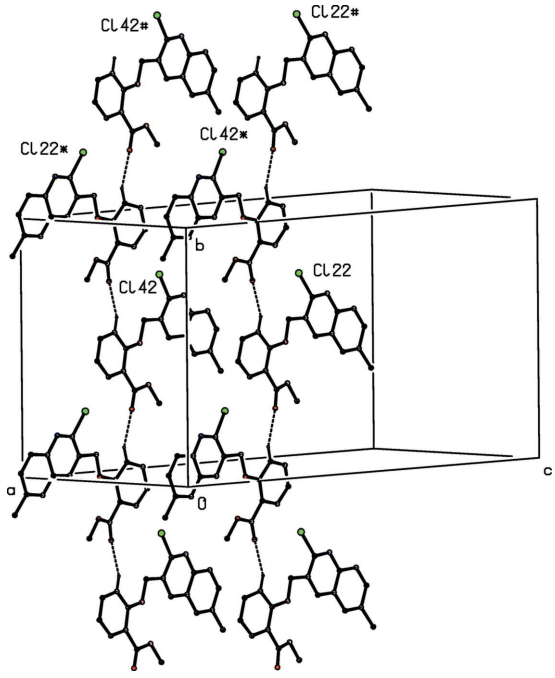


Figure 11
Part of the crystal structure of compound (III) showing the formation of a chain running parallel to the [010] direction and containing alternating molecules of types 2 and 4. For the sake of clarity, H atoms not involved in the motifs shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(-x+1, y+\frac{1}{2}, -z+\frac{1}{2})$ and $(x, y+1, z)$, respectively.

(III) has an H···N distance which is not significantly less than the sum of the van der Waals radii, but there are four independent C—H···O hydrogen bonds present in the structure although all are probably weak as they have quite small C—H···O angles (Table 2). However, the pattern of these contacts is of interest as it precludes the possibility of any additional crystallographic symmetry in this structure where $Z' = 4$. One of the C—H···O interactions involves only molecules of type 1 which are related by the 2_1 screw axis along $(0, y, \frac{1}{4})$, forming a $C(6)$ (Bernstein *et al.*, 1995) running parallel to the [010] direction (Fig. 10); an entirely similar chain is formed by type 3 molecules related to one another by the 2_1 screw axis along $(\frac{1}{2}, y, \frac{1}{4})$. However, the molecules of types 2 and 4 which are related by the 2_1 screw axis along $(\frac{1}{2}, y, \frac{1}{4})$ together form a $C_2^2(12)$ chain parallel to [010] (Fig. 11), which runs antiparallel to the chains formed by the molecules of types 1 and 3. Hence the patterns of supramolecular assembly in compounds (I)–(III), as well as their crystallization characteristics, show significant differences.

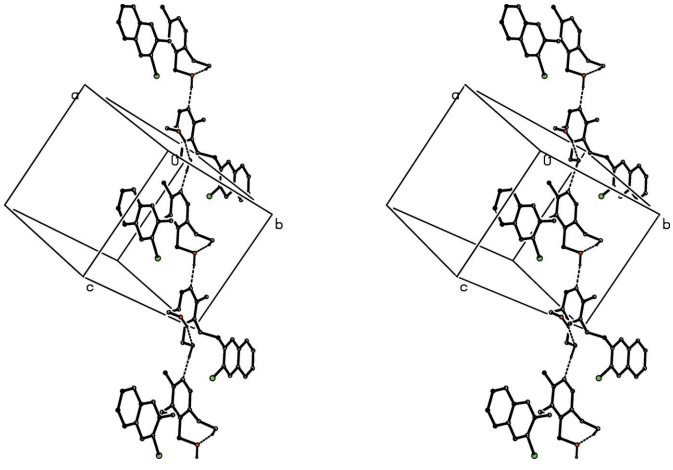


Figure 12
A stereoview of part of the crystal structure of compound (V) showing the formation of a $C(7)$ chain formed by O—H···N hydrogen bonds and running parallel to $[10\bar{1}]$. For the sake of clarity, H atoms bonded to C atoms have been omitted.

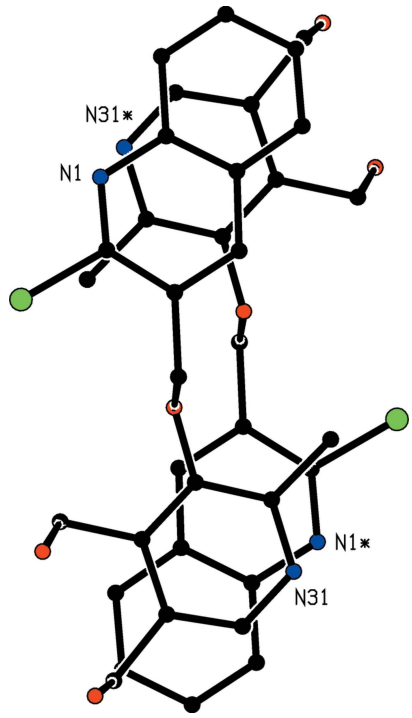


Figure 13
Part of the crystal structure of compound (V) showing the formation of a centrosymmetric π-stacked dimer. For the sake of clarity, H atoms have all been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(-x+1, -y+1, -z+1)$.

There are no hydrogen bonds of the C—H···N or C—H···O types in the crystal structure of compound (IV) and, despite the large number of independent aromatic rings, there are no π–π stacking interactions. The only direction-specific intermolecular interaction is a weak C—H···π(arene) contact involving molecules related by translation.

The supramolecular assembly in compound (V) is, however, rather more elaborate, resulting in part from the presence of additional hydrogen-bond donors and acceptors in the unfused pyridine unit. An intramolecular O—H···O hydrogen bond (Table 2) gives rise to an $S(7)$ (Bernstein *et al.*, 1995) motif, and an intermolecular O—H···N hydrogen bond links molecules related by the *n*-glide plane at $y = \frac{3}{4}$, forming a $C(7)$ chain running parallel to the $[10\bar{1}]$ direction (Fig. 12). In addition, inversion-related pairs of molecules are linked by π–π stacking interactions involving the unfused pyridine ring of one molecule and the quinoline unit of the other (Fig. 13). Thus the unfused pyridine ring of the molecule at (x, y, z) and

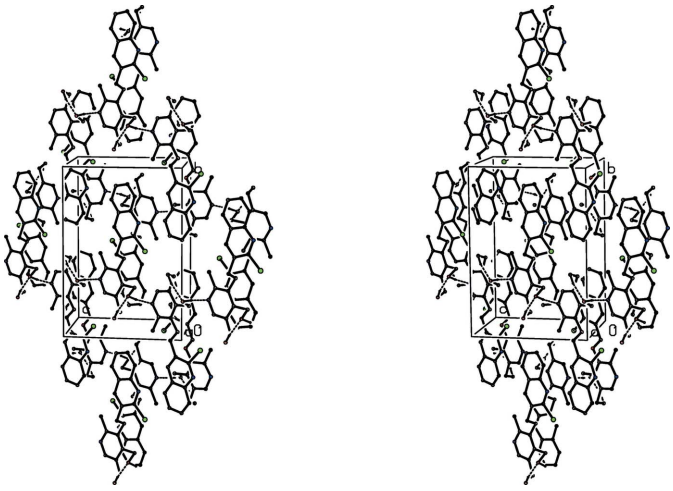


Figure 14
A stereoview of part of the crystal structure of compound (V) showing the formation of a π-stacked sheet of hydrogen bonded chains lying parallel to (101). For the sake of clarity, H atoms bonded to C atoms have been omitted.

the fused pyridine ring of the molecule at $(1-x, 1-y, 1-z)$ make a dihedral angle of 4.43 (8)°: the ring-centroid separation is 3.7499 (9) Å and the shortest perpendicular distance from the centroid of one ring to the plane of the other is 3.5077 (7) Å, corresponding to a ring-centroid offset of *ca* 1.33 Å. For the unfused pyridyl ring at (x, y, z) and the fused aryl ring at $(-x+1, -y+1, -z+1)$ the corresponding values are 1.73 (8)°, 3.7333 (10) Å, 3.4637 (8) Å and *ca* 1.39 Å, respectively. The effect of the hydrogen-bonded chains is to link the π-stacked dimer centered at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ directly to the four symmetry-related dimers centred at (1, 0, 0), (1, 1, 0), (0, 0, 1) and (0, 1, 1), thus forming a sheet of π-stacked hydrogen-bonded chains lying parallel to (101) [Fig. 14].

4. Database survey

The structures of a number of fairly simple 2-chloroquinolione derivatives related to compounds (I)–(V) have been reported in recent years. A structural study of a closely related group of six simply substituted 2-chloroquinolines (Hathwar *et al.*, 2010) focused on supramolecular aggregation *via* C—H···Cl hydrogen bonds and attractive Cl···Cl interactions. However, it must be pointed out firstly that it is now well established (Brammer *et al.*, 2001; Thallapally & Nangia, 2001) that Cl atoms bonded to C atoms are extremely poor acceptors of hydrogen bonds, even from strong donors such as O—H or N—H; and secondly, that for none of the compounds in this group were the shortest intermolecular Cl···Cl distances less than the sum of the van der Waals radii (Bondi, 1964; Nyburg & Faerman, 1985; Rowland & Taylor, 1996): indeed, the concept of the van der Waals radius was nowhere mentioned by the original authors. Two of the six compounds in this group contained 3-hydroxymethyl substituents and, in each of these, the molecules are linked into $C(6)$ chains by means of O—H···N hydrogen bonds.

Molecules of 2-[(2-chloroquinolin-3-yl)(hydroxy)methyl]-acrylonitrile (Anuradha *et al.*, 2013*a*) are also linked into $C(6)$ chains by O—H···N hydrogen bonds, while in the closely related methyl 2-[(2-chloroquinolin-3-yl)(hydroxy)methyl]-acrylate, where $Z' = 2$ (Anuradha *et al.*, 2013*b*), molecules of one type are linked by O—H···O hydrogen bonds, again forming $C(6)$ chains to which the molecules of the second type are linked by O—H···N hydrogen bonds. Chains of $C(6)$ type are formed also in *N*-{(2-chloro-3-quinlinyl)methyl]-4-fluoro-aniline (Jasinski *et al.*, 2010), which is closely related to compounds (I)–(V) except that an amino linkage replaces the ether linkage in (I)–(V), so that the chains are built from N—H···N hydrogen bonds.

In the esters (2-choloroquinolin-3-yl)methyl acetate and (2-chloro-6-methylquinolin-3-yl)methyl acetate (Tabassum *et al.*, 2014), there are no strong hydrogen bond donors: in the methylated compound, where $Z' = 2$, the only hydrogen bond, of C—H···O type, links the two independent molecules, while in the unmethylated compound, the molecules are linked into $C(5)$ chains by C—H···N hydrogen bonds. In the structure of 2-chloro-3-(dimethoxymethyl)-6-methoxyquinoline (Chandrika *et al.*, 2015), there are no hydrogen bonds of any kind.

5. Synthesis and crystallization

For the synthesis of compounds (I)–(V), a mixture of 0.4 mmol of the appropriate quinoline derivative, 2-chloro-3-(chloromethyl)quinoline for compounds (I), (IV) and (V) or 2-chloro-3-(chloromethyl)-5-methylquinoline for compounds (II) and (III) and 0.4 mmol of the appropriate hydroxy compound, methyl 5-bromo-2-hydroxybenzoate for (I) and (II), methyl 2-hydroxybenzoate for (III), 1-hydroxynaphthalene for (IV), or 3-hydroxy-4,5-bis(hydroxymethyl)-2-methylpyridinium chloride for (V), were dissolved in *N*,*N*-dimethylformamide (3–5 ml) together with potassium carbonate (2 mmol) and these mixtures were stirred at ambient temperature for 6–9 h, with monitoring by TLC. When each reaction was complete, ice-cold water (5 ml) was added and the resulting solid products were collected by filtration, washed with water and dried in air. Crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation, at ambient temperature and in the presence of air, of solutions in dichloromethane, with yields in the range 86–97%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were located in difference Fourier maps. C-bound H atoms were then treated as riding atoms in geometrically idealized positions: C—H distances 0.95–0.99 Å with $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl groups, which were permitted to rotate but not to tilt, and $1.2U_{eq}(C)$ for other C-bound H atoms.

The H atoms bonded to O atoms in compound (V) were permitted to ride at the positions located in the difference Fourier map, with $U_{iso}(H) = 1.5U_{eq}(O)$, giving O—H distances of 0.91 Å. For compound (III), the Flack *x* parameter (Flack,

Table 3
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{18}H_{13}BrClNO_3$	$C_{19}H_{15}BrClNO_3$	$C_{19}H_{16}ClNO_3$
M_r	406.64	420.67	341.78
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, $Pbca$	Orthorhombic, $P2_12_12_1$
Temperature (K)	173	173	173
a, b, c (Å)	7.3185 (4), 18.4177 (7), 11.7870 (5)	15.1920 (3), 11.98641 (19), 19.0307 (3)	13.5860 (3), 15.5857 (2), 30.9389 (5)
α, β, γ (°)	90, 93.609 (4), 90	90, 90, 90	90, 90, 90
V (Å^3)	1585.62 (13)	3465.44 (10)	6551.2 (2)
Z	4	8	16
Radiation type	Mo $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.78	4.81	2.21
Crystal size (mm)	0.44 × 0.23 × 0.12	0.24 × 0.16 × 0.08	0.48 × 0.26 × 0.14
Data collection			
Diffractometer	Agilent Eos Gemini	Agilent Eos Gemini	Agilent Eos Gemini
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)	Multi-scan (*SADABS*; Sheldrick, 2003)	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.335, 0.717	0.399, 0.680	0.472, 0.734
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17735, 4612, 3682	21861, 3421, 3062	45901, 12840, 11257
R_{int}	0.036	0.055	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703	0.618	0.619
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.071, 1.06	0.034, 0.093, 1.06	0.046, 0.129, 1.04
No. of reflections	4612	3421	12840
No. of parameters	218	229	874
No. of restraints	0	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.41	0.52, −0.49	0.42, −0.31
Absolute structure	–	–	Refined as an inversion twin
Absolute structure parameter	–	–	0.152 (16)

	(IV)	(V)
Crystal data		
Chemical formula	$C_{20}H_{14}ClNO$	$C_{18}H_{17}ClN_2O_3$
M_r	319.77	344.79
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1/n$
Temperature (K)	173	173
a, b, c (Å)	5.3165 (3), 10.5098 (4), 13.6201 (7)	9.7866 (3), 15.3336 (4), 10.6570 (3)
α, β, γ (°)	90, 98.527 (5), 90	90, 92.381 (3), 90
V (Å^3)	752.62 (6)	1597.85 (8)
Z	2	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.27	2.29
Crystal size (mm)	0.34 × 0.10 × 0.08	0.42 × 0.38 × 0.32
Data collection		
Diffractometer	Agilent Eos Gemini	Agilent Eos Gemini
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.551, 0.834	0.375, 0.481
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4606, 2014, 1938	9423, 3112, 2764
R_{int}	0.029	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619	0.618
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.090, 1.08	0.045, 0.127, 1.05
No. of reflections	2014	3112
No. of parameters	208	219
No. of restraints	1	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.19	0.32, −0.25
Absolute structure	Classical Flack method preferred over Parsons because s.u. lower	
Absolute structure parameter	−0.007 (18)	–

Computer programs: *CrysAlis PRO* and *CrysAlis RED* (Agilent, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

1983) for the crystal selected for data collection was x = 0.161 (1) calculated (Parsons *et al.*, 2013) using 4617 quotients of type $[(I^+)-(I^-)]/[(I^+)+(I^-)]$. Use of the TWIN/BASF instructions in *SHELXL2014* (Sheldrick, 2015) gave a value for the twin fraction of 0.152 (16). For compound (IV), the absolute configuration of the conformational enantiomer present in the crystal selected for data collection was established by means of the Flack x parameter calculated as x = −0.007 (18) by the standard method (Flack, 1983) and as x = 0.06 (2) calculated using 102 quotients of type $[(I^+)-(I^-)]/[(I^+)+(I^-)]$.

Acknowledgements

HBVS and THS thank the authorities of Jain University for their support and encouragement. HSY thanks the University of Mysore for research facilities. JPJ acknowledges the NSF–MRI program (grant No. 1039027) for funds to purchase the X-ray diffractometer.

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supporting information

Acta Cryst. (2015). E**71**, 609-617 [doi:10.1107/S2056989015008233]

Crystal structures of five (2-chloroquinolin-3-yl)methyl ethers: supramolecular assembly in one and two dimensions mediated by hydrogen bonding and π–π stacking

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Computing details

For all compounds, data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(I) Methyl 5-bromo-2-[(2-chloroquinolin-3-yl)methoxy]benzoate

Crystal data

$C_{18}H_{13}BrClNO_3$
M_r = 406.64
Monoclinic, $P2_1/n$
a = 7.3185 (4) Å
b = 18.4177 (7) Å
c = 11.7870 (5) Å
β = 93.609 (4)°
V = 1585.62 (13) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.703 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5443 reflections
θ = 3.0–33.0°
μ = 2.78 mm^{-1}
T = 173 K
Plate, colourles
0.44 × 0.23 × 0.12 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.335, T_{max} = 0.717
17735 measured reflections
4612 independent reflections
3682 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 30.0°, θ_{min} = 3.0°
h = −10→8
k = −24→25
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.071
S = 1.06
4612 reflections
218 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.6015P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3544 (2)	0.64638 (8)	0.75859 (12)	0.0228 (3)
C2	0.3622 (2)	0.57729 (10)	0.74061 (14)	0.0218 (4)
Cl2	0.44084 (7)	0.52448 (3)	0.85755 (4)	0.03157 (12)
C3	0.3125 (2)	0.54040 (10)	0.63773 (15)	0.0209 (4)
C4	0.2421 (2)	0.58250 (10)	0.55035 (15)	0.0219 (4)
H4	0.2034	0.5606	0.4799	0.026*
C4A	0.2265 (2)	0.65814 (10)	0.56389 (15)	0.0209 (4)
C5	0.1545 (3)	0.70490 (11)	0.47672 (16)	0.0257 (4)
H5	0.1115	0.6851	0.4055	0.031*
C6	0.1462 (3)	0.77791 (11)	0.49390 (17)	0.0303 (4)
H6	0.0952	0.8087	0.4354	0.036*
C7	0.2134 (3)	0.80793 (11)	0.59853 (18)	0.0315 (4)
H7	0.2101	0.8590	0.6093	0.038*
C8	0.2826 (3)	0.76456 (11)	0.68391 (17)	0.0276 (4)
H8	0.3271	0.7855	0.7539	0.033*
C8A	0.2888 (2)	0.68865 (10)	0.66944 (14)	0.0212 (4)
C37	0.3404 (3)	0.46017 (10)	0.62654 (15)	0.0246 (4)
H37A	0.4696	0.4471	0.6467	0.030*
H37B	0.2612	0.4333	0.6772	0.030*
O31	0.2926 (2)	0.44326 (7)	0.51108 (10)	0.0275 (3)
C31	0.2926 (2)	0.37331 (9)	0.47662 (14)	0.0203 (3)
C32	0.2264 (2)	0.35949 (9)	0.36438 (14)	0.0191 (3)
C33	0.2199 (2)	0.28798 (9)	0.32599 (14)	0.0203 (3)
H33	0.1751	0.2779	0.2502	0.024*
C34	0.2772 (3)	0.23189 (9)	0.39624 (15)	0.0212 (4)
Br34	0.26437 (3)	0.13590 (2)	0.33927 (2)	0.03066 (7)
C35	0.3456 (3)	0.24530 (10)	0.50667 (15)	0.0235 (4)
H35	0.3860	0.2064	0.5548	0.028*
C36	0.3543 (3)	0.31595 (10)	0.54578 (15)	0.0224 (4)
H36	0.4030	0.3255	0.6209	0.027*
C38	0.1676 (2)	0.41935 (10)	0.28586 (14)	0.0217 (4)
O38	0.1774 (2)	0.48297 (8)	0.30438 (12)	0.0415 (4)
O39	0.1018 (2)	0.39288 (7)	0.18579 (11)	0.0361 (4)
C39	0.0528 (3)	0.44627 (11)	0.10042 (18)	0.0380 (5)
H39A	−0.0067	0.4223	0.0336	0.057*
H39B	0.1633	0.4714	0.0786	0.057*

H39C	−0.0317	0.4815	0.1308	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0241 (8)	0.0260 (8)	0.0181 (7)	−0.0004 (6)	0.0007 (6)	−0.0038 (6)
C2	0.0222 (9)	0.0266 (9)	0.0164 (8)	0.0002 (7)	−0.0006 (7)	0.0005 (7)
Cl2	0.0414 (3)	0.0328 (3)	0.0196 (2)	0.0036 (2)	−0.00517 (19)	0.00316 (18)
C3	0.0220 (9)	0.0205 (9)	0.0202 (8)	−0.0018 (7)	0.0021 (7)	−0.0023 (7)
C4	0.0240 (9)	0.0237 (9)	0.0178 (8)	−0.0012 (7)	0.0002 (7)	−0.0028 (7)
C4A	0.0207 (9)	0.0222 (9)	0.0201 (8)	0.0005 (7)	0.0031 (7)	−0.0006 (7)
C5	0.0272 (10)	0.0282 (10)	0.0215 (8)	0.0036 (8)	0.0006 (7)	0.0006 (7)
C6	0.0314 (11)	0.0278 (10)	0.0320 (10)	0.0073 (8)	0.0048 (8)	0.0068 (8)
C7	0.0334 (11)	0.0228 (10)	0.0390 (11)	0.0045 (8)	0.0077 (9)	−0.0024 (8)
C8	0.0304 (11)	0.0242 (10)	0.0282 (9)	0.0009 (8)	0.0034 (8)	−0.0079 (8)
C8A	0.0199 (9)	0.0227 (9)	0.0213 (8)	0.0014 (7)	0.0036 (7)	−0.0029 (7)
C37	0.0354 (11)	0.0211 (9)	0.0170 (8)	0.0003 (7)	−0.0022 (7)	−0.0010 (7)
O31	0.0467 (9)	0.0168 (6)	0.0181 (6)	0.0019 (6)	−0.0048 (6)	−0.0020 (5)
C31	0.0231 (9)	0.0188 (9)	0.0191 (8)	−0.0002 (7)	0.0020 (7)	0.0000 (6)
C32	0.0215 (9)	0.0172 (8)	0.0186 (8)	0.0003 (6)	0.0009 (6)	0.0019 (6)
C33	0.0228 (9)	0.0187 (8)	0.0193 (8)	−0.0016 (7)	0.0003 (7)	0.0000 (6)
C34	0.0250 (9)	0.0158 (8)	0.0227 (8)	−0.0012 (6)	0.0008 (7)	0.0006 (7)
Br34	0.04557 (13)	0.01513 (9)	0.03011 (11)	−0.00002 (8)	−0.00682 (8)	−0.00001 (7)
C35	0.0284 (10)	0.0198 (9)	0.0224 (9)	0.0007 (7)	0.0010 (7)	0.0058 (7)
C36	0.0280 (10)	0.0209 (9)	0.0178 (8)	−0.0014 (7)	−0.0013 (7)	0.0026 (7)
C38	0.0247 (9)	0.0207 (9)	0.0197 (8)	0.0003 (7)	0.0011 (7)	0.0010 (7)
O38	0.0816 (12)	0.0175 (7)	0.0240 (7)	0.0027 (7)	−0.0074 (7)	0.0014 (6)
O39	0.0601 (10)	0.0178 (7)	0.0272 (7)	−0.0043 (6)	−0.0220 (7)	0.0050 (6)
C39	0.0540 (14)	0.0263 (11)	0.0307 (10)	−0.0027 (9)	−0.0207 (10)	0.0108 (8)

Geometric parameters (Å, º)

N1—C2	1.292 (2)	C37—H37B	0.9900
N1—C8A	1.370 (2)	O31—C31	1.351 (2)
C2—C3	1.417 (2)	C31—C36	1.392 (2)
C2—Cl2	1.7542 (18)	C31—C32	1.403 (2)
C3—C4	1.364 (2)	C32—C33	1.393 (2)
C3—C37	1.499 (2)	C32—C38	1.486 (2)
C4—C4A	1.408 (3)	C33—C34	1.373 (2)
C4—H4	0.9500	C33—H33	0.9500
C4A—C8A	1.414 (2)	C34—C35	1.387 (2)
C4A—C5	1.417 (3)	C34—Br34	1.8913 (18)
C5—C6	1.362 (3)	C35—C36	1.380 (3)
C5—H5	0.9500	C35—H35	0.9500
C6—C7	1.411 (3)	C36—H36	0.9500
C6—H6	0.9500	C38—O38	1.193 (2)
C7—C8	1.358 (3)	C38—O39	1.338 (2)
C7—H7	0.9500	O39—C39	1.436 (2)

C8—C8A	1.410 (3)	C39—H39A	0.9800
C8—H8	0.9500	C39—H39B	0.9800
C37—O31	1.418 (2)	C39—H39C	0.9800
C37—H37A	0.9900		

C2—N1—C8A	116.80 (15)	C3—C37—H37B	110.6
N1—C2—C3	126.94 (16)	H37A—C37—H37B	108.7
N1—C2—Cl2	115.65 (13)	C31—O31—C37	119.56 (14)
C3—C2—Cl2	117.41 (14)	O31—C31—C36	123.63 (15)
C4—C3—C2	115.97 (16)	O31—C31—C32	116.73 (15)
C4—C3—C37	122.75 (16)	C36—C31—C32	119.63 (16)
C2—C3—C37	121.27 (16)	C33—C32—C31	118.73 (15)
C3—C4—C4A	120.43 (16)	C33—C32—C38	119.78 (15)
C3—C4—H4	119.8	C31—C32—C38	121.48 (15)
C4A—C4—H4	119.8	C34—C33—C32	120.84 (16)
C4—C4A—C8A	117.96 (16)	C34—C33—H33	119.6
C4—C4A—C5	123.28 (16)	C32—C33—H33	119.6
C8A—C4A—C5	118.75 (17)	C33—C34—C35	120.69 (16)
C6—C5—C4A	120.70 (18)	C33—C34—Br34	118.86 (13)
C6—C5—H5	119.7	C35—C34—Br34	120.44 (13)
C4A—C5—H5	119.7	C36—C35—C34	119.18 (16)
C5—C6—C7	120.03 (18)	C36—C35—H35	120.4
C5—C6—H6	120.0	C34—C35—H35	120.4
C7—C6—H6	120.0	C35—C36—C31	120.88 (16)
C8—C7—C6	120.69 (19)	C35—C36—H36	119.6
C8—C7—H7	119.7	C31—C36—H36	119.6
C6—C7—H7	119.7	O38—C38—O39	122.23 (16)
C7—C8—C8A	120.48 (18)	O38—C38—C32	127.08 (16)
C7—C8—H8	119.8	O39—C38—C32	110.68 (15)
C8A—C8—H8	119.8	C38—O39—C39	115.37 (15)
N1—C8A—C8	118.90 (16)	O39—C39—H39A	109.5
N1—C8A—C4A	121.80 (16)	O39—C39—H39B	109.5
C8—C8A—C4A	119.31 (17)	H39A—C39—H39B	109.5
O31—C37—C3	105.92 (14)	O39—C39—H39C	109.5
O31—C37—H37A	110.6	H39A—C39—H39C	109.5
C3—C37—H37A	110.6	H39B—C39—H39C	109.5
O31—C37—H37B	110.6		

C8A—N1—C2—C3	1.0 (3)	C2—C3—C37—O31	−174.63 (17)
C8A—N1—C2—Cl2	−178.33 (13)	C3—C37—O31—C31	−175.71 (16)
N1—C2—C3—C4	−2.9 (3)	C37—O31—C31—C36	−6.4 (3)
Cl2—C2—C3—C4	176.39 (14)	C37—O31—C31—C32	173.73 (17)
N1—C2—C3—C37	175.89 (19)	O31—C31—C32—C33	−178.50 (16)
Cl2—C2—C3—C37	−4.8 (2)	C36—C31—C32—C33	1.6 (3)
C2—C3—C4—C4A	1.6 (3)	O31—C31—C32—C38	2.8 (3)
C37—C3—C4—C4A	−177.14 (17)	C36—C31—C32—C38	−177.03 (17)
C3—C4—C4A—C8A	1.1 (3)	C31—C32—C33—C34	−0.1 (3)
C3—C4—C4A—C5	−179.93 (18)	C38—C32—C33—C34	178.58 (17)

C4—C4A—C5—C6	−178.59 (19)	C32—C33—C34—C35	−1.0 (3)
C8A—C4A—C5—C6	0.3 (3)	C32—C33—C34—Br34	179.85 (14)
C4A—C5—C6—C7	1.4 (3)	C33—C34—C35—C36	0.5 (3)
C5—C6—C7—C8	−1.6 (3)	Br34—C34—C35—C36	179.65 (14)
C6—C7—C8—C8A	0.1 (3)	C34—C35—C36—C31	1.1 (3)
C2—N1—C8A—C8	−178.21 (17)	O31—C31—C36—C35	178.00 (17)
C2—N1—C8A—C4A	2.2 (3)	C32—C31—C36—C35	−2.2 (3)
C7—C8—C8A—N1	−178.03 (18)	C33—C32—C38—O38	−174.5 (2)
C7—C8—C8A—C4A	1.6 (3)	C31—C32—C38—O38	4.1 (3)
C4—C4A—C8A—N1	−3.2 (3)	C33—C32—C38—O39	4.3 (2)
C5—C4A—C8A—N1	177.82 (17)	C31—C32—C38—O39	−177.01 (17)
C4—C4A—C8A—C8	177.18 (17)	O38—C38—O39—C39	3.1 (3)
C5—C4A—C8A—C8	−1.8 (3)	C32—C38—O39—C39	−175.77 (17)
C4—C3—C37—O31	4.1 (3)		

(II) Methyl 5-bromo-2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate

Crystal data

$C_{19}H_{15}BrClNO_3$
M_r = 420.67
Orthorhombic, *Pbca*
a = 15.1920 (3) Å
b = 11.98641 (19) Å
c = 19.0307 (3) Å
V = 3465.44 (10) Å^3
Z = 8
$F(000)$ = 1696
D_x = 1.613 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3421 reflections
θ = 4.7–72.5°
μ = 4.81 mm^{-1}
T = 173 K
Block, colourless
0.24 × 0.16 × 0.08 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.399, T_{max} = 0.680
21861 measured reflections
3421 independent reflections
3062 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 72.5°, θ_{min} = 4.7°
h = −18→18
k = −14→12
l = −23→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.06
3421 reflections
229 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 1.8465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00048 (6)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.42983 (12)	0.87307 (15)	0.45790 (10)	0.0272 (4)
C2	0.42690 (13)	0.78272 (18)	0.42079 (11)	0.0249 (4)
Cl2	0.52936 (3)	0.72811 (5)	0.39507 (3)	0.03655 (16)
C3	0.35033 (14)	0.72343 (17)	0.40030 (10)	0.0226 (4)
C4	0.27189 (13)	0.76626 (18)	0.42260 (11)	0.0224 (4)
H4	0.2185	0.7297	0.4106	0.027*
C4A	0.26987 (13)	0.86525 (18)	0.46363 (11)	0.0219 (4)
C5	0.19142 (14)	0.91446 (18)	0.48888 (11)	0.0253 (4)
H5	0.1366	0.8805	0.4780	0.030*
C6	0.19242 (15)	1.00976 (18)	0.52857 (11)	0.0267 (4)
C7	0.27500 (15)	1.05991 (19)	0.54421 (12)	0.0302 (5)
H7	0.2765	1.1261	0.5716	0.036*
C8	0.35220 (15)	1.01485 (19)	0.52062 (12)	0.0299 (5)
H8	0.4066	1.0499	0.5316	0.036*
C8A	0.35123 (14)	0.91644 (17)	0.48007 (11)	0.0242 (4)
C37	0.35875 (13)	0.61865 (18)	0.35765 (11)	0.0243 (4)
H37A	0.3916	0.6338	0.3137	0.029*
H37B	0.3909	0.5610	0.3846	0.029*
O31	0.27182 (9)	0.58119 (13)	0.34187 (8)	0.0254 (3)
C31	0.26370 (13)	0.48636 (18)	0.30374 (11)	0.0224 (4)
C32	0.17885 (14)	0.45623 (18)	0.28094 (11)	0.0236 (4)
C33	0.16860 (15)	0.36086 (18)	0.23979 (11)	0.0267 (4)
H33	0.1116	0.3399	0.2240	0.032*
C34	0.24049 (16)	0.29669 (19)	0.22183 (11)	0.0271 (5)
Br34	0.22547 (2)	0.17010 (2)	0.16308 (2)	0.03596 (12)
C35	0.32387 (16)	0.32597 (18)	0.24421 (12)	0.0297 (5)
H35	0.3731	0.2813	0.2317	0.036*
C36	0.33537 (14)	0.42003 (18)	0.28463 (11)	0.0273 (5)
H36	0.3928	0.4401	0.2997	0.033*
C38	0.09631 (14)	0.5209 (2)	0.29458 (12)	0.0309 (5)
O38	0.03146 (13)	0.5097 (2)	0.25963 (13)	0.0739 (8)
O39	0.10112 (11)	0.59054 (16)	0.34798 (9)	0.0380 (4)
C39	0.02126 (19)	0.6494 (3)	0.36541 (18)	0.0522 (7)
H39A	0.0089	0.7052	0.3291	0.078*
H39B	0.0283	0.6866	0.4109	0.078*
H39C	−0.0277	0.5963	0.3680	0.078*
C61	0.10926 (16)	1.0618 (2)	0.55704 (13)	0.0365 (5)
H61A	0.0590	1.0382	0.5284	0.055*
H61B	0.1145	1.1432	0.5555	0.055*

H61C	0.1003	1.0376	0.6057	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0241 (9)	0.0257 (9)	0.0319 (10)	−0.0054 (7)	−0.0027 (7)	−0.0008 (8)
C2	0.0193 (10)	0.0264 (11)	0.0291 (11)	−0.0017 (8)	0.0002 (8)	0.0026 (8)
Cl2	0.0207 (3)	0.0373 (3)	0.0516 (4)	−0.0023 (2)	0.0022 (2)	−0.0088 (3)
C3	0.0236 (10)	0.0229 (10)	0.0214 (10)	−0.0037 (8)	−0.0022 (8)	0.0021 (8)
C4	0.0202 (10)	0.0249 (10)	0.0222 (10)	−0.0041 (8)	−0.0023 (7)	0.0023 (8)
C4A	0.0236 (10)	0.0226 (10)	0.0196 (10)	−0.0023 (8)	−0.0023 (7)	0.0033 (8)
C5	0.0248 (10)	0.0288 (11)	0.0224 (10)	−0.0030 (9)	−0.0021 (8)	0.0012 (8)
C6	0.0309 (11)	0.0263 (11)	0.0228 (10)	0.0025 (9)	−0.0017 (8)	0.0019 (8)
C7	0.0397 (13)	0.0231 (10)	0.0276 (11)	−0.0022 (9)	−0.0023 (9)	−0.0035 (9)
C8	0.0308 (11)	0.0263 (11)	0.0325 (11)	−0.0059 (9)	−0.0045 (9)	−0.0022 (9)
C8A	0.0262 (10)	0.0227 (10)	0.0238 (10)	−0.0040 (8)	−0.0038 (8)	0.0014 (8)
C37	0.0199 (10)	0.0245 (10)	0.0285 (11)	−0.0029 (8)	−0.0007 (8)	−0.0021 (9)
O31	0.0198 (7)	0.0252 (8)	0.0312 (8)	−0.0013 (6)	−0.0016 (5)	−0.0079 (6)
C31	0.0241 (10)	0.0226 (10)	0.0204 (10)	−0.0015 (8)	0.0002 (7)	0.0013 (8)
C32	0.0230 (10)	0.0237 (10)	0.0242 (10)	−0.0026 (8)	−0.0009 (8)	0.0037 (8)
C33	0.0283 (11)	0.0279 (11)	0.0238 (10)	−0.0068 (9)	−0.0032 (8)	0.0032 (9)
C34	0.0407 (12)	0.0212 (10)	0.0195 (10)	−0.0054 (9)	−0.0007 (9)	−0.0012 (8)
Br34	0.0551 (2)	0.02513 (16)	0.02764 (17)	−0.00542 (10)	−0.00230 (10)	−0.00488 (9)
C35	0.0322 (11)	0.0286 (12)	0.0283 (11)	0.0027 (9)	0.0045 (9)	−0.0016 (9)
C36	0.0225 (10)	0.0300 (12)	0.0294 (11)	−0.0023 (9)	0.0004 (8)	−0.0022 (9)
C38	0.0225 (10)	0.0334 (12)	0.0369 (12)	−0.0003 (9)	−0.0027 (9)	−0.0007 (10)
O38	0.0309 (10)	0.100 (2)	0.0905 (17)	0.0164 (11)	−0.0257 (11)	−0.0441 (16)
O39	0.0232 (8)	0.0460 (11)	0.0446 (10)	0.0068 (7)	0.0006 (7)	−0.0115 (8)
C39	0.0298 (13)	0.0636 (19)	0.0632 (19)	0.0151 (13)	0.0099 (13)	−0.0070 (16)
C61	0.0372 (13)	0.0366 (13)	0.0357 (13)	0.0042 (10)	0.0022 (10)	−0.0082 (10)

Geometric parameters (Å, º)

N1—C2	1.294 (3)	O31—C31	1.354 (3)
N1—C8A	1.369 (3)	C31—C36	1.396 (3)
C2—C3	1.418 (3)	C31—C32	1.407 (3)
C2—Cl2	1.758 (2)	C32—C33	1.394 (3)
C3—C4	1.365 (3)	C32—C38	1.497 (3)
C3—C37	1.501 (3)	C33—C34	1.379 (3)
C4—C4A	1.421 (3)	C33—H33	0.9500
C4—H4	0.9500	C34—C35	1.382 (3)
C4A—C5	1.414 (3)	C34—Br34	1.899 (2)
C4A—C8A	1.415 (3)	C35—C36	1.376 (3)
C5—C6	1.370 (3)	C35—H35	0.9500
C5—H5	0.9500	C36—H36	0.9500
C6—C7	1.423 (3)	C38—O38	1.196 (3)
C6—C61	1.509 (3)	C38—O39	1.317 (3)
C7—C8	1.367 (3)	O39—C39	1.442 (3)

C7—H7	0.9500	C39—H39A	0.9800
C8—C8A	1.410 (3)	C39—H39B	0.9800
C8—H8	0.9500	C39—H39C	0.9800
C37—O31	1.427 (2)	C61—H61A	0.9800
C37—H37A	0.9900	C61—H61B	0.9800
C37—H37B	0.9900	C61—H61C	0.9800

C2—N1—C8A	117.13 (18)	O31—C31—C36	123.12 (19)
N1—C2—C3	126.73 (19)	O31—C31—C32	117.66 (18)
N1—C2—Cl2	115.67 (15)	C36—C31—C32	119.2 (2)
C3—C2—Cl2	117.59 (16)	C33—C32—C31	119.1 (2)
C4—C3—C2	116.24 (19)	C33—C32—C38	115.38 (19)
C4—C3—C37	123.86 (18)	C31—C32—C38	125.50 (19)
C2—C3—C37	119.89 (19)	C34—C33—C32	120.5 (2)
C3—C4—C4A	120.25 (18)	C34—C33—H33	119.7
C3—C4—H4	119.9	C32—C33—H33	119.7
C4A—C4—H4	119.9	C33—C34—C35	120.5 (2)
C5—C4A—C8A	118.7 (2)	C33—C34—Br34	119.77 (17)
C5—C4A—C4	123.60 (18)	C35—C34—Br34	119.65 (18)
C8A—C4A—C4	117.70 (18)	C36—C35—C34	119.8 (2)
C6—C5—C4A	121.7 (2)	C36—C35—H35	120.1
C6—C5—H5	119.1	C34—C35—H35	120.1
C4A—C5—H5	119.1	C35—C36—C31	120.9 (2)
C5—C6—C7	118.5 (2)	C35—C36—H36	119.6
C5—C6—C61	122.2 (2)	C31—C36—H36	119.6
C7—C6—C61	119.2 (2)	O38—C38—O39	123.1 (2)
C8—C7—C6	121.4 (2)	O38—C38—C32	122.3 (2)
C8—C7—H7	119.3	O39—C38—C32	114.56 (18)
C6—C7—H7	119.3	C38—O39—C39	116.1 (2)
C7—C8—C8A	120.1 (2)	O39—C39—H39A	109.5
C7—C8—H8	120.0	O39—C39—H39B	109.5
C8A—C8—H8	120.0	H39A—C39—H39B	109.5
N1—C8A—C8	118.51 (19)	O39—C39—H39C	109.5
N1—C8A—C4A	121.94 (19)	H39A—C39—H39C	109.5
C8—C8A—C4A	119.5 (2)	H39B—C39—H39C	109.5
O31—C37—C3	107.35 (16)	C6—C61—H61A	109.5
O31—C37—H37A	110.2	C6—C61—H61B	109.5
C3—C37—H37A	110.2	H61A—C61—H61B	109.5
O31—C37—H37B	110.2	C6—C61—H61C	109.5
C3—C37—H37B	110.2	H61A—C61—H61C	109.5
H37A—C37—H37B	108.5	H61B—C61—H61C	109.5
C31—O31—C37	117.47 (16)		

C8A—N1—C2—C3	0.2 (3)	C4—C3—C37—O31	4.3 (3)
C8A—N1—C2—Cl2	−178.63 (15)	C2—C3—C37—O31	−176.93 (18)
N1—C2—C3—C4	−0.4 (3)	C3—C37—O31—C31	−179.57 (17)
Cl2—C2—C3—C4	178.35 (16)	C37—O31—C31—C36	5.4 (3)
N1—C2—C3—C37	−179.3 (2)	C37—O31—C31—C32	−172.62 (18)

Cl2—C2—C3—C37	−0.5 (3)	O31—C31—C32—C33	178.09 (18)
C2—C3—C4—C4A	0.3 (3)	C36—C31—C32—C33	0.0 (3)
C37—C3—C4—C4A	179.16 (19)	O31—C31—C32—C38	0.7 (3)
C3—C4—C4A—C5	−179.75 (19)	C36—C31—C32—C38	−177.4 (2)
C3—C4—C4A—C8A	0.0 (3)	C31—C32—C33—C34	0.2 (3)
C8A—C4A—C5—C6	0.0 (3)	C38—C32—C33—C34	177.8 (2)
C4—C4A—C5—C6	179.7 (2)	C32—C33—C34—C35	−0.1 (3)
C4A—C5—C6—C7	0.2 (3)	C32—C33—C34—Br34	−177.84 (16)
C4A—C5—C6—C61	−178.7 (2)	C33—C34—C35—C36	−0.1 (3)
C5—C6—C7—C8	−0.1 (3)	Br34—C34—C35—C36	177.58 (17)
C61—C6—C7—C8	178.9 (2)	C34—C35—C36—C31	0.3 (3)
C6—C7—C8—C8A	−0.2 (4)	O31—C31—C36—C35	−178.2 (2)
C2—N1—C8A—C8	180.0 (2)	C32—C31—C36—C35	−0.2 (3)
C2—N1—C8A—C4A	0.2 (3)	C33—C32—C38—O38	−18.0 (4)
C7—C8—C8A—N1	−179.4 (2)	C31—C32—C38—O38	159.5 (3)
C7—C8—C8A—C4A	0.4 (3)	C33—C32—C38—O39	161.8 (2)
C5—C4A—C8A—N1	179.49 (19)	C31—C32—C38—O39	−20.7 (3)
C4—C4A—C8A—N1	−0.3 (3)	O38—C38—O39—C39	3.5 (4)
C5—C4A—C8A—C8	−0.3 (3)	C32—C38—O39—C39	−176.4 (2)
C4—C4A—C8A—C8	179.95 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C36—H36···O38^{i}	0.95	2.53	3.277 (3)	136

Symmetry code: (i) *x*+1/2, *y*, −*z*+1/2.

(III) Methyl 2-[(2-chloro-6-methylquinolin-3-yl)methoxy]benzoate

Crystal data

$C_{19}H_{16}ClNO_3$
M_r = 341.78
Orthorhombic, $P2_12_12_1$
a = 13.5860 (3) Å
b = 15.5857 (2) Å
c = 30.9389 (5) Å
V = 6551.2 (2) Å^3
Z = 16
$F(000)$ = 2848
D_x = 1.386 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 12841 reflections
θ = 3.6–72.6°
μ = 2.21 mm^{-1}
T = 173 K
Block, colourless
0.48 × 0.26 × 0.14 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.472, T_{max} = 0.734
45901 measured reflections
12840 independent reflections
11257 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 72.6°, θ_{min} = 3.6°
h = −16→15
k = −19→15
l = −38→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.129$
$S = 1.04$
12840 reflections
874 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 0.9452P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.152 (16)

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N11	0.0311 (2)	0.26008 (18)	0.44748 (8)	0.0301 (6)
C12	0.0259 (3)	0.2694 (2)	0.40606 (10)	0.0293 (7)
Cl12	0.02044 (8)	0.17391 (5)	0.37626 (3)	0.0430 (2)
C13	0.0238 (2)	0.3474 (2)	0.38287 (10)	0.0268 (6)
C14	0.0259 (2)	0.4211 (2)	0.40728 (10)	0.0282 (7)
H14	0.0256	0.4756	0.3935	0.034*
C14A	0.0287 (2)	0.4159 (2)	0.45268 (11)	0.0282 (7)
C15	0.0243 (3)	0.4892 (2)	0.47997 (12)	0.0332 (7)
H15	0.0226	0.5447	0.4674	0.040*
C16	0.0225 (3)	0.4814 (3)	0.52403 (12)	0.0363 (8)
C17	0.0282 (3)	0.3981 (3)	0.54256 (11)	0.0382 (8)
H17	0.0286	0.3923	0.5731	0.046*
C18	0.0332 (3)	0.3261 (2)	0.51731 (11)	0.0348 (7)
H18	0.0371	0.2710	0.5304	0.042*
C18A	0.0325 (2)	0.3337 (2)	0.47186 (11)	0.0290 (7)
C137	0.0188 (3)	0.3476 (2)	0.33422 (10)	0.0302 (7)
H13A	0.0764	0.3171	0.3220	0.036*
H13B	−0.0418	0.3184	0.3243	0.036*
O131	0.0187 (2)	0.43457 (15)	0.32062 (7)	0.0346 (5)
C131	0.0188 (3)	0.4508 (2)	0.27728 (10)	0.0277 (7)
C132	0.0243 (3)	0.5371 (2)	0.26405 (10)	0.0284 (7)
C133	0.0259 (3)	0.5540 (2)	0.21978 (11)	0.0338 (8)
H133	0.0303	0.6119	0.2103	0.041*
C134	0.0215 (3)	0.4895 (3)	0.18938 (11)	0.0404 (9)
H134	0.0230	0.5027	0.1594	0.048*
C135	0.0147 (3)	0.4051 (3)	0.20307 (12)	0.0391 (8)
H135	0.0107	0.3602	0.1824	0.047*

C136	0.0138 (3)	0.3858 (2)	0.24656 (11)	0.0349 (8)
H136	0.0097	0.3276	0.2556	0.042*
C138	0.0272 (3)	0.6138 (2)	0.29250 (11)	0.0318 (7)
O138	0.0287 (3)	0.68600 (18)	0.27853 (9)	0.0590 (8)
O139	0.0286 (2)	0.59794 (16)	0.33477 (8)	0.0362 (6)
C139	0.0327 (3)	0.6724 (3)	0.36214 (12)	0.0412 (9)
H19A	0.0351	0.6543	0.3925	0.062*
H19B	−0.0259	0.7077	0.3574	0.062*
H19C	0.0917	0.7058	0.3553	0.062*
C161	0.0161 (4)	0.5585 (3)	0.55315 (13)	0.0489 (10)
H16A	0.0696	0.5566	0.5743	0.073*
H16B	−0.0473	0.5583	0.5683	0.073*
H16C	0.0217	0.6109	0.5358	0.073*
N21	0.2866 (2)	0.67705 (19)	0.53534 (10)	0.0345 (6)
C22	0.2884 (3)	0.6675 (2)	0.49411 (11)	0.0311 (7)
Cl22	0.30603 (8)	0.76266 (6)	0.46423 (3)	0.0463 (2)
C23	0.2803 (2)	0.5902 (2)	0.47028 (11)	0.0297 (7)
C24	0.2724 (3)	0.5170 (2)	0.49451 (11)	0.0312 (7)
H24	0.2675	0.4628	0.4806	0.037*
C24A	0.2716 (3)	0.5217 (2)	0.54036 (11)	0.0302 (7)
C25	0.2632 (3)	0.4488 (2)	0.56743 (12)	0.0359 (8)
H25	0.2604	0.3933	0.5548	0.043*
C26	0.2590 (3)	0.4568 (3)	0.61136 (13)	0.0406 (9)
C27	0.2650 (3)	0.5396 (3)	0.62980 (13)	0.0434 (9)
H27	0.2622	0.5453	0.6603	0.052*
C28	0.2746 (3)	0.6112 (3)	0.60521 (12)	0.0388 (8)
H28	0.2794	0.6660	0.6186	0.047*
C28A	0.2774 (3)	0.6041 (2)	0.55952 (12)	0.0332 (7)
C237	0.2795 (3)	0.5903 (2)	0.42186 (11)	0.0320 (7)
H23A	0.2233	0.6245	0.4110	0.038*
H23B	0.3411	0.6158	0.4106	0.038*
O231	0.2709 (2)	0.50396 (16)	0.40813 (8)	0.0375 (6)
C231	0.2748 (3)	0.4863 (2)	0.36514 (11)	0.0301 (7)
C232	0.2748 (3)	0.3993 (2)	0.35269 (11)	0.0294 (7)
C233	0.2777 (3)	0.3806 (2)	0.30865 (12)	0.0367 (8)
H233	0.2774	0.3223	0.2998	0.044*
C234	0.2811 (3)	0.4434 (3)	0.27777 (12)	0.0392 (9)
H234	0.2836	0.4286	0.2480	0.047*
C235	0.2810 (3)	0.5288 (3)	0.29027 (12)	0.0383 (8)
H235	0.2827	0.5727	0.2690	0.046*
C236	0.2782 (3)	0.5503 (2)	0.33367 (12)	0.0330 (7)
H236	0.2787	0.6090	0.3421	0.040*
C238	0.2727 (3)	0.3238 (2)	0.38217 (12)	0.0331 (8)
O238	0.2553 (3)	0.25274 (18)	0.36991 (10)	0.0546 (8)
O239	0.2936 (2)	0.34248 (17)	0.42314 (8)	0.0417 (6)
C239	0.2981 (3)	0.2700 (3)	0.45206 (13)	0.0485 (10)
H29A	0.3414	0.2260	0.4398	0.073*
H29B	0.2319	0.2462	0.4559	0.073*

H29C	0.3241	0.2885	0.4801	0.073*
C261	0.2477 (4)	0.3792 (3)	0.64007 (14)	0.0528 (11)
H26A	0.3075	0.3716	0.6574	0.079*
H26B	0.2372	0.3281	0.6222	0.079*
H26C	0.1912	0.3873	0.6593	0.079*
N31	0.5271 (2)	0.39181 (18)	0.44626 (9)	0.0282 (6)
C32	0.5293 (2)	0.3996 (2)	0.40484 (10)	0.0272 (7)
Cl32	0.53360 (8)	0.30319 (5)	0.37552 (3)	0.0403 (2)
C33	0.5300 (2)	0.4771 (2)	0.38069 (10)	0.0253 (6)
C34	0.5317 (2)	0.5512 (2)	0.40443 (10)	0.0272 (7)
H34	0.5335	0.6052	0.3902	0.033*
C34A	0.5309 (3)	0.5474 (2)	0.44993 (11)	0.0277 (7)
C35	0.5330 (3)	0.6216 (2)	0.47646 (12)	0.0345 (8)
H35	0.5362	0.6766	0.4633	0.041*
C36	0.5305 (3)	0.6157 (3)	0.52091 (12)	0.0387 (8)
C37	0.5264 (3)	0.5331 (3)	0.53988 (11)	0.0401 (8)
H37	0.5248	0.5285	0.5705	0.048*
C38	0.5248 (3)	0.4602 (3)	0.51574 (11)	0.0356 (8)
H38	0.5219	0.4057	0.5295	0.043*
C38A	0.5275 (3)	0.4658 (2)	0.46987 (10)	0.0279 (7)
C337	0.5297 (3)	0.4760 (2)	0.33200 (10)	0.0261 (6)
H33A	0.5895	0.4469	0.3210	0.031*
H33B	0.4711	0.4450	0.3211	0.031*
O331	0.5278 (2)	0.56258 (14)	0.31813 (7)	0.0317 (5)
C331	0.5256 (2)	0.5789 (2)	0.27513 (10)	0.0265 (6)
C332	0.5200 (3)	0.6657 (2)	0.26216 (10)	0.0299 (7)
C333	0.5204 (3)	0.6837 (2)	0.21809 (11)	0.0368 (8)
H333	0.5178	0.7418	0.2089	0.044*
C334	0.5244 (3)	0.6196 (3)	0.18732 (11)	0.0417 (9)
H334	0.5254	0.6336	0.1574	0.050*
C335	0.5269 (3)	0.5350 (2)	0.20050 (11)	0.0372 (8)
H335	0.5282	0.4905	0.1795	0.045*
C336	0.5277 (3)	0.5144 (2)	0.24398 (11)	0.0316 (7)
H336	0.5297	0.4560	0.2527	0.038*
C338	0.5135 (3)	0.7414 (2)	0.29139 (11)	0.0339 (7)
O338	0.4943 (3)	0.81240 (18)	0.27849 (10)	0.0545 (8)
O339	0.5325 (2)	0.72473 (16)	0.33255 (8)	0.0430 (6)
C339	0.5292 (4)	0.7983 (3)	0.36114 (13)	0.0584 (12)
H39A	0.5762	0.8417	0.3511	0.088*
H39B	0.5466	0.7803	0.3905	0.088*
H39C	0.4627	0.8226	0.3611	0.088*
C361	0.5325 (4)	0.6949 (3)	0.54871 (13)	0.0520 (11)
H36A	0.5506	0.7446	0.5310	0.078*
H36B	0.5810	0.6875	0.5719	0.078*
H36C	0.4673	0.7043	0.5614	0.078*
N41	0.7784 (2)	0.67216 (19)	0.35785 (9)	0.0312 (6)
C42	0.7768 (2)	0.6643 (2)	0.31639 (11)	0.0276 (7)
Cl42	0.77365 (8)	0.76085 (5)	0.28715 (3)	0.0395 (2)

C43	0.7776 (2)	0.5869 (2)	0.29224 (11)	0.0265 (7)
C44	0.7803 (2)	0.5131 (2)	0.31580 (11)	0.0283 (7)
H44	0.7824	0.4593	0.3014	0.034*
C44A	0.7802 (2)	0.5158 (2)	0.36136 (11)	0.0278 (7)
C45	0.7793 (3)	0.4418 (2)	0.38798 (12)	0.0338 (8)
H45	0.7787	0.3867	0.3749	0.041*
C46	0.7792 (3)	0.4481 (3)	0.43207 (13)	0.0371 (9)
C47	0.7801 (3)	0.5302 (3)	0.45138 (12)	0.0393 (9)
H47	0.7802	0.5347	0.4820	0.047*
C48	0.7811 (3)	0.6034 (3)	0.42712 (12)	0.0371 (8)
H48	0.7825	0.6578	0.4409	0.045*
C48A	0.7799 (2)	0.5982 (2)	0.38153 (10)	0.0284 (7)
C437	0.7759 (3)	0.5886 (2)	0.24373 (10)	0.0287 (7)
H43A	0.7172	0.6200	0.2333	0.034*
H43B	0.8355	0.6176	0.2325	0.034*
O431	0.77309 (19)	0.50187 (15)	0.22965 (8)	0.0334 (5)
C431	0.7656 (3)	0.4859 (2)	0.18670 (11)	0.0294 (7)
C432	0.7540 (2)	0.4005 (2)	0.17336 (11)	0.0314 (7)
C433	0.7493 (3)	0.3835 (2)	0.12886 (12)	0.0388 (8)
H433	0.7435	0.3257	0.1194	0.047*
C434	0.7528 (3)	0.4479 (3)	0.09854 (12)	0.0452 (10)
H434	0.7488	0.4348	0.0686	0.054*
C435	0.7621 (3)	0.5321 (3)	0.11217 (12)	0.0420 (9)
H435	0.7647	0.5770	0.0915	0.050*
C436	0.7678 (3)	0.5512 (2)	0.15565 (12)	0.0353 (8)
H436	0.7732	0.6093	0.1646	0.042*
C438	0.7472 (3)	0.3232 (2)	0.20179 (12)	0.0347 (8)
O438	0.7358 (3)	0.25227 (18)	0.18788 (10)	0.0560 (8)
O439	0.7541 (2)	0.33994 (16)	0.24416 (8)	0.0404 (6)
C439	0.7475 (4)	0.2656 (3)	0.27155 (13)	0.0501 (10)
H49A	0.7496	0.2835	0.3019	0.075*
H49B	0.8030	0.2272	0.2656	0.075*
H49C	0.6856	0.2355	0.2659	0.075*
C461	0.7757 (3)	0.3687 (3)	0.46052 (14)	0.0498 (11)
H46A	0.7075	0.3576	0.4693	0.075*
H46B	0.8163	0.3780	0.4863	0.075*
H46C	0.8009	0.3193	0.4444	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N11	0.0385 (15)	0.0228 (13)	0.0289 (13)	0.0008 (12)	−0.0018 (12)	0.0024 (11)
C12	0.0348 (17)	0.0208 (15)	0.0324 (16)	0.0002 (14)	−0.0029 (14)	−0.0009 (13)
Cl12	0.0731 (6)	0.0208 (4)	0.0351 (4)	−0.0022 (4)	−0.0056 (4)	−0.0023 (3)
C13	0.0278 (15)	0.0240 (16)	0.0286 (16)	0.0016 (13)	−0.0003 (13)	0.0023 (12)
C14	0.0306 (16)	0.0225 (16)	0.0315 (16)	−0.0009 (13)	−0.0002 (14)	0.0040 (13)
C14A	0.0254 (15)	0.0247 (16)	0.0345 (17)	−0.0018 (13)	−0.0005 (13)	−0.0019 (13)
C15	0.0321 (17)	0.0271 (17)	0.0404 (19)	0.0011 (14)	0.0004 (15)	−0.0037 (14)

C16	0.0306 (17)	0.040 (2)	0.039 (2)	−0.0001 (16)	−0.0027 (15)	−0.0103 (16)
C17	0.0402 (19)	0.048 (2)	0.0259 (16)	−0.0039 (18)	−0.0017 (15)	−0.0029 (15)
C18	0.0391 (19)	0.0345 (18)	0.0309 (17)	−0.0009 (16)	−0.0023 (15)	0.0030 (15)
C18A	0.0266 (16)	0.0276 (16)	0.0329 (17)	−0.0010 (13)	−0.0019 (13)	0.0001 (14)
C137	0.0413 (18)	0.0206 (15)	0.0287 (16)	0.0009 (14)	−0.0029 (14)	0.0027 (13)
O131	0.0548 (15)	0.0209 (11)	0.0282 (12)	0.0041 (11)	−0.0016 (11)	0.0038 (9)
C131	0.0296 (16)	0.0256 (16)	0.0279 (16)	0.0039 (13)	0.0008 (13)	0.0048 (13)
C132	0.0284 (16)	0.0270 (17)	0.0298 (17)	0.0045 (14)	0.0011 (13)	0.0042 (13)
C133	0.0373 (18)	0.0323 (18)	0.0316 (18)	0.0075 (15)	0.0034 (15)	0.0107 (14)
C134	0.049 (2)	0.046 (2)	0.0266 (17)	0.0104 (19)	0.0010 (16)	0.0043 (16)
C135	0.049 (2)	0.0355 (19)	0.0326 (18)	0.0083 (17)	−0.0029 (16)	−0.0056 (15)
C136	0.044 (2)	0.0251 (17)	0.0359 (18)	0.0066 (15)	0.0004 (15)	−0.0002 (14)
C138	0.0357 (18)	0.0251 (17)	0.0345 (17)	0.0045 (14)	−0.0010 (14)	0.0045 (14)
O138	0.108 (3)	0.0250 (14)	0.0440 (16)	0.0015 (16)	−0.0068 (17)	0.0038 (12)
O139	0.0511 (15)	0.0257 (12)	0.0318 (12)	−0.0007 (11)	−0.0024 (11)	−0.0004 (10)
C139	0.053 (2)	0.0323 (19)	0.0382 (19)	−0.0024 (18)	−0.0049 (17)	−0.0082 (16)
C161	0.054 (2)	0.049 (2)	0.044 (2)	0.003 (2)	0.0007 (19)	−0.0149 (19)
N21	0.0440 (17)	0.0262 (15)	0.0332 (15)	0.0035 (13)	−0.0030 (13)	−0.0036 (12)
C22	0.0377 (18)	0.0238 (16)	0.0318 (17)	0.0025 (14)	−0.0026 (13)	0.0006 (14)
Cl22	0.0791 (7)	0.0235 (4)	0.0363 (4)	0.0029 (4)	−0.0059 (4)	0.0019 (4)
C23	0.0307 (16)	0.0286 (17)	0.0297 (17)	0.0046 (14)	−0.0027 (13)	−0.0045 (14)
C24	0.0332 (17)	0.0237 (16)	0.0366 (19)	0.0004 (14)	−0.0022 (14)	−0.0045 (14)
C24A	0.0281 (16)	0.0295 (17)	0.0330 (18)	−0.0005 (14)	−0.0010 (14)	−0.0025 (14)
C25	0.0371 (19)	0.0314 (18)	0.039 (2)	−0.0024 (15)	−0.0011 (15)	0.0001 (15)
C26	0.040 (2)	0.045 (2)	0.037 (2)	−0.0038 (17)	−0.0008 (16)	0.0092 (17)
C27	0.046 (2)	0.054 (2)	0.0295 (18)	−0.0019 (19)	−0.0019 (16)	−0.0007 (17)
C28	0.048 (2)	0.039 (2)	0.0296 (18)	0.0000 (17)	−0.0002 (16)	−0.0060 (15)
C28A	0.0322 (17)	0.0314 (18)	0.0359 (18)	0.0022 (15)	−0.0013 (14)	−0.0021 (15)
C237	0.0403 (19)	0.0230 (16)	0.0328 (18)	0.0032 (14)	−0.0021 (14)	−0.0036 (14)
O231	0.0597 (16)	0.0244 (12)	0.0285 (13)	−0.0032 (11)	0.0045 (11)	−0.0034 (10)
C231	0.0297 (16)	0.0290 (17)	0.0316 (18)	−0.0023 (14)	−0.0020 (13)	−0.0035 (13)
C232	0.0286 (16)	0.0276 (17)	0.0321 (17)	−0.0028 (14)	−0.0032 (13)	−0.0032 (14)
C233	0.042 (2)	0.0306 (18)	0.0378 (19)	−0.0064 (16)	−0.0020 (16)	−0.0099 (15)
C234	0.048 (2)	0.043 (2)	0.0268 (18)	−0.0062 (18)	−0.0065 (15)	−0.0023 (16)
C235	0.041 (2)	0.040 (2)	0.0338 (19)	0.0003 (16)	−0.0053 (15)	0.0082 (16)
C236	0.0348 (18)	0.0275 (17)	0.0368 (19)	0.0012 (14)	−0.0039 (15)	0.0011 (14)
C238	0.0301 (16)	0.0297 (18)	0.039 (2)	−0.0025 (14)	0.0013 (14)	−0.0053 (15)
O238	0.088 (2)	0.0271 (14)	0.0490 (17)	−0.0156 (14)	−0.0052 (15)	−0.0007 (13)
O239	0.0632 (18)	0.0287 (13)	0.0330 (13)	0.0012 (12)	−0.0076 (12)	0.0028 (11)
C239	0.065 (3)	0.036 (2)	0.045 (2)	0.0049 (19)	−0.0081 (19)	0.0128 (18)
C261	0.061 (3)	0.049 (3)	0.048 (2)	−0.005 (2)	0.001 (2)	0.015 (2)
N31	0.0335 (14)	0.0237 (14)	0.0274 (13)	−0.0006 (12)	−0.0016 (11)	0.0024 (11)
C32	0.0324 (16)	0.0188 (15)	0.0302 (16)	−0.0016 (13)	−0.0026 (14)	−0.0014 (13)
Cl32	0.0723 (6)	0.0187 (4)	0.0299 (4)	−0.0005 (4)	−0.0027 (4)	−0.0015 (3)
C33	0.0249 (14)	0.0211 (15)	0.0300 (16)	0.0011 (12)	0.0012 (13)	0.0023 (13)
C34	0.0304 (16)	0.0203 (15)	0.0308 (16)	0.0017 (13)	0.0005 (14)	0.0026 (12)
C34A	0.0262 (16)	0.0268 (17)	0.0300 (17)	0.0016 (13)	−0.0013 (13)	−0.0033 (13)
C35	0.0377 (18)	0.0281 (17)	0.0377 (19)	0.0022 (15)	−0.0022 (15)	−0.0068 (15)

C36	0.0371 (19)	0.043 (2)	0.0364 (19)	0.0025 (17)	−0.0052 (15)	−0.0114 (16)
C37	0.042 (2)	0.053 (2)	0.0261 (17)	0.0016 (18)	−0.0019 (16)	−0.0059 (16)
C38	0.0412 (19)	0.039 (2)	0.0270 (17)	0.0004 (17)	−0.0025 (15)	0.0027 (15)
C38A	0.0277 (16)	0.0291 (17)	0.0268 (16)	−0.0011 (13)	−0.0015 (13)	0.0023 (13)
C337	0.0336 (16)	0.0178 (14)	0.0268 (16)	0.0008 (13)	0.0005 (13)	0.0026 (12)
O331	0.0517 (14)	0.0184 (11)	0.0251 (11)	−0.0017 (11)	0.0010 (11)	0.0016 (9)
C331	0.0296 (15)	0.0244 (16)	0.0254 (15)	−0.0011 (13)	−0.0001 (13)	0.0033 (12)
C332	0.0324 (17)	0.0255 (16)	0.0319 (17)	0.0009 (14)	−0.0019 (14)	0.0021 (13)
C333	0.045 (2)	0.0304 (18)	0.0345 (18)	0.0046 (16)	−0.0043 (16)	0.0113 (14)
C334	0.055 (2)	0.045 (2)	0.0244 (16)	0.007 (2)	−0.0042 (16)	0.0058 (16)
C335	0.045 (2)	0.038 (2)	0.0295 (17)	0.0029 (17)	−0.0036 (16)	−0.0040 (15)
C336	0.0418 (19)	0.0226 (16)	0.0304 (17)	−0.0010 (15)	0.0016 (15)	0.0016 (13)
C338	0.0391 (19)	0.0221 (16)	0.0406 (18)	0.0006 (15)	−0.0016 (15)	0.0046 (14)
O338	0.087 (2)	0.0234 (14)	0.0528 (17)	0.0118 (14)	−0.0069 (16)	0.0045 (12)
O339	0.0746 (19)	0.0206 (12)	0.0338 (13)	0.0021 (12)	−0.0089 (13)	−0.0035 (10)
C339	0.100 (4)	0.028 (2)	0.047 (2)	0.004 (2)	−0.007 (2)	−0.0121 (18)
C361	0.057 (3)	0.054 (3)	0.045 (2)	0.003 (2)	−0.003 (2)	−0.023 (2)
N41	0.0366 (16)	0.0262 (14)	0.0308 (14)	−0.0005 (12)	−0.0009 (12)	−0.0026 (12)
C42	0.0324 (17)	0.0205 (15)	0.0298 (16)	−0.0022 (13)	−0.0016 (13)	0.0015 (13)
Cl42	0.0676 (6)	0.0203 (4)	0.0306 (4)	−0.0046 (4)	−0.0026 (4)	0.0015 (3)
C43	0.0280 (16)	0.0233 (16)	0.0281 (16)	−0.0012 (13)	−0.0007 (13)	0.0007 (13)
C44	0.0307 (16)	0.0229 (16)	0.0313 (17)	0.0003 (13)	−0.0012 (13)	−0.0051 (13)
C44A	0.0241 (16)	0.0280 (17)	0.0314 (17)	0.0011 (13)	−0.0001 (13)	0.0028 (14)
C45	0.0330 (18)	0.0291 (18)	0.039 (2)	0.0034 (15)	−0.0007 (15)	0.0065 (15)
C46	0.0259 (17)	0.047 (2)	0.039 (2)	0.0050 (16)	−0.0011 (15)	0.0125 (17)
C47	0.040 (2)	0.052 (2)	0.0260 (17)	0.0009 (17)	−0.0003 (15)	0.0090 (16)
C48	0.041 (2)	0.039 (2)	0.0312 (18)	0.0008 (16)	−0.0028 (15)	−0.0050 (16)
C48A	0.0274 (16)	0.0318 (17)	0.0260 (16)	−0.0013 (13)	0.0010 (12)	0.0002 (14)
C437	0.0382 (18)	0.0207 (15)	0.0270 (16)	0.0016 (14)	0.0001 (13)	−0.0025 (13)
O431	0.0513 (15)	0.0210 (12)	0.0278 (12)	0.0010 (11)	−0.0005 (11)	−0.0040 (9)
C431	0.0322 (17)	0.0278 (17)	0.0282 (16)	0.0004 (14)	0.0012 (13)	−0.0039 (13)
C432	0.0329 (18)	0.0305 (18)	0.0307 (17)	−0.0020 (14)	0.0026 (13)	−0.0029 (14)
C433	0.049 (2)	0.0322 (18)	0.0356 (19)	−0.0055 (16)	0.0025 (16)	−0.0107 (16)
C434	0.061 (3)	0.048 (2)	0.0262 (18)	−0.004 (2)	0.0002 (17)	−0.0078 (16)
C435	0.056 (2)	0.041 (2)	0.0294 (19)	0.0004 (19)	0.0032 (17)	0.0040 (16)
C436	0.043 (2)	0.0286 (17)	0.0338 (19)	−0.0036 (16)	0.0031 (15)	−0.0020 (15)
C438	0.0402 (19)	0.0263 (18)	0.0376 (19)	0.0000 (15)	−0.0007 (14)	−0.0065 (14)
O438	0.092 (2)	0.0269 (14)	0.0488 (17)	−0.0053 (15)	−0.0008 (15)	−0.0079 (13)
O439	0.0629 (17)	0.0251 (12)	0.0332 (13)	−0.0066 (11)	−0.0010 (12)	0.0014 (10)
C439	0.078 (3)	0.0304 (19)	0.042 (2)	−0.007 (2)	−0.002 (2)	0.0069 (17)
C461	0.046 (2)	0.059 (3)	0.045 (2)	0.007 (2)	−0.0015 (19)	0.026 (2)

Geometric parameters (Å, º)

N11—C12	1.292 (4)	N31—C32	1.287 (4)
N11—C18A	1.373 (4)	N31—C38A	1.365 (4)
C12—C13	1.412 (4)	C32—C33	1.420 (4)
C12—Cl12	1.752 (3)	C32—Cl32	1.756 (3)

C13—C14	1.375 (4)	C33—C34	1.369 (4)
C13—C137	1.507 (4)	C33—C337	1.507 (4)
C14—C14A	1.408 (4)	C34—C34A	1.409 (4)
C14—H14	0.9500	C34—H34	0.9500
C14A—C18A	1.414 (5)	C34A—C38A	1.415 (5)
C14A—C15	1.421 (5)	C34A—C35	1.418 (5)
C15—C16	1.369 (5)	C35—C36	1.379 (5)
C15—H15	0.9500	C35—H35	0.9500
C16—C17	1.421 (6)	C36—C37	1.415 (6)
C16—C161	1.505 (5)	C36—C361	1.506 (5)
C17—C18	1.370 (5)	C37—C38	1.360 (5)
C17—H17	0.9500	C37—H37	0.9500
C18—C18A	1.411 (5)	C38—C38A	1.422 (5)
C18—H18	0.9500	C38—H38	0.9500
C137—O131	1.419 (4)	C337—O331	1.417 (4)
C137—H13A	0.9900	C337—H33A	0.9900
C137—H13B	0.9900	C337—H33B	0.9900
O131—C131	1.365 (4)	O331—C331	1.355 (4)
C131—C136	1.391 (5)	C331—C336	1.393 (5)
C131—C132	1.408 (5)	C331—C332	1.413 (4)
C132—C133	1.395 (4)	C332—C333	1.392 (5)
C132—C138	1.486 (5)	C332—C338	1.489 (5)
C133—C134	1.378 (5)	C333—C334	1.380 (5)
C133—H133	0.9500	C333—H333	0.9500
C134—C135	1.386 (6)	C334—C335	1.380 (5)
C134—H134	0.9500	C334—H334	0.9500
C135—C136	1.379 (5)	C335—C336	1.383 (5)
C135—H135	0.9500	C335—H335	0.9500
C136—H136	0.9500	C336—H336	0.9500
C138—O138	1.205 (4)	C338—O338	1.205 (5)
C138—O139	1.331 (4)	C338—O339	1.325 (4)
O139—C139	1.437 (4)	O339—C339	1.448 (4)
C139—H19A	0.9800	C339—H39A	0.9800
C139—H19B	0.9800	C339—H39B	0.9800
C139—H19C	0.9800	C339—H39C	0.9800
C161—H16A	0.9800	C361—H36A	0.9800
C161—H16B	0.9800	C361—H36B	0.9800
C161—H16C	0.9800	C361—H36C	0.9800
N21—C22	1.284 (4)	N41—C42	1.289 (4)
N21—C28A	1.367 (5)	N41—C48A	1.366 (4)
C22—C23	1.417 (5)	C42—C43	1.419 (5)
C22—Cl22	1.764 (4)	C42—Cl42	1.757 (3)
C23—C24	1.369 (5)	C43—C44	1.362 (5)
C23—C237	1.498 (5)	C43—C437	1.501 (4)
C24—C24A	1.420 (5)	C44—C44A	1.410 (5)
C24—H24	0.9500	C44—H44	0.9500
C24A—C25	1.415 (5)	C44A—C45	1.417 (5)
C24A—C28A	1.418 (5)	C44A—C48A	1.429 (5)

C25—C26	1.366 (5)	C45—C46	1.368 (5)
C25—H25	0.9500	C45—H45	0.9500
C26—C27	1.413 (6)	C46—C47	1.413 (6)
C26—C261	1.509 (5)	C46—C461	1.519 (5)
C27—C28	1.357 (6)	C47—C48	1.365 (5)
C27—H27	0.9500	C47—H47	0.9500
C28—C28A	1.419 (5)	C48—C48A	1.413 (5)
C28—H28	0.9500	C48—H48	0.9500
C237—O231	1.416 (4)	C437—O431	1.421 (4)
C237—H23A	0.9900	C437—H43A	0.9900
C237—H23B	0.9900	C437—H43B	0.9900
O231—C231	1.359 (4)	O431—C431	1.356 (4)
C231—C236	1.395 (5)	C431—C436	1.400 (5)
C231—C232	1.409 (5)	C431—C432	1.403 (5)
C232—C233	1.394 (5)	C432—C433	1.404 (5)
C232—C238	1.489 (5)	C432—C438	1.494 (5)
C233—C234	1.368 (5)	C433—C434	1.375 (6)
C233—H233	0.9500	C433—H433	0.9500
C234—C235	1.386 (6)	C434—C435	1.384 (6)
C234—H234	0.9500	C434—H434	0.9500
C235—C236	1.384 (5)	C435—C436	1.380 (5)
C235—H235	0.9500	C435—H435	0.9500
C236—H236	0.9500	C436—H436	0.9500
C238—O238	1.195 (4)	C438—O438	1.196 (5)
C238—O239	1.331 (4)	C438—O439	1.340 (4)
O239—C239	1.443 (4)	O439—C439	1.438 (4)
C239—H29A	0.9800	C439—H49A	0.9800
C239—H29B	0.9800	C439—H49B	0.9800
C239—H29C	0.9800	C439—H49C	0.9800
C261—H26A	0.9800	C461—H46A	0.9800
C261—H26B	0.9800	C461—H46B	0.9800
C261—H26C	0.9800	C461—H46C	0.9800
C12—N11—C18A	116.9 (3)	C32—N31—C38A	116.9 (3)
N11—C12—C13	127.0 (3)	N31—C32—C33	127.2 (3)
N11—C12—Cl12	115.4 (3)	N31—C32—Cl32	115.7 (2)
C13—C12—Cl12	117.6 (2)	C33—C32—Cl32	117.1 (2)
C14—C13—C12	116.1 (3)	C34—C33—C32	115.8 (3)
C14—C13—C137	123.2 (3)	C34—C33—C337	123.1 (3)
C12—C13—C137	120.7 (3)	C32—C33—C337	121.1 (3)
C13—C14—C14A	120.0 (3)	C33—C34—C34A	120.0 (3)
C13—C14—H14	120.0	C33—C34—H34	120.0
C14A—C14—H14	120.0	C34A—C34—H34	120.0
C14—C14A—C18A	118.2 (3)	C34—C34A—C38A	118.3 (3)
C14—C14A—C15	123.1 (3)	C34—C34A—C35	123.0 (3)
C18A—C14A—C15	118.7 (3)	C38A—C34A—C35	118.8 (3)
C16—C15—C14A	121.4 (3)	C36—C35—C34A	121.5 (3)
C16—C15—H15	119.3	C36—C35—H35	119.3

C14A—C15—H15	119.3	C34A—C35—H35	119.3
C15—C16—C17	118.8 (3)	C35—C36—C37	118.4 (3)
C15—C16—C161	121.8 (4)	C35—C36—C361	120.9 (4)
C17—C16—C161	119.4 (3)	C37—C36—C361	120.6 (3)
C18—C17—C16	121.4 (3)	C38—C37—C36	122.2 (3)
C18—C17—H17	119.3	C38—C37—H37	118.9
C16—C17—H17	119.3	C36—C37—H37	118.9
C17—C18—C18A	119.9 (3)	C37—C38—C38A	119.7 (4)
C17—C18—H18	120.0	C37—C38—H38	120.1
C18A—C18—H18	120.0	C38A—C38—H38	120.1
N11—C18A—C18	118.5 (3)	N31—C38A—C34A	121.8 (3)
N11—C18A—C14A	121.8 (3)	N31—C38A—C38	118.8 (3)
C18—C18A—C14A	119.7 (3)	C34A—C38A—C38	119.4 (3)
O131—C137—C13	107.4 (3)	O331—C337—C33	107.0 (3)
O131—C137—H13A	110.2	O331—C337—H33A	110.3
C13—C137—H13A	110.2	C33—C337—H33A	110.3
O131—C137—H13B	110.2	O331—C337—H33B	110.3
C13—C137—H13B	110.2	C33—C337—H33B	110.3
H13A—C137—H13B	108.5	H33A—C337—H33B	108.6
C131—O131—C137	117.9 (2)	C331—O331—C337	118.5 (2)
O131—C131—C136	122.4 (3)	O331—C331—C336	122.9 (3)
O131—C131—C132	117.6 (3)	O331—C331—C332	117.4 (3)
C136—C131—C132	120.0 (3)	C336—C331—C332	119.7 (3)
C133—C132—C131	117.8 (3)	C333—C332—C331	118.1 (3)
C133—C132—C138	115.4 (3)	C333—C332—C338	115.9 (3)
C131—C132—C138	126.8 (3)	C331—C332—C338	126.1 (3)
C134—C133—C132	122.1 (3)	C334—C333—C332	122.0 (3)
C134—C133—H133	119.0	C334—C333—H333	119.0
C132—C133—H133	119.0	C332—C333—H333	119.0
C133—C134—C135	119.2 (3)	C335—C334—C333	119.2 (3)
C133—C134—H134	120.4	C335—C334—H334	120.4
C135—C134—H134	120.4	C333—C334—H334	120.4
C136—C135—C134	120.4 (3)	C334—C335—C336	120.6 (3)
C136—C135—H135	119.8	C334—C335—H335	119.7
C134—C135—H135	119.8	C336—C335—H335	119.7
C135—C136—C131	120.5 (3)	C335—C336—C331	120.3 (3)
C135—C136—H136	119.8	C335—C336—H336	119.8
C131—C136—H136	119.8	C331—C336—H336	119.8
O138—C138—O139	121.7 (3)	O338—C338—O339	122.7 (3)
O138—C138—C132	122.6 (3)	O338—C338—C332	122.6 (3)
O139—C138—C132	115.6 (3)	O339—C338—C332	114.6 (3)
C138—O139—C139	115.4 (3)	C338—O339—C339	115.2 (3)
O139—C139—H19A	109.5	O339—C339—H39A	109.5
O139—C139—H19B	109.5	O339—C339—H39B	109.5
H19A—C139—H19B	109.5	H39A—C339—H39B	109.5
O139—C139—H19C	109.5	O339—C339—H39C	109.5
H19A—C139—H19C	109.5	H39A—C339—H39C	109.5
H19B—C139—H19C	109.5	H39B—C339—H39C	109.5

C16—C161—H16A	109.5	C36—C361—H36A	109.5
C16—C161—H16B	109.5	C36—C361—H36B	109.5
H16A—C161—H16B	109.5	H36A—C361—H36B	109.5
C16—C161—H16C	109.5	C36—C361—H36C	109.5
H16A—C161—H16C	109.5	H36A—C361—H36C	109.5
H16B—C161—H16C	109.5	H36B—C361—H36C	109.5
C22—N21—C28A	116.7 (3)	C42—N41—C48A	117.0 (3)
N21—C22—C23	127.9 (3)	N41—C42—C43	127.2 (3)
N21—C22—Cl22	115.2 (3)	N41—C42—Cl42	115.6 (3)
C23—C22—Cl22	116.9 (3)	C43—C42—Cl42	117.2 (2)
C24—C23—C22	115.5 (3)	C44—C43—C42	115.9 (3)
C24—C23—C237	123.2 (3)	C44—C43—C437	123.4 (3)
C22—C23—C237	121.3 (3)	C42—C43—C437	120.7 (3)
C23—C24—C24A	120.3 (3)	C43—C44—C44A	120.6 (3)
C23—C24—H24	119.8	C43—C44—H44	119.7
C24A—C24—H24	119.8	C44A—C44—H44	119.7
C25—C24A—C28A	119.0 (3)	C44—C44A—C45	123.8 (3)
C25—C24A—C24	123.4 (3)	C44—C44A—C48A	117.6 (3)
C28A—C24A—C24	117.6 (3)	C45—C44A—C48A	118.5 (3)
C26—C25—C24A	121.3 (4)	C46—C45—C44A	121.5 (4)
C26—C25—H25	119.4	C46—C45—H45	119.3
C24A—C25—H25	119.4	C44A—C45—H45	119.3
C25—C26—C27	118.8 (4)	C45—C46—C47	119.1 (3)
C25—C26—C261	121.1 (4)	C45—C46—C461	121.4 (4)
C27—C26—C261	120.0 (4)	C47—C46—C461	119.5 (4)
C28—C27—C26	122.0 (4)	C48—C47—C46	121.6 (3)
C28—C27—H27	119.0	C48—C47—H47	119.2
C26—C27—H27	119.0	C46—C47—H47	119.2
C27—C28—C28A	119.8 (4)	C47—C48—C48A	120.1 (4)
C27—C28—H28	120.1	C47—C48—H48	119.9
C28A—C28—H28	120.1	C48A—C48—H48	119.9
N21—C28A—C24A	122.0 (3)	N41—C48A—C48	119.2 (3)
N21—C28A—C28	118.9 (3)	N41—C48A—C44A	121.7 (3)
C24A—C28A—C28	119.1 (3)	C48—C48A—C44A	119.1 (3)
O231—C237—C23	107.4 (3)	O431—C437—C43	106.8 (3)
O231—C237—H23A	110.2	O431—C437—H43A	110.4
C23—C237—H23A	110.2	C43—C437—H43A	110.4
O231—C237—H23B	110.2	O431—C437—H43B	110.4
C23—C237—H23B	110.2	C43—C437—H43B	110.4
H23A—C237—H23B	108.5	H43A—C437—H43B	108.6
C231—O231—C237	118.9 (3)	C431—O431—C437	118.5 (3)
O231—C231—C236	122.7 (3)	O431—C431—C436	122.6 (3)
O231—C231—C232	117.5 (3)	O431—C431—C432	118.1 (3)
C236—C231—C232	119.8 (3)	C436—C431—C432	119.4 (3)
C233—C232—C231	117.9 (3)	C431—C432—C433	118.2 (3)
C233—C232—C238	115.7 (3)	C431—C432—C438	126.8 (3)
C231—C232—C238	126.3 (3)	C433—C432—C438	115.0 (3)
C234—C233—C232	122.2 (4)	C434—C433—C432	122.0 (3)

C234—C233—H233	118.9	C434—C433—H433	119.0
C232—C233—H233	118.9	C432—C433—H433	119.0
C233—C234—C235	119.5 (3)	C433—C434—C435	119.2 (3)
C233—C234—H234	120.3	C433—C434—H434	120.4
C235—C234—H234	120.3	C435—C434—H434	120.4
C236—C235—C234	120.2 (3)	C436—C435—C434	120.5 (4)
C236—C235—H235	119.9	C436—C435—H435	119.8
C234—C235—H235	119.9	C434—C435—H435	119.8
C235—C236—C231	120.3 (3)	C435—C436—C431	120.7 (3)
C235—C236—H236	119.8	C435—C436—H436	119.6
C231—C236—H236	119.8	C431—C436—H436	119.6
O238—C238—O239	123.2 (4)	O438—C438—O439	122.7 (4)
O238—C238—C232	122.8 (3)	O438—C438—C432	122.8 (3)
O239—C238—C232	114.0 (3)	O439—C438—C432	114.5 (3)
C238—O239—C239	115.4 (3)	C438—O439—C439	114.6 (3)
O239—C239—H29A	109.5	O439—C439—H49A	109.5
O239—C239—H29B	109.5	O439—C439—H49B	109.5
H29A—C239—H29B	109.5	H49A—C439—H49B	109.5
O239—C239—H29C	109.5	O439—C439—H49C	109.5
H29A—C239—H29C	109.5	H49A—C439—H49C	109.5
H29B—C239—H29C	109.5	H49B—C439—H49C	109.5
C26—C261—H26A	109.5	C46—C461—H46A	109.5
C26—C261—H26B	109.5	C46—C461—H46B	109.5
H26A—C261—H26B	109.5	H46A—C461—H46B	109.5
C26—C261—H26C	109.5	C46—C461—H46C	109.5
H26A—C261—H26C	109.5	H46A—C461—H46C	109.5
H26B—C261—H26C	109.5	H46B—C461—H46C	109.5

C18A—N11—C12—C13	1.6 (6)	C38A—N31—C32—C33	−1.5 (5)
C18A—N11—C12—Cl12	−178.1 (2)	C38A—N31—C32—Cl32	177.6 (2)
N11—C12—C13—C14	−1.1 (5)	N31—C32—C33—C34	2.3 (5)
Cl12—C12—C13—C14	178.6 (3)	Cl32—C32—C33—C34	−176.7 (3)
N11—C12—C13—C137	179.3 (3)	N31—C32—C33—C337	−178.2 (3)
Cl12—C12—C13—C137	−1.1 (5)	Cl32—C32—C33—C337	2.8 (4)
C12—C13—C14—C14A	−0.9 (5)	C32—C33—C34—C34A	−1.1 (5)
C137—C13—C14—C14A	178.8 (3)	C337—C33—C34—C34A	179.4 (3)
C13—C14—C14A—C18A	2.1 (5)	C33—C34—C34A—C38A	−0.5 (5)
C13—C14—C14A—C15	−175.6 (3)	C33—C34—C34A—C35	179.8 (3)
C14—C14A—C15—C16	176.9 (4)	C34—C34A—C35—C36	178.9 (3)
C18A—C14A—C15—C16	−0.7 (5)	C38A—C34A—C35—C36	−0.8 (6)
C14A—C15—C16—C17	1.9 (6)	C34A—C35—C36—C37	0.4 (6)
C14A—C15—C16—C161	−178.9 (3)	C34A—C35—C36—C361	−179.9 (4)
C15—C16—C17—C18	−1.5 (6)	C35—C36—C37—C38	−0.1 (6)
C161—C16—C17—C18	179.3 (4)	C361—C36—C37—C38	−179.8 (4)
C16—C17—C18—C18A	−0.1 (6)	C36—C37—C38—C38A	0.2 (6)
C12—N11—C18A—C18	176.9 (3)	C32—N31—C38A—C34A	−0.4 (5)
C12—N11—C18A—C14A	−0.2 (5)	C32—N31—C38A—C38	179.8 (3)
C17—C18—C18A—N11	−175.8 (3)	C34—C34A—C38A—N31	1.4 (5)

C17—C18—C18A—C14A	1.3 (5)	C35—C34A—C38A—N31	−178.9 (3)
C14—C14A—C18A—N11	−1.6 (5)	C34—C34A—C38A—C38	−178.9 (3)
C15—C14A—C18A—N11	176.2 (3)	C35—C34A—C38A—C38	0.9 (5)
C14—C14A—C18A—C18	−178.6 (3)	C37—C38—C38A—N31	179.2 (3)
C15—C14A—C18A—C18	−0.9 (5)	C37—C38—C38A—C34A	−0.6 (6)
C14—C13—C137—O131	0.9 (5)	C34—C33—C337—O331	−2.1 (4)
C12—C13—C137—O131	−179.4 (3)	C32—C33—C337—O331	178.4 (3)
C13—C137—O131—C131	177.2 (3)	C33—C337—O331—C331	−178.9 (3)
C137—O131—C131—C136	3.5 (5)	C337—O331—C331—C336	−1.8 (5)
C137—O131—C131—C132	−176.5 (3)	C337—O331—C331—C332	177.7 (3)
O131—C131—C132—C133	179.1 (3)	O331—C331—C332—C333	178.2 (3)
C136—C131—C132—C133	−0.9 (5)	C336—C331—C332—C333	−2.3 (5)
O131—C131—C132—C138	−1.9 (5)	O331—C331—C332—C338	−1.8 (5)
C136—C131—C132—C138	178.1 (3)	C336—C331—C332—C338	177.7 (3)
C131—C132—C133—C134	0.6 (6)	C331—C332—C333—C334	1.1 (6)
C138—C132—C133—C134	−178.6 (3)	C338—C332—C333—C334	−178.9 (4)
C132—C133—C134—C135	0.3 (6)	C332—C333—C334—C335	0.8 (6)
C133—C134—C135—C136	−0.9 (6)	C333—C334—C335—C336	−1.5 (6)
C134—C135—C136—C131	0.5 (6)	C334—C335—C336—C331	0.2 (6)
O131—C131—C136—C135	−179.6 (3)	O331—C331—C336—C335	−178.9 (3)
C132—C131—C136—C135	0.4 (6)	C332—C331—C336—C335	1.7 (5)
C133—C132—C138—O138	1.6 (6)	C333—C332—C338—O338	11.3 (6)
C131—C132—C138—O138	−177.5 (4)	C331—C332—C338—O338	−168.7 (4)
C133—C132—C138—O139	−178.1 (3)	C333—C332—C338—O339	−167.4 (3)
C131—C132—C138—O139	2.8 (6)	C331—C332—C338—O339	12.7 (5)
O138—C138—O139—C139	−0.5 (6)	O338—C338—O339—C339	−0.3 (6)
C132—C138—O139—C139	179.2 (3)	C332—C338—O339—C339	178.3 (4)
C28A—N21—C22—C23	1.2 (6)	C48A—N41—C42—C43	−0.9 (5)
C28A—N21—C22—Cl22	−177.2 (3)	C48A—N41—C42—Cl42	179.4 (2)
N21—C22—C23—C24	−2.1 (5)	N41—C42—C43—C44	0.0 (5)
Cl22—C22—C23—C24	176.4 (3)	Cl42—C42—C43—C44	179.8 (3)
N21—C22—C23—C237	177.4 (3)	N41—C42—C43—C437	−179.7 (3)
Cl22—C22—C23—C237	−4.2 (4)	Cl42—C42—C43—C437	0.1 (4)
C22—C23—C24—C24A	0.7 (5)	C42—C43—C44—C44A	1.3 (5)
C237—C23—C24—C24A	−178.7 (3)	C437—C43—C44—C44A	−179.0 (3)
C23—C24—C24A—C25	179.7 (3)	C43—C44—C44A—C45	177.5 (3)
C23—C24—C24A—C28A	1.1 (5)	C43—C44—C44A—C48A	−1.7 (5)
C28A—C24A—C25—C26	1.0 (5)	C44—C44A—C45—C46	−180.0 (3)
C24—C24A—C25—C26	−177.5 (4)	C48A—C44A—C45—C46	−0.8 (5)
C24A—C25—C26—C27	−1.1 (6)	C44A—C45—C46—C47	−0.1 (6)
C24A—C25—C26—C261	178.6 (4)	C44A—C45—C46—C461	178.5 (3)
C25—C26—C27—C28	0.1 (6)	C45—C46—C47—C48	0.1 (6)
C261—C26—C27—C28	−179.6 (4)	C461—C46—C47—C48	−178.5 (4)
C26—C27—C28—C28A	0.9 (6)	C46—C47—C48—C48A	0.8 (6)
C22—N21—C28A—C24A	1.0 (5)	C42—N41—C48A—C48	−179.6 (3)
C22—N21—C28A—C28	−179.7 (3)	C42—N41—C48A—C44A	0.4 (5)
C25—C24A—C28A—N21	179.3 (3)	C47—C48—C48A—N41	178.4 (3)
C24—C24A—C28A—N21	−2.1 (5)	C47—C48—C48A—C44A	−1.6 (5)

C25—C24A—C28A—C28	0.0 (5)	C44—C44A—C48A—N41	0.8 (5)
C24—C24A—C28A—C28	178.6 (3)	C45—C44A—C48A—N41	−178.4 (3)
C27—C28—C28A—N21	179.7 (4)	C44—C44A—C48A—C48	−179.2 (3)
C27—C28—C28A—C24A	−1.0 (6)	C45—C44A—C48A—C48	1.6 (5)
C24—C23—C237—O231	−0.8 (5)	C44—C43—C437—O431	2.7 (5)
C22—C23—C237—O231	179.8 (3)	C42—C43—C437—O431	−177.6 (3)
C23—C237—O231—C231	−175.9 (3)	C43—C437—O431—C431	176.4 (3)
C237—O231—C231—C236	−5.8 (5)	C437—O431—C431—C436	4.8 (5)
C237—O231—C231—C232	174.5 (3)	C437—O431—C431—C432	−174.4 (3)
O231—C231—C232—C233	179.3 (3)	O431—C431—C432—C433	−178.1 (3)
C236—C231—C232—C233	−0.3 (5)	C436—C431—C432—C433	2.7 (5)
O231—C231—C232—C238	−1.2 (5)	O431—C431—C432—C438	1.1 (5)
C236—C231—C232—C238	179.2 (3)	C436—C431—C432—C438	−178.1 (3)
C231—C232—C233—C234	0.3 (6)	C431—C432—C433—C434	−1.9 (6)
C238—C232—C233—C234	−179.2 (3)	C438—C432—C433—C434	178.8 (4)
C232—C233—C234—C235	−0.5 (6)	C432—C433—C434—C435	0.6 (6)
C233—C234—C235—C236	0.6 (6)	C433—C434—C435—C436	−0.1 (7)
C234—C235—C236—C231	−0.5 (6)	C434—C435—C436—C431	0.9 (6)
O231—C231—C236—C235	−179.2 (3)	O431—C431—C436—C435	178.5 (4)
C232—C231—C236—C235	0.4 (5)	C432—C431—C436—C435	−2.3 (6)
C233—C232—C238—O238	−14.2 (5)	C431—C432—C438—O438	178.9 (4)
C231—C232—C238—O238	166.4 (4)	C433—C432—C438—O438	−1.9 (6)
C233—C232—C238—O239	164.7 (3)	C431—C432—C438—O439	−0.7 (5)
C231—C232—C238—O239	−14.8 (5)	C433—C432—C438—O439	178.5 (3)
O238—C238—O239—C239	2.5 (6)	O438—C438—O439—C439	0.4 (6)
C232—C238—O239—C239	−176.4 (3)	C432—C438—O439—C439	−180.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C28—H28···N41^{i}	0.95	2.63	3.565 (5)	169
C136—H136···O138^{ii}	0.95	2.50	3.261 (4)	137
C236—H236···O438^{iii}	0.95	2.43	3.223 (4)	141
C336—H336···O338^{iv}	0.95	2.46	3.238 (4)	139
C436—H436···O238^{iii}	0.95	2.51	3.254 (4)	136
C337—H33*B*···*Cg*1	0.99	2.64	3.441 (4)	138
C437—H43*A*···*Cg*2	0.99	2.64	3.446 (4)	138

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

(IV) 2-Chloro-3-[(naphthalen-1-yloxy)methyl]quinoline

Crystal data

$C_{20}H_{14}ClNO$
M_r = 319.77
Monoclinic, $P2_1$
a = 5.3165 (3) Å
b = 10.5098 (4) Å
c = 13.6201 (7) Å
β = 98.527 (5)°
V = 752.62 (6) Å^3
Z = 2
F(000) = 332
D_x = 1.411 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 2014 reflections
θ = 3.3–72.6°

μ = 2.27 mm^{-1}
T = 173 K

Needle, colourless
0.34 × 0.10 × 0.08 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.551, T_{max} = 0.834
4606 measured reflections

2014 independent reflections
1938 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 72.6°, θ_{min} = 3.3°
h = −6→6
k = −8→12
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.08
2014 reflections
208 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Classical Flack method preferred over Parsons because s.u. lower.
Absolute structure parameter: −0.007 (18)

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}
N1	0.1678 (4)	0.8551 (2)	0.36307 (18)	0.0324 (5)
C2	0.3087 (5)	0.8457 (3)	0.29394 (19)	0.0300 (5)
Cl2	0.25067 (12)	0.95854 (7)	0.19826 (5)	0.04033 (19)
C3	0.5025 (5)	0.7539 (2)	0.28753 (19)	0.0291 (5)
C4	0.5420 (5)	0.6680 (3)	0.3636 (2)	0.0311 (5)
H4	0.6701	0.6049	0.3641	0.037*
C4A	0.3943 (5)	0.6721 (3)	0.4417 (2)	0.0301 (5)
C5	0.4220 (6)	0.5842 (3)	0.5210 (2)	0.0373 (6)
H5	0.5494	0.5202	0.5244	0.045*
C6	0.2686 (6)	0.5897 (3)	0.5927 (2)	0.0392 (6)
H6	0.2863	0.5284	0.6446	0.047*
C7	0.0835 (5)	0.6863 (3)	0.5899 (2)	0.0394 (6)
H7	−0.0216	0.6903	0.6404	0.047*
C8	0.0539 (5)	0.7742 (3)	0.5151 (2)	0.0375 (6)
H8	−0.0698	0.8396	0.5145	0.045*
C8A	0.2063 (5)	0.7682 (2)	0.4390 (2)	0.0301 (5)
C37A	0.6440 (5)	0.7514 (3)	0.20041 (19)	0.0309 (5)
H37A	0.5238	0.7395	0.1383	0.037*

H37B	0.7351	0.8329	0.1958	0.037*
O31	0.8208 (4)	0.64868 (19)	0.21392 (13)	0.0335 (4)
C31	0.9563 (5)	0.6249 (3)	0.13811 (19)	0.0300 (5)
C32	0.9293 (5)	0.6908 (3)	0.0506 (2)	0.0338 (6)
H32	0.8081	0.7576	0.0391	0.041*
C33	1.0815 (5)	0.6599 (3)	−0.0230 (2)	0.0359 (6)
H33	1.0579	0.7047	−0.0842	0.043*
C34	1.2606 (5)	0.5671 (3)	−0.0073 (2)	0.0372 (6)
H34	1.3650	0.5496	−0.0566	0.045*
C34A	1.2927 (5)	0.4962 (2)	0.0824 (2)	0.0323 (6)
C35	1.4795 (5)	0.3997 (3)	0.1028 (2)	0.0375 (6)
H35	1.5873	0.3812	0.0550	0.045*
C36	1.5078 (5)	0.3334 (3)	0.1892 (2)	0.0417 (7)
H36	1.6336	0.2687	0.2007	0.050*
C37	1.3522 (5)	0.3594 (3)	0.2622 (2)	0.0386 (6)
H37	1.3739	0.3127	0.3226	0.046*
C38	1.1692 (5)	0.4525 (3)	0.24564 (19)	0.0329 (5)
H38	1.0628	0.4690	0.2944	0.040*
C38A	1.1379 (5)	0.5238 (2)	0.1565 (2)	0.0288 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0306 (11)	0.0295 (11)	0.0363 (11)	0.0035 (9)	0.0022 (9)	−0.0015 (9)
C2	0.0298 (12)	0.0270 (12)	0.0313 (13)	−0.0002 (10)	−0.0016 (10)	0.0006 (10)
Cl2	0.0429 (3)	0.0359 (3)	0.0417 (3)	0.0079 (3)	0.0048 (2)	0.0091 (3)
C3	0.0259 (12)	0.0279 (12)	0.0319 (12)	−0.0018 (10)	−0.0011 (10)	−0.0042 (10)
C4	0.0276 (12)	0.0281 (12)	0.0365 (13)	0.0036 (10)	0.0016 (10)	−0.0036 (11)
C4A	0.0268 (11)	0.0267 (12)	0.0355 (13)	−0.0020 (10)	0.0007 (10)	−0.0045 (10)
C5	0.0376 (13)	0.0330 (14)	0.0403 (14)	0.0040 (11)	0.0029 (11)	0.0025 (11)
C6	0.0407 (15)	0.0389 (16)	0.0369 (14)	−0.0042 (13)	0.0023 (12)	0.0053 (12)
C7	0.0346 (14)	0.0493 (17)	0.0356 (14)	−0.0025 (13)	0.0090 (11)	−0.0027 (12)
C8	0.0321 (14)	0.0393 (15)	0.0410 (15)	0.0034 (12)	0.0050 (11)	−0.0038 (12)
C8A	0.0265 (11)	0.0286 (12)	0.0339 (13)	−0.0017 (10)	0.0006 (10)	−0.0046 (10)
C37A	0.0287 (12)	0.0285 (12)	0.0348 (13)	0.0013 (10)	0.0024 (10)	0.0010 (10)
O31	0.0363 (9)	0.0332 (10)	0.0320 (9)	0.0074 (8)	0.0078 (7)	0.0022 (7)
C31	0.0281 (12)	0.0308 (12)	0.0313 (12)	−0.0043 (10)	0.0053 (10)	−0.0024 (10)
C32	0.0327 (13)	0.0349 (14)	0.0331 (13)	0.0000 (11)	0.0027 (10)	−0.0005 (11)
C33	0.0386 (14)	0.0397 (15)	0.0287 (13)	−0.0083 (12)	0.0031 (11)	0.0006 (11)
C34	0.0365 (14)	0.0416 (15)	0.0348 (14)	−0.0083 (12)	0.0095 (11)	−0.0087 (12)
C34A	0.0290 (12)	0.0316 (14)	0.0355 (13)	−0.0061 (10)	0.0024 (10)	−0.0088 (10)
C35	0.0298 (13)	0.0373 (14)	0.0466 (15)	−0.0011 (11)	0.0095 (11)	−0.0108 (12)
C36	0.0313 (14)	0.0358 (15)	0.0571 (18)	0.0044 (12)	0.0033 (13)	−0.0027 (13)
C37	0.0358 (14)	0.0366 (14)	0.0423 (15)	0.0008 (12)	0.0023 (12)	0.0058 (13)
C38	0.0301 (11)	0.0324 (13)	0.0367 (12)	−0.0015 (12)	0.0063 (10)	−0.0015 (13)
C38A	0.0259 (11)	0.0270 (12)	0.0327 (12)	−0.0043 (9)	0.0013 (10)	−0.0039 (10)

Geometric parameters (Å, º)

N1—C2	1.291 (3)	C37A—H37B	0.9900
N1—C8A	1.372 (3)	O31—C31	1.367 (3)
C2—C3	1.424 (4)	C31—C32	1.368 (4)
C2—Cl2	1.755 (3)	C31—C38A	1.432 (4)
C3—C4	1.367 (4)	C32—C33	1.416 (4)
C3—C37A	1.497 (3)	C32—H32	0.9500
C4—C4A	1.413 (3)	C33—C34	1.357 (5)
C4—H4	0.9500	C33—H33	0.9500
C4A—C5	1.413 (4)	C34—C34A	1.420 (4)
C4A—C8A	1.418 (4)	C34—H34	0.9500
C5—C6	1.364 (4)	C34A—C35	1.417 (4)
C5—H5	0.9500	C34A—C38A	1.423 (4)
C6—C7	1.410 (4)	C35—C36	1.357 (4)
C6—H6	0.9500	C35—H35	0.9500
C7—C8	1.366 (4)	C36—C37	1.411 (4)
C7—H7	0.9500	C36—H36	0.9500
C8—C8A	1.409 (4)	C37—C38	1.375 (4)
C8—H8	0.9500	C37—H37	0.9500
C37A—O31	1.426 (3)	C38—C38A	1.416 (4)
C37A—H37A	0.9900	C38—H38	0.9500
C2—N1—C8A	117.4 (2)	H37A—C37A—H37B	108.4
N1—C2—C3	126.9 (2)	C31—O31—C37A	116.9 (2)
N1—C2—Cl2	115.61 (19)	O31—C31—C32	124.5 (2)
C3—C2—Cl2	117.5 (2)	O31—C31—C38A	114.9 (2)
C4—C3—C2	115.6 (2)	C32—C31—C38A	120.6 (2)
C4—C3—C37A	123.4 (2)	C31—C32—C33	120.2 (3)
C2—C3—C37A	120.9 (2)	C31—C32—H32	119.9
C3—C4—C4A	120.7 (2)	C33—C32—H32	119.9
C3—C4—H4	119.7	C34—C33—C32	121.0 (3)
C4A—C4—H4	119.7	C34—C33—H33	119.5
C4—C4A—C5	123.3 (2)	C32—C33—H33	119.5
C4—C4A—C8A	118.1 (2)	C33—C34—C34A	120.3 (2)
C5—C4A—C8A	118.6 (2)	C33—C34—H34	119.9
C6—C5—C4A	120.9 (3)	C34A—C34—H34	119.9
C6—C5—H5	119.5	C35—C34A—C34	122.4 (3)
C4A—C5—H5	119.5	C35—C34A—C38A	118.0 (3)
C5—C6—C7	120.0 (3)	C34—C34A—C38A	119.6 (3)
C5—C6—H6	120.0	C36—C35—C34A	121.5 (3)
C7—C6—H6	120.0	C36—C35—H35	119.3
C8—C7—C6	120.7 (3)	C34A—C35—H35	119.3
C8—C7—H7	119.7	C35—C36—C37	120.7 (3)
C6—C7—H7	119.7	C35—C36—H36	119.7
C7—C8—C8A	120.2 (3)	C37—C36—H36	119.7
C7—C8—H8	119.9	C38—C37—C36	119.8 (3)
C8A—C8—H8	119.9	C38—C37—H37	120.1

N1—C8A—C8	119.2 (2)	C36—C37—H37	120.1
N1—C8A—C4A	121.3 (2)	C37—C38—C38A	120.5 (2)
C8—C8A—C4A	119.5 (2)	C37—C38—H38	119.7
O31—C37A—C3	108.1 (2)	C38A—C38—H38	119.7
O31—C37A—H37A	110.1	C38—C38A—C34A	119.5 (2)
C3—C37A—H37A	110.1	C38—C38A—C31	122.2 (2)
O31—C37A—H37B	110.1	C34A—C38A—C31	118.2 (2)
C3—C37A—H37B	110.1		

C8A—N1—C2—C3	0.0 (4)	C3—C37A—O31—C31	175.4 (2)
C8A—N1—C2—Cl2	179.65 (19)	C37A—O31—C31—C32	−1.4 (4)
N1—C2—C3—C4	−0.5 (4)	C37A—O31—C31—C38A	177.9 (2)
Cl2—C2—C3—C4	179.83 (19)	O31—C31—C32—C33	179.2 (3)
N1—C2—C3—C37A	177.5 (2)	C38A—C31—C32—C33	−0.1 (4)
Cl2—C2—C3—C37A	−2.1 (3)	C31—C32—C33—C34	−1.7 (4)
C2—C3—C4—C4A	0.7 (4)	C32—C33—C34—C34A	2.1 (4)
C37A—C3—C4—C4A	−177.3 (2)	C33—C34—C34A—C35	−179.0 (2)
C3—C4—C4A—C5	178.4 (3)	C33—C34—C34A—C38A	−0.7 (4)
C3—C4—C4A—C8A	−0.5 (4)	C34—C34A—C35—C36	179.7 (3)
C4—C4A—C5—C6	−177.7 (3)	C38A—C34A—C35—C36	1.4 (4)
C8A—C4A—C5—C6	1.2 (4)	C34A—C35—C36—C37	−0.6 (4)
C4A—C5—C6—C7	−1.7 (4)	C35—C36—C37—C38	0.3 (4)
C5—C6—C7—C8	0.7 (5)	C36—C37—C38—C38A	−0.9 (4)
C6—C7—C8—C8A	0.9 (4)	C37—C38—C38A—C34A	1.8 (4)
C2—N1—C8A—C8	−179.1 (2)	C37—C38—C38A—C31	−177.5 (2)
C2—N1—C8A—C4A	0.3 (4)	C35—C34A—C38A—C38	−2.0 (4)
C7—C8—C8A—N1	178.0 (3)	C34—C34A—C38A—C38	179.6 (2)
C7—C8—C8A—C4A	−1.4 (4)	C35—C34A—C38A—C31	177.3 (2)
C4—C4A—C8A—N1	−0.1 (4)	C34—C34A—C38A—C31	−1.0 (3)
C5—C4A—C8A—N1	−179.0 (2)	O31—C31—C38A—C38	1.4 (3)
C4—C4A—C8A—C8	179.3 (2)	C32—C31—C38A—C38	−179.2 (2)
C5—C4A—C8A—C8	0.4 (4)	O31—C31—C38A—C34A	−177.9 (2)
C4—C3—C37A—O31	−1.1 (3)	C32—C31—C38A—C34A	1.4 (3)
C2—C3—C37A—O31	−179.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C37*A*—H37*A*···*Cg*3^{i}	0.99	2.74	3.552 (3)	139

Symmetry code: (i) *x*−1, *y*, *z*.

(V) {5-[(2-Chloroquinolin-3-yl)methoxy]-4-(hydroxymethyl)-6-methyl-pyridin-3-yl}methanol

Crystal data

$C_{18}H_{17}ClN_2O_3$	*b* = 15.3336 (4) Å
M_r = 344.79	*c* = 10.6570 (3) Å
Monoclinic, $P2_1/n$	*β* = 92.381 (3)°
a = 9.7866 (3) Å	*V* = 1597.85 (8) Å^3

$Z = 4$
$F(000) = 720$
$D_x = 1.433$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 3112 reflections
$\theta = 5.1–72.5°$
$\mu = 2.29$ mm^{-1}
$T = 173$ K
Block, colourless
0.42 × 0.38 × 0.32 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.375$, $T_{max} = 0.481$
9423 measured reflections
3112 independent reflections
2764 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 72.5°$, $\theta_{min} = 5.1°$
$h = -11 \rightarrow 9$
$k = -17 \rightarrow 18$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.127$
$S = 1.05$
3112 reflections
219 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0793P)^2 + 0.2783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.14131 (14)	0.33261 (9)	0.62337 (13)	0.0316 (3)
C2	0.16152 (16)	0.41138 (10)	0.58407 (15)	0.0285 (3)
Cl2	0.10286 (4)	0.49427 (3)	0.68208 (4)	0.03973 (18)
C3	0.22557 (16)	0.43634 (10)	0.47234 (16)	0.0289 (3)
C4	0.27768 (17)	0.36931 (11)	0.40445 (15)	0.0317 (4)
H4	0.3241	0.3818	0.3300	0.038*
C4A	0.26375 (17)	0.28188 (11)	0.44305 (16)	0.0310 (4)
C5	0.3168 (2)	0.21043 (12)	0.37582 (18)	0.0389 (4)
H5	0.3677	0.2203	0.3031	0.047*
C6	0.2941 (2)	0.12723 (12)	0.41650 (19)	0.0429 (5)
H6	0.3305	0.0795	0.3720	0.052*
C7	0.2183 (2)	0.11136 (12)	0.52249 (19)	0.0463 (5)
H7	0.2022	0.0530	0.5479	0.056*
C8	0.1668 (2)	0.17907 (12)	0.59013 (17)	0.0408 (4)
H8	0.1155	0.1677	0.6621	0.049*
C8A	0.19062 (18)	0.26579 (10)	0.55190 (16)	0.0313 (4)

C37	0.23683 (17)	0.52862 (11)	0.42748 (17)	0.0329 (4)
H37A	0.2336	0.5302	0.3345	0.039*
H37B	0.1596	0.5636	0.4573	0.039*
O31	0.36442 (11)	0.56428 (7)	0.47603 (10)	0.0276 (3)
N31	0.51999 (13)	0.70720 (9)	0.25268 (13)	0.0297 (3)
C32	0.47930 (15)	0.63485 (10)	0.30994 (15)	0.0259 (3)
C33	0.39991 (15)	0.64051 (10)	0.41634 (14)	0.0236 (3)
C34	0.36223 (15)	0.72095 (10)	0.46347 (14)	0.0258 (3)
C35	0.40670 (16)	0.79604 (10)	0.40161 (15)	0.0284 (3)
C36	0.48433 (17)	0.78469 (10)	0.29806 (16)	0.0311 (4)
H36	0.5145	0.8354	0.2561	0.037*
C321	0.52007 (17)	0.54887 (11)	0.25592 (17)	0.0329 (4)
H32A	0.5987	0.5572	0.2032	0.039*
H32B	0.4434	0.5249	0.2049	0.039*
H32C	0.5447	0.5084	0.3243	0.039*
C341	0.27452 (17)	0.72795 (11)	0.57607 (15)	0.0316 (4)
H41A	0.2588	0.6694	0.6119	0.038*
H41B	0.3204	0.7647	0.6416	0.038*
O341	0.14772 (13)	0.76632 (10)	0.53514 (12)	0.0437 (3)
H341	0.1027	0.7791	0.6056	0.066*
C351	0.36913 (19)	0.88673 (11)	0.44319 (18)	0.0371 (4)
H51A	0.3812	0.8906	0.5357	0.045*
H51B	0.4321	0.9293	0.4063	0.045*
O351	0.23190 (14)	0.90946 (8)	0.40706 (13)	0.0434 (3)
H351	0.1838	0.8642	0.4382	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0401 (7)	0.0246 (7)	0.0303 (7)	−0.0041 (5)	0.0016 (6)	0.0012 (5)
C2	0.0320 (7)	0.0220 (7)	0.0314 (8)	−0.0007 (6)	0.0000 (6)	−0.0026 (6)
Cl2	0.0436 (3)	0.0287 (2)	0.0476 (3)	0.00182 (15)	0.0100 (2)	−0.00770 (16)
C3	0.0312 (8)	0.0235 (8)	0.0318 (8)	−0.0028 (6)	−0.0022 (6)	0.0030 (6)
C4	0.0380 (8)	0.0295 (9)	0.0274 (8)	−0.0038 (6)	0.0000 (6)	0.0017 (6)
C4A	0.0377 (8)	0.0258 (8)	0.0290 (8)	−0.0007 (6)	−0.0044 (7)	−0.0014 (6)
C5	0.0460 (10)	0.0349 (9)	0.0353 (9)	0.0023 (7)	−0.0043 (8)	−0.0076 (7)
C6	0.0575 (11)	0.0270 (9)	0.0430 (10)	0.0059 (8)	−0.0132 (9)	−0.0105 (7)
C7	0.0708 (13)	0.0214 (8)	0.0453 (11)	−0.0039 (8)	−0.0149 (10)	−0.0006 (7)
C8	0.0602 (11)	0.0266 (9)	0.0350 (9)	−0.0081 (8)	−0.0051 (8)	0.0024 (7)
C8A	0.0413 (9)	0.0233 (8)	0.0285 (8)	−0.0029 (6)	−0.0068 (7)	0.0009 (6)
C37	0.0346 (8)	0.0255 (8)	0.0381 (9)	−0.0030 (6)	−0.0039 (7)	0.0081 (7)
O31	0.0319 (6)	0.0216 (5)	0.0292 (6)	−0.0012 (4)	0.0000 (4)	0.0060 (4)
N31	0.0299 (7)	0.0274 (7)	0.0324 (7)	−0.0012 (5)	0.0082 (5)	0.0014 (5)
C32	0.0255 (7)	0.0240 (8)	0.0280 (8)	0.0017 (6)	0.0018 (6)	−0.0011 (6)
C33	0.0254 (7)	0.0204 (7)	0.0251 (7)	−0.0004 (5)	0.0005 (6)	0.0025 (5)
C34	0.0284 (7)	0.0250 (8)	0.0240 (7)	0.0007 (5)	0.0012 (6)	−0.0002 (6)
C35	0.0333 (8)	0.0201 (7)	0.0318 (8)	−0.0005 (6)	0.0025 (6)	−0.0011 (6)
C36	0.0331 (8)	0.0256 (8)	0.0351 (9)	−0.0033 (6)	0.0064 (6)	0.0038 (6)

C321	0.0363 (8)	0.0274 (8)	0.0354 (9)	0.0056 (6)	0.0058 (7)	−0.0048 (7)
C341	0.0407 (9)	0.0304 (8)	0.0244 (8)	0.0032 (6)	0.0084 (6)	−0.0011 (6)
O341	0.0404 (7)	0.0575 (8)	0.0343 (7)	0.0124 (6)	0.0145 (5)	0.0018 (6)
C351	0.0481 (10)	0.0220 (8)	0.0415 (10)	0.0018 (7)	0.0067 (8)	−0.0035 (7)
O351	0.0531 (8)	0.0307 (7)	0.0467 (8)	0.0135 (6)	0.0046 (6)	−0.0013 (5)

Geometric parameters (Å, º)

N1—C2	1.296 (2)	N31—C36	1.335 (2)
N1—C8A	1.376 (2)	N31—C32	1.335 (2)
C2—C3	1.421 (2)	C32—C33	1.404 (2)
C2—Cl2	1.7566 (16)	C32—C321	1.499 (2)
C3—C4	1.368 (2)	C33—C34	1.388 (2)
C3—C37	1.499 (2)	C34—C35	1.405 (2)
C4—C4A	1.411 (2)	C34—C341	1.508 (2)
C4—H4	0.9500	C35—C36	1.377 (2)
C4A—C8A	1.410 (2)	C35—C351	1.510 (2)
C4A—C5	1.419 (2)	C36—H36	0.9500
C5—C6	1.368 (3)	C321—H32A	0.9800
C5—H5	0.9500	C321—H32B	0.9800
C6—C7	1.398 (3)	C321—H32C	0.9800
C6—H6	0.9500	C341—O341	1.425 (2)
C7—C8	1.372 (3)	C341—H41A	0.9900
C7—H7	0.9500	C341—H41B	0.9900
C8—C8A	1.413 (2)	O341—H341	0.9077
C8—H8	0.9500	C351—O351	1.425 (2)
C37—O31	1.4394 (19)	C351—H51A	0.9900
C37—H37A	0.9900	C351—H51B	0.9900
C37—H37B	0.9900	O351—H351	0.9093
O31—C33	1.3819 (18)		
C2—N1—C8A	116.95 (14)	N31—C32—C33	120.23 (14)
N1—C2—C3	126.88 (15)	N31—C32—C321	117.78 (14)
N1—C2—Cl2	115.09 (12)	C33—C32—C321	121.98 (14)
C3—C2—Cl2	118.02 (12)	O31—C33—C34	120.64 (14)
C4—C3—C2	115.34 (14)	O31—C33—C32	118.54 (13)
C4—C3—C37	120.45 (15)	C34—C33—C32	120.78 (13)
C2—C3—C37	124.21 (15)	C33—C34—C35	117.81 (14)
C3—C4—C4A	121.15 (15)	C33—C34—C341	121.33 (14)
C3—C4—H4	119.4	C35—C34—C341	120.85 (14)
C4A—C4—H4	119.4	C36—C35—C34	117.68 (14)
C8A—C4A—C4	117.69 (15)	C36—C35—C351	120.08 (15)
C8A—C4A—C5	119.29 (15)	C34—C35—C351	122.22 (15)
C4—C4A—C5	123.00 (16)	N31—C36—C35	124.36 (14)
C6—C5—C4A	119.48 (18)	N31—C36—H36	117.8
C6—C5—H5	120.3	C35—C36—H36	117.8
C4A—C5—H5	120.3	C32—C321—H32A	109.5
C5—C6—C7	121.11 (17)	C32—C321—H32B	109.5

C5—C6—H6	119.4	H32A—C321—H32B	109.5
C7—C6—H6	119.4	C32—C321—H32C	109.5
C8—C7—C6	120.77 (17)	H32A—C321—H32C	109.5
C8—C7—H7	119.6	H32B—C321—H32C	109.5
C6—C7—H7	119.6	O341—C341—C34	107.64 (13)
C7—C8—C8A	119.49 (18)	O341—C341—H41A	110.2
C7—C8—H8	120.3	C34—C341—H41A	110.2
C8A—C8—H8	120.3	O341—C341—H41B	110.2
N1—C8A—C4A	121.79 (15)	C34—C341—H41B	110.2
N1—C8A—C8	118.38 (16)	H41A—C341—H41B	108.5
C4A—C8A—C8	119.83 (16)	C341—O341—H341	106.4
O31—C37—C3	108.55 (12)	O351—C351—C35	112.61 (14)
O31—C37—H37A	110.0	O351—C351—H51A	109.1
C3—C37—H37A	110.0	C35—C351—H51A	109.1
O31—C37—H37B	110.0	O351—C351—H51B	109.1
C3—C37—H37B	110.0	C35—C351—H51B	109.1
H37A—C37—H37B	108.4	H51A—C351—H51B	107.8
C33—O31—C37	112.75 (11)	C351—O351—H351	102.2
C36—N31—C32	119.13 (14)		

C8A—N1—C2—C3	2.2 (2)	C3—C37—O31—C33	165.21 (13)
C8A—N1—C2—Cl2	−177.48 (11)	C36—N31—C32—C33	0.1 (2)
N1—C2—C3—C4	−4.1 (2)	C36—N31—C32—C321	179.48 (14)
Cl2—C2—C3—C4	175.57 (12)	C37—O31—C33—C34	92.25 (17)
N1—C2—C3—C37	175.40 (15)	C37—O31—C33—C32	−90.17 (17)
Cl2—C2—C3—C37	−4.9 (2)	N31—C32—C33—O31	−177.42 (13)
C2—C3—C4—C4A	1.8 (2)	C321—C32—C33—O31	3.2 (2)
C37—C3—C4—C4A	−177.78 (14)	N31—C32—C33—C34	0.2 (2)
C3—C4—C4A—C8A	1.9 (2)	C321—C32—C33—C34	−179.21 (14)
C3—C4—C4A—C5	−179.68 (15)	O31—C33—C34—C35	177.22 (13)
C8A—C4A—C5—C6	1.1 (3)	C32—C33—C34—C35	−0.3 (2)
C4—C4A—C5—C6	−177.29 (16)	O31—C33—C34—C341	−3.8 (2)
C4A—C5—C6—C7	0.7 (3)	C32—C33—C34—C341	178.71 (14)
C5—C6—C7—C8	−1.3 (3)	C33—C34—C35—C36	0.2 (2)
C6—C7—C8—C8A	0.1 (3)	C341—C34—C35—C36	−178.80 (14)
C2—N1—C8A—C4A	2.0 (2)	C33—C34—C35—C351	178.66 (14)
C2—N1—C8A—C8	−178.19 (15)	C341—C34—C35—C351	−0.4 (2)
C4—C4A—C8A—N1	−4.0 (2)	C32—N31—C36—C35	−0.2 (3)
C5—C4A—C8A—N1	177.53 (15)	C34—C35—C36—N31	0.0 (3)
C4—C4A—C8A—C8	176.21 (15)	C351—C35—C36—N31	−178.46 (15)
C5—C4A—C8A—C8	−2.3 (2)	C33—C34—C341—O341	−114.67 (16)
C7—C8—C8A—N1	−178.14 (16)	C35—C34—C341—O341	64.32 (19)
C7—C8—C8A—C4A	1.7 (3)	C36—C35—C351—O351	102.07 (19)
C4—C3—C37—O31	−88.42 (18)	C34—C35—C351—O351	−76.3 (2)
C2—C3—C37—O31	92.08 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O341—H341···N31^{i}	0.91	1.81	2.7098 (19)	174
O351—H351···O341	0.91	1.86	2.7299 (19)	158
C4—H4···O351^{ii}	0.95	2.60	3.374 (2)	139

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