Crystal structure of (RS)-(4-chlorophenyl)(pyridin-2-yl)methanol

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In the title racemic compound, $C_{12}H_{10}ClNO$, the dihedral angle between the benzene and pyridine rings is 74.34 (6)°. In the crystal, the molecules are linked by O—H···N hydrogen bonds, forming zigzag $C(5)$ [001] chains in which alternating R- and S-configuration molecules are related by c-glide symmetry. In addition, inversion-related pairs of molecules are linked into dimers by pairs of weak C—Cl···π(pyridyl) interactions, which link the hydrogen-bonded chains into (100) sheets. Structural comparisons are drawn with a number of related compounds.

1. Chemical context

Simply substituted diphenylmethanols, RPh_2COH, exhibit a very rich diversity of supramolecular arrangements, including isolated molecules, hydrogen-bonded dimers, trimers, tetramers and hexamers, as well as continuous hydrogen-bonded chains (Ferguson *et al.*, 1992, 1994, 1995). The predominant mode of molecular association in these structures involves O—H···O hydrogen bonds, although O—H···π(arene) interactions are sometimes present. It is therefore of considerable interest to investigate the influence of an addition potential acceptor of hydrogen bonds as achieved, for example, by the replacement of one of the phenyl rings by an isosteric pyridyl substituent. Here we report the molecular and supramolecular structure of (RS)-4-chlorophenyl(pyridin-2-yl)methanol (I) (Fig. 1), which shows some striking structural differences from the simpler, non-chlorinated analogue phenyl(pyridin-2-yl)methanol, whose structure has been reported recently (Kim & Kang, 2014; Tsang *et al.*, 2015).
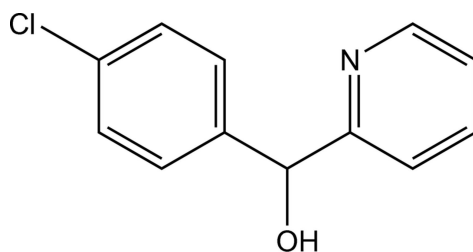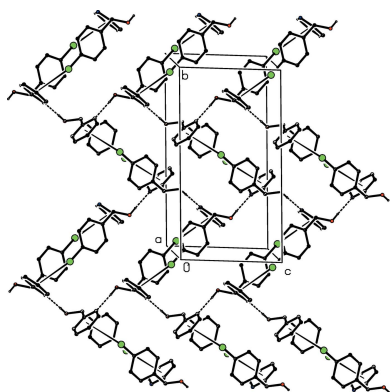
2. Structural commentary

The molecules of compound (I) contain a stereogenic centre at atom C1 (Fig. 1) and the reference molecule was selected as one having the R-configuration at atom C1. The centrosym-

Table 1
Selected torsion angles (°).

O1—C1—C11—C12	−51.14 (17)	C11—C1—O1—H1A	−180.0 (17)
O1—C1—C22—N21	−156.41 (13)		

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1A⋯N21^i	0.84 (2)	2.01 (2)	2.8444 (18)	176 (2)

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

metric space group confirms that compound (I) has crystallized as a racemic mixture.

Both of the rings are rotated out of the plane of the central C11–C1–C22 fragment, which makes dihedral angles of 70.69 (2) and 84.66 (9)° with the phenyl and pyridyl rings, respectively. The dihedral angle between the rings is 74.34 (6)°, and this value is very similar to the value of 71.42 (10)° reported (Kim & Kang, 2014) for the corresponding angle in the non-chlorinated analogue, compound (II). The general conformational similarity between the molecules of compounds (I) and (II) is shown by the torsional angles O—C—C—C and O—C—C—N (Table 1), where the corresponding angles for the *R*-enantiomer of (II) [the reference molecule was actually selected (Kim & Kang, 2014) as one having the *S*-configuration] are 49.0 (4) and −150.6 (2)°, respectively.

However, one point of difference between the conformations in compounds (I) and (II) centres on the locations of the hydroxyl H atoms. In compound (I), this atom is antiperiplanar to atom C11 (Table 1), but the corresponding torsional angle for the *R*-enantiomer of (II) is −67 (2)°. This difference in hydroxyl group conformations is probably associated with the different patterns of hydrogen-bonded supramolecular aggregation in compounds (I) and (II), as discussed below.

3. Supramolecular interactions

The molecules of compound (I) are linked by O—H⋯N hydrogen bonds (Table 2), forming zigzag $C(5)$ chains running parallel to the [001] direction. The chain containing the reference molecule at (x, y, z) consists of molecules which are related by the *c*-glide plane at $y = \frac{1}{4}$, so that molecules of *R*-configuration and *S*-configuration alternate along the chain
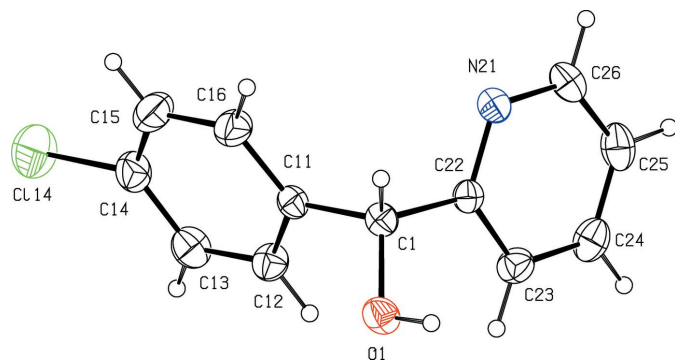
(Fig. 2). Two chains of this type, related to one another by inversion, pass through each unit cell.

The crystal structure of compound (I) contains neither C—H⋯π hydrogen bonds nor π–π stacking interactions. There is, however, a single short C—Cl⋯π contact with geometric parameters Cl⋯Cg^i = 3.5280 (10) Å, C⋯Cg^i = 5.1785 (19) Å and C—Cl⋯Cg^i = 157.79 (7)° [symmetry code: (i) $1 - x, -y, -z$] where Cg represents the centroid of the pyridine ring. This Cl⋯Cg distance is slightly shorter than the average distance, 3.6 Å, deduced (Imai *et al.*, 2008) from database analysis in a study which concluded that such interactions were attractive, with interaction energies of *ca* 2 kcal mol^{-1}, comparable to those typical of weak hydrogen bonds

Figure 1
The molecular structure of the *R*-enantiomer of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.
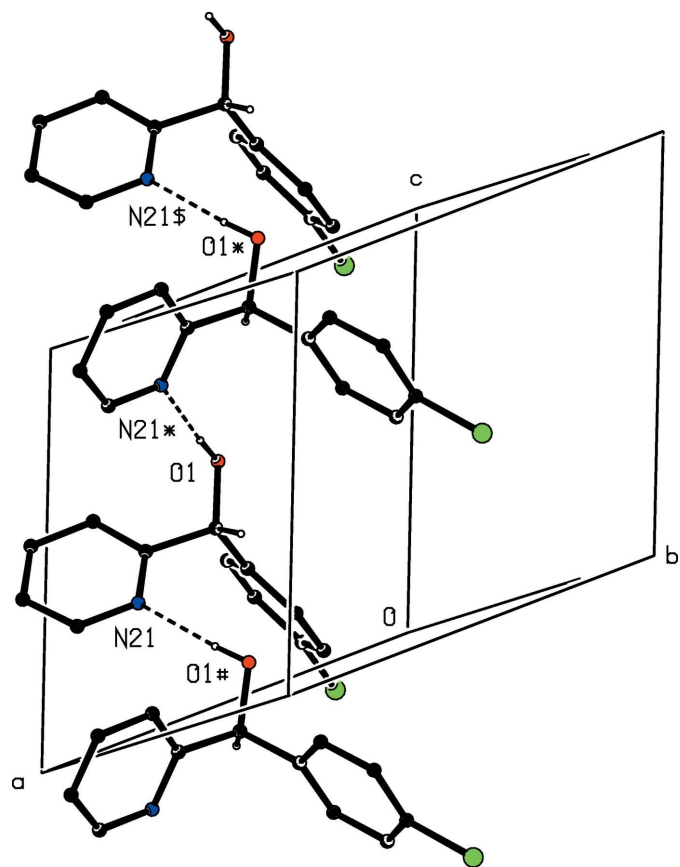
Figure 2
Part of the crystal structure of compound (I), showing the formation of a hydrogen-bonded $C(5)$ chain containing alternating enantiomers and running parallel to [001]. For the sake of clarity, the H atoms bonded to the ring C atoms have been omitted. The atoms marked with an asterisk (*), a hash (#) or a dollar sign ($) are at the symmetry positions $(x, \frac{1}{2} - y, \frac{1}{2} + z)$, $(x, \frac{1}{2} - y, -\frac{1}{2} + z)$ and $(x, y, 1 + z)$, respectively.
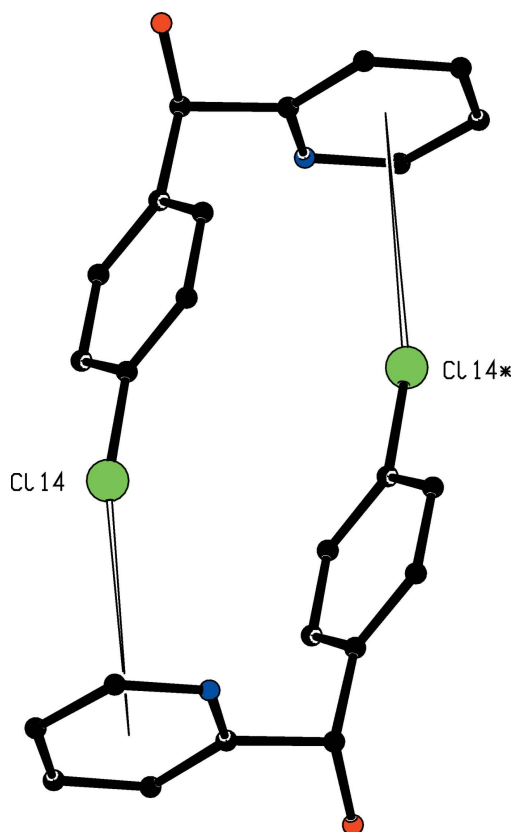
Figure 3
A centrosymmetric dimer in in the crystal of (I) in which the molecules are linked by C—Cl···π interactions, shown as hollow lines. For the sake of clarity, all of the H atoms have been omitted. The Cl atom marked with an asterisk (*) is at the symmetry position ($1 - x$, $-y$, $-z$).

Figure 4
A view of part of the crystal structure of (I), showing the formation of a sheet parallel to (001) built from hydrogen-bonded chains linked by C—Cl···π interactions. For the sake of clarity, the H atoms bonded to C atoms have all been omitted.

Figure 5
Related compounds.

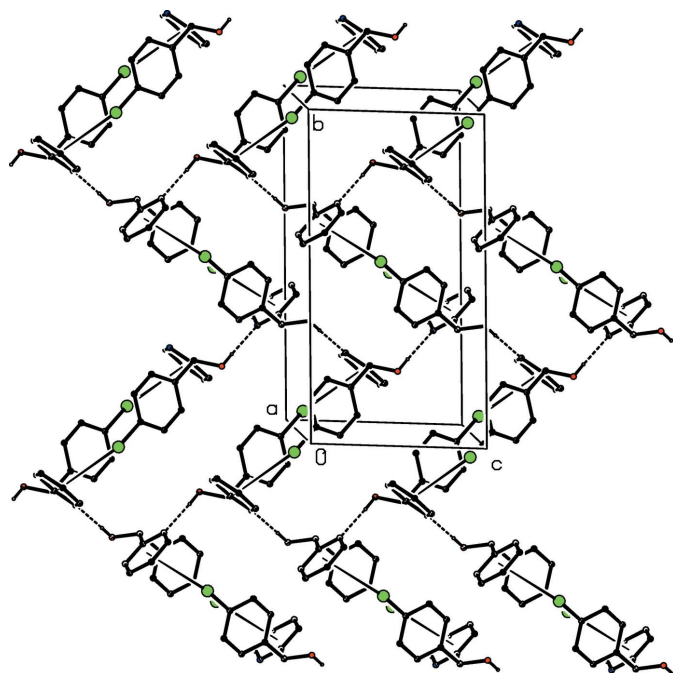(Desiraju & Steiner, 1999). In compound (I), this interaction links inversion-related pairs of molecules into cyclic centro-symmetric dimers (Fig. 3).

The overall effect of the C—Cl···π interaction in (I) is to link the hydrogen-bonded chain containing molecules related by the *c*-glide plane at $y = \frac{1}{4}$ directly to the two chains that contain molecules related by the glide planes at $y = -\frac{1}{4}$ and $y = \frac{3}{4}$, respectively, and propagation by translation of this interaction links the hydrogen-bonded chains along [001] into a sheet lying parallel to (100) (Fig. 4), but there are no direction-specific interactions between adjacent sheets.

4. Structural comparisons with related compounds

It is of interest briefly to compare the supramolecular assembly in compound (I), mediated by O—H···N hydrogen bonds and C—Cl···π interactions, with the assembly in some closely related compounds (II)–(VIII) (see Fig. 5), and particularly with compound (II), whose constitution differs from that of (I) only in lacking the chloro substituent.

The molecules of compound (II) are linked into *C*(5) chains by O—H···N hydrogen bonds (Kim & Kang, 2014; Tsang *et al.*, 2015), as in compound (I), but in (II) helical chains are

research communications

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{10}ClNO$
M_r	219.66
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	8.4309 (6), 16.1488 (11), 8.6878 (6)
β (°)	112.994 (2)
V (Å^3)	1088.85 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.32
Crystal size (mm)	$0.40 \times 0.30 \times 0.20$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.719, 0.938
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11481, 2510, 1860
R_{int}	0.030
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.118, 1.06
No. of reflections	2510
No. of parameters	139
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.21, −0.39

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

built from molecules related by 2_1 screw axes in space group $Pna2_1$, whereas in (I) zigzag chains are built from molecules related by glide planes. Hence in compound (II) each chain is homochiral, with equal numbers of chains built only from molecules having the *R*-configuration or only from molecules having the *S*-configuration: in (I), by contrast, each chain contains an alternation of the two enantiomers (*cf.* Fig. 2).

Similar homochiral $C(5)$ chains are formed in each of the three isomeric carborane derivatives (III)–(V) (Tsang *et al.*, 2015), regardless of whether they are crystallized as single enantiomers or as racemates. The structure of compound (VI), which is isomeric with (II) has been reported briefly (Shimada *et al.*, 2003) but, unfortunately, no atomic coordinates have been deposited in the Cambridge Structural Database (Groom & Allen, 2014). The structure report on (VI) concerns enantiomerically pure forms, in space group $P2_12_12_1$, so that the formation of homochiral helical chains of $C(7)$ type, seems plausible.

Compound (VII), which differs from (I) and (II) in containing two unsubstituted phenyl rings but no pyridyl ring, crystallizes with $Z' = 2$ in space group $P22_12_1$ (Ferguson *et al.*, 1995) and the molecules are linked by O—H···O hydrogen bonds to form $C_2^2(4)$ chains, but with no direction-specific interactions between adjacent chains. Compound (VIII) is the pentafluorophenyl analogue of (VII) and the molecules are

again linked by O—H···O hydrogen bonds, but now forming cyclic $R_6^6(12)$ hexamers having exact $\bar{3}$ (S_6) symmetry (Ferguson *et al.*, 1995).

5. Synthesis and crystallization

A sample of the title compound (I) was a gift from CAD Pharma, Bengaluru, India. Colourless blocks were grown by slow evaporation at room temperature of a solution in methanol, m.p. 478 K.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were located in difference maps. The H atoms bonded to C atoms were then treated as riding atoms in geometrically idealized position with C—H distances of 0.93 Å (aromatic and heteroaromatic) or 0.98 Å (aliphatic CH) and with $U_{iso}(H) = 1.2U_{eq}(C)$. For the hydroxyl H atom H1A, the atomic coordinates were refined with $U_{iso}(H) = 1.5U_{eq}(O)$, giving an O—H distance of 0.84 (2) Å. The analysis of variance reported a large value of K, 3.187, for the group of 252 very weak reflections having $F_c/F_c(max)$ in the range $0.000 < F_c/F_c(max) < 0.005$.

References

Bruker (2012). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. & Steiner, T. (1999). In *The Weak Hydrogen Bond*. Oxford University Press.
Ferguson, G., Carroll, C. D., Glidewell, C., Zakaria, C. M. & Lough, A. J. (1995). *Acta Cryst.* B**51**, 367–377.
Ferguson, G., Gallagher, J. F., Glidewell, C., Low, J. N. & Scrimgeour, S. N. (1992). *Acta Cryst.* C**48**, 1272–1275.
Ferguson, G., Gallagher, J. F., Glidewell, C. & Zakaria, C. M. (1994). *Acta Cryst.* C**50**, 70–73.
Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
Imai, Y. N., Inoue, Y., Nakanishi, I. & Kitaura, K. (2008). *Protein Sci.* **17**, 1129–1137.
Kim, H. & Kang, S. K. (2014). *Acta Cryst.* E**70**, o947.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Shimada, H., Fujiki, S., Oginuma, M., Asakawa, M., Okawara, T., Kato, K., Yamamura, S., Akita, H., Hara, A. & Imamura, Y. (2003). *J. Mol. Catal. B Enzym.* **23**, 29–35.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tsang, M. Y., Di Salvo, F., Teixidor, F., Viñas, C., Planas, J. G., Choquesillo-Lazarte, D. & Vanthuyne, N. (2015). *Cryst. Growth Des.* **15**, 935–945.

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT-Plus* (Bruker, 2012); data reduction: *SAINT-Plus* (Bruker, 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).

(*RS*)-(4-Chlorophenyl)(pyridin-2-yl)methanol

Crystal data

$C_{12}H_{10}ClNO$	$F(000) = 456$
$M_r = 219.66$	$D_x = 1.340$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.4309$ (6) Å	Cell parameters from 2785 reflections
$b = 16.1488$ (11) Å	$\theta = 2.5–28.6°$
$c = 8.6878$ (6) Å	$\mu = 0.32$ mm^{-1}
$\beta = 112.994$ (2)°	$T = 295$ K
$V = 1088.85$ (13) Å^3	Block, colourless
$Z = 4$	$0.40 \times 0.30 \times 0.20$ mm

Data collection

Bruker APEXII CCD diffractometer	11481 measured reflections
Radiation source: fine-focus sealed tube	2510 independent reflections
Graphite monochromator	1860 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.030$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$\theta_{max} = 27.6°$, $\theta_{min} = 2.5°$
	$h = -9 \rightarrow 10$
	$k = -21 \rightarrow 15$
$T_{min} = 0.719$, $T_{max} = 0.938$	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.045$	
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.2352P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
2510 reflections	$(\Delta/\sigma)_{max} < 0.001$
139 parameters	$\Delta\rho_{max} = 0.21$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.39$ 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}
C1	0.66425 (18)	0.19218 (9)	0.43123 (18)	0.0367 (3)
H1	0.6340	0.2499	0.3976	0.044*
O1	0.65282 (15)	0.17831 (8)	0.58744 (14)	0.0475 (3)
H1A	0.725 (3)	0.2105 (14)	0.655 (3)	0.071*
C11	0.53625 (18)	0.13554 (9)	0.30436 (19)	0.0358 (3)
C12	0.5356 (2)	0.05176 (10)	0.3383 (2)	0.0458 (4)
H12	0.6128	0.0313	0.4400	0.055*
C13	0.4232 (2)	−0.00168 (11)	0.2247 (2)	0.0533 (5)
H13	0.4239	−0.0578	0.2492	0.064*
C14	0.3099 (2)	0.02875 (12)	0.0747 (2)	0.0548 (5)
Cl14	0.16964 (9)	−0.03856 (4)	−0.07147 (8)	0.0922 (3)
C15	0.3058 (3)	0.11173 (14)	0.0391 (2)	0.0668 (6)
H15	0.2270	0.1321	−0.0619	0.080*
C16	0.4198 (2)	0.16462 (11)	0.1546 (2)	0.0538 (5)
H16	0.4175	0.2208	0.1304	0.065*
N21	0.88793 (16)	0.21277 (8)	0.32519 (16)	0.0414 (3)
C22	0.84457 (18)	0.17470 (9)	0.43935 (18)	0.0339 (3)
C23	0.9548 (2)	0.12092 (11)	0.5561 (2)	0.0461 (4)
H23	0.9219	0.0959	0.6353	0.055*
C24	1.1140 (2)	0.10498 (12)	0.5534 (2)	0.0537 (5)
H24	1.1899	0.0688	0.6304	0.064*
C25	1.1589 (2)	0.14314 (12)	0.4359 (3)	0.0570 (5)
H25	1.2658	0.1335	0.4314	0.068*
C26	1.0431 (2)	0.19599 (11)	0.3247 (2)	0.0523 (4)
H26	1.0741	0.2216	0.2446	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0359 (8)	0.0344 (8)	0.0421 (8)	0.0029 (6)	0.0178 (7)	0.0000 (6)
O1	0.0520 (7)	0.0526 (7)	0.0455 (7)	−0.0078 (6)	0.0272 (6)	−0.0106 (5)
C11	0.0323 (7)	0.0373 (8)	0.0411 (8)	0.0010 (6)	0.0177 (6)	−0.0001 (6)
C12	0.0452 (9)	0.0401 (9)	0.0485 (9)	0.0034 (7)	0.0142 (7)	0.0020 (7)
C13	0.0589 (11)	0.0406 (9)	0.0629 (12)	−0.0057 (9)	0.0265 (10)	−0.0055 (8)
C14	0.0524 (10)	0.0617 (12)	0.0497 (10)	−0.0168 (9)	0.0194 (8)	−0.0134 (9)
Cl14	0.0971 (5)	0.0942 (5)	0.0724 (4)	−0.0416 (4)	0.0190 (3)	−0.0316 (3)
C15	0.0667 (12)	0.0685 (13)	0.0465 (10)	−0.0118 (11)	0.0019 (9)	0.0068 (10)
C16	0.0554 (10)	0.0464 (10)	0.0502 (10)	−0.0044 (8)	0.0105 (8)	0.0095 (8)
N21	0.0390 (7)	0.0417 (7)	0.0450 (8)	−0.0018 (6)	0.0182 (6)	0.0005 (6)

C22	0.0341 (7)	0.0318 (7)	0.0351 (8)	−0.0016 (6)	0.0128 (6)	−0.0041 (6)
C23	0.0452 (9)	0.0492 (9)	0.0430 (9)	0.0064 (8)	0.0162 (7)	0.0031 (8)
C24	0.0418 (9)	0.0553 (11)	0.0563 (11)	0.0135 (8)	0.0108 (8)	−0.0005 (9)
C25	0.0357 (8)	0.0633 (12)	0.0748 (13)	0.0032 (9)	0.0245 (9)	−0.0093 (10)
C26	0.0459 (9)	0.0566 (11)	0.0637 (11)	−0.0050 (9)	0.0315 (9)	−0.0009 (9)

Geometric parameters (Å, º)

C1—O1	1.4154 (18)	C15—C16	1.381 (3)
C1—C11	1.512 (2)	C15—H15	0.9300
C1—C22	1.5206 (19)	C16—H16	0.9300
C1—H1	0.9800	N21—C22	1.3335 (19)
O1—H1A	0.84 (2)	N21—C26	1.338 (2)
C11—C16	1.371 (2)	C22—C23	1.382 (2)
C11—C12	1.385 (2)	C23—C24	1.376 (2)
C12—C13	1.373 (2)	C23—H23	0.9300
C12—H12	0.9300	C24—C25	1.367 (3)
C13—C14	1.371 (3)	C24—H24	0.9300
C13—H13	0.9300	C25—C26	1.370 (3)
C14—C15	1.373 (3)	C25—H25	0.9300
C14—Cl14	1.7376 (18)	C26—H26	0.9300
O1—C1—C11	107.86 (12)	C16—C15—H15	120.3
O1—C1—C22	111.56 (12)	C11—C16—C15	121.00 (17)
C11—C1—C22	109.72 (11)	C11—C16—H16	119.5
O1—C1—H1	109.2	C15—C16—H16	119.5
C11—C1—H1	109.2	C22—N21—C26	117.48 (14)
C22—C1—H1	109.2	N21—C22—C23	122.29 (13)
C1—O1—H1A	105.9 (15)	N21—C22—C1	116.07 (13)
C16—C11—C12	118.40 (15)	C23—C22—C1	121.63 (13)
C16—C11—C1	121.82 (14)	C24—C23—C22	119.09 (16)
C12—C11—C1	119.78 (14)	C24—C23—H23	120.5
C13—C12—C11	121.32 (16)	C22—C23—H23	120.5
C13—C12—H12	119.3	C25—C24—C23	119.03 (17)
C11—C12—H12	119.3	C25—C24—H24	120.5
C14—C13—C12	119.13 (17)	C23—C24—H24	120.5
C14—C13—H13	120.4	C24—C25—C26	118.56 (15)
C12—C13—H13	120.4	C24—C25—H25	120.7
C13—C14—C15	120.73 (17)	C26—C25—H25	120.7
C13—C14—Cl14	119.54 (15)	N21—C26—C25	123.55 (16)
C15—C14—Cl14	119.73 (15)	N21—C26—H26	118.2
C14—C15—C16	119.40 (18)	C25—C26—H26	118.2
C14—C15—H15	120.3		
O1—C1—C11—C16	129.16 (15)	C26—N21—C22—C23	1.2 (2)
C22—C1—C11—C16	−109.13 (16)	C26—N21—C22—C1	−177.31 (14)
O1—C1—C11—C12	−51.14 (17)	O1—C1—C22—N21	−156.41 (13)
C22—C1—C11—C12	70.57 (17)	C11—C1—C22—N21	84.12 (16)

C16—C11—C12—C13	0.9 (2)	O1—C1—C22—C23	25.1 (2)
C1—C11—C12—C13	−178.84 (14)	C11—C1—C22—C23	−94.42 (16)
C11—C12—C13—C14	0.2 (3)	N21—C22—C23—C24	−1.0 (2)
C12—C13—C14—C15	−1.3 (3)	C1—C22—C23—C24	177.48 (15)
C12—C13—C14—Cl14	178.90 (13)	C22—C23—C24—C25	0.3 (3)
C13—C14—C15—C16	1.4 (3)	C23—C24—C25—C26	0.0 (3)
Cl14—C14—C15—C16	−178.83 (15)	C22—N21—C26—C25	−0.9 (3)
C12—C11—C16—C15	−0.8 (3)	C24—C25—C26—N21	0.3 (3)
C1—C11—C16—C15	178.90 (16)	C11—C1—O1—H1A	−180.0 (17)
C14—C15—C16—C11	−0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N21[i]	0.84 (2)	2.01 (2)	2.8444 (18)	176 (2)

Symmetry code: (i) x, $-y+1/2$, $z+1/2$.