



Crystal structure of (*R*)-5-[(*R*)-3-(4-chlorophenyl)-5-methyl-4,5-dihydroisoxazol-5-yl]-2-methylcyclohex-2-enone

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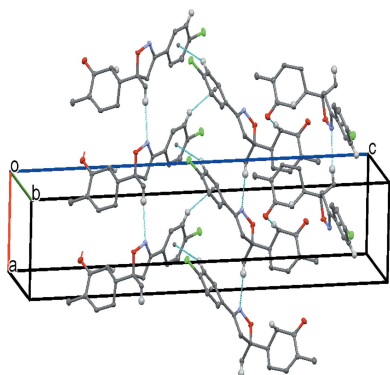
The title compound, C₁₇H₁₈ClNO₂, was prepared and isolated as a pure diastereoisomer, using column chromatography followed by a succession of fractional crystallizations. Its exact structure was fully identified *via* ¹H NMR and confirmed by X-ray diffraction. It is built up from a central five-membered dihydroisoxazole ring to which a *p*-chlorophenyl group and a cyclohex-2-enone ring are attached in the 3 and 5 positions. The cyclohex-2-one and isoxazoline rings each exhibit an envelope conformation. The crystal packing features C—H···O, C—H···N and C—H···π interactions, which generate a three-dimensional network.

1. Chemical context

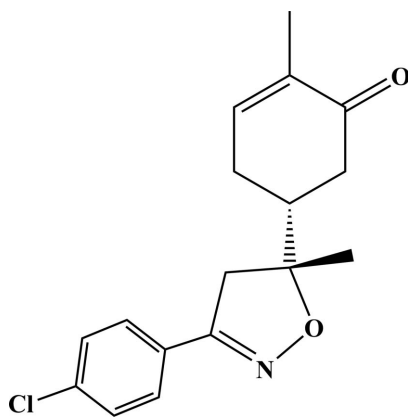
In recent years, isoxazole and isoxazoline derivatives have been considered to be good drug candidates because of their broad spectrum of pharmaceutical activities, such as anti-tumoral (Kamal *et al.*, 2010), antibacterial (Calí *et al.*, 2004), antiviral (Deng *et al.*, 2009) and anti-inflammatory (Pedada *et al.*, 2016). Cycloaddition and heterocyclization reactions have been widely used as synthetic methods for obtaining isoxazoles (Nieto *et al.*, 2019). In terms of selectivity, 1,3-dipolar cycloaddition reactions of nitrilimines with dipolarophiles, such as C=C, C=S or C=N, give high stereoselectivity (Ait Itto *et al.*, 2013), while nitrile oxides, which are less sterically hindered dipoles, lead to poor stereoselectivity (Feddouli *et al.*, 2006). This was confirmed in our recent work (Oubella *et al.*, 2019) in which the 1,3-cycloaddition reaction of diaryl-nitrilimines with (*R*)-carvone gave the corresponding pyrazoles isolated as the unique (3*aR*,5*R*,7*aR*) diastereoisomer, while the isoxazoles prepared with nitrile oxides were isolated as (*R,R*)/(*R,S*) diastereoisomeric mixtures with a slight predominance of (*R,R*). In the present work, we report the separation, identification by ¹H NMR spectroscopy, and X-ray structural analysis of the slightly major diastereoisomer of the isoxazole obtained by the 1,3-dipolar cycloaddition of 4-chlorobenzonitrile oxide with (*R*)-carvone.

2. Structural commentary

The title compound is built up from a central five-membered dihydroisoxazol ring to which a *p*-chlorophenyl group and a cyclohex-2-enone ring are attached to atoms C2 and C1 at the



3 and 5 positions, respectively (Fig. 1). Atom C1 also bears a methyl group. The absolute configuration of *R/R* at atoms C1 and C11 were confirmed by the Flack parameter (Parsons *et al.*, 2013). This structure is closely related to the previously reported isoxazole derivative having a methyl group in place of atom C1 3 (Oubella *et al.*, 2019). The isoxazole ring has an envelope conformation on C1 as indicated by the puckering parameters of $Q_2 = 0.145$ (3) Å and $\varphi_2 = 138.1$ (11)°. The puckering parameters for the cyclohexene ring, $Q = 0.449$ (3) Å, $\theta = 126.0$ (4)° and $\varphi = 189.2$ (5)°, agree with an envelope conformation on C11. The mean plane of the isoxazole ring makes a dihedral angle of 13.4 (2)° with the C21–C26 benzene ring, whereas it makes a dihedral angle of 66.2 (1)° with the mean plane of the C11–C16 ring.



3. Supramolecular features

The packing of the structure features weak C–H···N and C–H···O interactions (C4–H42···N1ⁱ and C12–H12B···O13ⁱⁱ; symmetry codes as in Table 1). The C–H···N interactions build up a linear chain along the *a*-axis direction, while the C–H···O interactions make a helical chain along the *b*-axis direction, forming a layer parallel to the *ab* plane (Fig. 2). Between the layers, a C–H··· π interaction is observed (C23–H23···Cg1ⁱⁱⁱ; Table 1), where Cg1 is the centroid of the C21–C26 benzene ring.

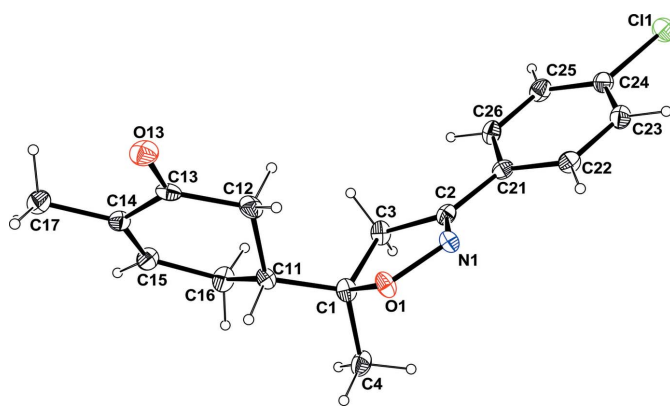


Figure 1
Molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles of arbitrary radii.

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

Cg1 is the centroid of the C21–C26 ring.

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C4–H42···N1 ⁱ	0.96	2.62	3.572 (4)	173
C12–H12B···O13 ⁱⁱ	0.97	2.54	3.488 (4)	165
C23–H23···Cg1 ⁱⁱⁱ	0.93	2.71	3.554 (3)	151

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

4. Database survey

A search in the Cambridge Structural Database (CSD, version 5.40, update August 2019; Groom *et al.*, 2016) for organic compounds with structures containing a 2-isoxazoline ring revealed 284 hits. Introducing a methyl group on position 5 reduced this number to 15 and searching for structures containing a phenyl ring attached to position 3 gave only seven hits. A comparison of related distances and angles within the 2-isoxazoline ring shows a good agreement between all these structures, with a systematically short C2–N1 bond with lengths ranging from 1.274 to 1.285 Å, corresponding to a C=N double bond. A larger discrepancy is observed for the dihedral angle between the isoxazol mean plane and the benzene ring in the (*S*)-3-(2,6-dichlorophenyl)-5-[(2,5-diphenylpyrrolidin-1-yl)carbonyl]-5-methyl-4,5-dihydroisoxazole compound (Houk *et al.*, 1984); at 66.8°, this is much larger than the value of 13.4 (2)° observed for the title compound. This larger dihedral angle is related to the occurrence of two Cl atoms in the 2 and 5 positions on the phenyl ring.

5. Synthesis and crystallization

As shown in Fig. 3, (*R*)-carvone, **1**, was reacted with nitrile oxide, **2**, generated *in situ* from the corresponding oxime

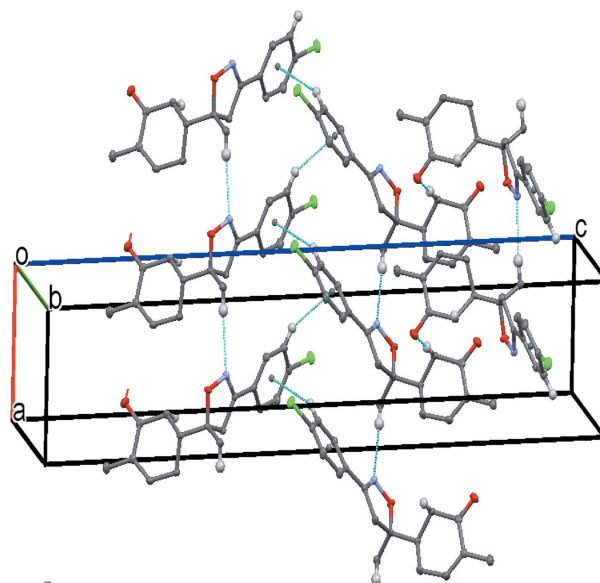


Figure 2
Partial packing diagram of the title compound, showing C–H···O, C–H···N and C–H··· π interactions.

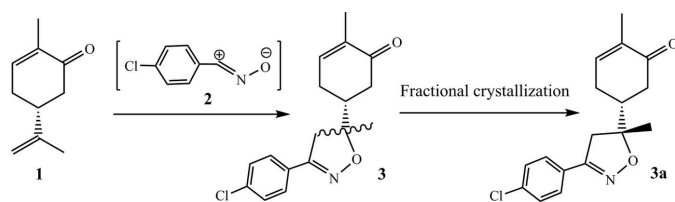


Figure 3
Synthesis pathway leading to the formation of the title compound, **3a**.

according to our recently described methodology (Oubella *et al.*, 2019). The corresponding isoxazole, **3**, was obtained in 80% yield, as an (*R,R*)/(*R,S*) diastereoisomeric mixture. The ^1H NMR spectrum of **3** clearly shows a splitting of both the methyl and methylene groups in the α position of the newly formed stereogenic center of the isoxazole nucleus (Fig. 4a). The former gave rise to two singlets at 1.44 ppm and 1.48 ppm, respectively, while the latter is seen as two pairs of doublets, one at 2.90 and 3.20 ppm ($J = 16.9$ Hz) and the other at 2.75 and 3.30 ppm ($J = 16.7$ Hz). Integrating the corresponding ^1H NMR signals allowed us to quantify the ratio of the diastereoisomeric mixture as 58:42. After several attempts at separation, either by column chromatography or a series of fractional crystallizations by slow evaporation from a chloroform solution of **3**, we managed to separate the diastereoisomer **3a**, the title compound, as pure single crystals suitable for crystallographic analysis. Its ^1H NMR spectrum (Fig. 4b) is mainly characterized by the isoxazolic methyl group resonating as a singlet at 1.44 ppm, and the methylene group appeared as two doublets at 2.90 ppm ($J = 16.9$ Hz) and 3.20 ppm ($J = 16.9$ Hz).

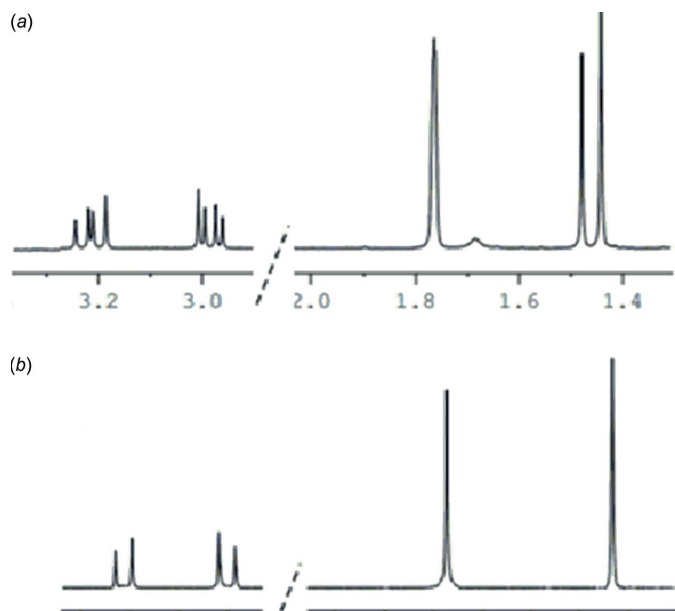


Figure 4
 ^1H NMR spectra of (a) the diastereoisomeric mixture **3** and (b) the pure separated (*5R,5'R*) diastereoisomer **3a**.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{17}\text{H}_{18}\text{ClNO}_2$
M_r	303.77
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	105
a, b, c (Å)	6.4590 (2), 7.3545 (3), 31.3436 (12)
V (Å ³)	1488.91 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.26
Crystal size (mm)	$0.31 \times 0.26 \times 0.18$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2015)
T_{\min}, T_{\max}	0.694, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16529, 3019, 2827
R_{int}	0.057
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.035, 0.105, 1.19
No. of reflections	3019
No. of parameters	193
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.40, -0.23
Absolute structure	Flack x determined using 1100 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.09 (4)

Computer programs: APEX2 and SAINT (Bruker, 2015), SHELXT (Sheldrick, 2015a), SHELXL2016 (Sheldrick, 2015b) and ORTEP-3 for Windows (Farrugia, 2012).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.99 Å (methylene), 0.98 Å (methyl) or 0.95 Å (methine), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene and methine or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

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Crystal structure of (R)-5-[(R)-3-(4-chlorophenyl)-5-methyl-4,5-dihydroisoxazol-5-yl]-2-methylcyclohex-2-enone

Ali Oubella, My Youssef Ait Itto, Aziz Auhmani, Abdelkhalek Riahi, Jean-Claude Daran and Abdelwahed Auhmani

Computing details

Data collection: *APEX2* (Bruker, 2015); cell refinement: *SAINTE* (Bruker, 2015); data reduction: *SAINTE* (Bruker, 2015); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015b).

(R)-5-[(R)-3-(4-Chlorophenyl)-5-methyl-4,5-dihydroisoxazol-5-yl]-2-methylcyclohex-2-enone

Crystal data

$C_{17}H_{18}ClNO_2$

$M_r = 303.77$

Orthorhombic, $P2_12_12_1$

$a = 6.4590$ (2) Å

$b = 7.3545$ (3) Å

$c = 31.3436$ (12) Å

$V = 1488.91$ (10) Å³

$Z = 4$

$F(000) = 640$

$D_x = 1.355$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5113 reflections

$\theta = 2.8$ – 27.9°

$\mu = 0.26$ mm⁻¹

$T = 105$ K

Box, colourless

$0.31 \times 0.26 \times 0.18$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: micro-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2015)

$T_{\min} = 0.694$, $T_{\max} = 0.746$

16529 measured reflections

3019 independent reflections

2827 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 1.3^\circ$

$h = -8 \rightarrow 8$

$k = -9 \rightarrow 9$

$l = -38 \rightarrow 39$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.105$

$S = 1.19$

3019 reflections

193 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.137P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.40$ e Å⁻³

$\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL2016
 (Sheldrick, 2015b),
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.014 (4)

Absolute structure: Flack x determined using
 1100 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
 Absolute structure parameter: -0.09 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6484 (4)	0.6566 (4)	0.64093 (9)	0.0150 (6)
C2	0.4125 (4)	0.4711 (4)	0.60439 (8)	0.0140 (6)
C3	0.6216 (4)	0.4598 (4)	0.62542 (9)	0.0158 (6)
H31	0.728644	0.425833	0.605242	0.019*
H32	0.621273	0.374475	0.649026	0.019*
C4	0.7886 (4)	0.7654 (4)	0.61166 (9)	0.0197 (6)
H41	0.739550	0.755866	0.582840	0.030*
H42	0.927089	0.718468	0.613353	0.030*
H43	0.787990	0.890632	0.620283	0.030*
C11	0.7057 (4)	0.6782 (4)	0.68816 (9)	0.0134 (6)
H11	0.713927	0.808792	0.694138	0.016*
C12	0.5419 (4)	0.5983 (4)	0.71777 (9)	0.0181 (6)
H12A	0.411443	0.660009	0.712739	0.022*
H12B	0.522661	0.470911	0.710757	0.022*
C13	0.5961 (4)	0.6140 (4)	0.76455 (9)	0.0155 (6)
C14	0.8176 (4)	0.6073 (4)	0.77632 (9)	0.0163 (6)
C15	0.9600 (4)	0.5958 (4)	0.74575 (9)	0.0175 (6)
H15	1.097590	0.587139	0.754279	0.021*
C16	0.9173 (4)	0.5956 (4)	0.69867 (9)	0.0182 (6)
H16A	0.922229	0.471584	0.688155	0.022*
H16B	1.024450	0.664296	0.684169	0.022*
C17	0.8694 (5)	0.6108 (4)	0.82302 (9)	0.0222 (6)
H17A	1.016154	0.596660	0.826631	0.033*
H17B	0.798826	0.513186	0.837226	0.033*
H17C	0.826500	0.724750	0.835047	0.033*
C21	0.3164 (4)	0.3268 (4)	0.57902 (8)	0.0146 (6)
C22	0.1345 (4)	0.3588 (4)	0.55578 (9)	0.0164 (6)
H22	0.077055	0.474733	0.555387	0.020*
C23	0.0396 (4)	0.2195 (4)	0.53343 (9)	0.0180 (6)
H23	-0.081403	0.240979	0.518175	0.022*
C24	0.1273 (5)	0.0476 (4)	0.53409 (9)	0.0176 (6)
C25	0.3067 (5)	0.0123 (4)	0.55656 (9)	0.0194 (6)
H25	0.364066	-0.103682	0.556670	0.023*
C26	0.3997 (4)	0.1524 (4)	0.57889 (9)	0.0181 (6)

H26	0.520399	0.129473	0.594145	0.022*
N1	0.3162 (3)	0.6195 (3)	0.61149 (7)	0.0152 (5)
O1	0.4384 (3)	0.7345 (3)	0.63657 (6)	0.0161 (4)
O13	0.4603 (3)	0.6257 (3)	0.79158 (6)	0.0220 (5)
Cl1	0.00864 (11)	-0.12745 (10)	0.50590 (2)	0.0242 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0094 (12)	0.0177 (14)	0.0179 (14)	0.0039 (11)	-0.0007 (11)	-0.0012 (11)
C2	0.0129 (13)	0.0170 (14)	0.0121 (13)	0.0026 (11)	0.0016 (10)	0.0016 (11)
C3	0.0132 (13)	0.0177 (14)	0.0166 (14)	0.0055 (11)	-0.0009 (11)	-0.0029 (11)
C4	0.0159 (13)	0.0272 (16)	0.0161 (14)	0.0024 (13)	-0.0020 (12)	0.0036 (12)
C11	0.0098 (12)	0.0144 (13)	0.0162 (13)	0.0015 (10)	-0.0007 (11)	-0.0021 (10)
C12	0.0111 (13)	0.0221 (15)	0.0210 (14)	-0.0027 (11)	0.0007 (11)	-0.0013 (11)
C13	0.0154 (13)	0.0098 (12)	0.0211 (14)	-0.0021 (11)	0.0037 (11)	-0.0003 (11)
C14	0.0185 (13)	0.0139 (13)	0.0164 (14)	-0.0008 (12)	0.0000 (11)	0.0009 (11)
C15	0.0119 (14)	0.0218 (14)	0.0188 (14)	0.0015 (12)	-0.0007 (11)	0.0027 (11)
C16	0.0113 (13)	0.0260 (16)	0.0172 (15)	0.0045 (12)	0.0018 (11)	-0.0002 (12)
C17	0.0230 (14)	0.0263 (16)	0.0171 (14)	-0.0038 (14)	0.0013 (12)	0.0018 (13)
C21	0.0156 (13)	0.0159 (14)	0.0123 (13)	0.0008 (11)	0.0037 (11)	0.0008 (10)
C22	0.0166 (12)	0.0152 (13)	0.0173 (13)	0.0021 (12)	0.0006 (11)	0.0004 (11)
C23	0.0167 (13)	0.0214 (14)	0.0161 (13)	0.0013 (12)	-0.0007 (11)	0.0004 (11)
C24	0.0215 (15)	0.0181 (14)	0.0131 (13)	-0.0032 (12)	0.0004 (12)	-0.0017 (11)
C25	0.0260 (15)	0.0151 (13)	0.0172 (14)	0.0031 (12)	-0.0007 (13)	0.0001 (11)
C26	0.0197 (14)	0.0191 (14)	0.0155 (14)	0.0038 (12)	-0.0032 (12)	0.0004 (11)
N1	0.0134 (10)	0.0162 (11)	0.0160 (11)	-0.0017 (11)	-0.0019 (9)	-0.0017 (10)
O1	0.0106 (9)	0.0156 (9)	0.0222 (10)	0.0035 (7)	-0.0048 (8)	-0.0048 (8)
O13	0.0191 (10)	0.0249 (10)	0.0220 (10)	-0.0008 (10)	0.0067 (8)	-0.0005 (9)
Cl1	0.0307 (4)	0.0197 (4)	0.0223 (4)	-0.0051 (3)	-0.0041 (3)	-0.0033 (3)

Geometric parameters (Å, °)

C1—O1	1.478 (3)	C14—C17	1.502 (4)
C1—C4	1.517 (4)	C15—C16	1.501 (4)
C1—C11	1.534 (4)	C15—H15	0.9300
C1—C3	1.537 (4)	C16—H16A	0.9700
C2—N1	1.276 (4)	C16—H16B	0.9700
C2—C21	1.464 (4)	C17—H17A	0.9600
C2—C3	1.505 (4)	C17—H17B	0.9600
C3—H31	0.9700	C17—H17C	0.9600
C3—H32	0.9700	C21—C26	1.391 (4)
C4—H41	0.9600	C21—C22	1.402 (4)
C4—H42	0.9600	C22—C23	1.384 (4)
C4—H43	0.9600	C22—H22	0.9300
C11—C12	1.525 (4)	C23—C24	1.386 (4)
C11—C16	1.532 (3)	C23—H23	0.9300
C11—H11	0.9800	C24—C25	1.380 (4)

C12—C13	1.512 (4)	C24—C11	1.740 (3)
C12—H12A	0.9700	C25—C26	1.383 (4)
C12—H12B	0.9700	C25—H25	0.9300
C13—O13	1.223 (3)	C26—H26	0.9300
C13—C14	1.478 (4)	N1—O1	1.398 (3)
C14—C15	1.331 (4)		
O1—C1—C4	106.7 (2)	C15—C14—C17	123.3 (3)
O1—C1—C11	105.7 (2)	C13—C14—C17	117.3 (2)
C4—C1—C11	112.6 (2)	C14—C15—C16	125.5 (3)
O1—C1—C3	103.4 (2)	C14—C15—H15	117.3
C4—C1—C3	111.9 (2)	C16—C15—H15	117.2
C11—C1—C3	115.5 (2)	C15—C16—C11	112.0 (2)
N1—C2—C21	120.6 (2)	C15—C16—H16A	109.2
N1—C2—C3	114.1 (2)	C11—C16—H16A	109.2
C21—C2—C3	125.3 (2)	C15—C16—H16B	109.2
C2—C3—C1	100.8 (2)	C11—C16—H16B	109.2
C2—C3—H31	111.6	H16A—C16—H16B	107.9
C1—C3—H31	111.6	C14—C17—H17A	109.5
C2—C3—H32	111.6	C14—C17—H17B	109.5
C1—C3—H32	111.6	H17A—C17—H17B	109.5
H31—C3—H32	109.4	C14—C17—H17C	109.5
C1—C4—H41	109.5	H17A—C17—H17C	109.5
C1—C4—H42	109.5	H17B—C17—H17C	109.5
H41—C4—H42	109.5	C26—C21—C22	118.5 (3)
C1—C4—H43	109.5	C26—C21—C2	120.4 (2)
H41—C4—H43	109.5	C22—C21—C2	121.0 (2)
H42—C4—H43	109.5	C23—C22—C21	120.6 (3)
C12—C11—C16	109.6 (2)	C23—C22—H22	119.7
C12—C11—C1	112.3 (2)	C21—C22—H22	119.7
C16—C11—C1	112.4 (2)	C22—C23—C24	119.1 (3)
C12—C11—H11	107.4	C22—C23—H23	120.4
C16—C11—H11	107.4	C24—C23—H23	120.4
C1—C11—H11	107.4	C25—C24—C23	121.5 (3)
C13—C12—C11	113.6 (2)	C25—C24—C11	119.3 (2)
C13—C12—H12A	108.9	C23—C24—C11	119.2 (2)
C11—C12—H12A	108.9	C24—C25—C26	118.9 (3)
C13—C12—H12B	108.9	C24—C25—H25	120.6
C11—C12—H12B	108.9	C26—C25—H25	120.6
H12A—C12—H12B	107.7	C25—C26—C21	121.4 (3)
O13—C13—C14	121.6 (3)	C25—C26—H26	119.3
O13—C13—C12	120.7 (2)	C21—C26—H26	119.3
C14—C13—C12	117.6 (2)	C2—N1—O1	109.9 (2)
C15—C14—C13	119.4 (2)	N1—O1—C1	109.61 (19)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C21–C26 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C4—H42···N1 ⁱ	0.96	2.62	3.572 (4)	173
C12—H12B···O13 ⁱⁱ	0.97	2.54	3.488 (4)	165
C23—H23···Cg1 ⁱⁱⁱ	0.93	2.71	3.554 (3)	151

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