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(Z)-N-(2,6-Diisopropylphenyl)-4-nitrobenzimidoyl chloride

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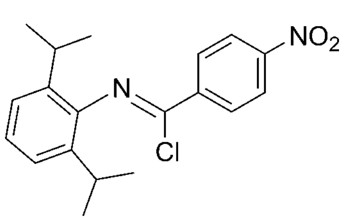
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.062; wR factor = 0.173; data-to-parameter ratio = 19.1.

In the title compound, $C_{19}H_{21}ClN_2O_2$, the aromatic rings are approximately perpendicular to each other, subtending a dihedral angle of 87.7 (1)°. In the crystal, the 4-nitrophenyl groups of pairs of neighbouring molecules are parallel and oriented head-to-tail with a ring centroid–centroid distance of 3.9247 (12) Å, leading to a π–π interaction between the pair. The faces of each phenyl ring of the 2,6-diisopropylphenyl group interact with two different groups, *viz*. a chloro group of an adjacent molecule on one side and the edge of the 4-nitrophenyl ring of a second molecule on the other side.

Related literature

For the synthesis and applications of imidoyl chlorides, see: Pelter *et al.* (1975); Manley & Bilodeau (2002); Cunico & Pandey (2005); Raussukana *et al.* (2006); Zheng & Alper (2008); Kuszpit *et al.* (2011). For a related structure of an imidoyl chloride, see: Seidelmann *et al.* (1998).



Experimental

Crystal data

$C_{19}H_{21}ClN_2O_2$
M_r = 344.83
Triclinic, $P\bar{1}$
a = 8.2988 (4) Å
b = 10.4667 (3) Å
c = 10.9665 (3) Å
α = 75.568 (2)°
β = 85.411 (2)°
γ = 74.145 (2)°
V = 887.33 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 150 K
0.35 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.924, T_{max} = 0.967
6021 measured reflections
4232 independent reflections
3108 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.173
S = 1.06
4232 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···$Cg2^{i}$	0.95	2.67	3.511 (2)	147
C16—H16B···$Cg1^{ii}$	0.98	2.79	3.663 (3)	149

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP99* for Windows (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5293).

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supplementary materials

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(*Z*)-*N*-(2,6-Diisopropylphenyl)-4-nitrobenzimidoyl chloride

Gamal A. El-Hiti, Keith Smith, Dyfyr Heulyn Jones, Ali Masmali and Benson M. Kariuki

1. Comment

The title compound I, a useful synthetic intermediate, was synthesized in good yield by the reaction of *N*-(2,6-diisopropylphenyl)-4-nitrobenzamide with phosphorus pentachloride. Imidoyl chlorides are useful reactive intermediates in syntheses of ketones from trialkylcyanoborates (Pelter *et al.*, 1975), of highly substituted 2-imidazolines *via* a ring-expansion reaction with aziridines (Kuszpit *et al.*, 2011), and by *in situ* reaction with pyridine-1-oxides to give 2-aminopyridine amides (Manley *et al.*, 2002). They have also been used as precursors to *α*-iminoamides (Cunico *et al.*, 2005), isoquinolin-1(2*H*)-ones *via* a palladium-catalyzed reaction with diethyl(2-iodoaryl)malonates (Zheng *et al.*, 2008), and 1,3-oxathiolanones and benzoxathianones by reaction with mercaptocarboxylic acids (Raussukana *et al.*, 2006). The X-ray crystal structure of *N*-(diethylaminothiocarbonyl)ferrocenecarbimidoyl chloride has been reported (Seidelmann *et al.*, 1998).

In the molecule (Fig. 1), the aromatic rings of the 2,6-diisopropylphenyl and 4-nitrophenyl groups are approximately perpendicular to each other; the dihedral angle between the least-squares planes through the rings is 87.7 (1)°. The molecule has no strong hydrogen bond donor and the crystal structure is shown in Figure 2. The 4-nitrophenyl groups of neighboring molecules are parallel and oriented head-to-tail with a ring centroid-centroid distance of 3.9247 (12) Å, leading to a π–π interaction (Fig. 3). One face of the phenyl ring of the 2,6-diisopropylphenyl group interacts with the chloro group of an adjacent molecule (C7—Cl1···*Cg*2) and the other face of the same ring interacts with the edge of the 4-nitrophenyl ring of a second molecule (C6—H6···*Cg*2; Fig. 4); *Cg*2 is the centroid of the C8–C13 ring. Another interaction, C16—H16B···*Cg*1, is also observed; *Cg*1 is the centroid of the C1–C6 ring.

2. Experimental

Synthesis of *N*-(2,6-diisopropylphenyl)-4-nitrobenzimidoyl chloride (I)

An oven dried two necked 100 ml flask equipped with a magnetic stirrer, septum-capped reflux condenser and septum was flushed with N_2 and phosphorus pentachloride (4.42 g, 21 mmol) and dry toluene (40 ml) were added. The mixture was stirred for 5 min then *N*-(2,6-diisopropylphenyl)-4-nitrobenzamide (6.90 g, 21 mmol) was quickly added to the flask under a fast stream of N_2, and the septum replaced by a stopper. The mixture was heated to reflux for 2 h, whereupon it became homogeneous and gas evolution was observed. Phosphorus oxychloride and toluene were removed under reduced pressure and the crude product was quickly extracted with hot diethyl ether (3 × 80 ml). The diethyl ether washings were evaporated under a fast stream of N_2 overnight, during which process bright yellow prisms of *N*-(2,6-diisopropylphenyl)-4-nitrobenzimidoyl chloride (6.93 g, 95%) separated; m.p. 144–146 °C. HREI$^+$–MS m/*z*: calcd for $C_{19}H_{21}N_2O_2$ ^{35}Cl 344.1292, found 344.1301.

3. Refinement

H atoms were positioned geometrically (C—H = 0.95–1.00 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C), allowing for free rotation of the methyl groups about the C—C bond.

Computing details

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP99* for Windows (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

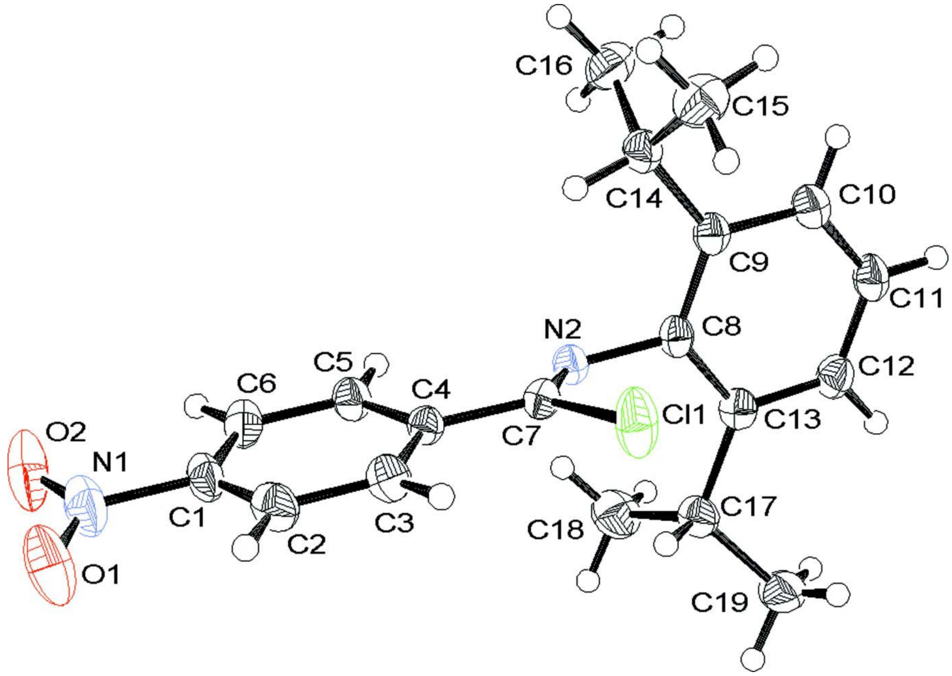

Figure 1

Molecular structure of the title compound, showing atom labels and 50% probability displacement ellipsoids for non-H atoms.

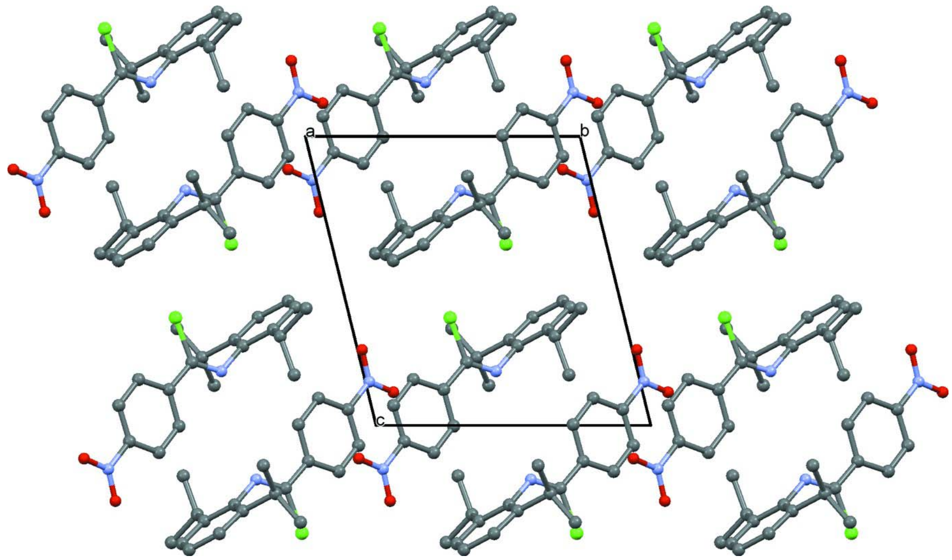

Figure 2

A packing view of the title compound along the *a* axis.

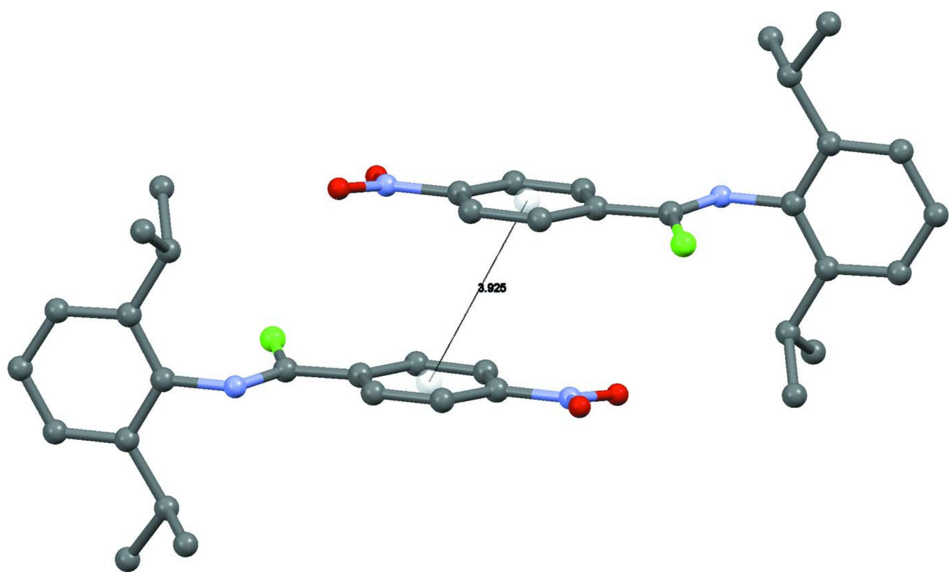

Figure 3

A pair of molecules showing the ring centroid-centroid distance for parallel 4-nitrobenzyl groups.

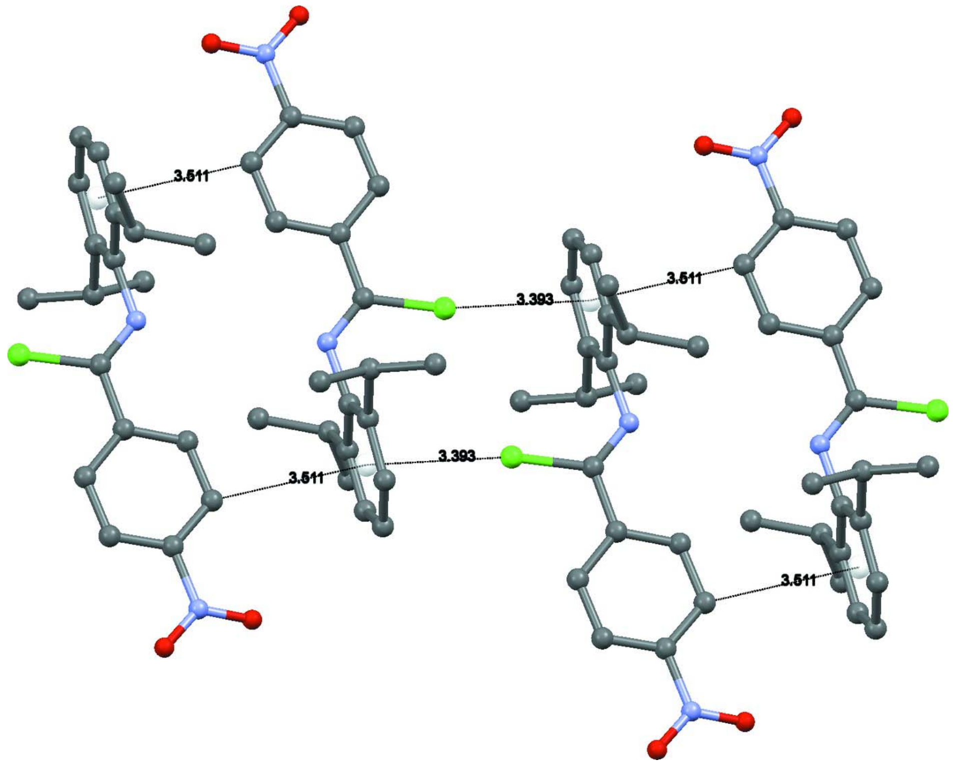

Figure 4

A segment showing edge-to-face and chloro-to-face contacts in the crystal structure.

(*Z*)-*N*-(2,6-Diisopropylphenyl)-4-nitrobenzimidoyl chloride

Crystal data

$C_{19}H_{21}ClN_2O_2$
M_r = 344.83
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.2988 (4) Å
b = 10.4667 (3) Å
c = 10.9665 (3) Å
α = 75.568 (2)°
β = 85.411 (2)°
γ = 74.145 (2)°
V = 887.33 (6) Å^3
Z = 2
F(000) = 364
D_x = 1.291 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3108 reflections
θ = 2.8–28.3°
μ = 0.23 mm^{-1}
T = 150 K
Block, yellow
0.35 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.924, T_{max} = 0.967
6021 measured reflections
4232 independent reflections
3108 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.3°, θ_{min} = 2.8°
h = −11→10
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.173$
$S = 1.06$
4232 reflections
222 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 0.589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.094 (10)

Special details

Experimental. ^{1}H (400 MHz; CDCl$_3$) δ: 8.25 (2 H, d, J = 8.4 Hz), 8.17 (2 H, d, J = 8.4 Hz), 7.05–7.12 (2 H, m), 6.97–7.04 (1 H, m), 2.66 (2 H, app. sept, J = 6.9 Hz), 1.11 (6 H, d, J = 6.6 Hz), 1.05 (6 H, d, J = 6.6 Hz) – the two 6 H doublets coalesced at 50 °C; ^{13}C (125 MHz; CDCl$_3$) δ: 149.9 (*s*), 143.4 (*s*), 141.8 (*s*), 140.1 (*s*), 136.3 (*s*), 130.3 (*d*), 125.5 (*d*), 123.7 (*d*), 123.3 (*d*), 28.8 (*d*), 23.3 (*q*), 22.8 (*q*); ν_{max} (thin film/cm^{-1}): 3017, 2966, 2929, 2871, 1662, 1605, 1529, 1349, 1216, 1168, 1461.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.2830 (3)	0.0882 (2)	1.0555 (2)	0.0319 (5)
C2	0.2874 (3)	0.0814 (2)	0.9309 (2)	0.0343 (5)
H2	0.2496	0.0132	0.9075	0.041*
C3	0.3483 (3)	0.1763 (2)	0.8410 (2)	0.0299 (5)
H3	0.3551	0.1720	0.7552	0.036*
C4	0.3996 (2)	0.27816 (19)	0.87595 (19)	0.0234 (4)
C5	0.3944 (3)	0.2816 (2)	1.0028 (2)	0.0277 (5)
H5	0.4310	0.3500	1.0269	0.033*
C6	0.3360 (3)	0.1857 (2)	1.0938 (2)	0.0320 (5)
H6	0.3326	0.1873	1.1803	0.038*
C7	0.4587 (3)	0.3856 (2)	0.78235 (18)	0.0237 (4)
C8	0.5521 (3)	0.5859 (2)	0.72503 (18)	0.0239 (4)
C9	0.7254 (3)	0.5618 (2)	0.70425 (19)	0.0259 (4)
C10	0.7851 (3)	0.6667 (2)	0.6259 (2)	0.0306 (5)
H10	0.9022	0.6527	0.6104	0.037*
C11	0.6771 (3)	0.7907 (2)	0.5702 (2)	0.0317 (5)
H11	0.7201	0.8614	0.5180	0.038*
C12	0.5055 (3)	0.8114 (2)	0.5911 (2)	0.0306 (5)
H12	0.4321	0.8961	0.5513	0.037*
C13	0.4386 (3)	0.7111 (2)	0.6689 (2)	0.0267 (5)

C14	0.8468 (3)	0.4269 (2)	0.7645 (2)	0.0307 (5)
H14	0.7792	0.3633	0.8100	0.037*
C15	0.9545 (3)	0.3613 (3)	0.6651 (3)	0.0427 (6)
H15A	0.8819	0.3544	0.6022	0.064*
H15B	1.0214	0.2697	0.7057	0.064*
H15C	1.0293	0.4178	0.6239	0.064*
C16	0.9550 (3)	0.4460 (3)	0.8613 (2)	0.0406 (6)
H16A	1.0282	0.5032	0.8185	0.061*
H16B	1.0235	0.3566	0.9054	0.061*
H16C	0.8827	0.4905	0.9222	0.061*
C17	0.2510 (3)	0.7304 (2)	0.6917 (2)	0.0308 (5)
H17	0.2250	0.6450	0.6838	0.037*
C18	0.2005 (3)	0.7468 (3)	0.8252 (3)	0.0446 (6)
H18A	0.2680	0.6693	0.8861	0.067*
H18B	0.0816	0.7497	0.8397	0.067*
H18C	0.2195	0.8320	0.8353	0.067*
C19	0.1440 (3)	0.8492 (3)	0.5950 (3)	0.0438 (6)
H19A	0.1614	0.9356	0.6032	0.066*
H19B	0.0255	0.8510	0.6101	0.066*
H19C	0.1766	0.8370	0.5099	0.066*
N1	0.2200 (3)	−0.0141 (2)	1.1512 (2)	0.0457 (6)
N2	0.4892 (2)	0.48451 (17)	0.81255 (16)	0.0246 (4)
O1	0.1607 (3)	−0.0925 (2)	1.1148 (2)	0.0716 (7)
O2	0.2325 (3)	−0.0162 (2)	1.2616 (2)	0.0651 (6)
Cl1	0.48157 (10)	0.36574 (7)	0.62743 (5)	0.0461 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0304 (11)	0.0202 (10)	0.0391 (12)	−0.0059 (8)	0.0081 (9)	0.0008 (9)
C2	0.0350 (12)	0.0224 (10)	0.0473 (14)	−0.0115 (9)	0.0001 (10)	−0.0074 (9)
C3	0.0334 (11)	0.0270 (11)	0.0312 (11)	−0.0100 (9)	0.0017 (9)	−0.0085 (9)
C4	0.0235 (10)	0.0192 (9)	0.0265 (10)	−0.0061 (7)	0.0001 (8)	−0.0031 (8)
C5	0.0318 (11)	0.0257 (10)	0.0269 (10)	−0.0105 (8)	0.0008 (9)	−0.0056 (8)
C6	0.0360 (12)	0.0272 (11)	0.0284 (11)	−0.0063 (9)	0.0046 (9)	−0.0023 (9)
C7	0.0267 (10)	0.0229 (9)	0.0205 (9)	−0.0056 (8)	−0.0003 (8)	−0.0043 (7)
C8	0.0308 (11)	0.0219 (9)	0.0210 (9)	−0.0102 (8)	0.0014 (8)	−0.0056 (7)
C9	0.0302 (11)	0.0233 (10)	0.0249 (10)	−0.0092 (8)	0.0009 (8)	−0.0050 (8)
C10	0.0328 (11)	0.0293 (11)	0.0304 (11)	−0.0125 (9)	0.0025 (9)	−0.0045 (9)
C11	0.0396 (12)	0.0267 (11)	0.0296 (11)	−0.0154 (9)	0.0027 (9)	−0.0017 (8)
C12	0.0359 (12)	0.0241 (10)	0.0296 (11)	−0.0086 (9)	−0.0027 (9)	−0.0010 (8)
C13	0.0312 (11)	0.0247 (10)	0.0260 (10)	−0.0095 (8)	0.0000 (8)	−0.0070 (8)
C14	0.0301 (11)	0.0264 (11)	0.0326 (11)	−0.0076 (9)	0.0018 (9)	−0.0018 (9)
C15	0.0432 (14)	0.0384 (13)	0.0435 (14)	−0.0016 (11)	−0.0010 (11)	−0.0143 (11)
C16	0.0391 (13)	0.0400 (13)	0.0367 (13)	−0.0010 (10)	−0.0049 (11)	−0.0070 (10)
C17	0.0302 (11)	0.0239 (10)	0.0377 (12)	−0.0081 (8)	−0.0002 (9)	−0.0051 (9)
C18	0.0389 (14)	0.0480 (15)	0.0462 (15)	−0.0086 (11)	0.0087 (11)	−0.0156 (12)
C19	0.0318 (12)	0.0367 (13)	0.0554 (16)	−0.0076 (10)	−0.0063 (11)	0.0028 (11)
N1	0.0472 (13)	0.0264 (10)	0.0566 (15)	−0.0112 (9)	0.0153 (11)	−0.0006 (10)
N2	0.0272 (9)	0.0228 (8)	0.0239 (8)	−0.0092 (7)	0.0009 (7)	−0.0035 (7)

O1	0.0921 (18)	0.0478 (12)	0.0828 (17)	−0.0473 (12)	0.0134 (14)	−0.0024 (11)
O2	0.0942 (17)	0.0485 (12)	0.0469 (12)	−0.0290 (12)	0.0254 (12)	0.0019 (9)
Cl1	0.0793 (5)	0.0479 (4)	0.0234 (3)	−0.0365 (3)	0.0067 (3)	−0.0110 (2)

Geometric parameters (Å, º)

C1—C6	1.379 (3)	C12—C13	1.391 (3)
C1—C2	1.382 (3)	C12—H12	0.9500
C1—N1	1.477 (3)	C13—C17	1.522 (3)
C2—C3	1.386 (3)	C14—C16	1.526 (3)
C2—H2	0.9500	C14—C15	1.529 (3)
C3—C4	1.393 (3)	C14—H14	1.0000
C3—H3	0.9500	C15—H15A	0.9800
C4—C5	1.397 (3)	C15—H15B	0.9800
C4—C7	1.485 (3)	C15—H15C	0.9800
C5—C6	1.388 (3)	C16—H16A	0.9800
C5—H5	0.9500	C16—H16B	0.9800
C6—H6	0.9500	C16—H16C	0.9800
C7—N2	1.254 (3)	C17—C18	1.529 (4)
C7—Cl1	1.752 (2)	C17—C19	1.533 (3)
C8—C9	1.400 (3)	C17—H17	1.0000
C8—C13	1.414 (3)	C18—H18A	0.9800
C8—N2	1.427 (3)	C18—H18B	0.9800
C9—C10	1.396 (3)	C18—H18C	0.9800
C9—C14	1.520 (3)	C19—H19A	0.9800
C10—C11	1.385 (3)	C19—H19B	0.9800
C10—H10	0.9500	C19—H19C	0.9800
C11—C12	1.390 (3)	N1—O2	1.218 (3)
C11—H11	0.9500	N1—O1	1.221 (3)
C6—C1—C2	122.8 (2)	C9—C14—C15	111.36 (19)
C6—C1—N1	118.8 (2)	C16—C14—C15	111.3 (2)
C2—C1—N1	118.4 (2)	C9—C14—H14	107.7
C1—C2—C3	118.5 (2)	C16—C14—H14	107.7
C1—C2—H2	120.7	C15—C14—H14	107.7
C3—C2—H2	120.7	C14—C15—H15A	109.5
C2—C3—C4	120.3 (2)	C14—C15—H15B	109.5
C2—C3—H3	119.9	H15A—C15—H15B	109.5
C4—C3—H3	119.9	C14—C15—H15C	109.5
C3—C4—C5	119.64 (19)	H15A—C15—H15C	109.5
C3—C4—C7	122.22 (19)	H15B—C15—H15C	109.5
C5—C4—C7	118.14 (18)	C14—C16—H16A	109.5
C6—C5—C4	120.5 (2)	C14—C16—H16B	109.5
C6—C5—H5	119.7	H16A—C16—H16B	109.5
C4—C5—H5	119.7	C14—C16—H16C	109.5
C1—C6—C5	118.2 (2)	H16A—C16—H16C	109.5
C1—C6—H6	120.9	H16B—C16—H16C	109.5
C5—C6—H6	120.9	C13—C17—C18	111.42 (19)
N2—C7—C4	121.94 (18)	C13—C17—C19	113.50 (19)
N2—C7—Cl1	122.36 (16)	C18—C17—C19	110.2 (2)

C4—C7—Cl1	115.70 (15)	C13—C17—H17	107.1
C9—C8—C13	122.16 (19)	C18—C17—H17	107.1
C9—C8—N2	118.85 (17)	C19—C17—H17	107.1
C13—C8—N2	118.84 (18)	C17—C18—H18A	109.5
C10—C9—C8	117.86 (19)	C17—C18—H18B	109.5
C10—C9—C14	120.20 (19)	H18A—C18—H18B	109.5
C8—C9—C14	121.94 (18)	C17—C18—H18C	109.5
C11—C10—C9	121.3 (2)	H18A—C18—H18C	109.5
C11—C10—H10	119.3	H18B—C18—H18C	109.5
C9—C10—H10	119.3	C17—C19—H19A	109.5
C10—C11—C12	119.7 (2)	C17—C19—H19B	109.5
C10—C11—H11	120.2	H19A—C19—H19B	109.5
C12—C11—H11	120.2	C17—C19—H19C	109.5
C11—C12—C13	121.6 (2)	H19A—C19—H19C	109.5
C11—C12—H12	119.2	H19B—C19—H19C	109.5
C13—C12—H12	119.2	O2—N1—O1	124.1 (2)
C12—C13—C8	117.3 (2)	O2—N1—C1	118.0 (2)
C12—C13—C17	122.60 (19)	O1—N1—C1	117.9 (2)
C8—C13—C17	120.03 (18)	C7—N2—C8	122.75 (18)
C9—C14—C16	110.82 (19)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···*Cg*2^{i}	0.95	2.67	3.511 (2)	147
C16—H16*B*···*Cg*1^{ii}	0.98	2.79	3.663 (3)	149

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