



Crystal structure and Hirshfeld surface analysis of dichlorido[2-(3-cyclopentyl-1,2,4-triazol-5-yl- κ N⁴)-pyridine- κ N]palladium(II) dimethylformamide monosolvate

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This study presents the synthesis, characterization and Hirshfeld surface analysis of the title mononuclear complex, [PdCl₂(C₁₂H₁₄N₄)]·C₃H₇NO. The compound crystallizes in the *P*2₁/*c* space group of the monoclinic system. The asymmetric unit contains one neutral complex Pd(HL^{c-Pe})Cl₂ [HL^{c-Pe} is 2-(3-cyclopentyl-1,2,4-triazol-5-yl)pyridine] and one molecule of DMF as a solvate. The Pd atom has a square-planar coordination. In the crystal, molecules are linked by intermolecular N—H···O and C—H···N hydrogen bonds, forming layers parallel to the *bc* plane. A Hirshfeld surface analysis showed that the H···H contacts dominate the crystal packing with a contribution of 41.4%. The contribution of the N···H/H···N and H···O/O···H interactions is somewhat smaller, amounting to 12.4% and 5%, respectively.

1. Chemical context

In recent years, square-planar coordination compounds of *d*⁸ metals with N-containing ligands have been widely investigated as effective catalysts and pre-catalysts in organic transformations (Kumbhar, 2017; Zakharchenko *et al.*, 2019; Jindabot *et al.*, 2014; Jiao *et al.*, 2020), components for optoelectronic devices (Cuerva *et al.*, 2014, 2018, 2023; Cuerva, Campo, Cano & Schmidt, 2019; Cuerva, Campo, Cano & Lodeiro, 2019), and analogs of anticancer drugs (Abu-Surrah & Kettunen, 2006; Ouellette *et al.*, 2019; Jakubowski *et al.*, 2020; Zakharchenko *et al.*, 2021; Ohorodnik *et al.*, 2023). Concurrently, functionalized pyridyl-azole-based ligands have been used in coordination chemistry as chelating polydentate ligands for obtaining various types of metal complexes with potential applications in similar fields. Complexes of dichloropalladium with functionalized pyridyl-1,2,3-triazole ligands were shown to be effective pre-catalysts with a broad functional group tolerance for cross-coupling reactions (Jindabot *et al.*, 2014; Jiao *et al.*, 2020). A series of metallomesogens of dihalide Pd^{II} and Pt^{II} compounds containing pyridyl-pyrazole ligands have been obtained in the context of the investigation of these complexes as 2D proton-conducting materials under anhydrous conditions (Cuerva *et al.*, 2014, 2018; Cuerva, Campo, Cano, & Schmidt, 2019). In subsequent studies, coordination compounds of this type were used as building blocks (precursors) for the synthesis of metallomesogens with structural asymmetry, which extends the known

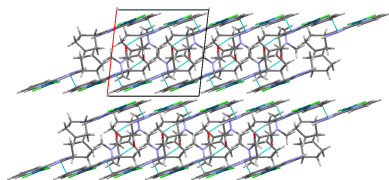
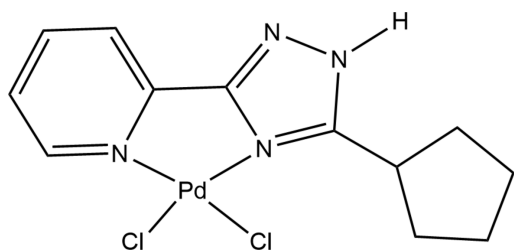


Table 1
Selected bond lengths (Å).

Pd1—C11	2.2811 (11)	Pd1—N1	2.061 (3)
Pd1—C12	2.2837 (10)	Pd1—N2	2.038 (3)

ranges of mesophases (Cuerva *et al.*, 2018, 2023; Cuerva, Campo, Cano, & Lodeiro, 2019). Furthermore, Pt^{II} metallo-mesogens exhibit photophysical multi-stimuli-responsive properties (Cuerva, Campo, Cano, & Lodeiro, 2019). The complexes of *d*⁸ metals with pyridyl-azole-based ligands have been explored in cancer therapy as analogues of cisplatin; their application is limited by the severe side effects and development of drug resistance. The combination of *d*⁸ metals and chelating pyridyl-azole-based ligands should lead to an increase in the stability of the corresponding complexes and to a decrease in hydrolysis in biological media and, as a result, to a decrease in the toxicity of the resulting compounds (Abu-Surrah & Kettunen, 2006). Previous studies demonstrated that the complexes of Pd and Pt with hydrophobic pyridyl-azole-based ligands have certain anticancer activity against various types of tumour cells *in vitro* (Ouellette *et al.*, 2019; Jakubowski *et al.*, 2020; Zakharchenko *et al.*, 2021; Ohorodnik *et al.*, 2023). Our previous research of six dichloride Pd^{II} complexes based on 5-substituted 3-(2-pyridyl)-5-alkyl-1,2,4-triazoles was reported. The evaluation of ¹H NMR spectroscopic data was focused on three types of proton signals of ligands and complexes located near the coordination centre and discussed in the context of the influence that cycloalkyl substituents have on intramolecular interactions, being also supported by X-ray data for Pd^{II} complexes (Ivanova *et al.*, 2024). We report herein the crystal structure, including characterization of the intermolecular contacts by Hirshfeld surface analysis, of a new mononuclear dichloropalladium(II) complex with 2-(3-cyclopentyl-1,2,4-triazol-5-yl)pyridine.



2. Structural commentary

The title compound crystallizes in the *P2*₁/*c* space group of the monoclinic system. The asymmetric unit contains one neutral complex Pd(HL^{c-Pc})Cl₂ [HL^{c-Pc} is 2-(3-cyclopentyl-1,2,4-triazol-5-yl)pyridine] and one molecule of DMF as a solvate. The molecular structure of title compound is shown in Fig. 1.

The Pd atom has a square-planar environment formed by the bidentate coordination of two nitrogen atoms of the HL^{c-Pc} ligand and two chlorine atoms. The deviation of the Pd atom from the mean-square plane defined by through the Cl1/Cl2/N1/N2 atoms (r.m.s.d. = 0.002 Å) is −0.0164 (11) Å. The Pd—N and Pd—Cl bond distances are 2.038 (3) and

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

<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>
N4—H4...O1	0.86	1.85	2.679 (4)	161
C3—H3...N3 ⁱ	0.93	2.66	3.471 (6)	146

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

2.061 (3) Å and 2.2811 (11) and 2.2837 (10) Å, respectively (Table 1). This structure of the title complex is in very good agreement with previously described Pd complexes with a similar coordination (Khomenko *et al.*, 2009; Zakharchenko *et al.*, 2021)

The five-membered ring is rotated relative to the plane of the pyridine-triazole fragment and is in the *ac* conformation relative to the C7—N4 bond of the triazole ring [the N4—C7—C8—C12 torsion angle is −91.1 (5)°]. The five-membered ring is in an envelope conformation. Atom C8 deviates by 0.564 (8) Å from the mean square plane through the remaining ring atoms (r.m.s.d. = 0.04Å).

3. Supramolecular features

In the crystal, Pd(HL^{c-Pc})Cl₂ complex molecules, and also molecules of the complex and molecules of DMF are linked by N—H...O and C—H...N hydrogen bonds (Table 2), forming layers parallel to the *bc* plane (Fig. 2).

4. Hirshfeld surface analysis and finger print plots

The intermolecular interactions in the crystal structure of the title compound have been analysed by means of the *d*_{norm} property (Fig. 3) mapped over the Hirshfeld surface (Spackman & Jayatilaka, 2009), which was calculated using the *CrystalExplorer21* program (Spackman *et al.*, 2021). The strongest contacts, which are visualized on the Hirshfeld

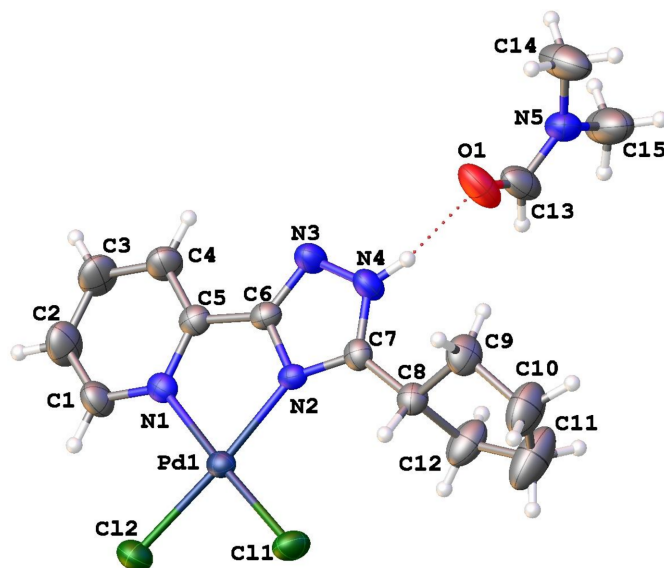


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

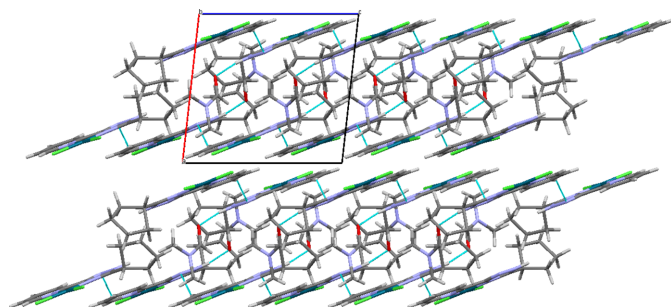


Figure 2
Crystal packing of the title compound.

surface as the dark-red spots, correspond to the N—H...O hydrogen bond between the complex molecule and the DMF solvent molecule. The lighter red spots correspond to H...N/N...H interactions. The majority of the intermolecular interactions of the title compound are weak, and are represented in blue on the Hirshfeld surface.

For further exploration of the intermolecular interactions, two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were generated, as shown in Fig. 4. The H...H interactions with a contribution of 41.4% have a significant effect on the consolidation in the solid state. The Cl...H/H...Cl (18.0%), N...H/H...N (12.4%), C...H/H...C (10.7%), O...H/H...O (5%), Cl...C/C...Cl (4.5%) and N...Cl/Cl...N (2.5%) interactions are less impactful in comparison.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.45, updated March 2024; Groom *et al.*, 2016) found only eleven structures containing the Pd atom coordinated to

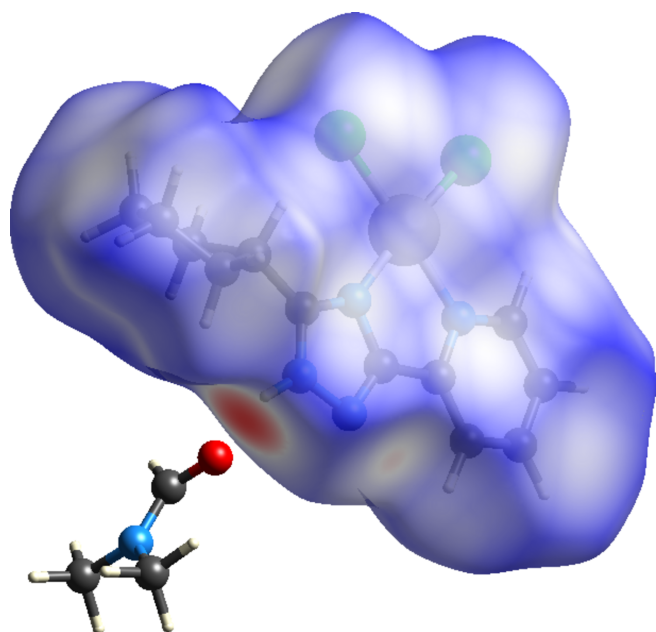


Figure 3
Three-dimensional Hirshfeld surface of title compound mapped over d_{norm} .

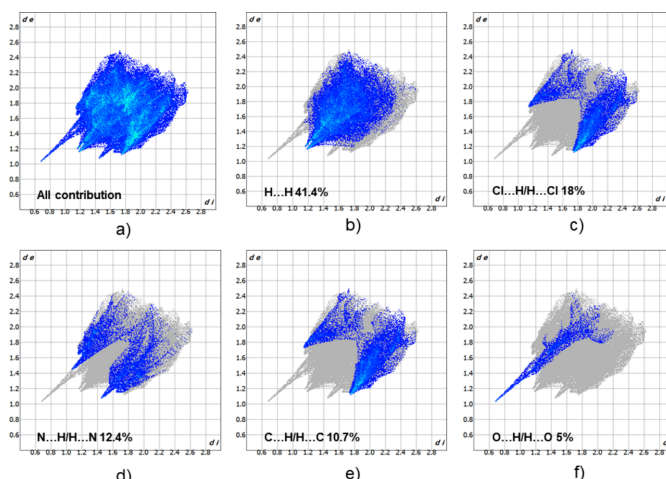


Figure 4
Two-dimensional fingerprint plots for title compound showing (a) all interactions, and (b)–(f) delineated into contributions from specific contacts (blue areas) [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

two Cl atoms and a pyridine-triazole fragment. Of these, seven structures contain a 1,2,3-triazol fragment (Ervithayasuporn *et al.*, 2015; Ervithayasuporn, 2016; Schweinfurth *et al.*, 2011; Yano *et al.*, 2012; Jindabot *et al.*, 2014; Schweinfurth *et al.*, 2009; Lang *et al.*, 2012) and four structures contain a 1,2,4-triazol fragment (Khomeiko *et al.*, 2009; Zakharchenko *et al.*, 2021; Ohorodnik *et al.*, 2023). All of the structures have a square-planar coordination of the Pd atom. The Pd—N and Pd—Cl bond distances vary from 1.999 (2)–2.066 (3) Å and 2.264 (2)–2.293 (2) Å, respectively.

6. Synthesis and crystallization

To obtain the complex Pd(HL^{c-Pe})Cl₂·DMF, 0.2 mmol of pre-synthesized Pd(HL^{c-Pe})Cl₂ (Ivanova *et al.*, 2024) was dissolved in 1 ml of DMF and salted out with 1 ml of MTBE (methyl *tert*-

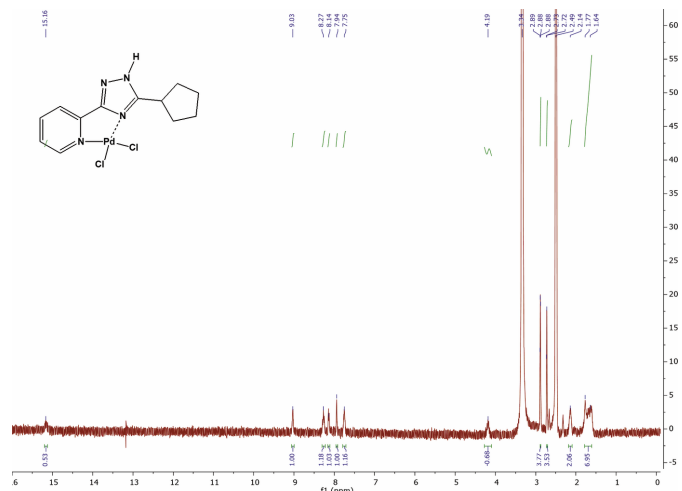


Figure 5
¹H NMR spectrum of Pd(HL^{c-Pe})Cl₂ in DMSO-*d*₆.

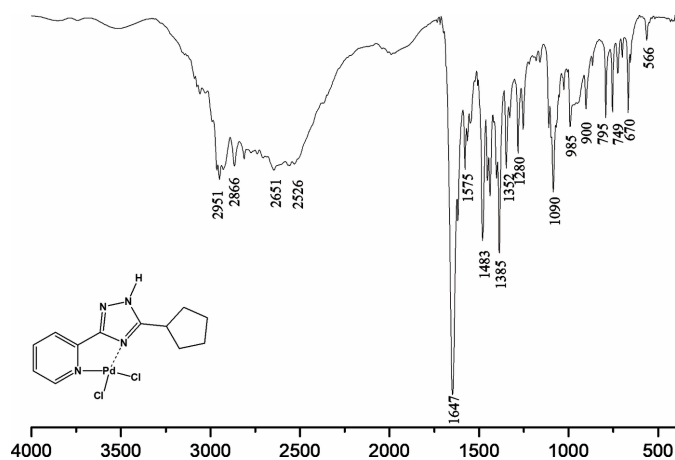


Figure 6
IR spectrum for Pd(HL^{c-Pe})Cl₂.

butyl ether) at room temperature for 72 h, affording yellow crystals. The crystals were collected by filtration.

Pd(HL^{c-Pe})Cl₂. Yield 66%. m. p. >523 K decomp. ¹H NMR (400 MHz, DMSO-*d*₆) δ: 15.17 (*br s*, 1H, NH), 9.04 (*d*, *J* = 5.6 Hz, 1H, Py-H⁶), 8.28 (*t*, *J* = 7.7 Hz, 1H, Py-H⁴), 8.15 (*d*, *J* = 8.1 Hz, 1H, Py-H³), 7.76 (*t*, *J* = 6.0 Hz, 1H, Py-H⁵), 4.20 (*m*, 1H, H⁹), 2.15 (*m*, 2H, H^{c-Pe}), 1.78–1.62 (*m*, 6H, H^{c-Pe}) ppm (Fig. 5). IR (KBr, cm⁻¹): 3457, 3250, 2945, 2873, 1621, 1543, 1470, 1287, 1090, 788, 723, 467 (Fig. 6). Elemental analysis: Analysis calculated for C₁₂H₁₄Cl₂N₄Pd (391.58): C, 36.81%; H, 3.60%; N, 14.31%. Found: C: 36.65% H: 3.52% N: 14.43%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms were placed in calculated positions and refined using a riding model with $U_{\text{iso}}(\text{H}) = nU_{\text{eq}}$ of the carrier atom ($n = 1.5$ for methyl groups and $n = 1.2$ for other hydrogen atoms). The U_{ij} values of the C atoms of the five-membered ring were restrained to be similar to each other (within a standard deviation of 0.02 Å²).

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Table 3

Experimental details.

Crystal data	[PdCl ₂ (C ₁₂ H ₁₄ N ₄)]·C ₃ H ₇ NO
Chemical formula	464.67
<i>M_r</i>	Monoclinic, <i>P</i> ₂ / <i>c</i>
Crystal system, space group	296
Temperature (K)	9.3964 (8), 20.2572 (16), 9.9822 (7)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	96.358 (2)
β (°)	1888.4 (3)
<i>V</i> (Å ³)	4
<i>Z</i>	Mo Kα
Radiation type	1.28
μ (mm ⁻¹)	0.4 × 0.2 × 0.15
Crystal size (mm)	
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.533, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	13789, 4304, 3345
<i>R</i> _{int}	0.046
(sin θ/λ) _{max} (Å ⁻¹)	0.650
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.051, 0.093, 1.12
No. of reflections	4304
No. of parameters	219
No. of restraints	30
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.64, −0.94

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2019/3* (Sheldrick, 2015b) and *OLEX2 1.5* (Dolomanov *et al.*, 2009).

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supporting information

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Crystal structure and Hirshfeld surface analysis of dichlorido[2-(3-cyclopentyl-1,2,4-triazol-5-yl- κ N⁴)pyridine- κ N]palladium(II) dimethylformamide monosolvate

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Computing details

Dichlorido[2-(3-cyclopentyl-1,2,4-triazol-5-yl- κ N⁴)pyridine- κ N]palladium(II) dimethylformamide monosolvate

Crystal data

[PdCl₂(C₁₂H₁₄N₄)]·C₃H₇NO

$M_r = 464.67$

Monoclinic, $P2_1/c$

$a = 9.3964$ (8) Å

$b = 20.2572$ (16) Å

$c = 9.9822$ (7) Å

$\beta = 96.358$ (2)°

$V = 1888.4$ (3) Å³

$Z = 4$

$F(000) = 936$

$D_x = 1.634$ Mg m⁻³

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

Cell parameters from 6028 reflections

$\theta = 2.3$ – 30.3 °

$\mu = 1.28$ mm⁻¹

$T = 296$ K

Block, orange

$0.4 \times 0.2 \times 0.15$ mm

Data collection

Bruker APEXII CCD
diffractometer

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.533$, $T_{\max} = 0.746$

13789 measured reflections

4304 independent reflections

3345 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.0$ °

$h = -12 \rightarrow 11$

$k = -23 \rightarrow 26$

$l = -10 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.093$

$S = 1.12$

4304 reflections

219 parameters

30 restraints

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.2719P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.64$ e Å⁻³

$\Delta\rho_{\min} = -0.94$ e Å⁻³

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.

Refinement. Using Olex2 (Dolomanov *et al.*, 2009), the structure was solved with the SHELXT (Sheldrick, 2018) structure solution program using Intrinsic Phasing and refined with the SHELXL (Sheldrick, 2015) refinement package. Full-matrix least-squares refinement against F^2 in anisotropic approximation was used for non-hydrogen atoms.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd1	0.14161 (3)	0.51528 (2)	0.63841 (3)	0.02837 (10)
Cl1	0.17109 (12)	0.61436 (5)	0.53648 (11)	0.0457 (3)
Cl2	0.06163 (12)	0.56975 (5)	0.81588 (11)	0.0475 (3)
N1	0.1217 (3)	0.42381 (15)	0.7248 (3)	0.0309 (7)
N2	0.2130 (3)	0.45857 (15)	0.4909 (3)	0.0261 (7)
N3	0.2590 (4)	0.35403 (16)	0.4333 (3)	0.0399 (8)
N4	0.2936 (4)	0.39792 (16)	0.3393 (3)	0.0382 (8)
H4	0.328939	0.386935	0.266629	0.046*
C1	0.0774 (5)	0.4111 (2)	0.8460 (4)	0.0450 (11)
H1	0.049967	0.446010	0.898062	0.054*
C2	0.0718 (5)	0.3477 (2)	0.8945 (5)	0.0596 (14)
H2	0.040242	0.339994	0.978152	0.072*
C3	0.1129 (5)	0.2958 (2)	0.8188 (5)	0.0582 (13)
H3	0.109421	0.252721	0.850674	0.070*
C4	0.1593 (5)	0.3083 (2)	0.6954 (4)	0.0469 (11)
H4A	0.188724	0.273951	0.642997	0.056*
C5	0.1612 (4)	0.37237 (19)	0.6510 (4)	0.0330 (9)
C6	0.2103 (4)	0.39271 (19)	0.5233 (4)	0.0312 (9)
C7	0.2667 (4)	0.4598 (2)	0.3727 (4)	0.0313 (8)
C8	0.2970 (4)	0.5186 (2)	0.2913 (4)	0.0344 (9)
H8	0.225634	0.552496	0.305020	0.041*
C9	0.2950 (5)	0.5072 (2)	0.1405 (4)	0.0501 (11)
H9A	0.345162	0.466919	0.122290	0.060*
H9B	0.197656	0.504772	0.096855	0.060*
C10	0.3716 (6)	0.5671 (3)	0.0933 (5)	0.0771 (16)
H10A	0.420108	0.556242	0.015282	0.093*
H10B	0.304162	0.602525	0.069144	0.093*
C11	0.4769 (6)	0.5871 (3)	0.2084 (6)	0.0959 (19)
H11A	0.468558	0.633999	0.225607	0.115*
H11B	0.573529	0.578154	0.187875	0.115*
C12	0.4455 (5)	0.5479 (3)	0.3309 (5)	0.0609 (13)
H12A	0.445256	0.576371	0.409077	0.073*
H12B	0.515995	0.513355	0.351091	0.073*
O1	0.4202 (4)	0.33801 (18)	0.1446 (3)	0.0690 (10)
N5	0.6183 (4)	0.28119 (17)	0.1094 (4)	0.0473 (9)
C13	0.5478 (6)	0.3255 (2)	0.1708 (4)	0.0543 (13)

H13	0.598512	0.349448	0.239900	0.065*
C14	0.5465 (6)	0.2439 (3)	-0.0011 (5)	0.0778 (18)
H14A	0.447518	0.256600	-0.014784	0.117*
H14B	0.553480	0.197671	0.019415	0.117*
H14C	0.590723	0.252728	-0.081424	0.117*
C15	0.7682 (6)	0.2678 (3)	0.1477 (6)	0.0799 (18)
H15A	0.803769	0.296598	0.220213	0.120*
H15B	0.820744	0.275203	0.071894	0.120*
H15C	0.779881	0.222732	0.176556	0.120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02677 (15)	0.02755 (16)	0.03033 (17)	-0.00105 (13)	0.00115 (11)	-0.00292 (13)
Cl1	0.0606 (7)	0.0298 (5)	0.0473 (6)	-0.0059 (5)	0.0080 (5)	-0.0003 (5)
Cl2	0.0589 (7)	0.0423 (6)	0.0431 (6)	-0.0010 (5)	0.0144 (5)	-0.0117 (5)
N1	0.0259 (16)	0.0341 (18)	0.0317 (18)	0.0024 (14)	-0.0002 (13)	-0.0026 (14)
N2	0.0241 (15)	0.0229 (15)	0.0306 (17)	0.0004 (13)	-0.0003 (13)	-0.0014 (13)
N3	0.049 (2)	0.0303 (19)	0.042 (2)	0.0047 (16)	0.0135 (17)	-0.0008 (16)
N4	0.046 (2)	0.037 (2)	0.0342 (19)	0.0060 (16)	0.0126 (16)	-0.0037 (15)
C1	0.056 (3)	0.048 (3)	0.033 (2)	0.005 (2)	0.013 (2)	-0.001 (2)
C2	0.077 (4)	0.059 (3)	0.046 (3)	0.007 (3)	0.020 (3)	0.019 (2)
C3	0.075 (4)	0.039 (3)	0.063 (3)	0.007 (3)	0.018 (3)	0.022 (2)
C4	0.057 (3)	0.033 (2)	0.052 (3)	0.006 (2)	0.012 (2)	0.007 (2)
C5	0.028 (2)	0.033 (2)	0.037 (2)	0.0005 (17)	-0.0003 (17)	0.0011 (18)
C6	0.030 (2)	0.028 (2)	0.035 (2)	-0.0012 (17)	0.0003 (17)	-0.0010 (17)
C7	0.0252 (19)	0.037 (2)	0.032 (2)	0.0006 (17)	0.0019 (16)	0.0001 (17)
C8	0.0318 (19)	0.040 (2)	0.031 (2)	-0.0023 (18)	0.0002 (16)	-0.0001 (18)
C9	0.055 (3)	0.062 (3)	0.033 (2)	-0.005 (2)	0.002 (2)	0.005 (2)
C10	0.077 (3)	0.098 (4)	0.056 (3)	-0.025 (3)	0.008 (3)	0.024 (3)
C11	0.080 (4)	0.124 (5)	0.080 (4)	-0.046 (3)	-0.009 (3)	0.043 (3)
C12	0.051 (3)	0.072 (3)	0.056 (3)	-0.024 (3)	-0.009 (2)	0.016 (3)
O1	0.085 (3)	0.071 (3)	0.056 (2)	0.029 (2)	0.026 (2)	-0.0065 (18)
N5	0.054 (2)	0.034 (2)	0.055 (2)	-0.0022 (18)	0.0126 (19)	-0.0088 (17)
C13	0.087 (4)	0.043 (3)	0.036 (3)	0.009 (3)	0.019 (3)	-0.002 (2)
C14	0.066 (4)	0.071 (4)	0.095 (5)	0.008 (3)	0.000 (3)	-0.038 (3)
C15	0.066 (4)	0.059 (4)	0.115 (5)	-0.006 (3)	0.012 (4)	-0.028 (3)

Geometric parameters (Å, °)

Pd1—Cl1	2.2811 (11)	C8—C12	1.528 (6)
Pd1—Cl2	2.2837 (10)	C9—H9A	0.9700
Pd1—N1	2.061 (3)	C9—H9B	0.9700
Pd1—N2	2.038 (3)	C9—C10	1.511 (6)
N1—C1	1.348 (5)	C10—H10A	0.9700
N1—C5	1.352 (5)	C10—H10B	0.9700
N2—C6	1.374 (5)	C10—C11	1.487 (7)
N2—C7	1.334 (4)	C11—H11A	0.9700

N3—N4	1.358 (4)	C11—H11B	0.9700
N3—C6	1.312 (5)	C11—C12	1.514 (7)
N4—H4	0.8600	C12—H12A	0.9700
N4—C7	1.328 (5)	C12—H12B	0.9700
C1—H1	0.9300	O1—C13	1.225 (6)
C1—C2	1.376 (6)	N5—C13	1.308 (5)
C2—H2	0.9300	N5—C14	1.440 (6)
C2—C3	1.376 (6)	N5—C15	1.444 (6)
C3—H3	0.9300	C13—H13	0.9300
C3—C4	1.375 (6)	C14—H14A	0.9600
C4—H4A	0.9300	C14—H14B	0.9600
C4—C5	1.373 (5)	C14—H14C	0.9600
C5—C6	1.462 (5)	C15—H15A	0.9600
C7—C8	1.487 (5)	C15—H15B	0.9600
C8—H8	0.9800	C15—H15C	0.9600
C8—C9	1.522 (5)		
C11—Pd1—C12	89.29 (4)	C8—C9—H9A	111.1
N1—Pd1—C11	177.27 (9)	C8—C9—H9B	111.1
N1—Pd1—C12	93.27 (9)	H9A—C9—H9B	109.0
N2—Pd1—C11	96.18 (9)	C10—C9—C8	103.5 (4)
N2—Pd1—C12	174.47 (9)	C10—C9—H9A	111.1
N2—Pd1—N1	81.25 (12)	C10—C9—H9B	111.1
C1—N1—Pd1	126.8 (3)	C9—C10—H10A	110.5
C1—N1—C5	118.3 (4)	C9—C10—H10B	110.5
C5—N1—Pd1	115.0 (2)	H10A—C10—H10B	108.7
C6—N2—Pd1	111.2 (2)	C11—C10—C9	106.1 (4)
C7—N2—Pd1	144.6 (3)	C11—C10—H10A	110.5
C7—N2—C6	104.2 (3)	C11—C10—H10B	110.5
C6—N3—N4	102.1 (3)	C10—C11—H11A	110.1
N3—N4—H4	123.9	C10—C11—H11B	110.1
C7—N4—N3	112.2 (3)	C10—C11—C12	108.0 (4)
C7—N4—H4	123.9	H11A—C11—H11B	108.4
N1—C1—H1	119.3	C12—C11—H11A	110.1
N1—C1—C2	121.4 (4)	C12—C11—H11B	110.1
C2—C1—H1	119.3	C8—C12—H12A	110.9
C1—C2—H2	120.1	C8—C12—H12B	110.9
C1—C2—C3	119.8 (4)	C11—C12—C8	104.4 (4)
C3—C2—H2	120.1	C11—C12—H12A	110.9
C2—C3—H3	120.4	C11—C12—H12B	110.9
C4—C3—C2	119.2 (4)	H12A—C12—H12B	108.9
C4—C3—H3	120.4	C13—N5—C14	120.0 (4)
C3—C4—H4A	120.7	C13—N5—C15	122.3 (4)
C5—C4—C3	118.7 (4)	C14—N5—C15	117.7 (4)
C5—C4—H4A	120.7	O1—C13—N5	125.2 (5)
N1—C5—C4	122.6 (4)	O1—C13—H13	117.4
N1—C5—C6	113.0 (3)	N5—C13—H13	117.4
C4—C5—C6	124.4 (4)	N5—C14—H14A	109.5

N2—C6—C5	119.6 (3)	N5—C14—H14B	109.5
N3—C6—N2	113.7 (3)	N5—C14—H14C	109.5
N3—C6—C5	126.6 (4)	H14A—C14—H14B	109.5
N2—C7—C8	127.7 (4)	H14A—C14—H14C	109.5
N4—C7—N2	107.8 (3)	H14B—C14—H14C	109.5
N4—C7—C8	124.4 (3)	N5—C15—H15A	109.5
C7—C8—H8	108.1	N5—C15—H15B	109.5
C7—C8—C9	116.0 (4)	N5—C15—H15C	109.5
C7—C8—C12	113.2 (3)	H15A—C15—H15B	109.5
C9—C8—H8	108.1	H15A—C15—H15C	109.5
C9—C8—C12	103.0 (3)	H15B—C15—H15C	109.5
C12—C8—H8	108.1		
Pd1—N1—C1—C2	-178.4 (3)	C2—C3—C4—C5	-0.8 (7)
Pd1—N1—C5—C4	177.8 (3)	C3—C4—C5—N1	1.2 (7)
Pd1—N1—C5—C6	-0.1 (4)	C3—C4—C5—C6	178.8 (4)
Pd1—N2—C6—N3	-178.2 (3)	C4—C5—C6—N2	-177.5 (4)
Pd1—N2—C6—C5	-0.5 (4)	C4—C5—C6—N3	0.0 (6)
Pd1—N2—C7—N4	177.4 (3)	C5—N1—C1—C2	-0.1 (6)
Pd1—N2—C7—C8	-1.0 (7)	C6—N2—C7—N4	-0.1 (4)
N1—C1—C2—C3	0.4 (8)	C6—N2—C7—C8	-178.5 (3)
N1—C5—C6—N2	0.4 (5)	C6—N3—N4—C7	0.1 (4)
N1—C5—C6—N3	177.8 (4)	C7—N2—C6—N3	0.2 (4)
N2—C7—C8—C9	-154.3 (4)	C7—N2—C6—C5	178.0 (3)
N2—C7—C8—C12	86.9 (5)	C7—C8—C9—C10	-163.2 (4)
N3—N4—C7—N2	0.0 (4)	C7—C8—C12—C11	158.7 (4)
N3—N4—C7—C8	178.4 (3)	C8—C9—C10—C11	30.6 (6)
N4—N3—C6—N2	-0.2 (4)	C9—C8—C12—C11	32.7 (5)
N4—N3—C6—C5	-177.7 (4)	C9—C10—C11—C12	-10.2 (7)
N4—C7—C8—C9	27.7 (5)	C10—C11—C12—C8	-14.2 (7)
N4—C7—C8—C12	-91.1 (5)	C12—C8—C9—C10	-39.0 (5)
C1—N1—C5—C4	-0.7 (6)	C14—N5—C13—O1	1.9 (8)
C1—N1—C5—C6	-178.6 (3)	C15—N5—C13—O1	-178.4 (5)
C1—C2—C3—C4	0.0 (8)		

Hydrogen-bond geometry (Å, °)

<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>
N4—H4...O1	0.86	1.85	2.679 (4)	161
C3—H3...N3 ⁱ	0.93	2.66	3.471 (6)	146

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