metal-organic compounds

Bis(hydrogen L-glutamato)palladium(II)

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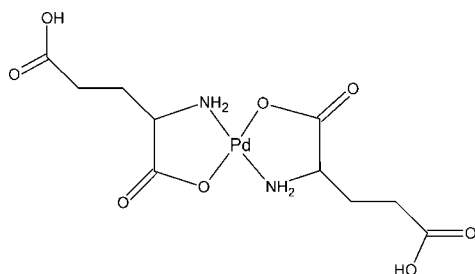Correspondence e-mail: kurt.merzweiler@chemie.uni-halle.de

In the title compound, $[Pd(C_5H_8NO_4)_2]$, the Pd(II) atom is coordinated by two O atoms and two N atoms of two *N,O*-chelating hydrogen L-glutatmate ligands in a square–planar geometry with the N and O atoms in a mutually *trans* arrangement. The complex units are embedded in a network of N—H⋯O and O—H⋯O hydrogen-bonding interactions that stabilize the three-dimensional crystal structure. The strongest hydrogen bonds are formed between the γ-COOH untis of adjacent glutamate ligands, leading to dimers of the type $R_2^2(8)$ with O⋯O separations of 2.640 (6) Å.

Related literature

For the synthesis of the title compound, see: Spacu & Scherzer (1962). For the structures of related palladium complexes with amino acid ligands, see: Vagg (1979); Jarzab *et al.* (1973); Sabat *et al.* (1979); Pletnev *et al.* (1992); Hao *et al.* (2007); Gao *et al.* (2008).

Experimental

Crystal data

$[Pd(C_5H_8NO_4)_2]$	γ = 104.245 (6)°
M_r = 398.66	V = 319.90 (4) Å^3
Triclinic, $P1$	Z = 1
a = 4.8858 (3) Å	Mo $K\alpha$ radiation
b = 5.1605 (4) Å	μ = 1.49 mm^{-1}
c = 13.3651 (9) Å	T = 200 K
α = 93.725 (6)°	0.17 × 0.06 × 0.04 mm
β = 99.734 (6)°	

Data collection

Stoe IPDS 2T diffractometer	4724 measured reflections
Absorption correction: integration (X-RED; Stoe & Cie, 2009)	2406 independent reflections
T_{min} = 0.806, T_{max} = 0.973	2389 reflections with $I > 2\sigma(I)$
	R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.066	
S = 1.04	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
2406 reflections	$\Delta\rho_{min}$ = −0.74 e Å^{-3}
208 parameters	Absolute structure: Flack (1983), 1146 Friedel pairs
9 restraints	Flack parameter: −0.02 (4)

Table 1
Selected bond lengths (Å).

Pd—N1	2.072 (9)	Pd—O1	1.976 (8)
Pd—N2	2.005 (11)	Pd—O5	2.024 (7)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H9⋯O6^i	0.85 (2)	2.15 (4)	2.979 (15)	162 (8)
N2—H10⋯O5^{ii}	0.85 (2)	2.43 (8)	3.121 (13)	138 (10)
O7—H16⋯O4^{iii}	0.85 (2)	1.80 (2)	2.639 (6)	169 (7)
O3—H8⋯O8^{iv}	0.86 (2)	1.79 (3)	2.640 (6)	167 (7)
N1—H1⋯O2^v	0.85 (2)	2.15 (3)	2.996 (15)	170 (9)
N1—H2⋯O1^{vi}	0.85 (2)	2.30 (8)	2.998 (15)	139 (10)
N1—H2⋯O5^{vii}	0.85 (2)	2.42 (7)	3.117 (13)	140 (10)

Symmetry codes: (i) $x + 1, y + 1, z$; (ii) $x, y + 1, z$; (iii) $x − 1, y + 1, z + 1$; (iv) $x + 1, y − 1, z − 1$; (v) $x − 1, y − 1, z$; (vi) $x, y − 1, z$; (vii) $x + 1, y, z$.

Data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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supporting information

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S1. Comment

The title compound, [Pd($C_5H_8NO_4$)$_2$] (I), consists of a palladium(II) atom which is coordinated by two N and two O atoms of two chelating hydrogen glutamate ligands. The metal atom adopts a distorted square–planar coordination with the two N atoms and the two O atoms in mutual *trans* arrangements. The maximum deviation from the least squares plane through the atoms Pd, N1, N2, O1 and O5 is 0.026 Å for N2. The distances Pd—O (1.976 (8), 2.024 (7) Å) and Pd—N (2.005 (11), 2.072 (9) Å) are in agreement with the values observed for other Pd(II) amino acid derivatives, like *cis*-bis(*L*-tyrosinato)-palladium(II) hemihydrate (Jarzab *et al.*, 1973), bis(*L*-tyrosinato)-palladium(II) (Sabat *et al.*, 1979), bis-(*L*-valinato)-palladium(II) monohydrate (Pletnev *et al.*, 1992); Hao *et al.*, 2007), *cis*-bis(*L*-aspartato-*N,O*)-palladium(II) (Gao *et al.*, 2008) or bis(*L*-serinato)-palladium(II) (Vagg, 1979). For both the hydrogen glutatmate ligands, the five membered PdNC$_2$O chelate rings adopt envelope conformations with a nearly coplanar arrangement of the Pd, O, C and N atoms at the flap positions.

The main conformational difference between both chelate rings arises from the orientation of the carboxyethyl groups. In the case of C2 the carboxyethyl group is in an axial position and for C7 an equatorially arrangend carboxyethyl group is observed (Fig. 1).

The packing of the complex units is supported by different types of hydrogen bonding interactions. The strongest hydrogen bridges are formed between the *γ*-carboxyl groups of neighbouring molecules. Consequently, $R_2^2(8)$ motifs are observed and the complex units are arranged in chains. Additionally, there are N—H⋯O hydrogen bridges of the type $C_1^1(4)$ and $C_1^1(5)$ which are formed between amino groups and oxygen atoms of adjacent *α*-carboxylate groups (Fig. 2)

S2. Experimental

The title compound was prepared from K$_2$PdCl$_4$ and sodium hydrogen glutamate according to a procedure described by Spacu & Scherzer (1962). For the growth of single crystals, the reaction mixture was stored at 278 K for several weeks.

S3. Refinement

C-bound H atoms of the hydrogen glutamate units were positioned geometrically and refinded using a riding model with $U_{iso}(H) = 1.2\ U_{eq}(C)$ [d(C—H) = 0.99 (for C–H) and 1.00 Å (for CH$_2$)]. H atoms attached to N and O were located from difference fourier maps and refined with N—H distances fixed at 0.85 (2) Å ($U_{iso}(H) = 1.2\ U_{eq}(N)$) and O—H distances fixed at 0.85 (2) and 0.86 (2) Å ($U_{iso}(H) = 1.2\ U_{eq}(O)$).
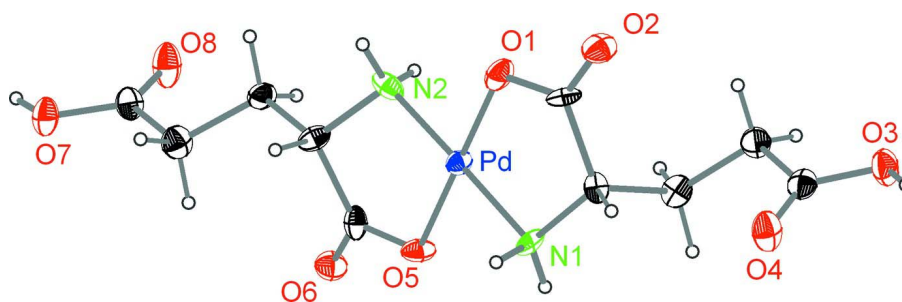
Figure 1

Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probabiltiy level.
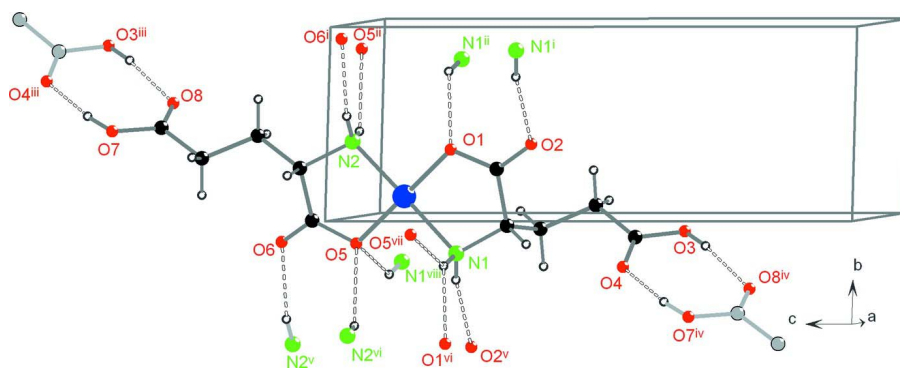

Figure 2

Arrangement of the hydrogen bonds around the complex unit. [Symmetry operators: (i) $x + 1, y + 1, z$; (ii) $x, y + 1, z$; (iii) $x - 1, y + 1, z + 1$; (iv) $x + 1, y - 1, z - 1$; (v) $x - 1, y - 1, z$; (vi) $x, y - 1, z$; (vii) $x + 1, y, z$; (viii) $x - 1, y, z$.]

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Crystal data

$[Pd(C_5H_8NO_4)_2]$	$Z = 1$
$M_r = 398.66$	$F(000) = 201$
Triclinic, $P1$	$D_x = 2.070$ Mg m^{-3}
Hall symbol: P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.8858$ (3) Å	Cell parameters from 7673 reflections
$b = 5.1605$ (4) Å	$\theta = 3.1–29.3°$
$c = 13.3651$ (9) Å	$\mu = 1.49$ mm^{-1}
$\alpha = 93.725$ (6)°	$T = 200$ K
$\beta = 99.734$ (6)°	Prism, yellow
$\gamma = 104.245$ (6)°	$0.17 \times 0.06 \times 0.04$ mm
$V = 319.90$ (4) Å^3	

Data collection

Stoe IPDS 2T diffractometer	$T_{min} = 0.806$, $T_{max} = 0.973$
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	4724 measured reflections
	2406 independent reflections
Plane graphite monochromator	2389 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.044$
ω–scans	$\theta_{max} = 26.0°$, $\theta_{min} = 3.1°$
Absorption correction: integration	$h = -6 \rightarrow 6$
(*X-RED*; Stoe & Cie, 2009)	$k = -6 \rightarrow 6$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.066$	
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.1842P]$ where $P = (F_o^2 + 2F_c^2)/3$
2406 reflections	
208 parameters	$(\Delta/\sigma)_{max} < 0.001$
9 restraints	$\Delta\rho_{max} = 0.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.74$ e Å^{-3}
	Absolute structure: Flack (1983), 1146 Friedel pairs
Secondary atom site location: difference Fourier map	Absolute structure parameter: −0.02 (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.

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 $F^2 > \sigma(F^2)$ 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	0.649 (3)	0.240 (2)	0.7428 (9)	0.020 (3)
C2	0.478 (2)	−0.043 (2)	0.7031 (8)	0.015 (2)
H3	0.6076	−0.1464	0.6791	0.017*
C3	0.2260 (11)	−0.0501 (11)	0.6139 (4)	0.0219 (11)
H4	0.1138	−0.2395	0.5939	0.026*
H5	0.0971	0.0487	0.6394	0.026*
C4	0.3130 (13)	0.0694 (11)	0.5184 (4)	0.0234 (11)
H6	0.1410	0.1014	0.4755	0.028*
H7	0.4546	0.2460	0.5398	0.028*
C5	0.4388 (11)	−0.1010 (11)	0.4554 (4)	0.0224 (11)
C6	−0.125 (2)	0.009 (2)	1.0111 (8)	0.018 (2)
C7	0.098 (2)	0.272 (2)	1.0603 (9)	0.019 (2)
H11	0.2662	0.2244	1.1017	0.023*
C8	−0.0210 (12)	0.4448 (10)	1.1299 (4)	0.0213 (11)
H12	−0.2096	0.4604	1.0938	0.026*
H13	0.1110	0.6279	1.1447	0.026*
C9	−0.0580 (13)	0.3289 (13)	1.2308 (4)	0.0249 (12)
H14	−0.1794	0.1414	1.2162	0.030*
H15	0.1325	0.3254	1.2694	0.030*
C10	−0.1944 (12)	0.4914 (11)	1.2950 (4)	0.0210 (11)
N1	0.345 (2)	−0.179 (2)	0.7842 (7)	0.018 (2)
H2	0.464 (16)	−0.25 (2)	0.820 (7)	0.022*
H1	0.196 (12)	−0.311 (12)	0.767 (7)	0.022*

N2	0.194 (2)	0.405 (2)	0.9716 (8)	0.020 (2)
H10	0.054 (15)	0.46 (2)	0.944 (8)	0.024*
H9	0.346 (13)	0.526 (13)	0.999 (7)	0.024*
O1	0.5808 (17)	0.3460 (16)	0.8246 (6)	0.023 (2)
O2	0.8325 (17)	0.3614 (16)	0.6976 (6)	0.0259 (16)
O3	0.3977 (9)	−0.0697 (8)	0.3575 (3)	0.0278 (8)
H8	0.503 (13)	−0.150 (12)	0.328 (5)	0.033*
O4	0.5723 (10)	−0.2598 (10)	0.4909 (3)	0.0289 (9)
O5	−0.0695 (16)	−0.1097 (14)	0.9320 (6)	0.0206 (18)
O6	−0.3437 (17)	−0.0908 (16)	1.0453 (6)	0.0237 (15)
O7	−0.1369 (9)	0.4718 (8)	1.3941 (3)	0.0267 (8)
H16	−0.220 (15)	0.553 (12)	1.432 (5)	0.032*
O8	−0.3538 (9)	0.6250 (9)	1.2573 (3)	0.0319 (9)
Pd	0.26234 (18)	0.11739 (15)	0.87796 (9)	0.01627 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.021 (6)	0.011 (5)	0.029 (6)	0.004 (4)	0.005 (5)	−0.001 (4)
C2	0.007 (4)	0.025 (4)	0.014 (4)	0.007 (3)	0.004 (3)	0.003 (3)
C3	0.017 (2)	0.026 (3)	0.023 (3)	0.007 (2)	0.003 (2)	0.000 (2)
C4	0.027 (3)	0.024 (3)	0.021 (3)	0.011 (2)	0.005 (2)	0.002 (2)
C5	0.017 (3)	0.025 (3)	0.022 (3)	−0.001 (2)	0.004 (2)	0.001 (2)
C6	0.014 (5)	0.024 (6)	0.015 (5)	0.009 (5)	−0.001 (4)	0.001 (4)
C7	0.012 (4)	0.016 (4)	0.027 (4)	0.000 (3)	0.002 (3)	−0.003 (3)
C8	0.028 (3)	0.017 (2)	0.020 (3)	0.004 (2)	0.010 (2)	−0.001 (2)
C9	0.027 (3)	0.027 (3)	0.023 (3)	0.009 (3)	0.008 (3)	0.001 (2)
C10	0.021 (3)	0.026 (3)	0.019 (3)	0.007 (2)	0.008 (2)	0.003 (2)
N1	0.020 (5)	0.016 (5)	0.018 (4)	0.004 (4)	0.006 (4)	−0.009 (3)
N2	0.015 (5)	0.022 (5)	0.027 (5)	0.005 (4)	0.006 (4)	0.013 (4)
O1	0.028 (4)	0.023 (5)	0.019 (4)	0.010 (4)	0.003 (3)	−0.006 (4)
O2	0.024 (3)	0.023 (3)	0.029 (3)	−0.001 (2)	0.011 (2)	−0.001 (2)
O3	0.037 (2)	0.033 (2)	0.0169 (18)	0.0129 (18)	0.0092 (16)	0.0034 (16)
O4	0.035 (3)	0.038 (3)	0.021 (2)	0.022 (2)	0.0092 (19)	0.003 (2)
O5	0.018 (4)	0.013 (4)	0.031 (4)	0.000 (3)	0.010 (3)	0.002 (3)
O6	0.021 (3)	0.024 (3)	0.026 (3)	0.003 (2)	0.007 (2)	0.004 (2)
O7	0.031 (2)	0.035 (2)	0.0165 (18)	0.0136 (18)	0.0065 (16)	−0.0001 (16)
O8	0.035 (2)	0.048 (3)	0.020 (2)	0.023 (2)	0.0071 (17)	0.0018 (18)
Pd	0.01683 (17)	0.01537 (15)	0.01715 (16)	0.00487 (11)	0.00451 (11)	−0.00026 (10)

Geometric parameters (Å, º)

C1—O2	1.231 (14)	C7—H11	1.0000
C1—O1	1.318 (14)	C8—C9	1.530 (7)
C1—C2	1.508 (17)	C8—H12	0.9900
C2—N1	1.483 (16)	C8—H13	0.9900
C2—C3	1.553 (11)	C9—C10	1.503 (8)
C2—H3	1.0000	C9—H14	0.9900

C3—C4	1.532 (7)	C9—H15	0.9900
C3—H4	0.9900	C10—O8	1.230 (7)
C3—H5	0.9900	C10—O7	1.323 (7)
C4—C5	1.485 (7)	Pd—N1	2.072 (9)
C4—H6	0.9900	N1—H2	0.85 (2)
C4—H7	0.9900	N1—H1	0.85 (2)
C5—O4	1.238 (7)	Pd—N2	2.005 (11)
C5—O3	1.316 (7)	N2—H10	0.85 (2)
C6—O6	1.243 (14)	N2—H9	0.85 (2)
C6—O5	1.289 (14)	Pd—O1	1.976 (8)
C6—C7	1.538 (16)	O3—H8	0.86 (2)
C7—N2	1.493 (16)	O5—Pd	2.024 (7)
C7—C8	1.529 (12)	O7—H16	0.85 (2)
O2—C1—O1	124.1 (11)	C9—C8—H12	109.1
O2—C1—C2	120.1 (10)	C7—C8—H13	109.1
O1—C1—C2	115.7 (11)	C9—C8—H13	109.1
N1—C2—C1	110.6 (9)	H12—C8—H13	107.8
N1—C2—C3	106.2 (8)	C10—C9—C8	111.8 (5)
C1—C2—C3	111.7 (9)	C10—C9—H14	109.3
N1—C2—H3	109.4	C8—C9—H14	109.3
C1—C2—H3	109.4	C10—C9—H15	109.3
C3—C2—H3	109.4	C8—C9—H15	109.3
C4—C3—C2	115.7 (5)	H14—C9—H15	107.9
C4—C3—H4	108.4	O8—C10—O7	123.0 (5)
C2—C3—H4	108.4	O8—C10—C9	122.2 (5)
C4—C3—H5	108.4	O7—C10—C9	114.8 (5)
C2—C3—H5	108.4	C2—N1—Pd	106.8 (8)
H4—C3—H5	107.4	C2—N1—H2	110 (6)
C5—C4—C3	114.6 (4)	Pd—N1—H2	108 (8)
C5—C4—H6	108.6	C2—N1—H1	119 (7)
C3—C4—H6	108.6	Pd—N1—H1	110 (7)
C5—C4—H7	108.6	H2—N1—H1	102 (9)
C3—C4—H7	108.6	C7—N2—Pd	106.3 (7)
H6—C4—H7	107.6	C7—N2—H10	105 (7)
O4—C5—O3	122.1 (5)	Pd—N2—H10	111 (9)
O4—C5—C4	123.5 (5)	C7—N2—H9	103 (7)
O3—C5—C4	114.5 (5)	Pd—N2—H9	114 (8)
O6—C6—O5	120.4 (11)	H10—N2—H9	115 (10)
O6—C6—C7	123.5 (10)	C1—O1—Pd	116.3 (8)
O5—C6—C7	116.1 (10)	C5—O3—H8	109 (5)
N2—C7—C8	114.0 (9)	C6—O5—Pd	113.1 (8)
N2—C7—C6	104.2 (10)	C10—O7—H16	117 (5)
C8—C7—C6	112.8 (8)	O1—Pd—N2	97.7 (4)
N2—C7—H11	108.6	O1—Pd—O5	178.6 (4)
C8—C7—H11	108.6	N2—Pd—O5	81.3 (4)
C6—C7—H11	108.6	O1—Pd—N1	81.7 (4)
C7—C8—C9	112.6 (6)	N2—Pd—N1	178.3 (6)

C7—C8—H12	109.1	O5—Pd—N1	99.3 (4)
O2—C1—C2—N1	161.2 (10)	C8—C9—C10—O7	−155.6 (5)
O1—C1—C2—N1	−20.8 (13)	C1—C2—N1—Pd	30.8 (10)
O2—C1—C2—C3	−80.7 (12)	C3—C2—N1—Pd	−90.6 (8)
O1—C1—C2—C3	97.3 (11)	C8—C7—N2—Pd	−168.6 (6)
N1—C2—C3—C4	−177.5 (6)	C6—C7—N2—Pd	−45.3 (9)
C1—C2—C3—C4	61.8 (10)	O2—C1—O1—Pd	176.4 (9)
C2—C3—C4—C5	74.0 (8)	C2—C1—O1—Pd	−1.5 (12)
C3—C4—C5—O4	−28.6 (8)	O6—C6—O5—Pd	171.2 (8)
C3—C4—C5—O3	151.5 (5)	C7—C6—O5—Pd	−10.6 (11)
O6—C6—C7—N2	−144.1 (10)	C1—O1—Pd—N2	−166.0 (8)
O5—C6—C7—N2	37.8 (12)	C1—O1—Pd—N1	15.7 (8)
O6—C6—C7—C8	−20.0 (15)	C7—N2—Pd—O1	−147.4 (7)
O5—C6—C7—C8	161.8 (8)	C7—N2—Pd—O5	33.7 (7)
N2—C7—C8—C9	−168.1 (8)	C6—O5—Pd—N2	−13.5 (7)
C6—C7—C8—C9	73.4 (10)	C6—O5—Pd—N1	164.8 (7)
C7—C8—C9—C10	−176.1 (6)	C2—N1—Pd—O1	−25.3 (7)
C8—C9—C10—O8	26.5 (8)	C2—N1—Pd—O5	153.7 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H9···O6[i]	0.85 (2)	2.15 (4)	2.979 (15)	162 (8)
N2—H10···O5[ii]	0.85 (2)	2.43 (8)	3.121 (13)	138 (10)
O7—H16···O4[iii]	0.85 (2)	1.80 (2)	2.639 (6)	169 (7)
O3—H8···O8[iv]	0.86 (2)	1.79 (3)	2.640 (6)	167 (7)
N1—H1···O2[v]	0.85 (2)	2.15 (3)	2.996 (15)	170 (9)
N1—H2···O1[vi]	0.85 (2)	2.30 (8)	2.998 (13)	139 (10)
N1—H2···O5[vii]	0.85 (2)	2.42 (7)	3.117 (13)	140 (10)

Symmetry codes: (i) *x*+1, *y*+1, *z*; (ii) *x*, *y*+1, *z*; (iii) *x*−1, *y*+1, *z*+1; (iv) *x*+1, *y*−1, *z*−1; (v) *x*−1, *y*−1, *z*; (vi) *x*, *y*−1, *z*; (vii) *x*+1, *y*, *z*.