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Bis(3,5-dinitrobenzoato-κO)bis(ethane-1,2-diamine-$\kappa^2 N,N'$)cadmium(II)

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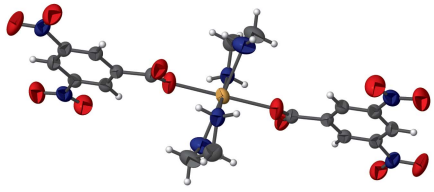
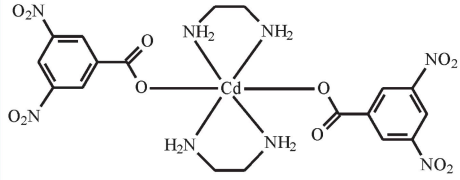
Structural data: full structural data are available from iucrdata.iucr.org

During systematic investigations of bioavailability and biological action enhancement of well known compounds with low bioactivity, a new mixed-ligand metal complex, $[Cd(DNBA)_2(en)_2]$ (DNBA = 3,5-dinitrobenzoate, $C_7H_3N_2O_6$; en = ethylendiamine, $C_2H_8N_2$), has been synthesized. The complex molecules are located on inversion centers. Two DNBA anions monodentately coordinate the Cd^{II} atom through an oxygen atom of the carboxylate group while two en molecules coordinate in a chelate fashion, resulting in a distorted O_2N_4 coordination set. There is a weak intramolecular hydrogen bond of 3.099 (4) Å between the non-coordinating oxygen atom of the carboxylate group and one of the en amine groups. Three relatively weak intermolecular N—H···O hydrogen bonds associate complex molecules into sheets extending parallel to $(0\bar{1}1)$, which are further stabilized by π–π interactions. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions to the crystal packing are from H···O/O···H (50.2%) and H···H (21.1%) interactions.

3D view



Chemical scheme



Structure description

DNBA (= 3,5-dinitrobenzoic acid) is an organic compound that is an important corrosion inhibitor applied in photography and is used by chemists to identify alcohol components in esters and in the fluorometric analysis of creatinine (Chandrasekaran *et al.*, 2013). DNBA demonstrates low antimicrobial activity against bacteria and yeasts with values of the half maximal inhibitory concentration (IC50) and minimum inhibition concentration (MIC) of more than 3 mmol l^{-1} but shows medium biological action against filamentous fungi *M. gypseum* with IC50 and MIC values of 2.1 and 3 mmol l^{-1} (microbicide effect), respectively (Vaskova *et al.*, 2009).

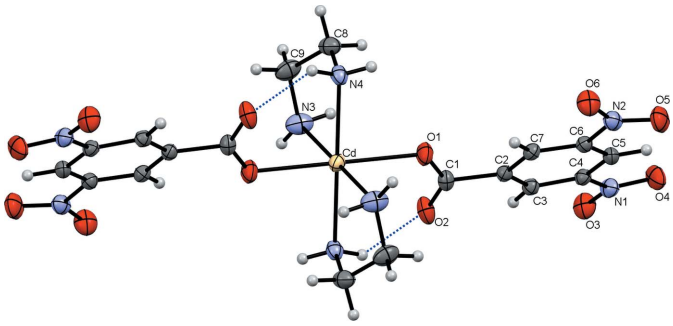


Figure 1
The molecular structure of the coordination complex $[Cd(DNBA)_2(en)_2]$ with displacement ellipsoids shown at the 30% probability level. The crystallographically independent part of the molecule is labelled, the atoms of the remaining part are generated by inversion symmetry. [Symmetry code: (i) $-x+2, -y+1, -z+2$].

En (ethylendiamine) is used in large quantities for the production of many industrial chemicals. It is a well known bidentate chelating ligand for coordination complexes (Matsushita & Taira, 1999). En itself is not biologically active against different strains of microorganisms, but its Co^{III} complex demonstrates a strong antifungal action against a broad spectrum of *Candida* species (Turecka *et al.*, 2018).

The water solubility of DNBA is low (1.35 g l^{-1} at 25°C; Rogers & Stovall, 2000). In order to enhance its water solubility and antimicrobial activity, we tried to apply some of the presently available approaches (Jain *et al.*, 2015). However, more encouraging is the combination of organic salts, DNBA and en as well as mixed-ligand complexes comprising respective ligands. Promising results have already been achieved in the case of 4-nitrobenzoic acid (Ibragimov *et al.*, 2017), 4-aminobenzoic acid (Ibragimov *et al.*, 2016) and 3-hydroxybenzoic acid (Ibragimov, 2016). A search of the Cambridge Structural Database (Groom *et al.*, 2016) has revealed that organic salts on the basis of DNBA have already been obtained [refcodes VUJXIH (Nethaji *et al.*, 1992) and FONCER (Jones *et al.*, 2005)] and therefore we made another attempt and synthesized a cadmium-based mixed-ligand complex. The choice of Cd is explained by the fact that compounds based on cadmium are toxic for living organisms including fungi.

In the crystal of the title compound, the complex molecules are located on inversion centers. Two symmetry-related

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2	0.92 (1)	2.32 (2)	3.099 (4)	143 (3)
N4—H4A···O4^{i}	0.92 (1)	2.56 (3)	3.268 (4)	134 (3)
N4—H4B···O4^{ii}	0.92 (1)	2.39 (2)	3.237 (4)	153 (4)
N3—H3B···O5^{iii}	0.92 (1)	2.52 (7)	3.312 (5)	145 (10)

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

DNBA anions monodentately coordinate to Cd^{II} through one of the oxygen atoms of the carboxylate group. The two en ligands coordinate in a chelate fashion through the two N atoms (Fig. 1). The bond lengths Cd—O1, Cd—N3 and Cd—N4 are 2.344 (2), 2.337 (4) and 2.322 (3) Å, respectively, and the *cis*-bond angles vary from 77.34 (12) to 102.66 (12)°, indicating a rather strong distortion from the ideal octahedral shape. The conformation of the complex molecule is stabilized through a weak intramolecular hydrogen bond [3.099 (4) Å and 143 (3)°] between the N4—H4A donor and the O2 acceptor (Table 1) defining a six-membered ring with graph-set notation $S(6)$. Most coplanar with the aromatic ring is the $N1O_2$ nitro group [dihedral angle of 3.873 (3)°] while the carboxylate group is considerably twisted from the aromatic ring [dihedral angle = 19.332 (9)°]. The arrangement of the $N2O_2$ nitro group is intermediate between the latter two, the corresponding dihedral angle being 13.529 (6)°.

There are three relatively weak intermolecular hydrogen bonds in the crystal structure (Table 1). N4—H4A···O4^{i} and N4—H4B···O4^{ii} hydrogen bonds define rings with graph-set notation $R_4^2(8)$. The rings are further connected *via* N3—H3B···O5^{iii} hydrogen bonds, forming sheets extending parallel to $(0\bar{1}1)$ (Fig. 2). The sheets are stabilized by π–π stacking interactions [$Cg1\cdots Cg1$ = 3.715 (3) Å, slippage = 1.608 Å, symmetry operation: $1-x, -y, 1-z$; $Cg1$ is the centroid of the phenyl (C1–C6) ring].

In order to visualize the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface (HS) analysis was carried out using *Crystal Explorer 17.5* (Turner *et al.*, 2017). The Hirshfeld surface mapped over d_{norm} (Fig. 3) shows the expected bright-red spots near atoms O2, O4, O5, H3B, H4A and H4B involved in the N—H···O hydrogen-bonding interactions described above. Fingerprint plots, Fig. 4,

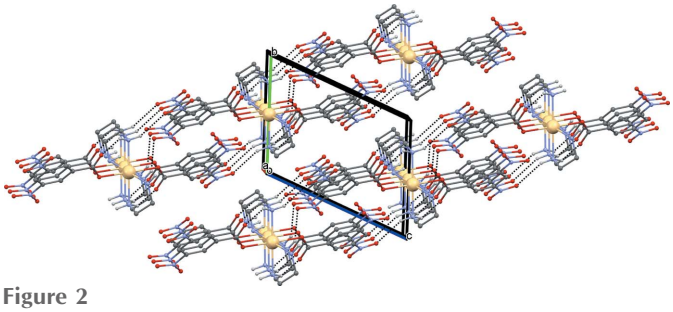


Figure 2
The crystal packing of the coordination complex $[Cd(DNBA)_2(en)_2]$ showing N—H···O hydrogen bonds as dashed lines. For clarity, H atoms not involved in hydrogen bonding are omitted.

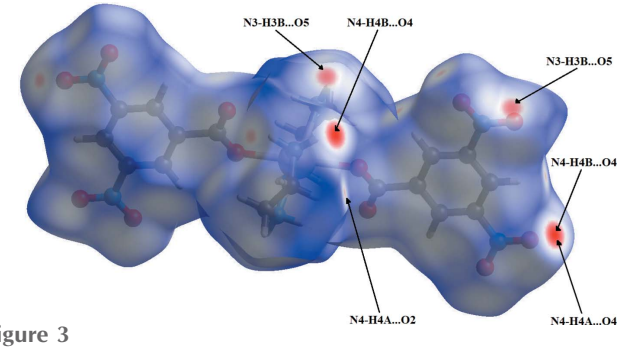


Figure 3
View of the three-dimensional Hirshfeld surface of the title compound plotted over d_{norm} in the range −0.2200 to 1.2846 a.u..

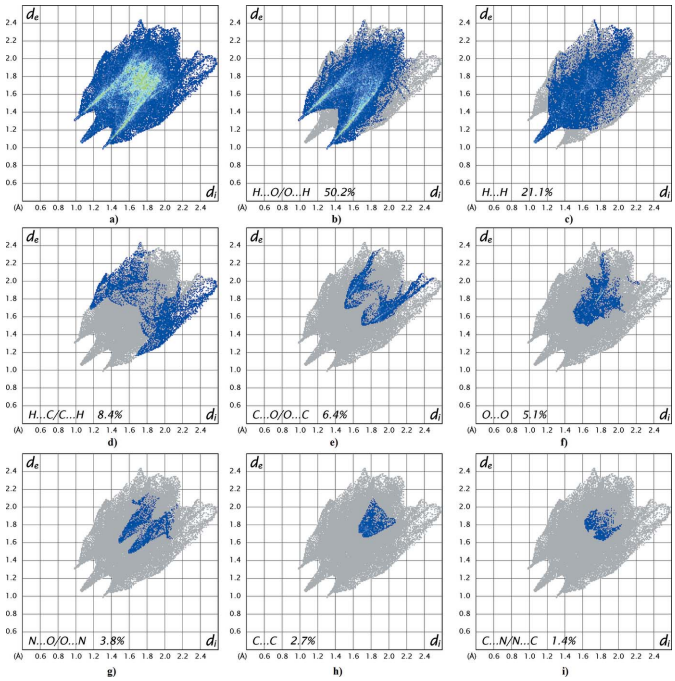


Figure 4
Full two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···O/O···H, (*c*) H···H, (*d*) H···C/C···H, (*e*) C···O/O···C, (*f*) O···O, (*g*) N···O/O···N, (*h*) C···C and (*i*) C···N/N···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from a given point on the Hirshfeld surface. Relative contributions are indicated.

reveal that while H···O/O···H interactions make the greatest contribution to the surface contacts, as would be expected for a molecule with such a predominance of O atoms, H···H and H···C/C···H contacts are also substantial. The C···O/O···C, O···O, N···O/O···N, C···C, C···N/N···C and H···N/N···H contacts are less significant.

A search of the Cambridge Structural Database (Version 5.41, November 2019; Groom *et al.*, 2016) attested that over 300 crystal structures based on DNBA are registered. Among these structures, eleven compounds are monoligand complexes while 120 ones belong to mixed-ligand coordination compounds. There are two mixed-ligand complexes closely related to the $[Cd(DNBA)_2(en)_2]$ complex. The silver complexes with refcodes EQOKEA (Zhu *et al.*, 2003) and EQOKEA01 (Qiu *et al.*, 2005) consist of discrete and polymeric components. In the discrete component, Ag^I is coordinated by two DNBA molecules in a monodentate mode whereas in the second component silver ions are associated by en ligands into polymeric chains. There are also DNBA, en and $–NO_2$ ligands in the Co^I complex with refcode KICCEF (Sharma *et al.*, 2007). In this complex, the metal ion is chelated by two en ligands, and one DNBA and one NO_2 molecules each in a monodentate mode.

Synthesis and crystallization

To an aqueous solution (2.5 ml) of $Cd(CH_3COO)_2$ (0.115 g, 0.5 mmol) was slowly added an ethanol solution (4 ml) containing en (60 μl) and DNBA (0.212 g, 1 mmol) under constant stirring. A colourless crystalline product was obtained at room temperature by slow solvent evaporation after 6 d. Single crystals for X-ray structure determination were selected from this product. Yield: 65%. Elemental analysis for $C_{18}H_{22}CdN_8O_{12}$ (654.83): calculated C 33.02; H 3.39; N 17.11%; found: C 32.96; H 3.32; N 17.08%.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_7H_3N_2O_6)_2(C_2H_8N_2)_2)]$
M_r	654.83
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	291
a, b, c (Å)	7.191 (5), 8.698 (5), 10.987 (5)
α, β, γ (°)	112.289 (5), 92.827 (5), 101.656 (5)
V (Å^3)	616.7 (6)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	7.81
Crystal size (mm)	0.22 × 0.18 × 0.16
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, Ruby
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.397, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4512, 2482, 2406
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.086, 1.06
No. of reflections	2482
No. of parameters	195
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.51

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2020). **5**, x200843 [https://doi.org/10.1107/S2414314620008433]

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Crystal data

$[Cd(C_7H_3N_2O_6)_2(C_2H_8N_2)_2)]$
M_r = 654.83
Triclinic, $P\overline{1}$
a = 7.191 (5) Å
b = 8.698 (5) Å
c = 10.987 (5) Å
α = 112.289 (5)°
β = 92.827 (5)°
γ = 101.656 (5)°
V = 616.7 (6) Å^3
Z = 1
$F(000)$ = 330
D_x = 1.763 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3166 reflections
θ = 4.4–75.1°
μ = 7.81 mm^{-1}
T = 291 K
Block, colorless
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku Oxford Diffraction Xcalibur, Ruby diffractometer
Radiation source: fine-focus sealed X-ray tube
Detector resolution: 10.2576 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.397, T_{max} = 1.000
4512 measured reflections
2482 independent reflections
2406 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 75.8°, θ_{min} = 4.4°
h = −8→8
k = −10→10
l = −11→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.086
S = 1.06
2482 reflections
195 parameters
5 restraints
Primary atom site location: Intrinsic-phasing
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.2183P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Extinction correction: SHELXL2018/3 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0032 (5)

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. N-bound H atoms were located in a difference Fourier map and were refined with bond-length restraints of 0.92 (1) Å.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	1.000000	0.500000	1.000000	0.04436 (14)
O2	0.6549 (4)	0.5433 (4)	0.7930 (3)	0.0651 (7)
O1	0.8216 (4)	0.3493 (3)	0.7881 (2)	0.0620 (7)
O3	0.1233 (4)	0.3373 (4)	0.4291 (3)	0.0715 (8)
O4	0.1282 (4)	0.1278 (4)	0.2450 (3)	0.0767 (9)
O6	0.8565 (4)	−0.0927 (4)	0.3594 (3)	0.0730 (8)
N1	0.1978 (4)	0.2284 (4)	0.3583 (3)	0.0517 (6)
N4	1.0222 (4)	0.7651 (3)	0.9904 (3)	0.0487 (6)
O5	0.6643 (5)	−0.1370 (4)	0.1882 (3)	0.0757 (8)
N2	0.7258 (4)	−0.0609 (4)	0.3057 (3)	0.0516 (6)
C2	0.6271 (4)	0.3000 (4)	0.5940 (3)	0.0381 (6)
C3	0.4603 (4)	0.3208 (4)	0.5398 (3)	0.0396 (6)
H3	0.402141	0.406126	0.589595	0.047*
C7	0.7155 (4)	0.1743 (4)	0.5164 (3)	0.0395 (6)
H7	0.827318	0.158989	0.551588	0.047*
C6	0.6340 (4)	0.0733 (4)	0.3869 (3)	0.0397 (6)
C4	0.3822 (4)	0.2132 (4)	0.4114 (3)	0.0401 (6)
C5	0.4662 (4)	0.0883 (4)	0.3320 (3)	0.0426 (6)
H5	0.411582	0.017367	0.245051	0.051*
N3	1.2449 (5)	0.5152 (5)	0.8698 (4)	0.0714 (10)
C1	0.7084 (4)	0.4101 (4)	0.7390 (3)	0.0443 (7)
C8	1.2033 (6)	0.8097 (5)	0.9427 (4)	0.0622 (9)
H8A	1.307671	0.851575	1.015179	0.075*
H8B	1.200122	0.900523	0.912486	0.075*
C9	1.2380 (7)	0.6594 (6)	0.8321 (5)	0.0725 (11)
H9A	1.136935	0.622053	0.758114	0.087*
H9B	1.358522	0.693491	0.802584	0.087*
H4A	0.922 (4)	0.747 (5)	0.928 (3)	0.050 (10)*
H4B	1.024 (6)	0.846 (4)	1.074 (2)	0.072 (13)*
H3A	1.336 (4)	0.586 (4)	0.940 (3)	0.053 (11)*
H3B	1.285 (10)	0.419 (8)	0.821 (8)	0.27 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0539 (2)	0.0461 (2)	0.03613 (18)	0.01547 (13)	0.00951 (12)	0.01752 (13)
O2	0.0524 (14)	0.0699 (16)	0.0509 (13)	0.0237 (12)	−0.0022 (10)	−0.0035 (12)

O1	0.0744 (17)	0.0650 (15)	0.0418 (12)	0.0244 (13)	−0.0096 (11)	0.0144 (11)
O3	0.0556 (15)	0.086 (2)	0.0744 (18)	0.0318 (14)	−0.0012 (13)	0.0279 (16)
O4	0.0756 (19)	0.0665 (17)	0.0712 (18)	0.0104 (14)	−0.0354 (15)	0.0181 (15)
O6	0.0684 (17)	0.0780 (19)	0.0744 (18)	0.0403 (15)	0.0103 (14)	0.0209 (15)
N1	0.0464 (14)	0.0535 (16)	0.0554 (16)	0.0080 (12)	−0.0075 (12)	0.0257 (13)
N4	0.0558 (16)	0.0437 (14)	0.0428 (14)	0.0192 (12)	0.0014 (11)	0.0099 (11)
O5	0.096 (2)	0.0711 (18)	0.0481 (15)	0.0316 (16)	0.0140 (13)	0.0040 (13)
N2	0.0561 (16)	0.0472 (15)	0.0494 (15)	0.0136 (12)	0.0162 (12)	0.0154 (12)
C2	0.0365 (13)	0.0420 (15)	0.0356 (13)	0.0062 (11)	0.0038 (10)	0.0169 (12)
C3	0.0384 (14)	0.0408 (15)	0.0400 (14)	0.0085 (11)	0.0056 (11)	0.0172 (12)
C7	0.0385 (14)	0.0437 (15)	0.0388 (14)	0.0109 (11)	0.0052 (11)	0.0185 (12)
C6	0.0446 (15)	0.0374 (14)	0.0381 (14)	0.0090 (11)	0.0086 (11)	0.0161 (12)
C4	0.0394 (14)	0.0412 (15)	0.0415 (14)	0.0063 (11)	−0.0018 (11)	0.0208 (12)
C5	0.0483 (16)	0.0400 (15)	0.0350 (13)	0.0043 (12)	0.0011 (11)	0.0139 (12)
N3	0.068 (2)	0.073 (2)	0.098 (3)	0.0355 (19)	0.038 (2)	0.047 (2)
C1	0.0386 (14)	0.0523 (17)	0.0350 (14)	0.0083 (12)	0.0034 (11)	0.0112 (13)
C8	0.064 (2)	0.052 (2)	0.074 (2)	0.0088 (16)	0.0048 (18)	0.0329 (19)
C9	0.074 (3)	0.086 (3)	0.082 (3)	0.029 (2)	0.035 (2)	0.052 (2)

Geometric parameters (Å, º)

Cd1—N4^{i}	2.322 (3)	C2—C7	1.397 (4)
Cd1—N4	2.322 (3)	C2—C1	1.524 (4)
Cd1—N3	2.337 (4)	C3—C4	1.374 (4)
Cd1—N3^{i}	2.337 (4)	C3—H3	0.9300
Cd1—O1	2.344 (2)	C7—C6	1.379 (4)
Cd1—O1^{i}	2.344 (2)	C7—H7	0.9300
O2—C1	1.235 (4)	C6—C5	1.375 (4)
O1—C1	1.257 (4)	C4—C5	1.380 (4)
O3—N1	1.216 (4)	C5—H5	0.9300
O4—N1	1.226 (4)	N3—C9	1.471 (6)
O6—N2	1.218 (4)	N3—H3A	0.914 (10)
N1—C4	1.473 (4)	N3—H3B	0.916 (10)
N4—C8	1.462 (5)	C8—C9	1.485 (6)
N4—H4A	0.916 (10)	C8—H8A	0.9700
N4—H4B	0.917 (10)	C8—H8B	0.9700
O5—N2	1.216 (4)	C9—H9A	0.9700
N2—C6	1.474 (4)	C9—H9B	0.9700
C2—C3	1.388 (4)		
N4^{i}—Cd1—N4	179.999 (11)	C6—C7—C2	118.8 (3)
N4^{i}—Cd1—N3	102.66 (12)	C6—C7—H7	120.6
N4—Cd1—N3	77.34 (12)	C2—C7—H7	120.6
N4^{i}—Cd1—N3^{i}	77.34 (12)	C5—C6—C7	122.6 (3)
N4—Cd1—N3^{i}	102.66 (12)	C5—C6—N2	118.6 (3)
N3—Cd1—N3^{i}	180.0	C7—C6—N2	118.8 (3)
N4^{i}—Cd1—O1	86.36 (10)	C3—C4—C5	122.8 (3)
N4—Cd1—O1	93.64 (10)	C3—C4—N1	118.4 (3)

N3—Cd1—O1	80.38 (15)	C5—C4—N1	118.8 (3)
N3^{i}—Cd1—O1	99.63 (15)	C6—C5—C4	117.1 (3)
N4^{i}—Cd1—O1^{i}	93.64 (10)	C6—C5—H5	121.5
N4—Cd1—O1^{i}	86.36 (10)	C4—C5—H5	121.5
N3—Cd1—O1^{i}	99.62 (15)	C9—N3—Cd1	106.2 (2)
N3^{i}—Cd1—O1^{i}	80.37 (15)	C9—N3—H3A	90 (3)
O1—Cd1—O1^{i}	180.00 (8)	Cd1—N3—H3A	95 (3)
C1—O1—Cd1	122.9 (2)	C9—N3—H3B	126 (8)
O3—N1—O4	124.1 (3)	Cd1—N3—H3B	121 (7)
O3—N1—C4	118.6 (3)	H3A—N3—H3B	110 (2)
O4—N1—C4	117.3 (3)	O2—C1—O1	128.6 (3)
C8—N4—Cd1	107.5 (2)	O2—C1—C2	117.4 (3)
C8—N4—H4A	109 (2)	O1—C1—C2	114.0 (3)
Cd1—N4—H4A	105 (2)	N4—C8—C9	111.1 (3)
C8—N4—H4B	109 (3)	N4—C8—H8A	109.4
Cd1—N4—H4B	110 (3)	C9—C8—H8A	109.4
H4A—N4—H4B	117 (4)	N4—C8—H8B	109.4
O5—N2—O6	123.1 (3)	C9—C8—H8B	109.4
O5—N2—C6	118.1 (3)	H8A—C8—H8B	108.0
O6—N2—C6	118.8 (3)	N3—C9—C8	112.9 (4)
C3—C2—C7	119.7 (3)	N3—C9—H9A	109.0
C3—C2—C1	119.7 (3)	C8—C9—H9A	109.0
C7—C2—C1	120.5 (3)	N3—C9—H9B	109.0
C4—C3—C2	118.9 (3)	C8—C9—H9B	109.0
C4—C3—H3	120.5	H9A—C9—H9B	107.8
C2—C3—H3	120.5		

C7—C2—C3—C4	1.8 (4)	O4—N1—C4—C5	0.0 (4)
C1—C2—C3—C4	−175.9 (3)	C7—C6—C5—C4	1.5 (4)
C3—C2—C7—C6	0.0 (4)	N2—C6—C5—C4	178.9 (3)
C1—C2—C7—C6	177.8 (3)	C3—C4—C5—C6	0.5 (4)
C2—C7—C6—C5	−1.8 (4)	N1—C4—C5—C6	−177.3 (3)
C2—C7—C6—N2	−179.2 (3)	Cd1—O1—C1—O2	−8.4 (5)
O5—N2—C6—C5	9.9 (4)	Cd1—O1—C1—C2	172.57 (19)
O6—N2—C6—C5	−168.6 (3)	C3—C2—C1—O2	−19.2 (4)
O5—N2—C6—C7	−172.6 (3)	C7—C2—C1—O2	163.0 (3)
O6—N2—C6—C7	8.9 (4)	C3—C2—C1—O1	159.9 (3)
C2—C3—C4—C5	−2.2 (4)	C7—C2—C1—O1	−17.8 (4)
C2—C3—C4—N1	175.6 (3)	Cd1—N4—C8—C9	42.2 (4)
O3—N1—C4—C3	1.3 (5)	Cd1—N3—C9—C8	41.0 (5)
O4—N1—C4—C3	−177.9 (3)	N4—C8—C9—N3	−59.1 (5)
O3—N1—C4—C5	179.2 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O2	0.92 (1)	2.32 (2)	3.099 (4)	143 (3)

N4—H4*A*···O4^{ii}	0.92 (1)	2.56 (3)	3.268 (4)	134 (3)
N4—H4*B*···O4^{iii}	0.92 (1)	2.39 (2)	3.237 (4)	153 (4)
N3—H3*B*···O5^{iv}	0.92 (1)	2.52 (7)	3.312 (5)	145 (10)

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

Percentage contributions to the Hirshfeld surface for (I).

Contacts	Included surface area %
H···O/O···H	50.2
H···H	21.1
H···C/C···H	8.4
C···O/O···C	6.4
O···O	5.1
N···O/O···N	3.8
C···C	2.7
C···N/N···C	1.4
H···N/N···H	1.0