

Crystal structure and Hirshfeld surface analysis of diiodido{*N'*-[(*E*)-(phenyl)(pyridin-2-yl- κ *N*)methylidene]pyridine-2-carbohydrazide- κ^2 *N',O*}-cadmium(II)}

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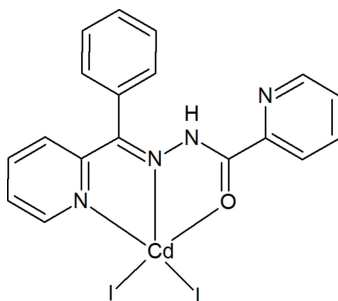
Supporting information: this article has supporting information at journals.iucr.org/e

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In each of the two independent molecules in the asymmetric unit of the title compound, [CdI₂(C₁₈H₁₄N₄O)], the *N,O,N'*-tridentate *N'*-[(*E*)-(phenyl)(pyridin-2-yl- κ *N*)methylidene]pyridine-2-carbohydrazide ligand and two iodide anions form an I₂N₂O pentacoordination sphere, with a distorted square-pyramidal geometry, with an I atom in the apical position. Both molecules feature an intramolecular N–H···N hydrogen bond. In the crystal, weak aromatic π – π stacking interactions [centroid–centroid separation = 3.830 (2) Å] link the molecules into dimers.

1. Chemical context

Hydrazone ligands show high efficiency in chelating transition-metal ions (Afkhami *et al.*, 2017*a*); such ligands obtained from pyridine carboxylic acids can act as ditopic ligands because of their two different donor sites, including an N-donor pyridine group and a tridentate coordination pocket, and have the potential to form mono-, di- and multinuclear structures (Afkhami *et al.*, 2017*b*). In this work, we report the synthesis, crystal structure and Hirshfeld surface analysis of the title Cd^{II} complex, (I), containing the tridentate hydrazone ligand *N'*-[(*E*)-(pyridin-2-yl)methylidene]pyridine-2-carbohydrazide.



2. Structural commentary

The molecular structure of (I), which contains two [CdI₂(C₁₈H₁₄N₄O)] molecules, *A* (with Cd1) and *B* (with Cd2), in the asymmetric unit is shown in Fig. 1. In both molecules, the Cd atom is pentacoordinated to two N, one O and two I

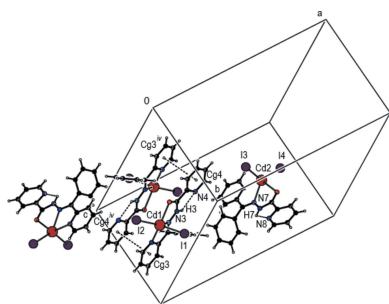


Table 1
Selected bond lengths (Å).

Cd1—N2	2.342 (3)	Cd2—N6	2.344 (3)
Cd1—N1	2.380 (3)	Cd2—N5	2.369 (3)
Cd1—O1	2.450 (2)	Cd2—O2	2.481 (3)
Cd1—I2	2.6917 (4)	Cd2—I4	2.6732 (4)
Cd1—I1	2.7509 (4)	Cd2—I3	2.7530 (4)

atoms (Table 1). The Addison τ parameter (Addison *et al.*, 1984) quantifies the distinction between trigonal-bipyramidal (ideally $\tau = 1$) and square-pyramidal (ideally $\tau = 0$) geometries. For the title complex, $\tau = 0.11$ for *A* and 0.09 for *B*, indicating a distorted square-pyramidal geometry (Fig. 2).

The dihedral angles between the planes of the pyridine rings are 4.44 (17)° for *A* and 15.63 (17)° for *B*. For *A*, the Cd1—I1 and Cd1—I2 bond lengths are 2.7509 (4) and 2.6917 (4) Å, respectively, and the Cd1—N2 bond length is 2.342 (3) Å. For *B*, the Cd2—I3 and Cd2—I4 bond lengths are 2.7530 (4) and 2.6732 (4) Å, respectively, and the Cd2—N6 bond length is 2.344 (3) Å. Both molecules feature an intramolecular N—H...N hydrogen bond with the pyridine-ring N atom as the acceptor (Table 2).

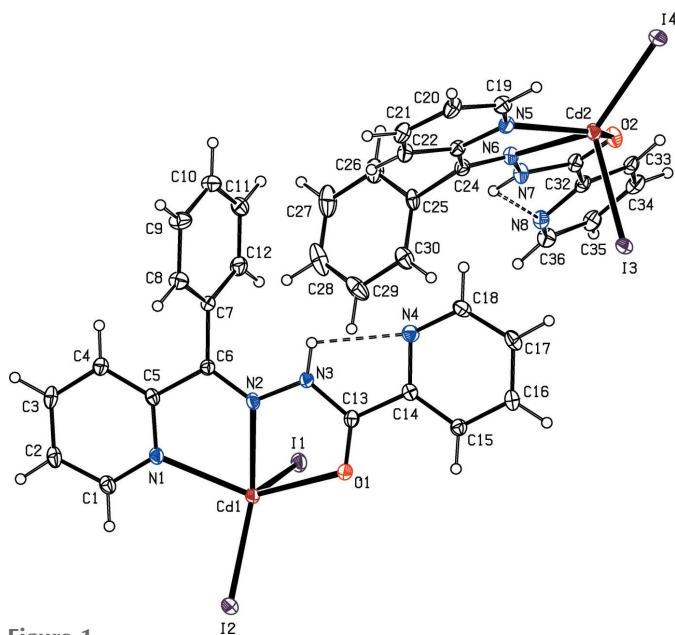


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

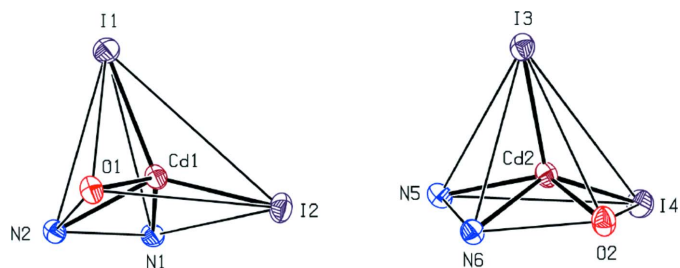


Figure 2
View of the coordination polyhedra about the Cd atoms in (I), showing their distorted square-based pyramidal geometries.

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>
N3—H3...N4	0.88	2.27	2.629 (4)	104
N7—H7...N8	0.88	2.28	2.640 (4)	104

3. Supramolecular features and Hirshfeld surface analysis

In the crystal of (I), molecules are linked into dimeric *A* + *B* associations by aromatic π – π stacking interactions [$Cg3 \cdots Cg4(-x, 1 - y, 1 - z) = 3.830$ (2) Å, where *Cg*3 and *Cg*4 are the centroids of the pyridine rings (N1/C1–C5) and (N4/C14–C18), respectively] (Fig. 3).

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) of (I) was performed using *CrystalExplorer3.1* (Wolff *et al.*, 2012) to generate d_{norm} surface plots and two-dimensional fingerprint plots (Spackman & McKinnon, 2002). Fig. 4*a* shows the overall two-dimensional fingerprint plot for the contacts contributing to the Hirshfeld surface. The percentage contributions and Hirshfeld surfaces for H...I/I...H contacts (30.5%), H...H (29.5%), C...H / H...C (13.3%), H...O / O...H (5.6%) and C...I/I...C (4.9%) are shown in Figs. 4*b–f*, respectively. The full list of percentage surface contributions in given in Table 3.

4. Database survey

All bond lengths and angles in (I) fall within their expected ranges and are comparable with those reported for related structures, such as bis{*N'*–[(*E*)-4-hydroxybenzylidene]-pyridine-4-carbohydrazide- κN^1 }diiododicadmium methanol disolvate (CCDC refcode: DADHIC; Afkhami *et al.*, 2017*c*), dibromido{*N'*–[1-(pyridin-2-yl)ethylidene]picolinohydrazide- $\kappa^2 N', O$ }cadmium (ACUDOT; Akkurt *et al.*, 2012), di- μ -

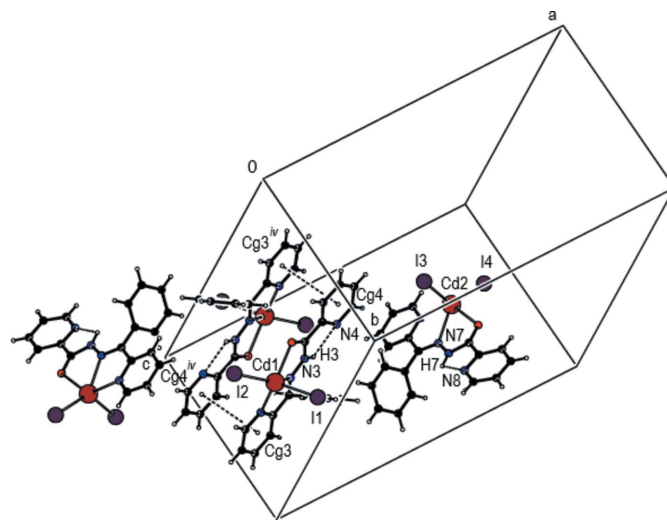


Figure 3
Partial packing diagram of (I) showing the *A* and *B* molecules linked by a pair of π – π stacking interactions. Symmetry operation: (iv) $-x, 1 - y, 1 - z$.

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface for (I).

Contact	Percentage contribution
H...I/I...H	30.5
H...H	29.5
C...H/H...C	13.3
H...O/O...H	5.6
C...I/I...C	4.9
C...C	3.3
N...H/H...N	2.9
C...N/N...C	2.8
H...Cd/Cd...H	2.1
N...I/I...N	1.7
N...O/O...N	1.5
I...I	0.6
N...N	0.4
C...O/O...C	0.4
C...Cd/Cd...C	0.3
N...Cd/Cd...N	0.2

chlorido-bis(chlorido[*N'*-(phenyl(pyridin-2-yl- κ N)methylidene)pyridine-2-carbohydrazide- κ^2 *N',O*]cadmium) (JOBTEB; Akkurt *et al.*, 2014), bis{2-[(2,4-dimethylphenyl)iminomethyl]pyridine- κ^2 *N,N'*}bis(thiocyanato- κ N)cadmium (GARTAW; Malekshahian *et al.*, 2012) and *cis*-diaquabis-[(*E*)-4-(2-hydroxybenzylideneamino)benzoato- κ^2 *O,O'*]cadmium (WEHSOS; Yao *et al.*, 2006) in which layers are built by strong O—H...O hydrogen bonds. In the crystal of diiodido-[*N'*-(pyridin-2-yl- κ N)methylidene]picolinohydrazide- κ^2 *N',O*]cadmium (WASCEB; Khandar *et al.*, 2017), the molecules are linked by N—H...I hydrogen bonds, forming chains propagating along [010].

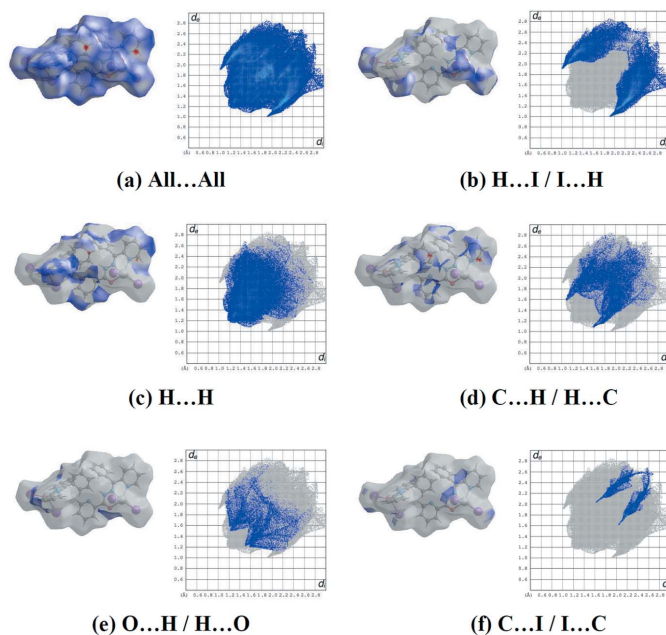


Figure 4
Hirshfeld surface representations and the two-dimensional fingerprint plots for (I), showing (a) all interactions, and delineated into (b) H...I/I...H, (c) H...H, (d) C...H/H...C, (e) H...O/O...H and (f) C...I/I...C interactions [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

Table 4
Experimental details.

Crystal data	
Chemical formula	[CdI ₂ (C ₁₈ H ₁₄ N ₄ O)]
M_r	668.53
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	19.9158 (15), 11.7252 (9), 17.8349 (14)
β (°)	104.207 (1)
V (Å ³)	4037.4 (5)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	4.16
Crystal size (mm)	0.34 × 0.33 × 0.17
Data collection	
Diffractometer	Bruker SMART APEX
Absorption correction	Multi-scan (SADABS; Bruker, 2009)
T_{\min}, T_{\max}	0.600, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24216, 9018, 7948
R_{int}	0.020
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.664
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.064, 1.03
No. of reflections	9018
No. of parameters	469
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.26, -0.56

Computer programs: APEX2 and SAINT (Bruker, 2009), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2015).

5. Synthesis and crystallization

The *N'*-(*E*)-(pyridin-2-yl)methylidene]pyridine-2-carbohydrazide ligand was synthesized according to the literature method (Abedi *et al.*, 2016). To prepare single crystals of (I), an equimolar mixture (1.0 mmol) of the hydrazone ligand and metal salt [CdI₂] were placed in the main arm of a branched tube, and methanol was carefully added to fill the arms (Khandar *et al.*, 2015). The tube was sealed and the mixture-containing arm was immersed in an oil bath at 333 K while the branched arm was kept at room temperature. After a couple of days, yellow prisms of (I) had been deposited in the cooler arm and these were isolated, filtered off, washed with diethyl ether and dried over P₄O₁₀ *in vacuo*.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were placed in calculated positions (C—H = 0.95 Å, N—H = 0.88 Å) and included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N,C})$.

Acknowledgements

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References

- Abedi, M., Yeşilel, O. Z., Mahmoudi, G., Bauzá, A., Lofland, S. E., Yerli, Y., Kaminsky, W., Garczarek, P., Zaręba, J. K., Ienco, A., Frontera, A. & Gargari, M. S. (2016). *Inorg. Chim. Acta*, **443**, 101–109.
- Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
- Afkhami, F. A., Khandar, A. A., Mahmoudi, G., Maniukiewicz, W., Gurbanov, A. V., Zubkov, F. I., Şahin, O., Yesilel, O. Z. & Frontera, A. (2017a). *CrystEngComm*, **19**, 1389–1399.
- Afkhami, F. A., Khandar, A. A., White, J. M., Guerri, A., Ienco, A., Bryant, J. T., Mhesn, N. & Lampropoulos, C. (2017b). *Inorg. Chim. Acta*, **457**, 150–159.
- Afkhami, F. A., Krautscheid, H., Atioğlu, Z. & Akkurt, M. (2017c). *Acta Cryst.* **E73**, 28–30.
- Akkurt, M., Khandar, A. A., Tahir, M. N., Afkhami, F. A. & Yazdi, S. A. H. (2014). *Acta Cryst.* **E70**, m213–m214.
- Akkurt, M., Khandar, A. A., Tahir, M. N., Yazdi, S. A. H. & Afkhami, F. A. (2012). *Acta Cryst.* **E68**, m842.
- Bruker (2009). *APEX2, SADABS and SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Khandar, A. A., Afkhami, F. A., Krautscheid, H., Kristoffersen, K. A., Atioğlu, Z., Akkurt, M. & Görbitz, C. H. (2017). *Acta Cryst.* **E73**, 698–701.
- Khandar, A. A., Ghosh, B. K., Lampropoulos, C., Gargari, M. S., Yilmaz, V. T., Bhar, K., Hosseini-Yazdi, S. A., Cain, J. M. & Mahmoudi, G. (2015). *Polyhedron*, **85**, 467–475.
- Malekshahian, M., Talei Babil Olyai, M. R. & Notash, B. (2012). *Acta Cryst.* **E68**, m218–m219.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
- Spackman, M. A. & McKinnon, J. J. (2002). *CrystEngComm*, **4**, 378–392.
- Spek, A. L. (2015). *Acta Cryst.* **C71**, 9–18.
- Wolff, S. K., Grimwood, D. J., McKinnon, J. J., Turner, M. J., Jayatilaka, D. & Spackman, M. A. (2012). *CrystalExplorer*. University of Western Australia.
- Yao, S.-Q., Zhu, M.-L., Lu, L.-P. & Gao, X.-L. (2006). *Acta Cryst.* **C62**, m183–m185.

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Acta Cryst. (2019). E75, 1061-1064 [https://doi.org/10.1107/S2056989019008831]

Crystal structure and Hirshfeld surface analysis of diiodido{*N'*-[(*E*)-(phenyl)(pyridin-2-yl- κ N)methylidene]pyridine-2-carbohydrazide- κ^2 *N',O*}cadmium(II)

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2015).

Diiodido{*N'*-[(*E*)-(phenyl)(pyridin-2-yl- κ N)methylidene]pyridine-2-carbohydrazide- κ^2 *N',O*}cadmium(II)

Crystal data

[CdI₂(C₁₈H₁₄N₄O)]
 $M_r = 668.53$
 Monoclinic, *P2₁/c*
 $a = 19.9158$ (15) Å
 $b = 11.7252$ (9) Å
 $c = 17.8349$ (14) Å
 $\beta = 104.207$ (1)°
 $V = 4037.4$ (5) Å³
 $Z = 8$

$F(000) = 2496$
 $D_x = 2.200$ Mg m⁻³
 Mo *K* α radiation, $\lambda = 0.71073$ Å
 Cell parameters from 9930 reflections
 $\theta = 2.2$ – 27.8°
 $\mu = 4.16$ mm⁻¹
 $T = 100$ K
 Hexagonal prism, yellow
 0.34 × 0.33 × 0.17 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.600$, $T_{\max} = 0.746$
 24216 measured reflections

9018 independent reflections
 7948 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\max} = 28.2^\circ$, $\theta_{\min} = 2.0^\circ$
 $h = -26 \rightarrow 25$
 $k = -15 \rightarrow 12$
 $l = -20 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.064$
 $S = 1.03$
 9018 reflections
 469 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 5.7109P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.26 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$$

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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.15988 (18)	0.7689 (3)	0.5679 (2)	0.0265 (8)
H1	-0.200797	0.761245	0.527529	0.032*
C2	-0.1651 (2)	0.8147 (3)	0.6379 (2)	0.0296 (8)
H2	-0.208603	0.839406	0.644720	0.036*
C3	-0.1066 (2)	0.8238 (3)	0.6971 (2)	0.0295 (8)
H3A	-0.108958	0.855873	0.745277	0.035*
C4	-0.04377 (18)	0.7855 (3)	0.6858 (2)	0.0245 (7)
H4	-0.002709	0.789869	0.726250	0.029*
C5	-0.04221 (17)	0.7409 (3)	0.6145 (2)	0.0218 (7)
C6	0.02285 (17)	0.6967 (3)	0.59802 (19)	0.0205 (7)
C7	0.08845 (17)	0.6963 (3)	0.65920 (19)	0.0210 (7)
C8	0.09709 (19)	0.6246 (3)	0.7225 (2)	0.0292 (8)
H8	0.060605	0.575262	0.727562	0.035*
C9	0.1594 (2)	0.6251 (4)	0.7788 (2)	0.0352 (9)
H9	0.165419	0.575842	0.822230	0.042*
C10	0.2129 (2)	0.6974 (4)	0.7716 (2)	0.0342 (9)
H10	0.255585	0.697081	0.809828	0.041*
C11	0.2035 (2)	0.7697 (4)	0.7086 (2)	0.0339 (9)
H11	0.239690	0.820040	0.703963	0.041*
C12	0.1420 (2)	0.7691 (3)	0.6523 (2)	0.0306 (8)
H12	0.136162	0.818266	0.608864	0.037*
C13	0.06053 (17)	0.5883 (3)	0.4289 (2)	0.0214 (7)
C14	0.12412 (17)	0.5528 (3)	0.4049 (2)	0.0216 (7)
C15	0.11899 (18)	0.5094 (3)	0.3316 (2)	0.0242 (7)
H15	0.075311	0.501950	0.295562	0.029*
C16	0.17994 (19)	0.4772 (3)	0.3122 (2)	0.0283 (8)
H16	0.178904	0.447717	0.262261	0.034*
C17	0.24142 (18)	0.4888 (3)	0.3667 (2)	0.0304 (8)
H17	0.283676	0.466404	0.355316	0.036*
C18	0.24135 (18)	0.5336 (3)	0.4386 (2)	0.0279 (8)
H18	0.284391	0.541529	0.475719	0.033*
Cd1	-0.08166 (2)	0.70487 (2)	0.42925 (2)	0.02325 (6)
I1	-0.02803 (2)	0.89997 (2)	0.38096 (2)	0.02834 (6)
I2	-0.20450 (2)	0.60932 (2)	0.36168 (2)	0.03106 (7)
N1	-0.09966 (14)	0.7350 (3)	0.55485 (17)	0.0232 (6)
N2	0.01685 (14)	0.6622 (2)	0.52758 (16)	0.0215 (6)
N3	0.07222 (14)	0.6208 (3)	0.50403 (16)	0.0226 (6)
H3	0.113503	0.615314	0.535951	0.027*

N4	0.18386 (15)	0.5661 (3)	0.45830 (18)	0.0253 (6)
O1	0.00248 (12)	0.5878 (2)	0.38410 (14)	0.0256 (5)
C19	0.47181 (19)	0.5871 (3)	0.5866 (2)	0.0270 (8)
H19	0.511452	0.549614	0.577806	0.032*
C20	0.4403 (2)	0.5409 (3)	0.6405 (2)	0.0314 (8)
H20	0.457550	0.472829	0.667323	0.038*
C21	0.3830 (2)	0.5955 (3)	0.6547 (2)	0.0303 (8)
H21	0.359945	0.565392	0.691081	0.036*
C22	0.36007 (19)	0.6954 (3)	0.6145 (2)	0.0261 (7)
H22	0.321326	0.735372	0.623582	0.031*
C23	0.39437 (17)	0.7359 (3)	0.5611 (2)	0.0224 (7)
C24	0.37348 (17)	0.8435 (3)	0.5184 (2)	0.0225 (7)
C25	0.30874 (18)	0.9009 (3)	0.5247 (2)	0.0255 (8)
C26	0.3113 (2)	0.9956 (4)	0.5723 (3)	0.0385 (10)
H26	0.354632	1.025469	0.599897	0.046*
C27	0.2505 (3)	1.0457 (4)	0.5790 (3)	0.0543 (13)
H27	0.251823	1.110396	0.611406	0.065*
C28	0.1876 (3)	1.0018 (4)	0.5387 (3)	0.0526 (14)
H28	0.145841	1.036347	0.544022	0.063*
C29	0.1845 (2)	0.9088 (4)	0.4909 (3)	0.0438 (11)
H29	0.140978	0.879841	0.462879	0.053*
C30	0.2457 (2)	0.8577 (4)	0.4840 (3)	0.0350 (9)
H30	0.244173	0.793135	0.451413	0.042*
C31	0.43945 (18)	1.0017 (3)	0.3850 (2)	0.0245 (7)
C32	0.41803 (18)	1.1068 (3)	0.3382 (2)	0.0238 (7)
C33	0.4640 (2)	1.1575 (3)	0.3007 (2)	0.0269 (8)
H33	0.508151	1.124917	0.303051	0.032*
C34	0.4431 (2)	1.2568 (3)	0.2598 (2)	0.0307 (8)
H34	0.472542	1.294272	0.233131	0.037*
C35	0.3784 (2)	1.3003 (3)	0.2587 (2)	0.0304 (8)
H35	0.363169	1.369376	0.232195	0.036*
C36	0.3361 (2)	1.2419 (3)	0.2967 (2)	0.0294 (8)
H36	0.291160	1.271413	0.293948	0.035*
Cd2	0.49190 (2)	0.75304 (2)	0.44240 (2)	0.02348 (6)
I3	0.39729 (2)	0.65574 (2)	0.32031 (2)	0.02644 (6)
I4	0.62809 (2)	0.71202 (2)	0.47863 (2)	0.03079 (7)
N5	0.44979 (15)	0.6813 (3)	0.54638 (17)	0.0241 (6)
N6	0.41289 (15)	0.8790 (2)	0.47642 (17)	0.0233 (6)
N7	0.39722 (15)	0.9746 (2)	0.43223 (17)	0.0246 (6)
H7	0.361299	1.017289	0.434038	0.030*
N8	0.35512 (15)	1.1468 (3)	0.33692 (18)	0.0266 (6)
O2	0.49091 (13)	0.9444 (2)	0.38286 (15)	0.0294 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0237 (17)	0.030 (2)	0.0272 (19)	0.0041 (15)	0.0095 (15)	0.0072 (15)
C2	0.0316 (19)	0.033 (2)	0.029 (2)	0.0070 (16)	0.0171 (16)	0.0084 (16)

C3	0.041 (2)	0.030 (2)	0.0241 (19)	0.0062 (16)	0.0192 (17)	0.0042 (15)
C4	0.0274 (17)	0.0256 (19)	0.0219 (18)	0.0009 (14)	0.0085 (14)	0.0011 (14)
C5	0.0210 (16)	0.0223 (17)	0.0244 (18)	-0.0003 (13)	0.0101 (14)	0.0030 (14)
C6	0.0209 (16)	0.0217 (17)	0.0199 (17)	-0.0009 (13)	0.0066 (13)	-0.0004 (13)
C7	0.0193 (15)	0.0247 (18)	0.0190 (16)	-0.0002 (13)	0.0049 (13)	-0.0033 (13)
C8	0.0287 (18)	0.029 (2)	0.029 (2)	-0.0017 (15)	0.0043 (15)	0.0055 (15)
C9	0.035 (2)	0.036 (2)	0.030 (2)	-0.0039 (17)	-0.0013 (17)	0.0058 (17)
C10	0.0255 (18)	0.042 (2)	0.032 (2)	-0.0019 (17)	0.0016 (16)	-0.0077 (18)
C11	0.0280 (19)	0.042 (2)	0.035 (2)	-0.0105 (17)	0.0130 (17)	-0.0033 (18)
C12	0.034 (2)	0.036 (2)	0.0242 (19)	-0.0050 (17)	0.0111 (16)	0.0030 (16)
C13	0.0248 (17)	0.0197 (17)	0.0212 (17)	0.0010 (13)	0.0084 (14)	0.0022 (13)
C14	0.0220 (16)	0.0196 (17)	0.0241 (18)	0.0013 (13)	0.0075 (14)	0.0027 (13)
C15	0.0246 (17)	0.0250 (18)	0.0234 (18)	-0.0014 (14)	0.0069 (14)	0.0001 (14)
C16	0.0298 (18)	0.028 (2)	0.031 (2)	0.0020 (15)	0.0164 (16)	0.0002 (16)
C17	0.0232 (17)	0.028 (2)	0.043 (2)	0.0032 (15)	0.0142 (16)	-0.0020 (17)
C18	0.0197 (16)	0.0265 (19)	0.037 (2)	-0.0008 (14)	0.0063 (15)	-0.0052 (16)
Cd1	0.01973 (12)	0.03217 (15)	0.01853 (13)	0.00340 (10)	0.00597 (10)	0.00226 (10)
I1	0.02828 (12)	0.03337 (14)	0.02603 (13)	0.00073 (10)	0.01178 (10)	0.00283 (10)
I2	0.02091 (11)	0.04454 (16)	0.02837 (13)	-0.00209 (10)	0.00728 (9)	-0.00054 (11)
N1	0.0219 (14)	0.0293 (16)	0.0201 (15)	0.0026 (12)	0.0087 (12)	0.0045 (12)
N2	0.0196 (13)	0.0252 (15)	0.0218 (15)	0.0054 (11)	0.0087 (11)	0.0014 (12)
N3	0.0195 (13)	0.0299 (16)	0.0186 (14)	0.0059 (12)	0.0052 (11)	-0.0005 (12)
N4	0.0235 (14)	0.0240 (15)	0.0282 (16)	0.0021 (12)	0.0056 (12)	-0.0024 (12)
O1	0.0227 (12)	0.0337 (14)	0.0206 (12)	0.0040 (10)	0.0057 (10)	-0.0023 (10)
C19	0.0298 (18)	0.0232 (18)	0.0265 (19)	0.0055 (15)	0.0038 (15)	0.0003 (14)
C20	0.044 (2)	0.029 (2)	0.0211 (18)	0.0063 (17)	0.0077 (16)	0.0018 (15)
C21	0.041 (2)	0.030 (2)	0.0222 (19)	0.0011 (16)	0.0106 (16)	0.0025 (15)
C22	0.0300 (18)	0.0263 (19)	0.0239 (18)	0.0039 (15)	0.0100 (15)	0.0004 (15)
C23	0.0252 (17)	0.0218 (17)	0.0198 (17)	0.0017 (14)	0.0046 (14)	-0.0012 (13)
C24	0.0243 (16)	0.0219 (17)	0.0219 (17)	0.0028 (14)	0.0067 (14)	-0.0026 (14)
C25	0.0300 (18)	0.0250 (19)	0.0268 (19)	0.0060 (14)	0.0172 (15)	0.0085 (14)
C26	0.047 (2)	0.031 (2)	0.042 (2)	0.0089 (18)	0.019 (2)	-0.0008 (18)
C27	0.073 (3)	0.042 (3)	0.061 (3)	0.023 (3)	0.042 (3)	0.004 (2)
C28	0.052 (3)	0.046 (3)	0.075 (4)	0.025 (2)	0.045 (3)	0.033 (3)
C29	0.027 (2)	0.048 (3)	0.059 (3)	0.0041 (18)	0.017 (2)	0.027 (2)
C30	0.0312 (19)	0.034 (2)	0.044 (2)	0.0024 (17)	0.0165 (18)	0.0093 (18)
C31	0.0306 (18)	0.0219 (18)	0.0230 (18)	-0.0023 (14)	0.0102 (15)	-0.0020 (14)
C32	0.0310 (18)	0.0215 (18)	0.0196 (17)	-0.0063 (14)	0.0076 (14)	-0.0062 (13)
C33	0.0352 (19)	0.0255 (19)	0.0213 (18)	-0.0065 (15)	0.0098 (15)	-0.0066 (14)
C34	0.043 (2)	0.027 (2)	0.0218 (19)	-0.0086 (17)	0.0082 (16)	-0.0013 (15)
C35	0.042 (2)	0.0246 (19)	0.0251 (19)	0.0006 (16)	0.0099 (17)	0.0026 (15)
C36	0.0334 (19)	0.0263 (19)	0.029 (2)	0.0031 (15)	0.0077 (16)	0.0028 (15)
Cd2	0.02161 (12)	0.02587 (14)	0.02434 (13)	0.00368 (10)	0.00830 (10)	-0.00026 (10)
I3	0.01929 (11)	0.03300 (13)	0.02632 (12)	0.00173 (9)	0.00425 (9)	0.00129 (10)
I4	0.02047 (11)	0.03842 (15)	0.03207 (14)	0.00249 (10)	0.00375 (10)	-0.00371 (10)
N5	0.0261 (15)	0.0262 (16)	0.0203 (15)	0.0034 (12)	0.0061 (12)	0.0000 (12)
N6	0.0266 (15)	0.0211 (15)	0.0233 (15)	0.0016 (12)	0.0086 (12)	0.0016 (12)
N7	0.0315 (15)	0.0195 (15)	0.0266 (16)	0.0056 (12)	0.0143 (13)	0.0052 (12)

N8	0.0280 (15)	0.0262 (16)	0.0277 (16)	-0.0005 (13)	0.0107 (13)	-0.0019 (13)
O2	0.0292 (13)	0.0266 (14)	0.0361 (15)	0.0038 (11)	0.0152 (11)	0.0024 (11)

Geometric parameters (Å, °)

C1—N1	1.337 (4)	C19—N5	1.331 (5)
C1—C2	1.385 (5)	C19—C20	1.382 (5)
C1—H1	0.9500	C19—H19	0.9500
C2—C3	1.371 (5)	C20—C21	1.384 (5)
C2—H2	0.9500	C20—H20	0.9500
C3—C4	1.389 (5)	C21—C22	1.391 (5)
C3—H3A	0.9500	C21—H21	0.9500
C4—C5	1.381 (5)	C22—C23	1.385 (5)
C4—H4	0.9500	C22—H22	0.9500
C5—N1	1.360 (4)	C23—N5	1.356 (4)
C5—C6	1.491 (5)	C23—C24	1.480 (5)
C6—N2	1.297 (4)	C24—N6	1.280 (5)
C6—C7	1.482 (4)	C24—C25	1.483 (5)
C7—C8	1.385 (5)	C25—C30	1.383 (5)
C7—C12	1.395 (5)	C25—C26	1.391 (6)
C8—C9	1.391 (5)	C26—C27	1.377 (6)
C8—H8	0.9500	C26—H26	0.9500
C9—C10	1.392 (6)	C27—C28	1.382 (8)
C9—H9	0.9500	C27—H27	0.9500
C10—C11	1.385 (6)	C28—C29	1.376 (7)
C10—H10	0.9500	C28—H28	0.9500
C11—C12	1.380 (5)	C29—C30	1.391 (6)
C11—H11	0.9500	C29—H29	0.9500
C12—H12	0.9500	C30—H30	0.9500
C13—O1	1.233 (4)	C31—O2	1.234 (4)
C13—N3	1.357 (4)	C31—N7	1.366 (4)
C13—C14	1.492 (5)	C31—C32	1.491 (5)
C14—N4	1.338 (4)	C32—N8	1.332 (5)
C14—C15	1.384 (5)	C32—C33	1.393 (5)
C15—C16	1.394 (5)	C33—C34	1.382 (5)
C15—H15	0.9500	C33—H33	0.9500
C16—C17	1.371 (5)	C34—C35	1.380 (6)
C16—H16	0.9500	C34—H34	0.9500
C17—C18	1.387 (5)	C35—C36	1.385 (5)
C17—H17	0.9500	C35—H35	0.9500
C18—N4	1.333 (4)	C36—N8	1.330 (5)
C18—H18	0.9500	C36—H36	0.9500
Cd1—N2	2.342 (3)	Cd2—N6	2.344 (3)
Cd1—N1	2.380 (3)	Cd2—N5	2.369 (3)
Cd1—O1	2.450 (2)	Cd2—O2	2.481 (3)
Cd1—I2	2.6917 (4)	Cd2—I4	2.6732 (4)
Cd1—I1	2.7509 (4)	Cd2—I3	2.7530 (4)
N2—N3	1.362 (4)	N6—N7	1.362 (4)

N3—H3	0.8800	N7—H7	0.8800
N1—C1—C2	122.7 (3)	N5—C19—C20	123.7 (3)
N1—C1—H1	118.6	N5—C19—H19	118.1
C2—C1—H1	118.6	C20—C19—H19	118.1
C3—C2—C1	119.1 (3)	C19—C20—C21	118.8 (4)
C3—C2—H2	120.4	C19—C20—H20	120.6
C1—C2—H2	120.4	C21—C20—H20	120.6
C2—C3—C4	119.2 (3)	C20—C21—C22	118.5 (4)
C2—C3—H3A	120.4	C20—C21—H21	120.8
C4—C3—H3A	120.4	C22—C21—H21	120.8
C5—C4—C3	118.7 (3)	C23—C22—C21	119.2 (3)
C5—C4—H4	120.7	C23—C22—H22	120.4
C3—C4—H4	120.7	C21—C22—H22	120.4
N1—C5—C4	122.3 (3)	N5—C23—C22	122.3 (3)
N1—C5—C6	115.6 (3)	N5—C23—C24	116.2 (3)
C4—C5—C6	122.0 (3)	C22—C23—C24	121.5 (3)
N2—C6—C7	124.6 (3)	N6—C24—C23	116.3 (3)
N2—C6—C5	115.0 (3)	N6—C24—C25	124.4 (3)
C7—C6—C5	120.5 (3)	C23—C24—C25	119.2 (3)
C8—C7—C12	119.9 (3)	C30—C25—C26	120.3 (4)
C8—C7—C6	120.8 (3)	C30—C25—C24	119.2 (3)
C12—C7—C6	119.3 (3)	C26—C25—C24	120.4 (4)
C7—C8—C9	119.7 (4)	C27—C26—C25	119.5 (4)
C7—C8—H8	120.1	C27—C26—H26	120.2
C9—C8—H8	120.1	C25—C26—H26	120.2
C8—C9—C10	120.3 (4)	C26—C27—C28	120.0 (5)
C8—C9—H9	119.9	C26—C27—H27	120.0
C10—C9—H9	119.9	C28—C27—H27	120.0
C11—C10—C9	119.6 (4)	C29—C28—C27	121.0 (4)
C11—C10—H10	120.2	C29—C28—H28	119.5
C9—C10—H10	120.2	C27—C28—H28	119.5
C12—C11—C10	120.4 (4)	C28—C29—C30	119.3 (4)
C12—C11—H11	119.8	C28—C29—H29	120.4
C10—C11—H11	119.8	C30—C29—H29	120.4
C11—C12—C7	120.1 (4)	C25—C30—C29	119.9 (4)
C11—C12—H12	120.0	C25—C30—H30	120.1
C7—C12—H12	120.0	C29—C30—H30	120.1
O1—C13—N3	123.2 (3)	O2—C31—N7	122.3 (3)
O1—C13—C14	122.7 (3)	O2—C31—C32	124.0 (3)
N3—C13—C14	114.1 (3)	N7—C31—C32	113.7 (3)
N4—C14—C15	124.2 (3)	N8—C32—C33	124.6 (3)
N4—C14—C13	115.7 (3)	N8—C32—C31	116.0 (3)
C15—C14—C13	120.2 (3)	C33—C32—C31	119.3 (3)
C14—C15—C16	117.9 (3)	C34—C33—C32	117.6 (4)
C14—C15—H15	121.1	C34—C33—H33	121.2
C16—C15—H15	121.1	C32—C33—H33	121.2
C17—C16—C15	118.5 (3)	C35—C34—C33	118.6 (4)

C17—C16—H16	120.7	C35—C34—H34	120.7
C15—C16—H16	120.7	C33—C34—H34	120.7
C16—C17—C18	119.4 (3)	C34—C35—C36	119.2 (4)
C16—C17—H17	120.3	C34—C35—H35	120.4
C18—C17—H17	120.3	C36—C35—H35	120.4
N4—C18—C17	123.2 (3)	N8—C36—C35	123.5 (4)
N4—C18—H18	118.4	N8—C36—H36	118.3
C17—C18—H18	118.4	C35—C36—H36	118.3
N2—Cd1—N1	67.60 (9)	N6—Cd2—N5	68.41 (10)
N2—Cd1—O1	67.15 (9)	N6—Cd2—O2	66.77 (9)
N1—Cd1—O1	131.72 (9)	N5—Cd2—O2	133.56 (9)
N2—Cd1—I2	138.47 (7)	N6—Cd2—I4	139.16 (7)
N1—Cd1—I2	98.79 (7)	N5—Cd2—I4	106.26 (7)
O1—Cd1—I2	103.85 (6)	O2—Cd2—I4	99.62 (6)
N2—Cd1—I1	95.38 (7)	N6—Cd2—I3	95.35 (7)
N1—Cd1—I1	109.34 (7)	N5—Cd2—I3	99.61 (7)
O1—Cd1—I1	90.77 (6)	O2—Cd2—I3	95.99 (6)
I2—Cd1—I1	125.873 (12)	I4—Cd2—I3	124.998 (12)
C1—N1—C5	117.8 (3)	C19—N5—C23	117.6 (3)
C1—N1—Cd1	123.8 (2)	C19—N5—Cd2	125.7 (2)
C5—N1—Cd1	116.9 (2)	C23—N5—Cd2	116.4 (2)
C6—N2—N3	121.4 (3)	C24—N6—N7	121.4 (3)
C6—N2—Cd1	121.3 (2)	C24—N6—Cd2	119.5 (2)
N3—N2—Cd1	116.0 (2)	N7—N6—Cd2	116.2 (2)
C13—N3—N2	116.7 (3)	N6—N7—C31	117.4 (3)
C13—N3—H3	121.7	N6—N7—H7	121.3
N2—N3—H3	121.7	C31—N7—H7	121.3
C18—N4—C14	116.8 (3)	C36—N8—C32	116.5 (3)
C13—O1—Cd1	113.1 (2)	C31—O2—Cd2	113.5 (2)
N1—C1—C2—C3	-1.4 (6)	N5—C19—C20—C21	-0.9 (6)
C1—C2—C3—C4	-0.9 (6)	C19—C20—C21—C22	-0.6 (6)
C2—C3—C4—C5	1.0 (5)	C20—C21—C22—C23	0.9 (6)
C3—C4—C5—N1	1.1 (5)	C21—C22—C23—N5	0.1 (5)
C3—C4—C5—C6	-179.2 (3)	C21—C22—C23—C24	-178.2 (3)
N1—C5—C6—N2	2.6 (4)	N5—C23—C24—N6	-5.3 (5)
C4—C5—C6—N2	-177.1 (3)	C22—C23—C24—N6	173.1 (3)
N1—C5—C6—C7	-178.6 (3)	N5—C23—C24—C25	173.1 (3)
C4—C5—C6—C7	1.7 (5)	C22—C23—C24—C25	-8.5 (5)
N2—C6—C7—C8	-112.8 (4)	N6—C24—C25—C30	101.6 (4)
C5—C6—C7—C8	68.6 (5)	C23—C24—C25—C30	-76.6 (4)
N2—C6—C7—C12	67.0 (5)	N6—C24—C25—C26	-79.8 (5)
C5—C6—C7—C12	-111.7 (4)	C23—C24—C25—C26	101.9 (4)
C12—C7—C8—C9	-0.4 (6)	C30—C25—C26—C27	0.4 (6)
C6—C7—C8—C9	179.4 (4)	C24—C25—C26—C27	-178.1 (4)
C7—C8—C9—C10	0.1 (6)	C25—C26—C27—C28	0.0 (7)
C8—C9—C10—C11	0.6 (6)	C26—C27—C28—C29	-0.6 (7)
C9—C10—C11—C12	-1.0 (6)	C27—C28—C29—C30	0.8 (7)

C10—C11—C12—C7	0.8 (6)	C26—C25—C30—C29	-0.2 (6)
C8—C7—C12—C11	-0.1 (6)	C24—C25—C30—C29	178.3 (4)
C6—C7—C12—C11	-179.8 (3)	C28—C29—C30—C25	-0.4 (6)
O1—C13—C14—N4	175.1 (3)	O2—C31—C32—N8	168.5 (3)
N3—C13—C14—N4	-5.0 (4)	N7—C31—C32—N8	-12.5 (5)
O1—C13—C14—C15	-4.8 (5)	O2—C31—C32—C33	-12.7 (5)
N3—C13—C14—C15	175.1 (3)	N7—C31—C32—C33	166.3 (3)
N4—C14—C15—C16	0.3 (5)	N8—C32—C33—C34	0.7 (5)
C13—C14—C15—C16	-179.8 (3)	C31—C32—C33—C34	-178.0 (3)
C14—C15—C16—C17	0.7 (5)	C32—C33—C34—C35	0.2 (5)
C15—C16—C17—C18	-0.9 (6)	C33—C34—C35—C36	-1.6 (6)
C16—C17—C18—N4	0.3 (6)	C34—C35—C36—N8	2.2 (6)
C2—C1—N1—C5	3.4 (5)	C20—C19—N5—C23	1.9 (5)
C2—C1—N1—Cd1	-162.4 (3)	C20—C19—N5—Cd2	-171.9 (3)
C4—C5—N1—C1	-3.3 (5)	C22—C23—N5—C19	-1.5 (5)
C6—C5—N1—C1	177.1 (3)	C24—C23—N5—C19	176.9 (3)
C4—C5—N1—Cd1	163.5 (3)	C22—C23—N5—Cd2	172.8 (3)
C6—C5—N1—Cd1	-16.2 (4)	C24—C23—N5—Cd2	-8.8 (4)
C7—C6—N2—N3	0.6 (5)	C23—C24—N6—N7	177.4 (3)
C5—C6—N2—N3	179.3 (3)	C25—C24—N6—N7	-0.9 (5)
C7—C6—N2—Cd1	-165.7 (3)	C23—C24—N6—Cd2	17.4 (4)
C5—C6—N2—Cd1	13.0 (4)	C25—C24—N6—Cd2	-160.9 (3)
O1—C13—N3—N2	-4.9 (5)	C24—N6—N7—C31	-175.4 (3)
C14—C13—N3—N2	175.2 (3)	Cd2—N6—N7—C31	-14.7 (4)
C6—N2—N3—C13	-179.2 (3)	O2—C31—N7—N6	-1.6 (5)
Cd1—N2—N3—C13	-12.2 (4)	C32—C31—N7—N6	179.4 (3)
C17—C18—N4—C14	0.6 (5)	C35—C36—N8—C32	-1.3 (6)
C15—C14—N4—C18	-0.9 (5)	C33—C32—N8—C36	-0.2 (5)
C13—C14—N4—C18	179.1 (3)	C31—C32—N8—C36	178.6 (3)
N3—C13—O1—Cd1	18.3 (4)	N7—C31—O2—Cd2	15.8 (4)
C14—C13—O1—Cd1	-161.9 (3)	C32—C31—O2—Cd2	-165.3 (3)

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>
N3—H3...N4	0.88	2.27	2.629 (4)	104
N7—H7...N8	0.88	2.28	2.640 (4)	104