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Diaquabis[*N*,*N*′-(ethane-1,2-diyl)bis(isonicotinamide)-κ*N*]bis(hydrogen phthalato-κ*O*)nickel(II) hexahydrate

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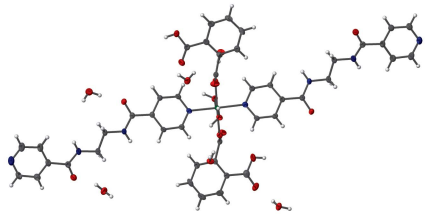
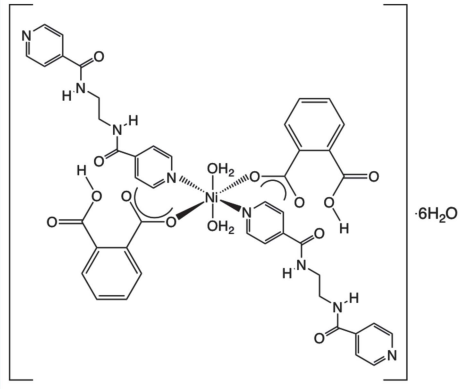
In the title solvated coordination complex, $[Ni(C_8H_5O_4)_2(C_{14}H_{14}N_4O_2)_2(H_2O)_2]\cdot 6H_2O$, the Ni^{II} cation is octahedrally coordinated by *trans* carboxylate O-atom donors from two crystallographically distinct monodentate hydrogen phthalate ($Hpht^-$) ligands, two *trans* aqua ligands, and *trans* pyridyl N-atom donors from two crystallographically distinct *N*,*N*′-(ethane-1,2-diyl)bis(isonicotinamide) (ebin) ligands. Extensive O—H···O and O—H···N hydrogen-bonding patterns involving the water molecules of crystallization anchor neighboring coordination complexes into a three-dimensional network.

3D view



Chemical scheme



Structure description

The title coordination complex was isolated during an attempt to prepare a nickel phthalate (pht) coordination polymer containing *N*,*N*′-(ethane-1,2-diyl)bis(isonicotinamide) (ebin) co-ligands. Nickel phthalate coordination polymers have displayed different structural topologies and property behavior depending on the nature of the neutral nitrogen-base co-ligand. For example, $\{[(pht)_2Ni(dpa)_2Ni(H_2O)_4]\cdot H_2O\}_n$ (dpa = 4,4′-dipyridylamine) displays a chain structure (Braverman *et al.*, 2007). The compound $[Ni(pht)(4\text{-meim})_2(H_2O]_n$ (4-meim = 4-methylimidazole), likewise with a one-dimensional structure, shows a negative influence on protease enzyme synthesis in fungal cultures *in vivo* (Filippova *et al.*, 2010). $[Ni(pht)(1,4\text{-bib})]_n$ [1,4-bib = 1,4-bis(imidazol-1-ylmethyl)benzene] exhibits a two-dimensional 6^3 herringbone topology and has nonlinear optical behavior (Zhao *et al.*, 2015). $[Ni(pht)(bbi)]_n$ [bbi = 1,1′-(1,4-butanediyl)bis(imidazole)] manifests a 4-connected three-dimensional 6^58 **cds** topology (Qi *et al.*, 2008).

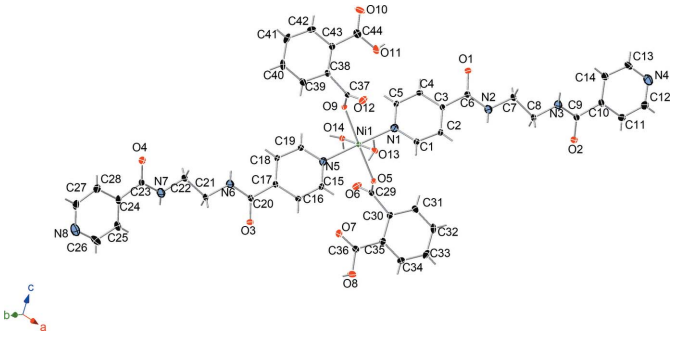


Figure 1
The coordination complex of the title compound, showing octahedral coordination at the Ni^{II} cation. Displacement ellipsoids are drawn at the 50% probability level and H atom positions are shown as gray sticks.

The asymmetric unit of the title compound contains one Ni^{II} cation, two $Hpht^{-}$ ligands, two aqua ligands, two ebin ligands, thus forming the coordination complex $[Ni(Hpht)_2(ebin)_2(H_2O)_2]$ (Fig. 1). Six water molecules of crystallization also reside in the asymmetric unit. The Ni^{II} cation is octahedrally coordinated by *trans* carboxylate O atom donors from two monodentate hydrogenphthalato (Hpht) ligands, two *trans* aqua ligands, and *trans* pyridyl N atom donors from two *N*,*N*′-(ethane-1,2-diyl)bis(isonicotinamide) (ebin) ligands. The two ebin ligands have an *anti*-conformation at their central (ethane-1,2-diyl)diamine moieties [N—C—C—N torsion angles = 179.68 (19) and 179.87 (19)°]. Bond lengths (Table 1) and angles confirm an octahedral coordination environment for the Ni^{II} atom.

Within the complex, intramolecular O—H···O hydrogen bonding is observed between the aqua ligands and the unbound O atoms belonging to the ligated and deprotonated $Hpht^{-}$ carboxylate groups (Table 2). Supramolecular layers parallel to (011) are constructed by O—H···N hydrogen bonding between unligated and protonated $Hpht^{-}$ carboxylate groups and unligated ebin pyridyl N atoms (Fig. 2). Water molecule pairs are anchored to the supramolecular layers by N—H···O hydrogen-bonding acceptance from ebin amide N—H groups, and O—H···O hydrogen-bonding donation to ebin amide C═O groups. Adjacent supramolecular layers aggregate and stack in an *ABAB* pattern along [010] (Fig. 3) by means of N—H···O hydrogen bonding from ebin amide N—H groups to isolated water molecules of crystallization, which in turn provide O—H···O hydrogen-bonding donation to ligated Hpht carboxylate O atoms (Table 2).

Table 1
Selected bond lengths (Å).

Ni1—O13	2.0643 (15)	Ni1—O9	2.1274 (15)
Ni1—O14	2.0563 (15)	Ni1—N1	2.1105 (18)
Ni1—O5	2.1045 (15)	Ni1—N5	2.1146 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8···N4^{i}	0.84	1.78	2.609 (3)	171
O11—H11···N8^{ii}	0.84	1.82	2.660 (3)	176
O13—H13*A*···O2*W*	0.88	1.90	2.706 (2)	150
O13—H13*B*···O12	0.88	1.94	2.733 (2)	149
O14—H14*B*···O6	0.88	1.87	2.668 (2)	149
N2—H2···O1*W*^{iii}	0.88	2.02	2.887 (3)	166
N3—H3···O3*W*^{ii}	0.88	2.02	2.874 (3)	164
N6—H6···O6*W*^{iv}	0.88	1.99	2.844 (3)	164
O1*W*—H1*WA*···O12^{v}	0.87	1.93	2.801 (2)	177
O1*W*—H1*WB*···O5	0.87	2.12	2.967 (2)	165
O2*W*—H2*WA*···O12^{v}	0.87	2.02	2.840 (2)	158
O2*W*—H2*WB*···O2^{iii}	0.87	1.90	2.757 (2)	169
O3*W*—H3*WA*···O5*W*^{iv}	0.87	1.98	2.849 (3)	173
O3*W*—H3*WB*···O3	0.87	1.91	2.777 (2)	175
O4*W*—H4*WA*···O4	0.87	1.96	2.800 (2)	161
O4*W*—H4*WB*···O14^{iv}	0.87	1.86	2.706 (2)	165
O5*W*—H5*WA*···O10	0.87	1.98	2.821 (3)	162
O5*W*—H5*WB*···O1^{vi}	0.87	1.92	2.776 (2)	169
O6*W*—H6*WA*···O6^{vii}	0.87	1.90	2.770 (2)	178
O6*W*—H6*WB*···O9	0.87	2.12	2.977 (2)	167

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

Synthesis and crystallization

$Ni(NO_3)_2{\cdot}6H_2O$ (108 mg, 0.37 mmol), phthalic acid (61 mg, 0.37 mol), ebin (100 mg, 0.37 mol) and 0.75 ml of a 1.0 *M*

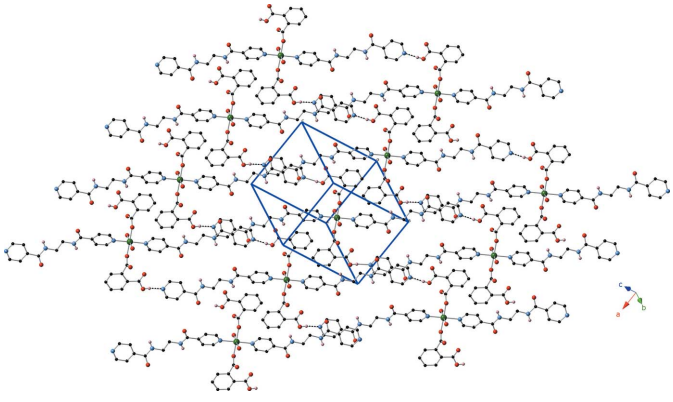


Figure 2
Supramolecular layer parallel to (011) in the title compound formed by O—H···N hydrogen bonding interactions between unligated $Hpht^{-}$ carboxylate groups and unligated ebin pyridyl nitrogen atoms. H-atom positions were omitted for clarity.

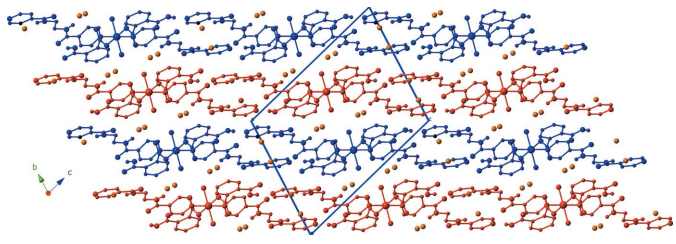


Figure 3
ABAB stacking pattern of supramolecular layer motifs in the title compound, mediated by N—H···O and O–H···O hydrogen bonding patterns involving the water molecules of crystallization situated in the interlamellar regions. H-atom positions were omitted for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_8H_5O_4)_2(C_{14}H_{14}N_4O_2)_2(H_2O)_2]\cdot 6H_2O$
M_r	1073.64
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	10.2857 (12), 14.3250 (17), 17.794 (2)
α, β, γ (°)	71.528 (1), 79.919 (1), 72.784 (1)
V (Å^3)	2365.7 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.50
Crystal size (mm)	0.27 × 0.21 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.711, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36698, 8669, 6860
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.115, 1.05
No. of reflections	8669
No. of parameters	680
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.64, −0.64

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *Crystal Maker* (Palmer, 2013).

NaOH solution were placed into 10 ml distilled water in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 393 K for 48 h, and then cooled slowly to 278 K. Green crystals of the title compound (106 mg, 53% yield based on ebin) were isolated after washing with distilled water and acetone, and drying in air.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

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full crystallographic data

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Diaquabis[*N*,*N*′-(ethane-1,2-diyl)bis(isonicotinamide)-κN]bis(hydrogen phthalato-κO)nickel(II) hexahydrate

Crystal data

$[Ni(C_8H_5O_4)_2(C_{14}H_{14}N_4O_2)_2(H_2O)_2]\cdot 6H_2O$
M_r = 1073.64
Triclinic, $P\overline{1}$
a = 10.2857 (12) Å
b = 14.3250 (17) Å
c = 17.794 (2) Å
α = 71.528 (1)°
β = 79.919 (1)°
γ = 72.784 (1)°
V = 2365.7 (5) Å^3
Z = 2
$F(000)$ = 1124
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9906 reflections
θ = 2.3–25.3°
μ = 0.50 mm^{-1}
T = 173 K
Block, green
0.27 × 0.21 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 836.6 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.711, T_{max} = 0.745
36698 measured reflections
8669 independent reflections
6860 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.4°, θ_{min} = 1.6°
h = −12→12
k = −17→17
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.05
8669 reflections
680 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 1.3935P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.49745 (3)	0.74721 (2)	0.50914 (2)	0.01646 (10)
O1	0.82860 (17)	0.45611 (14)	0.85737 (10)	0.0331 (4)
O2	1.51830 (17)	0.27370 (13)	0.80397 (10)	0.0325 (4)
O3	0.19602 (17)	1.05743 (14)	0.15603 (10)	0.0352 (5)
O4	−0.50372 (17)	1.22484 (13)	0.17927 (10)	0.0318 (4)
O5	0.67444 (15)	0.75127 (11)	0.42961 (9)	0.0183 (3)
O6	0.70332 (17)	0.90064 (12)	0.42718 (11)	0.0308 (4)
O7	0.69349 (17)	0.91897 (13)	0.25517 (10)	0.0330 (4)
O8	0.86509 (18)	0.92196 (16)	0.15992 (10)	0.0391 (5)
H8	0.8015	0.9572	0.1310	0.059*
O9	0.32138 (15)	0.74082 (11)	0.59165 (9)	0.0189 (3)
O10	0.0904 (2)	0.57849 (15)	0.86281 (10)	0.0404 (5)
O11	0.27474 (18)	0.57567 (14)	0.77595 (10)	0.0351 (4)
H11	0.3138	0.5379	0.8167	0.053*
O12	0.29879 (17)	0.58649 (12)	0.60231 (10)	0.0290 (4)
O13	0.50251 (16)	0.61563 (11)	0.48298 (9)	0.0215 (4)
H13A	0.4871	0.6295	0.4328	0.032*
H13B	0.4390	0.5874	0.5137	0.032*
O14	0.49020 (16)	0.87908 (11)	0.53467 (9)	0.0215 (4)
H14A	0.4099	0.9230	0.5253	0.032*
H14B	0.5544	0.9071	0.5047	0.032*
N1	0.62369 (18)	0.65432 (14)	0.60069 (11)	0.0189 (4)
N2	1.01031 (19)	0.41926 (14)	0.77027 (11)	0.0229 (4)
H2	1.0458	0.4305	0.7205	0.028*
N3	1.3188 (2)	0.24783 (15)	0.86972 (12)	0.0257 (5)
H3	1.2765	0.2163	0.9135	0.031*
N4	1.6880 (2)	0.03666 (17)	1.05794 (13)	0.0340 (5)
N5	0.37401 (18)	0.83994 (14)	0.41590 (11)	0.0184 (4)
N6	0.00097 (19)	1.07507 (14)	0.23624 (11)	0.0215 (4)
H6	−0.0409	1.0584	0.2842	0.026*
N7	−0.2954 (2)	1.24525 (15)	0.12505 (12)	0.0266 (5)
H7	−0.2473	1.2755	0.0835	0.032*
N8	−0.6137 (2)	1.45381 (16)	−0.09158 (13)	0.0354 (5)
C1	0.7449 (2)	0.59222 (17)	0.58465 (14)	0.0222 (5)
H1	0.7707	0.5898	0.5312	0.027*
C2	0.8340 (2)	0.53179 (17)	0.64121 (13)	0.0214 (5)
H2A	0.9198	0.4908	0.6264	0.026*
C3	0.7964 (2)	0.53183 (16)	0.72011 (13)	0.0194 (5)
C4	0.6697 (2)	0.59523 (17)	0.73731 (14)	0.0225 (5)
H4	0.6400	0.5975	0.7905	0.027*
C5	0.5880 (2)	0.65450 (17)	0.67687 (13)	0.0204 (5)
H5	0.5025	0.6974	0.6897	0.025*
C6	0.8811 (2)	0.46600 (17)	0.78795 (14)	0.0219 (5)
C7	1.0928 (2)	0.34900 (18)	0.83455 (14)	0.0246 (5)
H7A	1.0571	0.2880	0.8585	0.030*

H7B	1.0858	0.3825	0.8765	0.030*
C8	1.2404 (2)	0.31724 (18)	0.80369 (14)	0.0247 (5)
H8A	1.2482	0.2829	0.7622	0.030*
H8B	1.2767	0.3780	0.7797	0.030*
C9	1.4533 (2)	0.23228 (18)	0.86387 (14)	0.0235 (5)
C10	1.5292 (2)	0.16153 (17)	0.93421 (14)	0.0244 (5)
C11	1.6701 (3)	0.1322 (2)	0.92201 (16)	0.0360 (7)
H11A	1.7150	0.1548	0.8708	0.043*
C12	1.7447 (3)	0.0699 (2)	0.98459 (16)	0.0413 (7)
H12	1.8414	0.0496	0.9751	0.050*
C13	1.5523 (3)	0.06410 (19)	1.07036 (15)	0.0289 (6)
H13	1.5106	0.0403	1.1223	0.035*
C14	1.4696 (3)	0.12619 (18)	1.01016 (14)	0.0269 (6)
H14	1.3730	0.1442	1.0210	0.032*
C15	0.4203 (2)	0.84744 (17)	0.33952 (14)	0.0211 (5)
H15	0.5086	0.8070	0.3278	0.025*
C16	0.3449 (2)	0.91165 (18)	0.27709 (14)	0.0230 (5)
H16	0.3829	0.9168	0.2237	0.028*
C17	0.2134 (2)	0.96857 (17)	0.29281 (13)	0.0197 (5)
C18	0.1646 (2)	0.95989 (17)	0.37186 (13)	0.0209 (5)
H18	0.0749	0.9969	0.3853	0.025*
C19	0.2478 (2)	0.89696 (17)	0.43065 (14)	0.0222 (5)
H19	0.2142	0.8936	0.4844	0.027*
C20	0.1352 (2)	1.03773 (17)	0.22313 (14)	0.0227 (5)
C21	−0.0749 (2)	1.14415 (18)	0.16946 (14)	0.0240 (5)
H21A	−0.0615	1.1101	0.1272	0.029*
H21B	−0.0392	1.2053	0.1473	0.029*
C22	−0.2266 (2)	1.17618 (19)	0.19489 (14)	0.0258 (5)
H22A	−0.2637	1.1156	0.2165	0.031*
H22B	−0.2413	1.2110	0.2368	0.031*
C23	−0.4296 (2)	1.26325 (17)	0.12320 (14)	0.0235 (5)
C24	−0.4899 (2)	1.33226 (18)	0.04703 (15)	0.0254 (5)
C25	−0.4141 (3)	1.3655 (2)	−0.02330 (15)	0.0330 (6)
H25	−0.3171	1.3472	−0.0254	0.040*
C26	−0.4795 (3)	1.4256 (2)	−0.09107 (16)	0.0382 (7)
H26	−0.4253	1.4472	−0.1390	0.046*
C27	−0.6881 (3)	1.4218 (2)	−0.02409 (16)	0.0344 (6)
H27	−0.7848	1.4414	−0.0241	0.041*
C28	−0.6311 (3)	1.3610 (2)	0.04669 (16)	0.0327 (6)
H28	−0.6878	1.3397	0.0936	0.039*
C29	0.7415 (2)	0.81806 (17)	0.41064 (13)	0.0196 (5)
C30	0.8842 (2)	0.78887 (16)	0.37059 (14)	0.0190 (5)
C31	0.9853 (2)	0.72325 (18)	0.41893 (15)	0.0243 (5)
H31	0.9616	0.6968	0.4741	0.029*
C32	1.1202 (2)	0.69546 (18)	0.38840 (16)	0.0283 (6)
H32	1.1883	0.6519	0.4227	0.034*
C33	1.1552 (2)	0.73139 (19)	0.30775 (16)	0.0285 (6)
H33	1.2472	0.7122	0.2863	0.034*

C34	1.0555 (2)	0.79525 (18)	0.25885 (15)	0.0265 (5)
H34	1.0796	0.8193	0.2034	0.032*
C35	0.9196 (2)	0.82543 (17)	0.28905 (14)	0.0213 (5)
C36	0.8142 (2)	0.89364 (18)	0.23390 (14)	0.0232 (5)
C37	0.2565 (2)	0.67276 (17)	0.61349 (13)	0.0195 (5)
C38	0.1105 (2)	0.70516 (16)	0.64827 (13)	0.0181 (5)
C39	0.0192 (2)	0.77089 (18)	0.59354 (15)	0.0246 (5)
H39	0.0522	0.7923	0.5392	0.030*
C40	−0.1189 (2)	0.80629 (18)	0.61587 (16)	0.0289 (6)
H40	−0.1794	0.8498	0.5770	0.035*
C41	−0.1671 (2)	0.77775 (19)	0.69473 (16)	0.0298 (6)
H41	−0.2606	0.8028	0.7109	0.036*
C42	−0.0782 (2)	0.71239 (19)	0.75005 (15)	0.0271 (5)
H42	−0.1120	0.6927	0.8044	0.032*
C43	0.0599 (2)	0.67453 (17)	0.72839 (14)	0.0207 (5)
C44	0.1433 (3)	0.60501 (18)	0.79508 (15)	0.0278 (6)
O4W	−0.49901 (19)	1.07984 (13)	0.32827 (10)	0.0323 (4)
H4WA	−0.4802	1.1218	0.2829	0.048*
H4WB	−0.4931	1.1032	0.3668	0.048*
O3W	0.1356 (2)	1.17819 (17)	0.00369 (11)	0.0541 (6)
H3WA	0.0704	1.2325	0.0054	0.081*
H3WB	0.1499	1.1397	0.0519	0.081*
O1W	0.83173 (16)	0.56557 (13)	0.38217 (10)	0.0274 (4)
H1WA	0.7929	0.5169	0.3887	0.041*
H1WB	0.7728	0.6161	0.3964	0.041*
O5W	0.0946 (2)	0.65345 (14)	0.99086 (10)	0.0366 (5)
H5WA	0.0906	0.6184	0.9597	0.055*
H5WB	0.1169	0.6123	1.0371	0.055*
O2W	0.48153 (18)	0.58540 (14)	0.34348 (10)	0.0329 (4)
H2WA	0.5469	0.5297	0.3480	0.049*
H2WB	0.4933	0.6283	0.2974	0.049*
O6W	0.17069 (16)	0.94119 (13)	0.61888 (10)	0.0261 (4)
H6WA	0.2117	0.9901	0.6035	0.039*
H6WB	0.2260	0.8865	0.6090	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01450 (16)	0.01641 (16)	0.01615 (17)	−0.00139 (12)	−0.00291 (11)	−0.00300 (12)
O13	0.0255 (9)	0.0189 (8)	0.0199 (8)	−0.0066 (7)	−0.0021 (7)	−0.0043 (7)
O1	0.0246 (9)	0.0459 (11)	0.0160 (9)	0.0034 (8)	−0.0024 (7)	−0.0027 (8)
O14	0.0180 (8)	0.0185 (8)	0.0253 (9)	−0.0025 (6)	−0.0008 (7)	−0.0051 (7)
O2	0.0245 (9)	0.0380 (10)	0.0236 (10)	−0.0010 (8)	−0.0017 (8)	0.0000 (8)
O12	0.0252 (9)	0.0218 (9)	0.0394 (11)	−0.0065 (7)	0.0058 (8)	−0.0122 (8)
O3	0.0251 (9)	0.0472 (11)	0.0170 (9)	0.0041 (8)	−0.0021 (7)	0.0009 (8)
O4	0.0224 (9)	0.0372 (10)	0.0278 (10)	−0.0011 (8)	−0.0028 (8)	−0.0039 (8)
O5	0.0147 (8)	0.0184 (8)	0.0197 (8)	−0.0039 (6)	−0.0012 (6)	−0.0029 (6)
O6	0.0314 (10)	0.0231 (9)	0.0383 (11)	−0.0099 (8)	0.0106 (8)	−0.0137 (8)

O7	0.0204 (9)	0.0369 (10)	0.0299 (10)	0.0001 (8)	−0.0027 (8)	−0.0001 (8)
O8	0.0274 (10)	0.0565 (13)	0.0185 (9)	−0.0002 (9)	−0.0046 (8)	0.0015 (9)
O9	0.0156 (8)	0.0175 (8)	0.0220 (8)	−0.0048 (6)	−0.0019 (6)	−0.0029 (6)
O10	0.0447 (12)	0.0505 (12)	0.0189 (10)	−0.0125 (10)	−0.0028 (8)	0.0001 (9)
O11	0.0278 (10)	0.0392 (11)	0.0286 (10)	−0.0014 (8)	−0.0122 (8)	0.0022 (8)
N1	0.0173 (10)	0.0184 (10)	0.0206 (10)	−0.0040 (8)	−0.0012 (8)	−0.0057 (8)
N2	0.0206 (10)	0.0265 (11)	0.0164 (10)	−0.0004 (9)	−0.0056 (8)	−0.0019 (8)
N3	0.0204 (11)	0.0264 (11)	0.0213 (11)	−0.0007 (9)	−0.0041 (8)	0.0018 (9)
N4	0.0329 (13)	0.0377 (13)	0.0256 (12)	−0.0008 (10)	−0.0106 (10)	−0.0045 (10)
N5	0.0151 (9)	0.0181 (10)	0.0209 (10)	−0.0025 (8)	−0.0017 (8)	−0.0056 (8)
N6	0.0180 (10)	0.0247 (10)	0.0164 (10)	−0.0017 (8)	−0.0044 (8)	−0.0003 (8)
N7	0.0236 (11)	0.0284 (11)	0.0210 (11)	−0.0025 (9)	−0.0079 (9)	0.0015 (9)
N8	0.0419 (14)	0.0304 (12)	0.0319 (13)	−0.0065 (11)	−0.0149 (11)	−0.0024 (10)
C1	0.0207 (12)	0.0231 (12)	0.0195 (12)	−0.0008 (10)	−0.0018 (10)	−0.0059 (10)
C2	0.0183 (12)	0.0213 (12)	0.0210 (12)	0.0005 (9)	−0.0027 (9)	−0.0056 (10)
C3	0.0193 (12)	0.0172 (11)	0.0195 (12)	−0.0041 (9)	−0.0028 (9)	−0.0022 (9)
C4	0.0220 (12)	0.0254 (13)	0.0166 (12)	−0.0034 (10)	0.0008 (9)	−0.0052 (10)
C5	0.0156 (11)	0.0221 (12)	0.0205 (12)	−0.0009 (9)	−0.0011 (9)	−0.0057 (10)
C6	0.0209 (12)	0.0224 (12)	0.0196 (12)	−0.0032 (10)	−0.0029 (10)	−0.0038 (10)
C7	0.0227 (13)	0.0256 (13)	0.0201 (12)	−0.0014 (10)	−0.0073 (10)	−0.0007 (10)
C8	0.0218 (12)	0.0246 (13)	0.0208 (12)	0.0007 (10)	−0.0056 (10)	−0.0011 (10)
C9	0.0258 (13)	0.0214 (12)	0.0195 (13)	0.0000 (10)	−0.0033 (10)	−0.0054 (10)
C10	0.0275 (13)	0.0214 (12)	0.0223 (13)	0.0000 (10)	−0.0074 (10)	−0.0066 (10)
C11	0.0246 (14)	0.0495 (17)	0.0231 (14)	0.0003 (12)	−0.0030 (11)	−0.0040 (12)
C12	0.0268 (15)	0.0543 (18)	0.0294 (15)	0.0038 (13)	−0.0063 (12)	−0.0048 (13)
C13	0.0376 (15)	0.0273 (13)	0.0209 (13)	−0.0082 (11)	−0.0066 (11)	−0.0035 (10)
C14	0.0266 (13)	0.0272 (13)	0.0251 (13)	−0.0055 (11)	−0.0052 (11)	−0.0048 (11)
C15	0.0158 (11)	0.0216 (12)	0.0229 (12)	−0.0007 (9)	−0.0019 (9)	−0.0061 (10)
C16	0.0195 (12)	0.0276 (13)	0.0173 (12)	−0.0015 (10)	−0.0015 (9)	−0.0042 (10)
C17	0.0204 (12)	0.0179 (11)	0.0196 (12)	−0.0040 (9)	−0.0043 (9)	−0.0033 (9)
C18	0.0161 (11)	0.0217 (12)	0.0206 (12)	0.0000 (9)	−0.0013 (9)	−0.0049 (10)
C19	0.0198 (12)	0.0240 (12)	0.0194 (12)	−0.0017 (10)	−0.0010 (10)	−0.0056 (10)
C20	0.0233 (13)	0.0217 (12)	0.0186 (12)	−0.0017 (10)	−0.0043 (10)	−0.0022 (10)
C21	0.0216 (12)	0.0261 (13)	0.0194 (12)	−0.0011 (10)	−0.0069 (10)	−0.0016 (10)
C22	0.0239 (13)	0.0275 (13)	0.0191 (12)	−0.0015 (10)	−0.0059 (10)	0.0005 (10)
C23	0.0239 (13)	0.0212 (12)	0.0227 (13)	0.0005 (10)	−0.0054 (10)	−0.0068 (10)
C24	0.0269 (13)	0.0227 (12)	0.0276 (14)	−0.0009 (10)	−0.0114 (11)	−0.0088 (10)
C25	0.0321 (15)	0.0357 (15)	0.0284 (14)	−0.0087 (12)	−0.0116 (12)	−0.0006 (11)
C26	0.0398 (16)	0.0424 (17)	0.0288 (15)	−0.0149 (13)	−0.0115 (12)	0.0032 (12)
C27	0.0244 (14)	0.0378 (16)	0.0385 (16)	0.0027 (12)	−0.0125 (12)	−0.0122 (13)
C28	0.0260 (14)	0.0362 (15)	0.0315 (15)	−0.0005 (12)	−0.0048 (11)	−0.0093 (12)
C29	0.0191 (12)	0.0207 (12)	0.0171 (12)	−0.0039 (10)	−0.0031 (9)	−0.0030 (9)
C30	0.0166 (11)	0.0175 (11)	0.0243 (12)	−0.0060 (9)	−0.0018 (9)	−0.0064 (9)
C31	0.0252 (13)	0.0224 (12)	0.0245 (13)	−0.0064 (10)	−0.0047 (10)	−0.0038 (10)
C32	0.0206 (13)	0.0244 (13)	0.0377 (15)	−0.0011 (10)	−0.0115 (11)	−0.0053 (11)
C33	0.0161 (12)	0.0289 (14)	0.0397 (16)	−0.0049 (10)	0.0005 (11)	−0.0110 (12)
C34	0.0227 (13)	0.0289 (13)	0.0258 (13)	−0.0085 (11)	0.0018 (10)	−0.0054 (11)
C35	0.0194 (12)	0.0211 (12)	0.0244 (13)	−0.0058 (10)	−0.0028 (10)	−0.0070 (10)

C36	0.0249 (13)	0.0224 (12)	0.0209 (13)	−0.0067 (10)	−0.0022 (10)	−0.0035 (10)
C37	0.0202 (12)	0.0197 (12)	0.0158 (11)	−0.0022 (10)	−0.0036 (9)	−0.0029 (9)
C38	0.0180 (11)	0.0154 (11)	0.0218 (12)	−0.0058 (9)	−0.0047 (9)	−0.0034 (9)
C39	0.0241 (13)	0.0241 (12)	0.0240 (13)	−0.0069 (10)	−0.0060 (10)	−0.0019 (10)
C40	0.0207 (13)	0.0236 (13)	0.0421 (16)	−0.0007 (10)	−0.0150 (11)	−0.0067 (11)
C41	0.0154 (12)	0.0284 (14)	0.0467 (17)	−0.0037 (10)	−0.0019 (11)	−0.0143 (12)
C42	0.0243 (13)	0.0324 (14)	0.0253 (13)	−0.0109 (11)	0.0051 (10)	−0.0100 (11)
C43	0.0191 (12)	0.0198 (12)	0.0228 (12)	−0.0063 (9)	−0.0031 (10)	−0.0039 (10)
C44	0.0304 (14)	0.0247 (13)	0.0302 (15)	−0.0092 (11)	−0.0078 (11)	−0.0056 (11)
O4W	0.0384 (11)	0.0338 (10)	0.0227 (9)	−0.0029 (8)	−0.0055 (8)	−0.0099 (8)
O3W	0.0371 (12)	0.0618 (15)	0.0275 (11)	0.0107 (10)	0.0018 (9)	0.0124 (10)
O1W	0.0231 (9)	0.0268 (9)	0.0323 (10)	−0.0067 (7)	0.0031 (7)	−0.0109 (8)
O5W	0.0392 (11)	0.0400 (11)	0.0198 (9)	−0.0005 (9)	−0.0067 (8)	−0.0004 (8)
O2W	0.0363 (11)	0.0298 (10)	0.0230 (10)	0.0019 (8)	−0.0049 (8)	−0.0027 (8)
O6W	0.0214 (9)	0.0245 (9)	0.0307 (10)	−0.0071 (7)	0.0035 (7)	−0.0074 (8)

Geometric parameters (Å, º)

Ni1—O13	2.0643 (15)	C12—H12	0.9500
Ni1—O14	2.0563 (15)	C13—H13	0.9500
Ni1—O5	2.1045 (15)	C13—C14	1.389 (3)
Ni1—O9	2.1274 (15)	C14—H14	0.9500
Ni1—N1	2.1105 (18)	C15—H15	0.9500
Ni1—N5	2.1146 (18)	C15—C16	1.383 (3)
O13—H13A	0.8839	C16—H16	0.9500
O13—H13B	0.8835	C16—C17	1.390 (3)
O1—C6	1.240 (3)	C17—C18	1.387 (3)
O14—H14A	0.8832	C17—C20	1.505 (3)
O14—H14B	0.8831	C18—H18	0.9500
O2—C9	1.233 (3)	C18—C19	1.377 (3)
O12—C37	1.250 (3)	C19—H19	0.9500
O3—C20	1.235 (3)	C21—H21A	0.9900
O4—C23	1.230 (3)	C21—H21B	0.9900
O5—C29	1.269 (3)	C21—C22	1.519 (3)
O6—C29	1.243 (3)	C22—H22A	0.9900
O7—C36	1.213 (3)	C22—H22B	0.9900
O8—H8	0.8400	C23—C24	1.510 (3)
O8—C36	1.311 (3)	C24—C25	1.379 (4)
O9—C37	1.265 (3)	C24—C28	1.388 (3)
O10—C44	1.223 (3)	C25—H25	0.9500
O11—H11	0.8400	C25—C26	1.390 (3)
O11—C44	1.309 (3)	C26—H26	0.9500
N1—C1	1.344 (3)	C27—H27	0.9500
N1—C5	1.342 (3)	C27—C28	1.396 (4)
N2—H2	0.8800	C28—H28	0.9500
N2—C6	1.332 (3)	C29—C30	1.515 (3)
N2—C7	1.465 (3)	C30—C31	1.389 (3)
N3—H3	0.8800	C30—C35	1.399 (3)

N3—C8	1.462 (3)	C31—H31	0.9500
N3—C9	1.326 (3)	C31—C32	1.387 (3)
N4—C12	1.332 (3)	C32—H32	0.9500
N4—C13	1.331 (3)	C32—C33	1.384 (4)
N5—C15	1.340 (3)	C33—H33	0.9500
N5—C19	1.346 (3)	C33—C34	1.378 (3)
N6—H6	0.8800	C34—H34	0.9500
N6—C20	1.332 (3)	C34—C35	1.399 (3)
N6—C21	1.457 (3)	C35—C36	1.494 (3)
N7—H7	0.8800	C37—C38	1.516 (3)
N7—C22	1.462 (3)	C38—C39	1.390 (3)
N7—C23	1.332 (3)	C38—C43	1.405 (3)
N8—C26	1.320 (3)	C39—H39	0.9500
N8—C27	1.332 (4)	C39—C40	1.392 (3)
C1—H1	0.9500	C40—H40	0.9500
C1—C2	1.380 (3)	C40—C41	1.377 (4)
C2—H2A	0.9500	C41—H41	0.9500
C2—C3	1.389 (3)	C41—C42	1.380 (3)
C3—C4	1.397 (3)	C42—H42	0.9500
C3—C6	1.505 (3)	C42—C43	1.395 (3)
C4—H4	0.9500	C43—C44	1.496 (3)
C4—C5	1.378 (3)	O4W—H4WA	0.8702
C5—H5	0.9500	O4W—H4WB	0.8704
C7—H7A	0.9900	O3W—H3WA	0.8695
C7—H7B	0.9900	O3W—H3WB	0.8701
C7—C8	1.507 (3)	O1W—H1WA	0.8696
C8—H8A	0.9900	O1W—H1WB	0.8703
C8—H8B	0.9900	O5W—H5WA	0.8698
C9—C10	1.507 (3)	O5W—H5WB	0.8699
C10—C11	1.383 (3)	O2W—H2WA	0.8698
C10—C14	1.385 (3)	O2W—H2WB	0.8693
C11—H11A	0.9500	O6W—H6WA	0.8703
C11—C12	1.374 (3)	O6W—H6WB	0.8695

O13—Ni1—O5	85.98 (6)	C17—C16—H16	120.2
O13—Ni1—O9	93.90 (6)	C16—C17—C20	117.9 (2)
O13—Ni1—N1	87.30 (7)	C18—C17—C16	117.6 (2)
O13—Ni1—N5	92.43 (7)	C18—C17—C20	124.4 (2)
O14—Ni1—O13	179.32 (6)	C17—C18—H18	120.4
O14—Ni1—O5	94.34 (6)	C19—C18—C17	119.2 (2)
O14—Ni1—O9	85.80 (6)	C19—C18—H18	120.4
O14—Ni1—N1	93.30 (7)	N5—C19—C18	123.5 (2)
O14—Ni1—N5	86.97 (7)	N5—C19—H19	118.3
O5—Ni1—O9	178.69 (6)	C18—C19—H19	118.3
O5—Ni1—N1	88.57 (7)	O3—C20—N6	122.1 (2)
O5—Ni1—N5	90.42 (6)	O3—C20—C17	119.6 (2)
N1—Ni1—O9	90.12 (7)	N6—C20—C17	118.2 (2)
N1—Ni1—N5	178.97 (7)	N6—C21—H21A	109.4

N5—Ni1—O9	90.89 (6)	N6—C21—H21B	109.4
Ni1—O13—H13A	110.3	N6—C21—C22	111.26 (19)
Ni1—O13—H13B	109.9	H21A—C21—H21B	108.0
H13A—O13—H13B	108.6	C22—C21—H21A	109.4
Ni1—O14—H14A	110.1	C22—C21—H21B	109.4
Ni1—O14—H14B	110.2	N7—C22—C21	108.02 (19)
H14A—O14—H14B	108.7	N7—C22—H22A	110.1
C29—O5—Ni1	126.89 (14)	N7—C22—H22B	110.1
C36—O8—H8	109.5	C21—C22—H22A	110.1
C37—O9—Ni1	127.79 (14)	C21—C22—H22B	110.1
C44—O11—H11	109.5	H22A—C22—H22B	108.4
C1—N1—Ni1	120.89 (15)	O4—C23—N7	123.1 (2)
C5—N1—Ni1	122.14 (15)	O4—C23—C24	119.8 (2)
C5—N1—C1	116.97 (19)	N7—C23—C24	117.0 (2)
C6—N2—H2	120.4	C25—C24—C23	124.5 (2)
C6—N2—C7	119.3 (2)	C25—C24—C28	117.6 (2)
C7—N2—H2	120.4	C28—C24—C23	117.9 (2)
C8—N3—H3	119.9	C24—C25—H25	120.0
C9—N3—H3	119.9	C24—C25—C26	120.0 (3)
C9—N3—C8	120.2 (2)	C26—C25—H25	120.0
C13—N4—C12	118.0 (2)	N8—C26—C25	122.7 (3)
C15—N5—Ni1	121.35 (14)	N8—C26—H26	118.6
C15—N5—C19	117.24 (19)	C25—C26—H26	118.6
C19—N5—Ni1	121.35 (15)	N8—C27—H27	118.4
C20—N6—H6	120.7	N8—C27—C28	123.3 (2)
C20—N6—C21	118.59 (19)	C28—C27—H27	118.4
C21—N6—H6	120.7	C24—C28—C27	118.6 (2)
C22—N7—H7	119.4	C24—C28—H28	120.7
C23—N7—H7	119.4	C27—C28—H28	120.7
C23—N7—C22	121.2 (2)	O5—C29—C30	115.87 (19)
C26—N8—C27	117.9 (2)	O6—C29—O5	125.4 (2)
N1—C1—H1	118.1	O6—C29—C30	118.5 (2)
N1—C1—C2	123.9 (2)	C31—C30—C29	117.1 (2)
C2—C1—H1	118.1	C31—C30—C35	118.8 (2)
C1—C2—H2A	120.5	C35—C30—C29	124.1 (2)
C1—C2—C3	119.0 (2)	C30—C31—H31	119.3
C3—C2—H2A	120.5	C32—C31—C30	121.4 (2)
C2—C3—C4	117.4 (2)	C32—C31—H31	119.3
C2—C3—C6	124.3 (2)	C31—C32—H32	120.1
C4—C3—C6	118.3 (2)	C33—C32—C31	119.8 (2)
C3—C4—H4	120.1	C33—C32—H32	120.1
C5—C4—C3	119.8 (2)	C32—C33—H33	120.3
C5—C4—H4	120.1	C34—C33—C32	119.4 (2)
N1—C5—C4	123.0 (2)	C34—C33—H33	120.3
N1—C5—H5	118.5	C33—C34—H34	119.3
C4—C5—H5	118.5	C33—C34—C35	121.4 (2)
O1—C6—N2	122.6 (2)	C35—C34—H34	119.3
O1—C6—C3	119.5 (2)	C30—C35—C36	121.1 (2)

N2—C6—C3	117.8 (2)	C34—C35—C30	119.1 (2)
N2—C7—H7A	109.5	C34—C35—C36	119.8 (2)
N2—C7—H7B	109.5	O7—C36—O8	123.4 (2)
N2—C7—C8	110.80 (19)	O7—C36—C35	123.5 (2)
H7A—C7—H7B	108.1	O8—C36—C35	113.1 (2)
C8—C7—H7A	109.5	O12—C37—O9	125.5 (2)
C8—C7—H7B	109.5	O12—C37—C38	118.8 (2)
N3—C8—C7	108.93 (19)	O9—C37—C38	115.42 (19)
N3—C8—H8A	109.9	C39—C38—C37	115.1 (2)
N3—C8—H8B	109.9	C39—C38—C43	118.1 (2)
C7—C8—H8A	109.9	C43—C38—C37	126.81 (19)
C7—C8—H8B	109.9	C38—C39—H39	119.0
H8A—C8—H8B	108.3	C38—C39—C40	122.0 (2)
O2—C9—N3	122.9 (2)	C40—C39—H39	119.0
O2—C9—C10	118.9 (2)	C39—C40—H40	120.3
N3—C9—C10	118.1 (2)	C41—C40—C39	119.5 (2)
C11—C10—C9	116.9 (2)	C41—C40—H40	120.3
C11—C10—C14	117.7 (2)	C40—C41—H41	120.3
C14—C10—C9	125.4 (2)	C40—C41—C42	119.4 (2)
C10—C11—H11A	120.3	C42—C41—H41	120.3
C12—C11—C10	119.4 (2)	C41—C42—H42	119.1
C12—C11—H11A	120.3	C41—C42—C43	121.8 (2)
N4—C12—C11	123.1 (3)	C43—C42—H42	119.1
N4—C12—H12	118.4	C38—C43—C44	125.3 (2)
C11—C12—H12	118.4	C42—C43—C38	119.1 (2)
N4—C13—H13	118.8	C42—C43—C44	115.6 (2)
N4—C13—C14	122.4 (2)	O10—C44—O11	123.0 (2)
C14—C13—H13	118.8	O10—C44—C43	121.3 (2)
C10—C14—C13	119.4 (2)	O11—C44—C43	115.7 (2)
C10—C14—H14	120.3	H4WA—O4W—H4WB	109.4
C13—C14—H14	120.3	H3WA—O3W—H3WB	109.5
N5—C15—H15	118.6	H1WA—O1W—H1WB	109.5
N5—C15—C16	122.7 (2)	H5WA—O5W—H5WB	109.5
C16—C15—H15	118.6	H2WA—O2W—H2WB	109.6
C15—C16—H16	120.2	H6WA—O6W—H6WB	109.4
C15—C16—C17	119.7 (2)		

Ni1—O5—C29—O6	−10.8 (3)	C15—N5—C19—C18	1.4 (3)
Ni1—O5—C29—C30	163.86 (14)	C15—C16—C17—C18	1.6 (3)
Ni1—O9—C37—O12	14.7 (3)	C15—C16—C17—C20	179.8 (2)
Ni1—O9—C37—C38	−158.76 (14)	C16—C17—C18—C19	0.6 (3)
Ni1—N1—C1—C2	178.04 (17)	C16—C17—C20—O3	−13.8 (3)
Ni1—N1—C5—C4	−179.25 (17)	C16—C17—C20—N6	165.5 (2)
Ni1—N5—C15—C16	−176.37 (17)	C17—C18—C19—N5	−2.2 (4)
Ni1—N5—C19—C18	178.78 (17)	C18—C17—C20—O3	164.2 (2)
O2—C9—C10—C11	−11.9 (3)	C18—C17—C20—N6	−16.4 (3)
O2—C9—C10—C14	166.1 (2)	C19—N5—C15—C16	1.0 (3)
O12—C37—C38—C39	−101.6 (2)	C20—N6—C21—C22	178.2 (2)

O12—C37—C38—C43	77.4 (3)	C20—C17—C18—C19	−177.4 (2)
O4—C23—C24—C25	−168.7 (2)	C21—N6—C20—O3	−2.2 (4)
O4—C23—C24—C28	8.5 (3)	C21—N6—C20—C17	178.4 (2)
O5—C29—C30—C31	−77.1 (3)	C22—N7—C23—O4	0.9 (4)
O5—C29—C30—C35	104.3 (3)	C22—N7—C23—C24	−177.5 (2)
O6—C29—C30—C31	98.0 (3)	C23—N7—C22—C21	161.1 (2)
O6—C29—C30—C35	−80.7 (3)	C23—C24—C25—C26	177.3 (2)
O9—C37—C38—C39	72.3 (3)	C23—C24—C28—C27	−177.8 (2)
O9—C37—C38—C43	−108.7 (3)	C24—C25—C26—N8	0.5 (4)
N1—C1—C2—C3	2.0 (4)	C25—C24—C28—C27	−0.3 (4)
N2—C7—C8—N3	179.68 (19)	C26—N8—C27—C28	0.5 (4)
N3—C9—C10—C11	168.7 (2)	C27—N8—C26—C25	−0.8 (4)
N3—C9—C10—C14	−13.3 (4)	C28—C24—C25—C26	0.1 (4)
N4—C13—C14—C10	−0.1 (4)	C29—C30—C31—C32	−177.3 (2)
N5—C15—C16—C17	−2.5 (4)	C29—C30—C35—C34	178.4 (2)
N6—C21—C22—N7	179.87 (19)	C29—C30—C35—C36	−3.2 (3)
N7—C23—C24—C25	9.7 (4)	C30—C31—C32—C33	−1.7 (4)
N7—C23—C24—C28	−173.1 (2)	C30—C35—C36—O7	−2.0 (4)
N8—C27—C28—C24	0.0 (4)	C30—C35—C36—O8	179.0 (2)
C1—N1—C5—C4	0.4 (3)	C31—C30—C35—C34	−0.3 (3)
C1—C2—C3—C4	−1.0 (3)	C31—C30—C35—C36	178.1 (2)
C1—C2—C3—C6	177.0 (2)	C31—C32—C33—C34	0.6 (4)
C2—C3—C4—C5	−0.1 (3)	C32—C33—C34—C35	0.6 (4)
C2—C3—C6—O1	−165.9 (2)	C33—C34—C35—C30	−0.8 (4)
C2—C3—C6—N2	13.2 (3)	C33—C34—C35—C36	−179.2 (2)
C3—C4—C5—N1	0.4 (4)	C34—C35—C36—O7	176.4 (2)
C4—C3—C6—O1	12.2 (3)	C34—C35—C36—O8	−2.6 (3)
C4—C3—C6—N2	−168.8 (2)	C35—C30—C31—C32	1.5 (3)
C5—N1—C1—C2	−1.7 (3)	C37—C38—C39—C40	179.0 (2)
C6—N2—C7—C8	−171.2 (2)	C37—C38—C43—C42	179.8 (2)
C6—C3—C4—C5	−178.3 (2)	C37—C38—C43—C44	1.4 (4)
C7—N2—C6—O1	3.3 (4)	C38—C39—C40—C41	1.6 (4)
C7—N2—C6—C3	−175.7 (2)	C38—C43—C44—O10	−176.8 (2)
C8—N3—C9—O2	−0.5 (4)	C38—C43—C44—O11	3.5 (3)
C8—N3—C9—C10	178.9 (2)	C39—C38—C43—C42	−1.2 (3)
C9—N3—C8—C7	−160.6 (2)	C39—C38—C43—C44	−179.6 (2)
C9—C10—C11—C12	178.3 (2)	C39—C40—C41—C42	−1.7 (4)
C9—C10—C14—C13	−177.6 (2)	C40—C41—C42—C43	0.3 (4)
C10—C11—C12—N4	−0.9 (5)	C41—C42—C43—C38	1.2 (4)
C11—C10—C14—C13	0.4 (4)	C41—C42—C43—C44	179.7 (2)
C12—N4—C13—C14	−0.6 (4)	C42—C43—C44—O10	4.8 (3)
C13—N4—C12—C11	1.1 (4)	C42—C43—C44—O11	−174.9 (2)
C14—C10—C11—C12	0.1 (4)	C43—C38—C39—C40	−0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8···N4^{i}	0.84	1.78	2.609 (3)	171

O11—H11···N8^{ii}	0.84	1.82	2.660 (3)	176
O13—H13*A*···O2*W*	0.88	1.90	2.706 (2)	150
O13—H13*B*···O12	0.88	1.94	2.733 (2)	149
O14—H14*B*···O6	0.88	1.87	2.668 (2)	149
N2—H2···O1*W*^{iii}	0.88	2.02	2.887 (3)	166
N3—H3···O3*W*^{ii}	0.88	2.02	2.874 (3)	164
N6—H6···O6*W*^{iv}	0.88	1.99	2.844 (3)	164
O1*W*—H1*WA*···O12^{v}	0.87	1.93	2.801 (2)	177
O1*W*—H1*WB*···O5	0.87	2.12	2.967 (2)	165
O2*W*—H2*WA*···O12^{v}	0.87	2.02	2.840 (2)	158
O2*W*—H2*WB*···O2^{iii}	0.87	1.90	2.757 (2)	169
O3*W*—H3*WA*···O5*W*^{iv}	0.87	1.98	2.849 (3)	173
O3*W*—H3*WB*···O3	0.87	1.91	2.777 (2)	175
O4*W*—H4*WA*···O4	0.87	1.96	2.800 (2)	161
O4*W*—H4*WB*···O14^{iv}	0.87	1.86	2.706 (2)	165
O5*W*—H5*WA*···O10	0.87	1.98	2.821 (3)	162
O5*W*—H5*WB*···O1^{vi}	0.87	1.92	2.776 (2)	169
O6*W*—H6*WA*···O6^{vii}	0.87	1.90	2.770 (2)	178
O6*W*—H6*WB*···O9	0.87	2.12	2.977 (2)	167

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