Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaqua[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato-κ^2O,O']nickel(II)]-μ-4,4′-oxydibenzoato-$\kappa^2O:O'$]

Jun Hong

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China
Correspondence e-mail: junhong000@hotmail.com

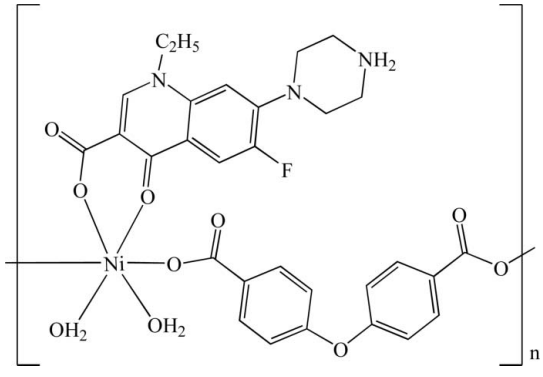
Received 6 November 2007; accepted 22 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.112; data-to-parameter ratio = 12.6.

In the title compound, $[Ni(C_{16}H_{18}FN_3O_3)(C_{14}H_8O_5)(H_2O)_2]_n$, the Ni^{II} atom exhibits a distorted octahedral geometry that is defined by four O atoms and two water molecules. Ni atoms are connected *via* the 4,4′-oxydibenzoate anions into a one-dimensional chain running along the crystallographic [$\bar{2}$30] direction. In the crystal structure, the one-dimensional chains are connected *via* N—H···O and O—H···O hydrogen bonding to form a three-dimensional supramolecular network.

Related literature

For general background, see: Xiao *et al.* (2005). For a related structure, see: An *et al.* (2005).



Experimental

Crystal data

$[Ni(C_{16}H_{18}FN_3O_3)(C_{14}H_8O_5)(H_2O)_2]$
M_r = 670.28
Triclinic, $P\bar{1}$
a = 10.105 (2) Å
b = 12.230 (2) Å
c = 13.052 (3) Å
α = 72.50 (3)°
β = 73.13 (3)°
γ = 77.57 (3)°
V = 1457.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 298 (2) K
0.32 × 0.24 × 0.22 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.798, T_{max} = 0.855
11571 measured reflections
5134 independent reflections
4210 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.02
5134 reflections
406 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H4···O2	0.85	1.93	2.695 (3)	149
O2W—H4···O1	0.85	2.55	2.965 (3)	111
N3—H3B···O2^{i}	0.90	1.82	2.714 (3)	170
N3—H3C···O8^{ii}	0.90	1.85	2.719 (3)	162
O1W—H1···O1^{iii}	0.85	2.03	2.761 (3)	144
O1W—H2···O4^{iv}	0.85	1.99	2.834 (3)	173
O2W—H3···O5^{v}	0.85	1.82	2.615 (3)	155

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The author thanks Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2047).

References

An, Z., Huang, J. & Qi, W. (2007). *Acta Cryst.* E**63**, m2009.
Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97 and SHELXL97*. University of Göttingen, Germany.
Xiao, D.-R., Wang, E.-B., An, H.-Y., Su, Z.-M., Li, Y.-G., Gao, L., Sun, C.-Y. & Xu, L. (2005). *Chem. Eur. J.* **11**, 6673–6686.

 doi:10.1107/S1600536807062216 © 2008 International Union of Crystallography

supplementary materials

Acta Cryst. (2008). E**64**, m17 [**doi:10.1107/S1600536807062216**]

catena-Poly[[diaqua[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato-κ^2O,O']nickel(II)]-μ-4,4'-oxydibenzoato-$\kappa^2O:O'$]

J. Hong

Comment

Norfloxacin [1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(piperazin-1-yl)quinoline-3-carboxylic acid, Hcf] is a member of a class of quinolones that is used to treat infections (Xiao *et al.* 2005; An *et al.* 2005), As a part of our ongoing investigations in this field we report here the crystal structure of the title compound. In the crystal structure of the title compound, the Ni atoms are coordinated by three oxygen atoms of two Hcf ligand and one 4,4'-oxy-bisbenzoate, one oxygen atom from one symmetry related 4,4'-oxy-bisbenzoate and two water molecules within a distorted octahedral geometry (Figure 1). The nickel atoms are linked by the 4,4'-oxy-bisbenzoate anions into a one-dimensional chain running along crystallographic [-1, 1.5, 0] direction. The adjacent chains are further extended into a two-dimensional supramolecular network by N—H···O and O—H···O hydrogen bonds(Tab. 1).

Experimental

Compound (I) was prepared by a hydrothermal method. A mixture of $Ni(NO_3)_2.6H_2O$ (0.15 g 0.5 mmol), norfloxacin (0.16 g 0.5 mmol), 4,4'-oxy-bisbenzoic acid (0.13 g 0.5 mmol) and water (10 ml) was stirred for 20 min and then transferred to a 23 ml Teflon reactor. The reactor was kept at 433 K for 72 h under autogenous pressure. Single crystals of (I) were obtained after cooling to room temperature.

Refinement

H atoms were placed in calculated positions with C—H = 0.93, 0.96 and 0.97 Å and N—H = 0.90 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C, N, O), H atoms of water molecule were located in difference maps and refined isotropically with O - H = 0.85 Å and U_{iso}(H) = 1.5 U_{eq}(O)

Figures

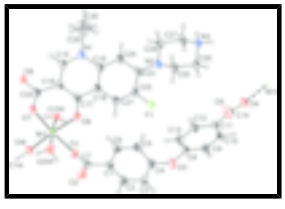


Fig. 1. Crystal structure of (I) with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: i = x + 1,y - 1,z

catena-Poly[[diaqua[1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4- dihydroquinoline-3-carboxylato-κ^2O,O']nickel(II)]-μ-4,4'-oxydibenzoato- $\kappa^2O:O'$]

Crystal data

$[Ni(C_{16}H_{18}F_1N_3O_3)(C_{14}H_8O_5)(H_2O)_2]$	$Z = 2$
$M_r = 670.28$	$F_{000} = 696$
Triclinic, $P\overline{1}$	$D_x = 1.527$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.105$ (2) Å	Cell parameters from 11571 reflections
$b = 12.230$ (2) Å	$\theta = 3.0$–25.0º
$c = 13.052$ (3) Å	$\mu = 0.74$ mm^{-1}
$\alpha = 72.50$ (3)º	$T = 298$ (2) K
$\beta = 73.13$ (3)º	Block, green
$\gamma = 77.57$ (3)º	0.32 × 0.24 × 0.22 mm
$V = 1457.7$ (5) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	5134 independent reflections
Radiation source: fine-focus sealed tube	4210 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 298$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.798$, $T_{max} = 0.855$	$k = -14 \rightarrow 14$
11571 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.5873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
5134 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
406 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Ni1	0.55118 (3)	0.06895 (3)	0.29346 (3)	0.02717 (12)
F1	0.11227 (19)	0.57062 (15)	0.2085 (2)	0.0690 (7)
C1	0.1138 (3)	0.1404 (2)	0.3988 (2)	0.0293 (6)
C2	−0.0181 (3)	0.1367 (3)	0.3899 (3)	0.0407 (7)
H2A	−0.0297	0.0864	0.3532	0.049*
C3	−0.1329 (3)	0.2070 (3)	0.4349 (3)	0.0409 (7)
H3A	−0.2216	0.2037	0.4295	0.049*
C4	−0.1139 (3)	0.2818 (2)	0.4879 (2)	0.0339 (6)
C5	0.0162 (3)	0.2876 (2)	0.4971 (3)	0.0390 (7)
H5A	0.0276	0.3396	0.5322	0.047*
C6	0.1296 (3)	0.2156 (2)	0.4539 (2)	0.0351 (6)
H6A	0.2175	0.2175	0.4618	0.042*
C7	0.2412 (3)	0.0689 (2)	0.3475 (2)	0.0296 (6)
C8	−0.2530 (3)	0.4649 (2)	0.4784 (2)	0.0314 (6)
C9	−0.3601 (3)	0.5352 (2)	0.5311 (2)	0.0362 (7)
H9AA	−0.4120	0.5051	0.6021	0.043*
C10	−0.3900 (3)	0.6506 (2)	0.4779 (3)	0.0376 (7)
H10A	−0.4615	0.6979	0.5139	0.045*
C11	−0.3143 (3)	0.6967 (2)	0.3712 (2)	0.0311 (6)
C12	−0.2076 (3)	0.6244 (2)	0.3210 (2)	0.0370 (7)
H12A	−0.1554	0.6541	0.2500	0.044*
C13	−0.1759 (3)	0.5093 (2)	0.3730 (3)	0.0401 (7)
H13A	−0.1035	0.4622	0.3375	0.048*
C14	−0.3468 (3)	0.8187 (2)	0.3084 (2)	0.0338 (6)
C15	0.7543 (3)	0.4092 (2)	0.1121 (3)	0.0388 (7)
H15A	0.8511	0.4014	0.0884	0.047*
C16	0.6950 (3)	0.3094 (2)	0.1539 (2)	0.0302 (6)
C17	0.5467 (3)	0.3187 (2)	0.1938 (2)	0.0285 (6)
C18	0.4717 (3)	0.4358 (2)	0.1767 (2)	0.0299 (6)
C19	0.5390 (3)	0.5341 (2)	0.1316 (2)	0.0317 (6)
C20	0.7920 (3)	0.1960 (2)	0.1557 (2)	0.0291 (6)
C21	0.3258 (3)	0.4520 (2)	0.2061 (3)	0.0380 (7)
H21A	0.2780	0.3882	0.2377	0.046*

C22	0.2540 (3)	0.5596 (2)	0.1887 (3)	0.0406 (7)
C23	0.3163 (3)	0.6614 (2)	0.1475 (2)	0.0317 (6)
C24	0.4612 (3)	0.6458 (2)	0.1191 (2)	0.0340 (6)
H24A	0.5080	0.7102	0.0914	0.041*
C25	0.1290 (3)	0.7917 (2)	0.2333 (2)	0.0378 (7)
H25A	0.1751	0.8083	0.2815	0.045*
H25B	0.0842	0.7233	0.2734	0.045*
C26	0.0199 (3)	0.8933 (2)	0.2016 (3)	0.0389 (7)
H26A	−0.0283	0.8761	0.1552	0.047*
H26B	−0.0483	0.9074	0.2676	0.047*
C27	0.1966 (3)	0.9750 (2)	0.0411 (2)	0.0391 (7)
H27A	0.2439	1.0425	0.0034	0.047*
H27B	0.1515	0.9616	−0.0095	0.047*
C28	0.3032 (3)	0.8699 (2)	0.0731 (2)	0.0363 (7)
H28A	0.3698	0.8545	0.0069	0.044*
H28B	0.3539	0.8856	0.1186	0.044*
C29	0.7665 (4)	0.6173 (3)	0.0620 (3)	0.0503 (9)
H29A	0.7179	0.6750	0.1024	0.060*
H29B	0.8569	0.5905	0.0795	0.060*
C30	0.7883 (5)	0.6721 (4)	−0.0552 (4)	0.0830 (14)
H30A	0.8412	0.7348	−0.0738	0.124*
H30B	0.6996	0.7015	−0.0733	0.124*
H30C	0.8385	0.6165	−0.0963	0.124*
N1	0.6856 (3)	0.51763 (19)	0.1020 (2)	0.0386 (6)
N2	0.2331 (2)	0.76972 (18)	0.13355 (19)	0.0316 (5)
N3	0.0891 (2)	0.99712 (18)	0.14108 (18)	0.0300 (5)
H3B	0.1298	1.0151	0.1856	0.036*
H3C	0.0252	1.0575	0.1207	0.036*
O1	0.34733 (19)	0.05291 (16)	0.38500 (15)	0.0317 (4)
O2	0.2384 (2)	0.0318 (2)	0.26830 (19)	0.0491 (6)
O3	−0.2308 (2)	0.35044 (16)	0.53603 (17)	0.0446 (5)
O4	−0.3916 (2)	0.89556 (15)	0.36257 (16)	0.0332 (4)
O5	−0.3263 (3)	0.83834 (18)	0.20552 (17)	0.0509 (6)
O6	0.4769 (2)	0.23599 (15)	0.23930 (18)	0.0385 (5)
O7	0.7459 (2)	0.10163 (15)	0.20642 (17)	0.0360 (5)
O8	0.9162 (2)	0.20092 (16)	0.10377 (18)	0.0407 (5)
O1W	0.5830 (2)	0.10404 (15)	0.43009 (15)	0.0325 (4)
H1	0.6392	0.0565	0.4655	0.049*
H2	0.5204	0.1036	0.4899	0.049*
O2W	0.5096 (2)	0.03404 (17)	0.16040 (15)	0.0380 (5)
H3	0.5639	−0.0287	0.1553	0.057*
H4	0.4342	0.0066	0.1966	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0245 (2)	0.01742 (18)	0.0365 (2)	0.00159 (13)	−0.00766 (14)	−0.00538 (14)
F1	0.0262 (10)	0.0311 (10)	0.138 (2)	0.0047 (8)	−0.0149 (11)	−0.0157 (12)

C1	0.0265 (14)	0.0263 (13)	0.0341 (14)	0.0016 (11)	−0.0103 (11)	−0.0071 (12)
C2	0.0313 (16)	0.0398 (17)	0.0594 (19)	0.0024 (13)	−0.0171 (14)	−0.0244 (15)
C3	0.0245 (15)	0.0416 (17)	0.0572 (19)	0.0005 (13)	−0.0128 (14)	−0.0143 (15)
C4	0.0314 (16)	0.0246 (13)	0.0334 (14)	0.0030 (11)	−0.0005 (12)	−0.0012 (12)
C5	0.0419 (18)	0.0313 (15)	0.0444 (16)	−0.0016 (13)	−0.0073 (14)	−0.0162 (13)
C6	0.0284 (15)	0.0361 (15)	0.0440 (16)	−0.0022 (12)	−0.0107 (13)	−0.0149 (13)
C7	0.0252 (14)	0.0247 (13)	0.0373 (14)	−0.0033 (11)	−0.0074 (12)	−0.0061 (12)
C8	0.0299 (15)	0.0236 (13)	0.0380 (15)	0.0003 (11)	−0.0072 (12)	−0.0080 (12)
C9	0.0347 (16)	0.0298 (14)	0.0351 (15)	−0.0009 (12)	0.0019 (12)	−0.0078 (12)
C10	0.0341 (16)	0.0254 (14)	0.0486 (17)	0.0035 (12)	−0.0003 (13)	−0.0172 (13)
C11	0.0313 (15)	0.0215 (13)	0.0414 (15)	−0.0003 (11)	−0.0100 (12)	−0.0104 (12)
C12	0.0378 (16)	0.0288 (14)	0.0343 (15)	0.0023 (12)	−0.0025 (13)	−0.0044 (12)
C13	0.0377 (17)	0.0283 (14)	0.0440 (17)	0.0081 (12)	−0.0015 (13)	−0.0112 (13)
C14	0.0296 (15)	0.0248 (13)	0.0421 (16)	0.0007 (11)	−0.0047 (12)	−0.0084 (13)
C15	0.0280 (15)	0.0281 (14)	0.0558 (18)	0.0033 (12)	−0.0069 (13)	−0.0125 (14)
C16	0.0296 (14)	0.0203 (13)	0.0385 (14)	0.0036 (11)	−0.0100 (12)	−0.0076 (11)
C17	0.0298 (15)	0.0220 (13)	0.0315 (13)	0.0013 (11)	−0.0093 (11)	−0.0051 (11)
C18	0.0297 (15)	0.0196 (13)	0.0366 (14)	0.0027 (11)	−0.0086 (12)	−0.0056 (11)
C19	0.0293 (15)	0.0236 (13)	0.0378 (15)	0.0043 (11)	−0.0062 (12)	−0.0091 (12)
C20	0.0275 (15)	0.0218 (13)	0.0384 (14)	0.0050 (11)	−0.0124 (12)	−0.0098 (12)
C21	0.0292 (16)	0.0205 (13)	0.0578 (18)	0.0000 (11)	−0.0088 (14)	−0.0046 (13)
C22	0.0243 (15)	0.0273 (15)	0.065 (2)	0.0028 (12)	−0.0099 (14)	−0.0092 (14)
C23	0.0355 (16)	0.0207 (13)	0.0325 (14)	0.0049 (11)	−0.0063 (12)	−0.0058 (11)
C24	0.0320 (16)	0.0210 (13)	0.0423 (15)	0.0006 (11)	−0.0040 (12)	−0.0062 (12)
C25	0.0360 (16)	0.0260 (14)	0.0393 (15)	0.0028 (12)	−0.0004 (13)	−0.0042 (13)
C26	0.0301 (16)	0.0286 (15)	0.0543 (18)	0.0039 (12)	−0.0087 (14)	−0.0123 (14)
C27	0.0502 (19)	0.0229 (14)	0.0338 (15)	0.0068 (13)	−0.0050 (13)	−0.0053 (12)
C28	0.0371 (16)	0.0234 (14)	0.0365 (15)	0.0039 (12)	0.0016 (13)	−0.0064 (12)
C29	0.0393 (18)	0.0307 (16)	0.074 (2)	−0.0037 (13)	−0.0025 (17)	−0.0153 (16)
C30	0.088 (3)	0.074 (3)	0.079 (3)	−0.038 (3)	−0.003 (3)	−0.006 (2)
N1	0.0310 (13)	0.0212 (11)	0.0551 (15)	0.0002 (10)	−0.0009 (11)	−0.0092 (11)
N2	0.0316 (13)	0.0190 (11)	0.0361 (12)	0.0060 (9)	−0.0057 (10)	−0.0046 (10)
N3	0.0279 (12)	0.0234 (11)	0.0384 (12)	0.0072 (9)	−0.0133 (10)	−0.0096 (10)
O1	0.0242 (10)	0.0338 (10)	0.0353 (10)	0.0003 (8)	−0.0091 (8)	−0.0073 (8)
O2	0.0320 (11)	0.0685 (15)	0.0625 (14)	0.0049 (11)	−0.0154 (10)	−0.0441 (13)
O3	0.0400 (12)	0.0256 (10)	0.0474 (12)	0.0098 (9)	0.0040 (10)	−0.0032 (9)
O4	0.0358 (11)	0.0200 (9)	0.0412 (10)	0.0031 (8)	−0.0084 (9)	−0.0097 (8)
O5	0.0719 (16)	0.0305 (11)	0.0384 (12)	0.0122 (11)	−0.0074 (11)	−0.0107 (10)
O6	0.0259 (10)	0.0200 (9)	0.0609 (13)	0.0017 (8)	−0.0084 (9)	−0.0030 (9)
O7	0.0287 (10)	0.0183 (9)	0.0529 (12)	0.0031 (8)	−0.0060 (9)	−0.0054 (9)
O8	0.0239 (11)	0.0249 (10)	0.0624 (13)	0.0040 (8)	−0.0038 (10)	−0.0069 (10)
O1W	0.0312 (10)	0.0279 (10)	0.0402 (10)	−0.0021 (8)	−0.0123 (9)	−0.0095 (9)
O2W	0.0382 (12)	0.0347 (11)	0.0350 (10)	−0.0016 (9)	−0.0046 (9)	−0.0067 (9)

Geometric parameters (Å, °)

Ni1—O6	2.0039 (19)	C17—C18	1.455 (3)
Ni1—O7	2.022 (2)	C18—C19	1.396 (4)
Ni1—O4^{i}	2.0663 (19)	C18—C21	1.397 (4)

Ni1—O1	2.077 (2)	C19—N1	1.404 (4)
Ni1—O1W	2.0786 (19)	C19—C24	1.410 (4)
Ni1—O2W	2.079 (2)	C20—O8	1.246 (3)
F1—C22	1.363 (3)	C20—O7	1.257 (3)
C1—C2	1.382 (4)	C21—C22	1.347 (4)
C1—C6	1.384 (4)	C21—H21A	0.9300
C1—C7	1.496 (4)	C22—C23	1.406 (4)
C2—C3	1.381 (4)	C23—C24	1.387 (4)
C2—H2A	0.9300	C23—N2	1.400 (3)
C3—C4	1.372 (4)	C24—H24A	0.9300
C3—H3A	0.9300	C25—N2	1.473 (3)
C4—C5	1.373 (4)	C25—C26	1.516 (4)
C4—O3	1.398 (3)	C25—H25A	0.9700
C5—C6	1.377 (4)	C25—H25B	0.9700
C5—H5A	0.9300	C26—N3	1.477 (4)
C6—H6A	0.9300	C26—H26A	0.9700
C7—O2	1.257 (3)	C26—H26B	0.9700
C7—O1	1.259 (3)	C27—N3	1.490 (3)
C8—O3	1.381 (3)	C27—C28	1.526 (4)
C8—C13	1.381 (4)	C27—H27A	0.9700
C8—C9	1.381 (4)	C27—H27B	0.9700
C9—C10	1.382 (4)	C28—N2	1.447 (4)
C9—H9AA	0.9300	C28—H28A	0.9700
C10—C11	1.393 (4)	C28—H28B	0.9700
C10—H10A	0.9300	C29—C30	1.446 (6)
C11—C12	1.379 (4)	C29—N1	1.492 (4)
C11—C14	1.488 (4)	C29—H29A	0.9700
C12—C13	1.379 (4)	C29—H29B	0.9700
C12—H12A	0.9300	C30—H30A	0.9600
C13—H13A	0.9300	C30—H30B	0.9600
C14—O5	1.253 (4)	C30—H30C	0.9600
C14—O4	1.273 (3)	N3—H3B	0.9000
C15—N1	1.345 (4)	N3—H3C	0.9000
C15—C16	1.368 (4)	O4—Ni1^{ii}	2.0663 (19)
C15—H15A	0.9300	O1W—H1	0.8500
C16—C17	1.428 (4)	O1W—H2	0.8501
C16—C20	1.515 (3)	O2W—H3	0.8500
C17—O6	1.255 (3)	O2W—H4	0.8499
O6—Ni1—O7	89.94 (8)	O8—C20—C16	117.4 (2)
O6—Ni1—O4^{i}	173.89 (8)	O7—C20—C16	120.1 (2)
O7—Ni1—O4^{i}	95.85 (8)	C22—C21—C18	120.3 (3)
O6—Ni1—O1	84.98 (8)	C22—C21—H21A	119.9
O7—Ni1—O1	173.98 (7)	C18—C21—H21A	119.9
O4^{i}—Ni1—O1	89.13 (8)	C21—C22—F1	118.1 (3)
O6—Ni1—O1W	90.05 (8)	C21—C22—C23	124.1 (3)
O7—Ni1—O1W	90.44 (8)	F1—C22—C23	117.8 (2)
O4^{i}—Ni1—O1W	87.94 (8)	C24—C23—N2	124.1 (3)
O1—Ni1—O1W	86.35 (8)	C24—C23—C22	115.7 (2)

O6—Ni1—O2W	89.40 (9)	N2—C23—C22	120.1 (3)
O7—Ni1—O2W	92.15 (9)	C23—C24—C19	121.3 (3)
$O4^{i}$—Ni1—O2W	92.34 (8)	C23—C24—H24A	119.3
O1—Ni1—O2W	91.02 (8)	C19—C24—H24A	119.3
O1W—Ni1—O2W	177.35 (7)	N2—C25—C26	110.2 (2)
C2—C1—C6	119.0 (2)	N2—C25—H25A	109.6
C2—C1—C7	122.3 (2)	C26—C25—H25A	109.6
C6—C1—C7	118.6 (2)	N2—C25—H25B	109.6
C3—C2—C1	120.8 (3)	C26—C25—H25B	109.6
C3—C2—H2A	119.6	H25A—C25—H25B	108.1
C1—C2—H2A	119.6	N3—C26—C25	109.2 (2)
C2—C3—C4	118.9 (3)	N3—C26—H26A	109.8
C2—C3—H3A	120.5	C25—C26—H26A	109.8
C4—C3—H3A	120.5	N3—C26—H26B	109.8
C5—C4—C3	121.3 (3)	C25—C26—H26B	109.8
C5—C4—O3	119.9 (3)	H26A—C26—H26B	108.3
C3—C4—O3	118.8 (3)	N3—C27—C28	110.7 (2)
C4—C5—C6	119.3 (3)	N3—C27—H27A	109.5
C4—C5—H5A	120.3	C28—C27—H27A	109.5
C6—C5—H5A	120.3	N3—C27—H27B	109.5
C5—C6—C1	120.6 (3)	C28—C27—H27B	109.5
C5—C6—H6A	119.7	H27A—C27—H27B	108.1
C1—C6—H6A	119.7	N2—C28—C27	110.0 (2)
O2—C7—O1	123.9 (2)	N2—C28—H28A	109.7
O2—C7—C1	119.1 (2)	C27—C28—H28A	109.7
O1—C7—C1	116.9 (2)	N2—C28—H28B	109.7
O3—C8—C13	123.3 (2)	C27—C28—H28B	109.7
O3—C8—C9	116.5 (2)	H28A—C28—H28B	108.2
C13—C8—C9	120.3 (3)	C30—C29—N1	114.9 (3)
C8—C9—C10	119.8 (3)	C30—C29—H29A	108.5
C8—C9—H9AA	120.1	N1—C29—H29A	108.5
C10—C9—H9AA	120.1	C30—C29—H29B	108.5
C9—C10—C11	120.8 (2)	N1—C29—H29B	108.5
C9—C10—H10A	119.6	H29A—C29—H29B	107.5
C11—C10—H10A	119.6	C29—C30—H30A	109.5
C12—C11—C10	118.0 (3)	C29—C30—H30B	109.5
C12—C11—C14	119.1 (3)	H30A—C30—H30B	109.5
C10—C11—C14	122.9 (2)	C29—C30—H30C	109.5
C13—C12—C11	122.0 (3)	H30A—C30—H30C	109.5
C13—C12—H12A	119.0	H30B—C30—H30C	109.5
C11—C12—H12A	119.0	C15—N1—C19	119.0 (2)
C12—C13—C8	119.2 (3)	C15—N1—C29	119.4 (3)
C12—C13—H13A	120.4	C19—N1—C29	121.5 (2)
C8—C13—H13A	120.4	C23—N2—C28	117.2 (2)
O5—C14—O4	124.8 (3)	C23—N2—C25	115.8 (2)
O5—C14—C11	117.4 (2)	C28—N2—C25	110.8 (2)
O4—C14—C11	117.9 (2)	C26—N3—C27	110.1 (2)
N1—C15—C16	126.1 (3)	C26—N3—H3B	109.6
N1—C15—H15A	116.9	C27—N3—H3B	109.6

C16—C15—H15A	116.9	C26—N3—H3C	109.6
C15—C16—C17	118.2 (2)	C27—N3—H3C	109.6
C15—C16—C20	117.5 (2)	H3B—N3—H3C	108.2
C17—C16—C20	124.4 (2)	C7—O1—Ni1	126.74 (17)
O6—C17—C16	126.2 (2)	C8—O3—C4	116.6 (2)
O6—C17—C18	118.1 (2)	C14—O4—Ni1^{ii}	124.49 (18)
C16—C17—C18	115.7 (2)	C17—O6—Ni1	126.84 (18)
C19—C18—C21	117.9 (2)	C20—O7—Ni1	130.58 (17)
C19—C18—C17	122.9 (2)	Ni1—O1W—H1	118.9
C21—C18—C17	119.2 (2)	Ni1—O1W—H2	123.4
C18—C19—N1	117.8 (2)	H1—O1W—H2	90.7
C18—C19—C24	120.6 (3)	Ni1—O2W—H3	102.1
N1—C19—C24	121.6 (3)	Ni1—O2W—H4	96.0
O8—C20—O7	122.5 (2)	H3—O2W—H4	99.5

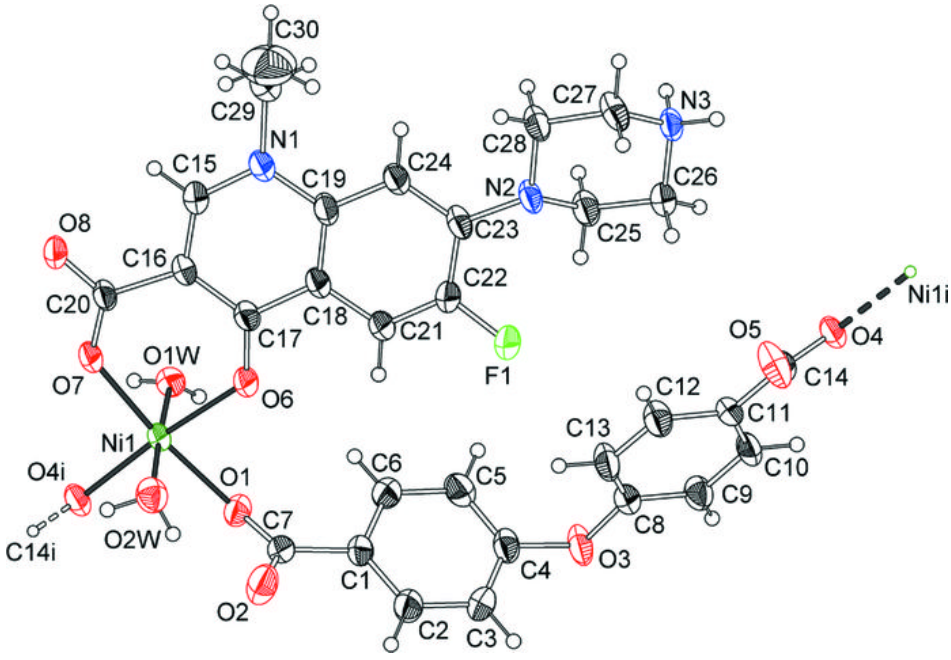
Symmetry codes: (i) *x*+1, *y*−1, *z*; (ii) *x*−1, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2W—H4···O2	0.85	1.93	2.695 (3)	149
O2W—H4···O1	0.85	2.55	2.965 (3)	111
N3—H3B···O2^{iii}	0.90	1.82	2.714 (3)	170
N3—H3C···O8^{ii}	0.90	1.85	2.719 (3)	162
O1W—H1···O1^{iv}	0.85	2.03	2.761 (3)	144
O1W—H2···O4^{v}	0.85	1.99	2.834 (3)	173
O2W—H3···O5^{i}	0.85	1.82	2.615 (3)	155

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

Fig. 1


C30
C29
N1
C15
C19
C24
C27
N3
C28
N2
C26
C23
C25
O8
C16
C22
Ni1i
C20
C18
C21
O5
O4
O1W
C17
F1
C12
C14
O7
O6
C13
C11
Ni1
C10
C6
C5
O4i
O1
C9
C7
C8
C14i
O2W
O3
C1
C4
O2
C2
C3