Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[bis[μ-1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato]nickel(II)] dihydrate]

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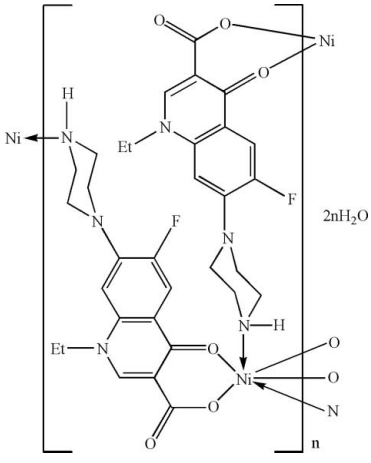
Received 10 November 2007; accepted 19 November 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; H-atom completeness 90%; disorder in solvent or counterion; R factor = 0.035; wR factor = 0.108; data-to-parameter ratio = 13.1.

In the title compound, $\{[Ni(C_{16}H_{17}FN_3O_3)_2]\cdot 2H_2O\}_n$, the Ni^{II} atom (site symmetry $\bar{1}$) exists in a distorted *trans*-NiN_2O_4 octahedral geometry defined by two monodentate *N*-bonded and two bidentate *O*,*O*-bonded 1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate (norf) monoanions. The extended two-dimensional structure is a square grid. N—H···O hydrogen bonds are present in the crystal structure. The water O atom is disordered over two positions; the site occupancy factors are *ca.* 0.77 and 0.23.

Related literature

For the cadmium and zinc complexes of the norf anion, see: Chen *et al.* (2001); Wang *et al.*(2004). For background on the medicinal uses of Norfloxacin, see: Mizuki *et al.* (1996).



Experimental

Crystal data

$[Ni(C_{16}H_{17}FN_3O_3)_2]\cdot 2H_2O$
M_r = 727.36
Monoclinic, $P2_1/c$
a = 5.8389 (2) Å
b = 21.5704 (8) Å
c = 13.2408 (4) Å
β = 100.763 (1)°
V = 1638.31 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 295 (2) K
0.32 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.816, T_{max} = 0.890
8473 measured reflections
3037 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.108
S = 0.97
3037 reflections
232 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.0415 (15)	Ni1—N3^{i}	2.1908 (16)
Ni1—O3	2.0552 (13)		

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*N*···O2^{ii}	0.852 (10)	2.425 (17)	3.159 (2)	145 (2)

Symmetry code: (ii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Innovation Science Foundation of Harbin Medical University (grant No. 060041).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2657).

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supplementary materials

Acta Cryst. (2007). E**63**, m3157 [**doi:10.1107/S1600536807060813**]

Poly[[bis[μ-1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato]nickel(II)] dihydrate]

W. Xu and Z. An

Comment

Norfloxacin (Hnorf, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl) −3-quinoline carboxylic acid) is member of the class of quinolones that is used to treat infections (Mizuki *et al.*, 1996). Cadmium(II) and zinc(II) derivatives of norf have been reported (Chen *et al.*, 2001; Wang *et al.*, 2004). The title nickel(II) derivative, (I), a two-dimensional coordination polymer in which the anion acts in a bridging mode, is reported here (Fig. 1).

The Ni(II) atom in (I) is coordinated by four oxygen atoms and two N atoms from four norfloxacin ligands (two mono-dentate-N and two O,*O*-bidentate) to form a square grid propagating in (100) (Fig. 2). The disordered, uncoordinated, water molecules occupy the cavities.

Experimental

A mixture of $Ni(NO_3)_2{\cdot}6H_2O$ (0.07 g, 0.25 mmol), Hnorf (0.16 g, 0.5 mmol), and water (12 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon-lined hydrothermal bomb. The bomb was kept at 433 K for 72 h under autogenous pressure. After cooling, green prisms of (I) were obtained from the reaction mixture.

Refinement

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U(H) = 1.2Ueq(C). The H on Nitrogen atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = 0.86 (1) /%A and with U_{iso}(H) = 1.2Ueq(N).

The water molecules is disordered over two sites in a 0.771 (7):0.229 (7) ratio. The water H atoms could not be located in the present study.

Figures

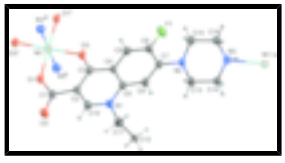

Fig. 1. The asymmetric unit of (I), extended to show the Ni coordination, showing 50% displacement ellipsoids for the non-hydrogen atoms. Symmetry codes: (i) *x*, *y*, *z*; (ii) −*x*, *y* + 1/2, −*z* + 1/2; (iii) −*x*, −*y*, −*z*; (iv) *x*, −*y* − 1/2, *z* − 1/2.

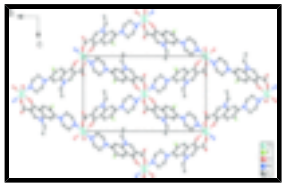

Fig. 2. A view of part of a two-dimensional polymeric sheet in (I) showing the square-grid connectivity (H atoms and water molecule O atoms omitted for clarity).

Poly[[bis[μ-1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline- 3-carboxylato]nickel(II)] dihydrate]

Crystal data

$[Ni(C_{16}H_{17}FN_3O_3)_2]\cdot 2H_2O$	$F_{000} = 756$
$M_r = 727.36$	$D_x = 1.474$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 8072 reflections
$a = 5.8389$ (2) Å	$\theta = 1.8$–25.5º
$b = 21.5704$ (8) Å	$\mu = 0.66$ mm^{-1}
$c = 13.2408$ (4) Å	$T = 295$ (2) K
$\beta = 100.763$ (1)º	Prism, green
$V = 1638.31$ (10) Å^3	0.32 × 0.26 × 0.18 mm
$Z = 2$	

Data collection

Bruker SMART CCD diffractometer	3037 independent reflections
Radiation source: fine-focus sealed tube	2766 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 295$(2) K	$\theta_{max} = 25.5$º
ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6\rightarrow 7$
$T_{min} = 0.816$, $T_{max} = 0.890$	$k = -26\rightarrow 20$
8473 measured reflections	$l = -16\rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 1.1691P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} < 0.001$
3037 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
232 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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.

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# 8. REFINEMENT DATA

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1W	−0.212 (3)	0.5083 (3)	0.9619 (4)	0.269 (7)	0.771 (7)
O2W	−0.530 (7)	0.4676 (10)	0.9199 (13)	0.269 (7)	0.229 (7)
Ni1	0.0000	0.5000	0.5000	0.02183 (14)	
F1	0.6987 (2)	0.25278 (6)	0.66313 (11)	0.0456 (4)	
O1	−0.2244 (3)	0.50862 (6)	0.60039 (12)	0.0278 (3)	
O2	−0.3489 (4)	0.50317 (7)	0.74766 (15)	0.0507 (5)	
O3	0.1702 (2)	0.43116 (6)	0.59199 (10)	0.0270 (3)	
N1	−0.0082 (3)	0.34446 (8)	0.84271 (12)	0.0288 (4)	
N2	0.5781 (3)	0.18573 (8)	0.82650 (13)	0.0282 (4)	
N3	0.7581 (3)	0.06548 (7)	0.90923 (13)	0.0260 (4)	
H3N	0.633 (3)	0.0444 (11)	0.893 (2)	0.046 (7)*	
C1	−0.2232 (4)	0.48474 (9)	0.68784 (16)	0.0276 (4)	
C2	−0.0695 (3)	0.42936 (8)	0.72119 (14)	0.0259 (4)	
C3	0.1112 (3)	0.40744 (8)	0.67023 (14)	0.0236 (4)	
C4	0.2286 (3)	0.35113 (8)	0.71319 (14)	0.0244 (4)	
C5	0.4086 (3)	0.32589 (9)	0.66939 (15)	0.0279 (4)	
H5	0.4551	0.3462	0.6146	0.034*	
C6	0.5158 (3)	0.27262 (9)	0.70514 (16)	0.0281 (4)	
C7	0.4534 (3)	0.23790 (9)	0.78697 (15)	0.0260 (4)	
C8	0.2748 (3)	0.26310 (9)	0.83045 (15)	0.0285 (4)	
H8	0.2258	0.2419	0.8838	0.034*	
C9	0.1661 (3)	0.31940 (9)	0.79669 (15)	0.0257 (4)	
C10	−0.1149 (3)	0.39704 (9)	0.80463 (15)	0.0285 (4)	
H10	−0.2294	0.4129	0.8377	0.034*	
C11	−0.0729 (4)	0.31627 (11)	0.93573 (17)	0.0370 (5)	
H11A	−0.0875	0.2718	0.9260	0.044*	
H11B	−0.2239	0.3321	0.9438	0.044*	
C12	0.1007 (6)	0.32911 (15)	1.0321 (2)	0.0613 (8)	
H12A	0.2522	0.3153	1.0236	0.092*	
H12B	0.0557	0.3074	1.0886	0.092*	
H12C	0.1054	0.3728	1.0459	0.092*	
C13	0.5224 (5)	0.16096 (11)	0.92160 (18)	0.0445 (6)	

H13A	0.3755	0.1387	0.9065	0.053*
H13B	0.5053	0.1948	0.9678	0.053*
C14	0.7127 (5)	0.11770 (11)	0.97288 (17)	0.0428 (6)
H14A	0.8555	0.1413	0.9925	0.051*
H14B	0.6702	0.1017	1.0353	0.051*
C15	0.6156 (4)	0.13449 (10)	0.75747 (16)	0.0351 (5)
H15A	0.6624	0.1512	0.6964	0.042*
H15B	0.4710	0.1119	0.7362	0.042*
C16	0.8036 (4)	0.09047 (10)	0.81179 (16)	0.0353 (5)
H16A	0.8185	0.0562	0.7661	0.042*
H16B	0.9515	0.1123	0.8250	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1W	0.64 (2)	0.116 (4)	0.061 (3)	0.061 (7)	0.082 (6)	−0.012 (3)
O2W	0.64 (2)	0.116 (4)	0.061 (3)	0.061 (7)	0.082 (6)	−0.012 (3)
Ni1	0.0265 (2)	0.0140 (2)	0.0229 (2)	−0.00066 (11)	−0.00080 (14)	0.00301 (11)
F1	0.0492 (8)	0.0390 (7)	0.0566 (8)	0.0183 (6)	0.0304 (7)	0.0168 (6)
O1	0.0312 (8)	0.0212 (7)	0.0292 (8)	0.0046 (5)	0.0007 (6)	0.0038 (5)
O2	0.0658 (13)	0.0475 (11)	0.0436 (11)	0.0328 (8)	0.0230 (9)	0.0142 (7)
O3	0.0312 (7)	0.0203 (7)	0.0287 (7)	0.0025 (5)	0.0036 (5)	0.0078 (5)
N1	0.0328 (9)	0.0266 (9)	0.0280 (8)	0.0069 (7)	0.0085 (7)	0.0076 (7)
N2	0.0378 (9)	0.0207 (8)	0.0262 (8)	0.0095 (7)	0.0062 (7)	0.0048 (6)
N3	0.0290 (9)	0.0182 (8)	0.0291 (8)	0.0020 (6)	0.0009 (7)	0.0012 (6)
C1	0.0309 (10)	0.0218 (9)	0.0288 (10)	0.0043 (8)	0.0022 (8)	0.0000 (8)
C2	0.0293 (9)	0.0198 (9)	0.0264 (9)	0.0036 (7)	−0.0005 (7)	0.0014 (7)
C3	0.0266 (9)	0.0190 (9)	0.0226 (9)	−0.0014 (7)	−0.0016 (7)	0.0001 (7)
C4	0.0274 (9)	0.0200 (9)	0.0246 (9)	0.0020 (7)	0.0015 (7)	0.0029 (7)
C5	0.0331 (10)	0.0245 (10)	0.0269 (10)	0.0014 (8)	0.0075 (8)	0.0063 (8)
C6	0.0293 (10)	0.0253 (10)	0.0308 (10)	0.0056 (8)	0.0086 (8)	0.0034 (8)
C7	0.0303 (10)	0.0207 (9)	0.0254 (10)	0.0017 (7)	0.0011 (8)	0.0028 (7)
C8	0.0342 (10)	0.0247 (10)	0.0272 (10)	0.0048 (8)	0.0074 (8)	0.0082 (8)
C9	0.0288 (10)	0.0226 (9)	0.0249 (9)	0.0028 (7)	0.0030 (7)	0.0035 (7)
C10	0.0313 (10)	0.0252 (10)	0.0288 (10)	0.0064 (8)	0.0048 (8)	0.0013 (8)
C11	0.0414 (12)	0.0368 (12)	0.0365 (12)	0.0077 (9)	0.0171 (9)	0.0132 (9)
C12	0.076 (2)	0.071 (2)	0.0359 (13)	0.0055 (16)	0.0105 (13)	0.0087 (13)
C13	0.0620 (15)	0.0395 (13)	0.0373 (12)	0.0287 (11)	0.0227 (11)	0.0183 (10)
C14	0.0663 (15)	0.0355 (12)	0.0274 (11)	0.0278 (11)	0.0113 (10)	0.0083 (9)
C15	0.0493 (13)	0.0261 (10)	0.0279 (10)	0.0076 (9)	0.0026 (9)	0.0011 (8)
C16	0.0465 (12)	0.0287 (11)	0.0312 (11)	0.0124 (9)	0.0089 (9)	0.0022 (9)

Geometric parameters (Å, °)

Ni1—O1^{i}	2.0415 (15)	C4—C9	1.405 (3)
Ni1—O1	2.0415 (15)	C5—C6	1.351 (3)
Ni1—O3	2.0552 (13)	C5—H5	0.9300
Ni1—O3^{i}	2.0552 (13)	C6—C7	1.419 (3)

Ni1—N3^{ii}	2.1908 (16)	C7—C8	1.392 (3)
Ni1—N3^{iii}	2.1908 (16)	C8—C9	1.404 (3)
F1—C6	1.362 (2)	C8—H8	0.9300
O1—C1	1.266 (3)	C10—H10	0.9300
O2—C1	1.241 (3)	C11—C12	1.500 (4)
O3—C3	1.260 (2)	C11—H11A	0.9700
N1—C10	1.346 (2)	C11—H11B	0.9700
N1—C9	1.389 (2)	C12—H12A	0.9600
N1—C11	1.484 (2)	C12—H12B	0.9600
N2—C7	1.389 (2)	C12—H12C	0.9600
N2—C13	1.460 (3)	C13—C14	1.512 (3)
N2—C15	1.476 (3)	C13—H13A	0.9700
N3—C14	1.461 (3)	C13—H13B	0.9700
N3—C16	1.468 (3)	C14—H14A	0.9700
N3—Ni1^{iv}	2.1908 (16)	C14—H14B	0.9700
N3—H3N	0.852 (10)	C15—C16	1.526 (3)
C1—C2	1.510 (3)	C15—H15A	0.9700
C2—C10	1.373 (3)	C15—H15B	0.9700
C2—C3	1.435 (3)	C16—H16A	0.9700
C3—C4	1.457 (3)	C16—H16B	0.9700
C4—C5	1.401 (3)		
O1^{i}—Ni1—O1	180.0	N2—C7—C6	121.60 (18)
O1^{i}—Ni1—O3	91.26 (5)	C8—C7—C6	115.36 (18)
O1—Ni1—O3	88.74 (5)	C7—C8—C9	122.36 (18)
O1^{i}—Ni1—O3^{i}	88.74 (5)	C7—C8—H8	118.8
O1—Ni1—O3^{i}	91.26 (5)	C9—C8—H8	118.8
O3—Ni1—O3^{i}	180.0	N1—C9—C8	121.44 (17)
O1^{i}—Ni1—N3^{ii}	90.60 (6)	N1—C9—C4	118.35 (17)
O1—Ni1—N3^{ii}	89.40 (6)	C8—C9—C4	120.20 (18)
O3—Ni1—N3^{ii}	92.88 (6)	N1—C10—C2	125.71 (18)
O3^{i}—Ni1—N3^{ii}	87.12 (6)	N1—C10—H10	117.1
O1^{i}—Ni1—N3^{iii}	89.40 (6)	C2—C10—H10	117.1
O1—Ni1—N3^{iii}	90.60 (6)	N1—C11—C12	113.2 (2)
O3—Ni1—N3^{iii}	87.12 (6)	N1—C11—H11A	108.9
O3^{i}—Ni1—N3^{iii}	92.88 (6)	C12—C11—H11A	108.9
N3^{ii}—Ni1—N3^{iii}	180.0	N1—C11—H11B	108.9
C1—O1—Ni1	131.60 (13)	C12—C11—H11B	108.9
C3—O3—Ni1	127.19 (12)	H11A—C11—H11B	107.8
C10—N1—C9	119.29 (16)	C11—C12—H12A	109.5
C10—N1—C11	118.96 (16)	C11—C12—H12B	109.5
C9—N1—C11	121.70 (16)	H12A—C12—H12B	109.5
C7—N2—C13	115.85 (16)	C11—C12—H12C	109.5
C7—N2—C15	120.08 (16)	H12A—C12—H12C	109.5
C13—N2—C15	110.05 (17)	H12B—C12—H12C	109.5
C14—N3—C16	107.83 (16)	N2—C13—C14	110.48 (18)

C14—N3—Ni1^{iv}	110.40 (12)	N2—C13—H13A	109.6
C16—N3—Ni1^{iv}	121.00 (13)	C14—C13—H13A	109.6
C14—N3—H3N	108.2 (18)	N2—C13—H13B	109.6
C16—N3—H3N	105.5 (18)	C14—C13—H13B	109.6
Ni1^{iv}—N3—H3N	103.1 (18)	H13A—C13—H13B	108.1
O2—C1—O1	123.41 (18)	N3—C14—C13	114.48 (19)
O2—C1—C2	117.17 (18)	N3—C14—H14A	108.6
O1—C1—C2	119.38 (18)	C13—C14—H14A	108.6
C10—C2—C3	118.71 (17)	N3—C14—H14B	108.6
C10—C2—C1	116.33 (17)	C13—C14—H14B	108.6
C3—C2—C1	124.92 (17)	H14A—C14—H14B	107.6
O3—C3—C2	126.23 (17)	N2—C15—C16	110.53 (16)
O3—C3—C4	118.58 (17)	N2—C15—H15A	109.5
C2—C3—C4	115.15 (16)	C16—C15—H15A	109.5
C5—C4—C9	117.48 (17)	N2—C15—H15B	109.5
C5—C4—C3	119.79 (17)	C16—C15—H15B	109.5
C9—C4—C3	122.71 (17)	H15A—C15—H15B	108.1
C6—C5—C4	121.30 (18)	N3—C16—C15	114.23 (17)
C6—C5—H5	119.4	N3—C16—H16A	108.7
C4—C5—H5	119.4	C15—C16—H16A	108.7
C5—C6—F1	118.13 (17)	N3—C16—H16B	108.7
C5—C6—C7	123.23 (19)	C15—C16—H16B	108.7
F1—C6—C7	118.58 (17)	H16A—C16—H16B	107.6
N2—C7—C8	122.76 (18)		
O3—Ni1—O1—C1	7.83 (18)	F1—C6—C7—N2	1.9 (3)
N3^{ii}—Ni1—O1—C1	100.72 (18)	C5—C6—C7—C8	−1.2 (3)
N3^{iii}—Ni1—O1—C1	−79.28 (18)	F1—C6—C7—C8	176.00 (17)
O1^{i}—Ni1—O3—C3	−174.28 (15)	N2—C7—C8—C9	173.20 (18)
O1—Ni1—O3—C3	5.72 (15)	C6—C7—C8—C9	−0.8 (3)
N3^{ii}—Ni1—O3—C3	−83.62 (15)	C10—N1—C9—C8	−176.91 (19)
N3^{iii}—Ni1—O3—C3	96.38 (15)	C11—N1—C9—C8	5.8 (3)
Ni1—O1—C1—O2	166.39 (17)	C10—N1—C9—C4	1.7 (3)
Ni1—O1—C1—C2	−16.1 (3)	C11—N1—C9—C4	−175.62 (18)
O2—C1—C2—C10	12.3 (3)	C7—C8—C9—N1	−178.50 (19)
O1—C1—C2—C10	−165.38 (19)	C7—C8—C9—C4	2.9 (3)
O2—C1—C2—C3	−170.1 (2)	C5—C4—C9—N1	178.51 (17)
O1—C1—C2—C3	12.2 (3)	C3—C4—C9—N1	−2.9 (3)
Ni1—O3—C3—C2	−9.7 (3)	C5—C4—C9—C8	−2.9 (3)
Ni1—O3—C3—C4	168.14 (12)	C3—C4—C9—C8	175.70 (18)
C10—C2—C3—O3	178.57 (18)	C9—N1—C10—C2	0.8 (3)
C1—C2—C3—O3	1.0 (3)	C11—N1—C10—C2	178.1 (2)
C10—C2—C3—C4	0.7 (3)	C3—C2—C10—N1	−2.0 (3)
C1—C2—C3—C4	−176.88 (17)	C1—C2—C10—N1	175.80 (19)
O3—C3—C4—C5	2.2 (3)	C10—N1—C11—C12	−101.8 (2)
C2—C3—C4—C5	−179.76 (17)	C9—N1—C11—C12	75.5 (3)
O3—C3—C4—C9	−176.37 (17)	C7—N2—C13—C14	−163.1 (2)
C2—C3—C4—C9	1.7 (3)	C15—N2—C13—C14	56.5 (3)

C9—C4—C5—C6	0.9 (3)	C16—N3—C14—C13	53.9 (3)
C3—C4—C5—C6	−177.74 (19)	Ni1^{iv}—N3—C14—C13	−171.88 (17)
C4—C5—C6—F1	−176.03 (18)	N2—C13—C14—N3	−57.8 (3)
C4—C5—C6—C7	1.2 (3)	C7—N2—C15—C16	166.05 (18)
C13—N2—C7—C8	−4.2 (3)	C13—N2—C15—C16	−55.5 (2)
C15—N2—C7—C8	131.9 (2)	C14—N3—C16—C15	−52.7 (2)
C13—N2—C7—C6	169.5 (2)	Ni1^{iv}—N3—C16—C15	178.92 (14)
C15—N2—C7—C6	−54.4 (3)	N2—C15—C16—N3	55.4 (2)
C5—C6—C7—N2	−175.37 (18)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*−1, −*y*+1/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+3/2; (iv) −*x*+1, *y*−1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O2^{v}	0.852 (10)	2.425 (17)	3.159 (2)	145 (2)

Symmetry codes: (v) −*x*, *y*−1/2, −*z*+3/2.

Fig. 1

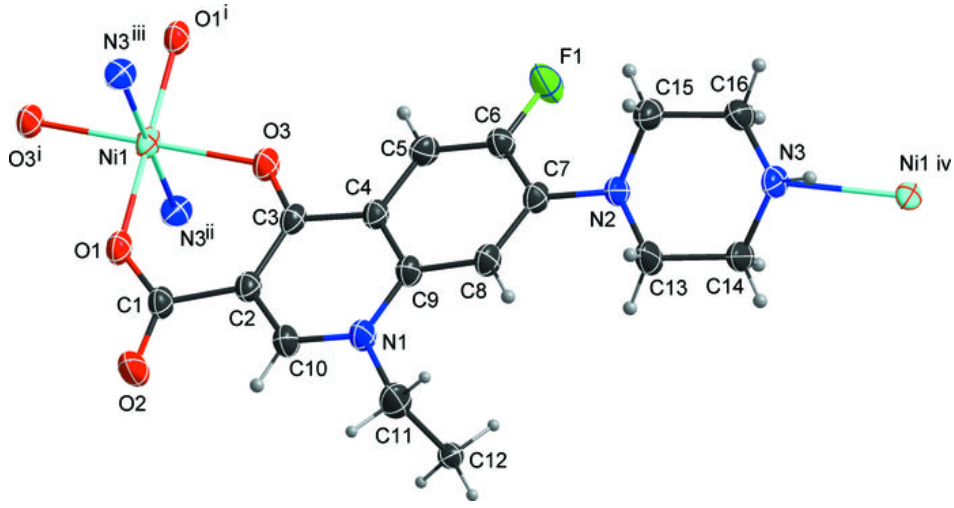
O1i
N3iii
F1
C15
C16
O3
C6
O3i
Ni1
C5
N3
Ni1 iv
C4
C7
C3
N2
N3ii
O1
C1
C2
C9
C8
C13
C14
N1
C10
O2
C11
C12

Fig. 2