Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[1-ethyl-6-fluoro-7-(4-methylpiperazin-4-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylato]cobalt(II) octahydrate

Zhe An,* Jing Huang and Wei Qi

School of Pharmaceutical Science, Harbin Medical University, Harbin 150086, People's Republic of China
Correspondence e-mail: anzhe6409@sina.com

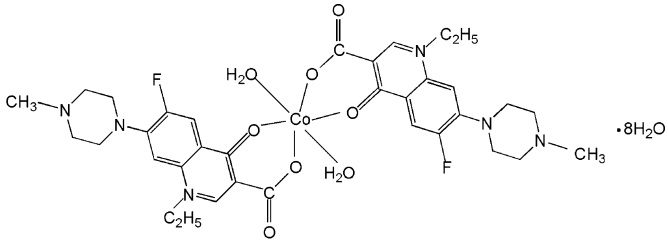
Received 22 June 2007; accepted 23 June 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.103; data-to-parameter ratio = 12.5.

In the title compound, $[Co(C_{17}H_{19}FN_3O_3)_2(H_2O)_2]\cdot 8H_2O$, the Co^{II} atom (site symmetry $\overline{1}$) exhibits a distorted octahedral geometry that is defined by two bidentate *O*,*O*-bonded 1-ethyl-6-fluoro-7-(4-methylpiperazin-4-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylate (pef) monoanions and two water molecules. A network of O—H···O and O—H···N hydrogen bonds help to establish the crystal packing.

Related literature

For a silver complex of the same ligand, see: Baenziger *et al.* (1986). For background on the medicinal uses of the free ligand, see Mizuki *et al.* (1996).



Experimental

Crystal data

$[Co(C_{17}H_{19}FN_3O_3)_2(H_2O)_2]\cdot 8H_2O$
M_r = 903.79
Triclinic, $P\overline{1}$
a = 8.889 (5) Å
b = 10.231 (5) Å
c = 12.911 (5) Å
α = 73.287 (5)°
β = 72.040 (5)°
γ = 85.603 (5)°
V = 1069.7 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 295 (2) K
0.34 × 0.26 × 0.17 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.853, T_{max} = 0.922
5428 measured reflections
3756 independent reflections
3380 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.103
S = 1.10
3756 reflections
300 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O3	2.0206 (15)	Co1—O5*W*	2.180 (2)
Co1—O1	2.0598 (16)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4*W*—H4*W*1···O1*W*	0.844 (10)	2.083 (12)	2.879 (3)	157 (2)
O3*W*—H3*W*1···O1*W*^{i}	0.848 (10)	2.035 (12)	2.859 (3)	164 (3)
O3*W*—H3*W*2···O2^{ii}	0.851 (10)	1.899 (10)	2.747 (2)	174 (3)
O1*W*—H1*W*1···O1^{iii}	0.846 (10)	1.911 (11)	2.754 (2)	175 (2)
O1*W*—H1*W*2···O3*W*^{iv}	0.849 (10)	2.129 (18)	2.877 (3)	147 (2)
O2*W*—H2*W*1···O3*W*	0.840 (9)	1.979 (11)	2.813 (3)	171 (3)
O2*W*—H2*W*2···O5*W*	0.840 (9)	2.066 (11)	2.904 (3)	175 (2)
O5*W*—H5*W*1···N3^{v}	0.862 (10)	2.029 (12)	2.870 (3)	165 (3)
O5*W*—H5*W*2···O4*W*^{vi}	0.856 (10)	2.064 (11)	2.918 (3)	175 (2)
O4*W*—H4*W*2···O2*W*^{vii}	0.835 (10)	1.980 (11)	2.787 (3)	162 (2)

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

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 thank the Innovation Science Foundation of Harbin Medical University for financial support (**grant No.** 060041).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2455).

References

Baenziger, N. C., Fox, C. L. & Modak, S. L. (1986). *Acta Cryst.* C**42**, 1505–1509.
Bruker (1998). *SMART*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Mizuki, Y., Fujiwara, I. & Yamaguchi, T. (1996). *J. Antimicrob. Chemother.* **37**, Suppl. A, 41–45.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m2009 [**doi:10.1107/S1600536807030681**]

Diaquabis[1-ethyl-6-fluoro-7-(4-methylpiperazin-4-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylato]cobalt(II) octahydrate

Z. An, J. Huang and W. Qi

Comment

Pefloxacin (Hpef, 1-ethyl-6-fluoro-7-(4-methylpiperazin-1-yl)-4-oxoquinoline-3-carboxylic acid) is member of a class of quinolones used to treat infections (Mizuki *et al.*, 1996). The silver(I) derivative of pefloxacin have been reported (Baenziger *et al.*, 1986). The title cobalt(II) derivative, (I), is reported here.

The Co^{II} atom (site symmetry $\bar{1}$) in (I) exhibits a distorted octahedral geometry, defined by six oxygen atoms from two pefloxacin ligands and two water (Table 1, Fig. 1). The component species in (I) are linked by the O—H···O and O—H···N hydrogen bonds involving all the potential donors, generating a three-dimensional supramolecular network.

Experimental

A mixture of $Co(CH_3COO)_2{\cdot}4H_2O$ (0.062 g, 0.25 mmol), Hpef (0.17 g, 0.5 mmol) and water (12 ml) was stirred for 30 min in air. The mixture was then transferred to a 23 ml Teflon-lined hydrothermal bomb. The bomb was heated to 433 K for 72 h under autogenous pressure. Pink blocks of (I) suitable for X-ray analysis were obtained from the reaction mixture upon cooling.

Refinement

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms on the water molecules were located in a difference map and refined with a distance restraint of 0.85 (1)Å and the constraint $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

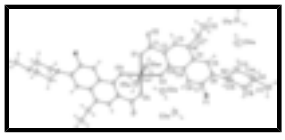


Fig. 1. The molecular structure of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry code: (i) $1-x, 1-y, -z$.

Diaquabis[1-ethyl-6-fluoro-7-(4-methylpiperazin-4-yl)-4-oxo-1,4- dihydroquinoline-3-carboxylato]cobalt(II) octahydrate

Crystal data

$[Co(C_{17}H_{19}FN_3O_3)_2(H_2O)_2]{\cdot}8H_2O$	$Z = 1$
$M_r = 903.79$	$F_{000} = 477$

Triclinic, $P\bar{1}$	D_x = 1.403 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 8.889 (5) Å	Cell parameters from 2882 reflections
b = 10.231 (5) Å	θ = 1.7–25.0º
c = 12.911 (5) Å	μ = 0.48 mm^{-1}
α = 73.287 (5)º	T = 295 (2) K
β = 72.040 (5)º	Block, pink
γ = 85.603 (5)º	0.34 × 0.26 × 0.17 mm
V = 1069.7 (9) Å^3	

Data collection

Bruker SMART CCD diffractometer	3756 independent reflections
Radiation source: fine-focus sealed tube	3380 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.015
T = 295(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −6→10
T_{min} = 0.853, T_{max} = 0.922	k = −12→11
5428 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.103	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.3439P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
3756 reflections	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
300 parameters	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
15 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.0000	0.02908 (14)
C1	0.5131 (2)	0.2447 (2)	0.19334 (17)	0.0301 (4)
C2	0.4572 (2)	0.3295 (2)	0.27595 (16)	0.0283 (4)
C3	0.4449 (2)	0.2636 (2)	0.38738 (17)	0.0307 (4)
H3	0.4774	0.1733	0.4036	0.037*
C4	0.3317 (2)	0.45088 (19)	0.45597 (16)	0.0273 (4)

C5	0.2592 (2)	0.5077 (2)	0.54588 (16)	0.0296 (4)
H5	0.2524	0.4571	0.6197	0.036*
C6	0.1977 (2)	0.6377 (2)	0.52631 (16)	0.0296 (4)
C7	0.2172 (3)	0.7112 (2)	0.41160 (18)	0.0347 (5)
C8	0.2845 (2)	0.6589 (2)	0.32356 (17)	0.0328 (4)
H8	0.2920	0.7108	0.2500	0.039*
C9	0.3434 (2)	0.52531 (19)	0.34378 (16)	0.0273 (4)
C10	0.4125 (2)	0.4693 (2)	0.24821 (16)	0.0274 (4)
C11	0.3830 (3)	0.2310 (2)	0.58984 (17)	0.0361 (5)
H11A	0.4012	0.2874	0.6338	0.043*
H11B	0.4663	0.1640	0.5843	0.043*
C12	0.2252 (4)	0.1581 (3)	0.6505 (2)	0.0605 (7)
H12A	0.1427	0.2241	0.6585	0.091*
H12B	0.2258	0.1022	0.7242	0.091*
H12C	0.2069	0.1018	0.6075	0.091*
C13	0.1324 (2)	0.6346 (2)	0.72586 (17)	0.0333 (4)
H13A	0.2394	0.6045	0.7229	0.040*
H13B	0.0627	0.5552	0.7595	0.040*
C14	0.0828 (3)	0.7342 (2)	0.79736 (18)	0.0399 (5)
H14A	0.0900	0.6906	0.8730	0.048*
H14B	0.1540	0.8127	0.7642	0.048*
C15	−0.0391 (3)	0.7464 (2)	0.61697 (19)	0.0386 (5)
H15A	−0.1096	0.6675	0.6488	0.046*
H15B	−0.0455	0.7914	0.5413	0.046*
C16	−0.0896 (3)	0.8433 (2)	0.68983 (19)	0.0393 (5)
H16A	−0.0223	0.9242	0.6556	0.047*
H16B	−0.1975	0.8713	0.6937	0.047*
C17	−0.1262 (4)	0.8792 (3)	0.8708 (2)	0.0576 (7)
H17A	−0.0605	0.9595	0.8328	0.086*
H17B	−0.1137	0.8398	0.9446	0.086*
H17C	−0.2348	0.9033	0.8782	0.086*
F1	0.16971 (19)	0.84283 (13)	0.38897 (11)	0.0547 (4)
N1	0.3904 (2)	0.31782 (16)	0.47450 (13)	0.0301 (4)
N2	0.12440 (19)	0.70204 (17)	0.61093 (14)	0.0304 (4)
N3	−0.0797 (2)	0.77955 (18)	0.80430 (15)	0.0380 (4)
O1	0.53493 (18)	0.30345 (14)	0.08824 (12)	0.0374 (3)
O2	0.5324 (2)	0.12126 (15)	0.23227 (13)	0.0464 (4)
O3	0.42376 (18)	0.54564 (14)	0.14985 (11)	0.0358 (3)
O1W	0.6676 (2)	0.14217 (17)	0.94617 (14)	0.0480 (4)
O2W	0.7499 (2)	0.66234 (18)	0.16054 (15)	0.0491 (4)
O3W	0.5779 (2)	0.90613 (18)	0.13899 (16)	0.0523 (4)
O4W	0.9208 (2)	0.3290 (2)	0.9021 (2)	0.0768 (7)
O5W	0.74297 (18)	0.55369 (16)	−0.02246 (13)	0.0414 (4)
H4W1	0.867 (2)	0.263 (2)	0.904 (2)	0.062*
H3W1	0.493 (2)	0.889 (3)	0.128 (2)	0.062*
H3W2	0.561 (3)	0.969 (2)	0.172 (2)	0.062*
H1W1	0.628 (3)	0.1962 (19)	0.9860 (18)	0.062*
H1W2	0.680 (3)	0.0644 (14)	0.9890 (18)	0.062*
H2W1	0.708 (3)	0.7396 (15)	0.151 (2)	0.062*

H2W2	0.752 (3)	0.627 (2)	0.1088 (18)	0.062*
H5W1	0.781 (3)	0.6243 (15)	−0.0782 (16)	0.062*
H5W2	0.792 (3)	0.4842 (15)	−0.041 (2)	0.062*
H4W2	1.0178 (12)	0.314 (2)	0.884 (2)	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0346 (2)	0.0295 (2)	0.0213 (2)	0.00173 (15)	−0.00322 (15)	−0.01031 (15)
C1	0.0304 (10)	0.0307 (11)	0.0299 (11)	0.0019 (8)	−0.0058 (8)	−0.0135 (9)
C2	0.0277 (10)	0.0298 (10)	0.0279 (10)	0.0008 (8)	−0.0054 (8)	−0.0119 (8)
C3	0.0336 (11)	0.0263 (10)	0.0323 (11)	0.0036 (8)	−0.0083 (9)	−0.0110 (8)
C4	0.0281 (10)	0.0274 (10)	0.0265 (10)	−0.0013 (8)	−0.0063 (8)	−0.0093 (8)
C5	0.0332 (11)	0.0311 (10)	0.0228 (9)	−0.0004 (8)	−0.0051 (8)	−0.0083 (8)
C6	0.0300 (10)	0.0328 (10)	0.0257 (10)	−0.0007 (8)	−0.0041 (8)	−0.0119 (8)
C7	0.0434 (12)	0.0265 (10)	0.0310 (11)	0.0065 (9)	−0.0073 (9)	−0.0091 (8)
C8	0.0412 (12)	0.0307 (11)	0.0226 (10)	0.0004 (9)	−0.0057 (8)	−0.0058 (8)
C9	0.0291 (10)	0.0272 (10)	0.0245 (10)	−0.0018 (8)	−0.0039 (8)	−0.0093 (8)
C10	0.0263 (10)	0.0306 (10)	0.0248 (10)	−0.0028 (8)	−0.0044 (8)	−0.0095 (8)
C11	0.0495 (13)	0.0325 (11)	0.0284 (11)	0.0055 (9)	−0.0165 (9)	−0.0078 (9)
C12	0.0781 (19)	0.0554 (16)	0.0415 (14)	−0.0244 (14)	−0.0235 (14)	0.0088 (12)
C13	0.0349 (11)	0.0365 (11)	0.0264 (10)	0.0047 (9)	−0.0061 (8)	−0.0103 (8)
C14	0.0455 (13)	0.0460 (13)	0.0294 (11)	−0.0001 (10)	−0.0080 (10)	−0.0158 (10)
C15	0.0357 (11)	0.0454 (13)	0.0379 (12)	0.0105 (10)	−0.0116 (9)	−0.0185 (10)
C16	0.0369 (12)	0.0361 (12)	0.0402 (12)	0.0077 (9)	−0.0033 (9)	−0.0139 (10)
C17	0.0745 (18)	0.0459 (14)	0.0454 (14)	0.0048 (13)	0.0045 (13)	−0.0272 (12)
F1	0.0874 (11)	0.0312 (7)	0.0354 (7)	0.0207 (7)	−0.0088 (7)	−0.0094 (6)
N1	0.0369 (9)	0.0278 (8)	0.0248 (8)	0.0038 (7)	−0.0082 (7)	−0.0082 (7)
N2	0.0307 (9)	0.0346 (9)	0.0254 (8)	0.0057 (7)	−0.0046 (7)	−0.0129 (7)
N3	0.0420 (10)	0.0338 (9)	0.0326 (9)	0.0018 (8)	0.0026 (8)	−0.0157 (8)
O1	0.0512 (9)	0.0331 (8)	0.0268 (8)	0.0062 (7)	−0.0065 (6)	−0.0137 (6)
O2	0.0740 (11)	0.0291 (8)	0.0368 (8)	0.0121 (7)	−0.0158 (8)	−0.0143 (7)
O3	0.0518 (9)	0.0302 (7)	0.0214 (7)	0.0047 (6)	−0.0051 (6)	−0.0086 (6)
O1W	0.0664 (11)	0.0362 (9)	0.0383 (9)	0.0063 (8)	−0.0065 (8)	−0.0170 (7)
O2W	0.0560 (11)	0.0459 (10)	0.0481 (10)	0.0083 (8)	−0.0200 (8)	−0.0141 (8)
O3W	0.0652 (12)	0.0428 (10)	0.0590 (11)	0.0121 (8)	−0.0257 (9)	−0.0248 (8)
O4W	0.0406 (10)	0.0666 (14)	0.1171 (19)	−0.0018 (9)	−0.0131 (12)	−0.0269 (13)
O5W	0.0394 (9)	0.0383 (8)	0.0421 (9)	−0.0033 (7)	−0.0068 (7)	−0.0096 (7)

Geometric parameters (Å, °)

Co1—O3^{i}	2.0206 (15)	C12—H12B	0.9600
Co1—O3	2.0206 (15)	C12—H12C	0.9600
Co1—O1	2.0598 (16)	C13—N2	1.467 (3)
Co1—O1^{i}	2.0598 (16)	C13—C14	1.519 (3)
Co1—O5W	2.180 (2)	C13—H13A	0.9700
Co1—O5W^{i}	2.180 (2)	C13—H13B	0.9700
C1—O2	1.237 (3)	C14—N3	1.467 (3)

C1—O1	1.275 (2)	C14—H14A	0.9700
C1—C2	1.509 (3)	C14—H14B	0.9700
C2—C3	1.376 (3)	C15—N2	1.475 (3)
C2—C10	1.428 (3)	C15—C16	1.509 (3)
C3—N1	1.338 (3)	C15—H15A	0.9700
C3—H3	0.9300	C15—H15B	0.9700
C4—N1	1.401 (3)	C16—N3	1.461 (3)
C4—C5	1.403 (3)	C16—H16A	0.9700
C4—C9	1.405 (3)	C16—H16B	0.9700
C5—C6	1.383 (3)	C17—N3	1.472 (3)
C5—H5	0.9300	C17—H17A	0.9600
C6—N2	1.400 (2)	C17—H17B	0.9600
C6—C7	1.418 (3)	C17—H17C	0.9600
C7—C8	1.348 (3)	O1W—H1W1	0.846 (10)
C7—F1	1.356 (2)	O1W—H1W2	0.849 (10)
C8—C9	1.407 (3)	O2W—H2W1	0.840 (19)
C8—H8	0.9300	O2W—H2W2	0.84 (2)
C9—C10	1.454 (3)	O3W—H3W1	0.848 (10)
C10—O3	1.263 (2)	O3W—H3W2	0.851 (10)
C11—N1	1.483 (3)	O4W—H4W1	0.844 (10)
C11—C12	1.511 (3)	O4W—H4W2	0.835 (10)
C11—H11A	0.9700	O5W—H5W1	0.862 (10)
C11—H11B	0.9700	O5W—H5W2	0.856 (10)
C12—H12A	0.9600		

$O3^{i}$—Co1—O3	180.0	H12A—C12—H12B	109.5
$O3^{i}$—Co1—O1	92.09 (6)	C11—C12—H12C	109.5
O3—Co1—O1	87.91 (6)	H12A—C12—H12C	109.5
$O3^{i}$—Co1—$O1^{i}$	87.91 (6)	H12B—C12—H12C	109.5
O3—Co1—$O1^{i}$	92.09 (6)	N2—C13—C14	109.25 (17)
O1—Co1—$O1^{i}$	180.0	N2—C13—H13A	109.8
$O3^{i}$—Co1—O5W	88.65 (6)	C14—C13—H13A	109.8
O3—Co1—O5W	91.35 (6)	N2—C13—H13B	109.8
O1—Co1—O5W	90.07 (6)	C14—C13—H13B	109.8
$O1^{i}$—Co1—O5W	89.93 (6)	H13A—C13—H13B	108.3
$O3^{i}$—Co1—$O5W^{i}$	91.35 (6)	N3—C14—C13	110.74 (17)
O3—Co1—$O5W^{i}$	88.65 (6)	N3—C14—H14A	109.5
O1—Co1—$O5W^{i}$	89.93 (6)	C13—C14—H14A	109.5
$O1^{i}$—Co1—$O5W^{i}$	90.07 (6)	N3—C14—H14B	109.5
O5W—Co1—$O5W^{i}$	180.0	C13—C14—H14B	109.5
O2—C1—O1	123.93 (18)	H14A—C14—H14B	108.1
O2—C1—C2	117.69 (18)	N2—C15—C16	110.02 (18)
O1—C1—C2	118.37 (17)	N2—C15—H15A	109.7
C3—C2—C10	118.28 (17)	C16—C15—H15A	109.7
C3—C2—C1	116.25 (17)	N2—C15—H15B	109.7
C10—C2—C1	125.44 (17)	C16—C15—H15B	109.7
N1—C3—C2	125.78 (18)	H15A—C15—H15B	108.2

N1—C3—H3	117.1	N3—C16—C15	111.24 (18)
C2—C3—H3	117.1	N3—C16—H16A	109.4
N1—C4—C5	121.73 (17)	C15—C16—H16A	109.4
N1—C4—C9	117.70 (17)	N3—C16—H16B	109.4
C5—C4—C9	120.55 (18)	C15—C16—H16B	109.4
C6—C5—C4	120.95 (18)	H16A—C16—H16B	108.0
C6—C5—H5	119.5	N3—C17—H17A	109.5
C4—C5—H5	119.5	N3—C17—H17B	109.5
C5—C6—N2	124.57 (18)	H17A—C17—H17B	109.5
C5—C6—C7	116.71 (17)	N3—C17—H17C	109.5
N2—C6—C7	118.67 (18)	H17A—C17—H17C	109.5
C8—C7—F1	118.16 (18)	H17B—C17—H17C	109.5
C8—C7—C6	123.67 (18)	C3—N1—C4	119.52 (16)
F1—C7—C6	118.13 (17)	C3—N1—C11	118.58 (16)
C7—C8—C9	119.53 (18)	C4—N1—C11	121.75 (16)
C7—C8—H8	120.2	C6—N2—C13	117.51 (16)
C9—C8—H8	120.2	C6—N2—C15	115.44 (16)
C4—C9—C8	118.51 (17)	C13—N2—C15	109.06 (16)
C4—C9—C10	122.62 (17)	C16—N3—C14	109.00 (16)
C8—C9—C10	118.87 (17)	C16—N3—C17	109.03 (18)
O3—C10—C2	126.05 (18)	C14—N3—C17	110.79 (19)
O3—C10—C9	118.16 (18)	C1—O1—Co1	132.96 (12)
C2—C10—C9	115.76 (17)	C10—O3—Co1	129.04 (13)
N1—C11—C12	112.06 (18)	H1W1—O1W—H1W2	109.4 (15)
N1—C11—H11A	109.2	H2W1—O2W—H2W2	112.1 (16)
C12—C11—H11A	109.2	H3W1—O3W—H3W2	109.2 (15)
N1—C11—H11B	109.2	H4W1—O4W—H4W2	112.0 (16)
C12—C11—H11B	109.2	Co1—O5W—H5W1	114.6 (19)
H11A—C11—H11B	107.9	Co1—O5W—H5W2	100.6 (18)
C11—C12—H12A	109.5	H5W1—O5W—H5W2	107.0 (15)
C11—C12—H12B	109.5		
O2—C1—C2—C3	5.2 (3)	C2—C3—N1—C4	3.5 (3)
O1—C1—C2—C3	−176.05 (18)	C2—C3—N1—C11	179.04 (19)
O2—C1—C2—C10	−172.9 (2)	C5—C4—N1—C3	173.72 (18)
O1—C1—C2—C10	5.9 (3)	C9—C4—N1—C3	−4.4 (3)
C10—C2—C3—N1	1.8 (3)	C5—C4—N1—C11	−1.7 (3)
C1—C2—C3—N1	−176.44 (18)	C9—C4—N1—C11	−179.82 (17)
N1—C4—C5—C6	−178.05 (18)	C12—C11—N1—C3	−91.1 (2)
C9—C4—C5—C6	0.1 (3)	C12—C11—N1—C4	84.3 (2)
C4—C5—C6—N2	−179.66 (18)	C5—C6—N2—C13	8.6 (3)
C4—C5—C6—C7	−2.3 (3)	C7—C6—N2—C13	−168.65 (18)
C5—C6—C7—C8	3.2 (3)	C5—C6—N2—C15	−122.3 (2)
N2—C6—C7—C8	−179.29 (19)	C7—C6—N2—C15	60.4 (2)
C5—C6—C7—F1	−174.77 (18)	C14—C13—N2—C6	166.40 (17)
N2—C6—C7—F1	2.7 (3)	C14—C13—N2—C15	−59.8 (2)
F1—C7—C8—C9	176.32 (19)	C16—C15—N2—C6	−165.98 (18)
C6—C7—C8—C9	−1.7 (3)	C16—C15—N2—C13	59.2 (2)
N1—C4—C9—C8	179.74 (17)	C15—C16—N3—C14	57.5 (2)
C5—C4—C9—C8	1.6 (3)	C15—C16—N3—C17	178.60 (19)

N1—C4—C9—C10	0.4 (3)	C13—C14—N3—C16	−58.4 (2)
C5—C4—C9—C10	−177.81 (17)	C13—C14—N3—C17	−178.33 (19)
C7—C8—C9—C4	−0.8 (3)	O2—C1—O1—Co1	175.48 (15)
C7—C8—C9—C10	178.62 (19)	C2—C1—O1—Co1	−3.2 (3)
C3—C2—C10—O3	176.41 (18)	O3^{i}—Co1—O1—C1	−179.59 (18)
C1—C2—C10—O3	−5.5 (3)	O3—Co1—O1—C1	0.41 (18)
C3—C2—C10—C9	−5.5 (3)	O5W—Co1—O1—C1	91.75 (19)
C1—C2—C10—C9	172.50 (17)	O5W^{i}—Co1—O1—C1	−88.25 (19)
C4—C9—C10—O3	−177.22 (18)	C2—C10—O3—Co1	2.1 (3)
C8—C9—C10—O3	3.4 (3)	C9—C10—O3—Co1	−175.93 (13)
C4—C9—C10—C2	4.6 (3)	O1—Co1—O3—C10	0.37 (17)
C8—C9—C10—C2	−174.79 (18)	O1^{i}—Co1—O3—C10	−179.63 (17)
N2—C13—C14—N3	60.3 (2)	O5W—Co1—O3—C10	−89.65 (17)
N2—C15—C16—N3	−58.6 (2)	O5W^{i}—Co1—O3—C10	90.35 (17)

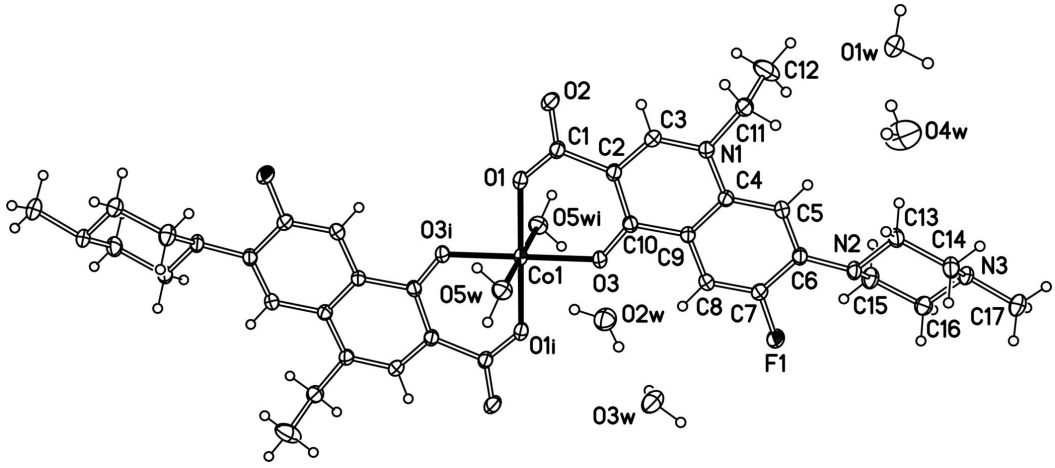
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4W—H4W1···O1W	0.844 (10)	2.083 (12)	2.879 (3)	157 (2)
O3W—H3W1···O1W^{ii}	0.848 (10)	2.035 (12)	2.859 (3)	164 (3)
O3W—H3W2···O2^{iii}	0.851 (10)	1.899 (10)	2.747 (2)	174 (3)
O1W—H1W1···O1^{iv}	0.846 (10)	1.911 (11)	2.754 (2)	175 (2)
O1W—H1W2···O3W^{v}	0.849 (10)	2.129 (18)	2.877 (3)	147 (2)
O2W—H2W1···O3W	0.840 (9)	1.979 (11)	2.813 (3)	171 (3)
O2W—H2W2···O5W	0.840 (9)	2.066 (11)	2.904 (3)	175 (2)
O5W—H5W1···N3^{vi}	0.862 (10)	2.029 (12)	2.870 (3)	165 (3)
O5W—H5W2···O4W^{vii}	0.856 (10)	2.064 (11)	2.918 (3)	175 (2)
O4W—H4W2···O2W^{viii}	0.835 (10)	1.980 (11)	2.787 (3)	162 (2)

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

Fig. 1


O1w
C12
O2
C3
C11
O4w
C1
C2
N1
O1
C4
C5
C13
O3i
O5wi
C10
C9
N2
C14
N3
Co1
O3
C6
O5w
O2w
C8
C7
C15
C16
C17
O1i
F1
O3w