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Poly[[[(1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato)manganese(II)]-μ_3-4,4′-oxydibenzoato] monohydrate]

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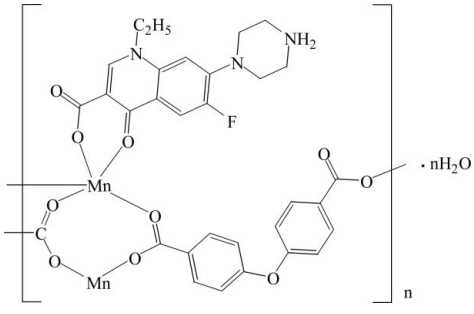
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.038; wR factor = 0.129; data-to-parameter ratio = 15.3.

In the title compound, $\{[Mn(C_{16}H_{18}N_3O_3)(C_{14}H_8O_5)]\cdot H_2O\}_n$, the unique Mn^{II} ion is coordinated by two O atoms from a chelating 1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate ligand and three O atoms from three 4,4′-oxydibenzoate ligands, forming a distorted square-pyramidal coordination environment. In the crystal structure, centrosymmetric dinuclear manganese units are linked *via* 4,4′-oxydibenzoate ligands into one-dimensional chains; these chains are, in turn, connected *via* intermolecular N—H···O and O—H···O hydrogen bonds to form a two-dimensional supramolecular network. The O atom of the solvent water molecule is disordered over two sites with equal occupancies; the attached H atoms are common to both sites.

Related literature

For general background, see: Xiao *et al.* (2005). For a related structure, see: An *et al.* (2007).



Experimental

Crystal data

$[Mn(C_{16}H_{18}N_3O_3)(C_{14}H_8O_5)]\cdot H_2O$
M_r = 648.49
Triclinic, $P\overline{1}$
a = 10.208 (5) Å
b = 11.915 (5) Å
c = 13.202 (5) Å
α = 100.751 (5)°
β = 112.010 (5)°
γ = 102.318 (5)°
V = 1390.1 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.885, T_{max} = 0.908
13533 measured reflections
6236 independent reflections
5434 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.129
S = 1.05
6236 reflections
407 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W′—H2···O3^{i}	1.16	2.40	3.359 (14)	138
O1W′—H2···O4^{i}	1.16	1.87	2.874 (12)	142
N3—H3B···O8^{i}	0.90	1.80	2.694 (3)	169
N3—H3C···O4^{ii}	0.90	1.83	2.716 (3)	169

Symmetry codes: (i) $x-1, y-1, z$; (ii) $x-1, y-2, z$.

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 authors thank Jilin Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2564).

References

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supplementary materials

Acta Cryst. (2008). E**64**, m21 [**doi:10.1107/S1600536807060825**]

Poly[[[(1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylato)manganese(II)]-μ_3-4,4'-oxydibenzoato] monohydrate]

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.* 2007). 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 Mn atoms are coordinated by three oxygen atoms of one Hcf ligand, one 4,4'-oxydibenzoate ligand and one oxygen atom from one symmetry related 4,4'-oxydibenzoate within a distorted square-pyramidal geometry (Figure 1). In the crystal structure, dinuclear manganese units are linked *via* the 4,4'-oxydibenzoate anions into a one-dimensional chain running along [-2, -3, 2]. Finally, one-dimensional chains are connected with N—H···O and O—H···O hydrogen bonds to form a two-dimensional supramolecular network.

Experimental

The title compound was prepared by a hydrothermal method. A mixture of $MnCl_2$ (0.07 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 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 but were included as riding with O - H = 0.85 Å and U_{iso}(H) = 1.5 U_{eq}(O). The O atom of the water molecule is disordered over two sites with the ratio of refined occupancies being 0.50 (2):0.50 (2). The H atoms of this water molecule are common to both sites.

Figures

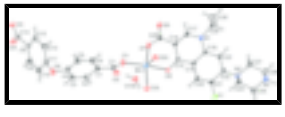


Fig. 1. Part of the crystal structure with labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: i = *x* - 1,*y* - 1,*z*; ii = -*x* + 2,-*y* + 1,-*z* + 1]. The disorder is not showm.

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

Crystal data

$[Mn(C_{16}H_{18}N_3O_3)(C_{14}H_8O_5)]\cdot H_2O$ $Z = 2$

M_r = 648.49	F_{000} = 670
Triclinic, $P\bar{1}$	D_x = 1.549 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.208 (5) Å	Cell parameters from 13533 reflections
b = 11.915 (5) Å	θ = 3.2–27.5º
c = 13.202 (5) Å	μ = 0.55 mm^{-1}
α = 100.751 (5)º	T = 298 (2) K
β = 112.010 (5)º	Block, colorless
γ = 102.318 (5)º	0.23 × 0.20 × 0.18 mm
V = 1390.1 (10) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6236 independent reflections
Radiation source: fine-focus sealed tube	5434 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 298(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→13
T_{min} = 0.885, T_{max} = 0.908	k = −14→15
13533 measured reflections	l = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.0863P)^2 + 0.3678P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
6236 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
407 parameters	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
Mn1	0.87296 (3)	0.44003 (2)	0.32348 (2)	0.02128 (10)	
C1	1.1128 (2)	0.82195 (16)	0.49788 (16)	0.0247 (4)	
C2	1.1270 (2)	0.90958 (17)	0.59100 (16)	0.0264 (4)	
H2A	1.0997	0.8865	0.6456	0.032*	
C3	1.1812 (2)	1.03007 (17)	0.60306 (16)	0.0273 (4)	
H3A	1.1903	1.0879	0.6654	0.033*	
C4	1.2219 (2)	1.06439 (16)	0.52159 (17)	0.0262 (4)	
C5	1.2094 (2)	0.97946 (18)	0.42831 (18)	0.0314 (4)	
H5A	1.2378	1.0029	0.3743	0.038*	
C6	1.1536 (2)	0.85872 (17)	0.41711 (18)	0.0297 (4)	
H6A	1.1432	0.8010	0.3541	0.036*	
C7	1.0531 (2)	0.69147 (17)	0.48503 (18)	0.0264 (4)	
C8	1.4875 (2)	1.36779 (17)	0.38123 (17)	0.0265 (4)	
C9	1.3520 (2)	1.37948 (19)	0.37526 (19)	0.0323 (4)	
H9A	1.3122	1.4316	0.3380	0.039*	
C10	1.2758 (2)	1.31470 (19)	0.42401 (19)	0.0315 (4)	
H10A	1.1860	1.3237	0.4205	0.038*	
C11	1.3354 (2)	1.23664 (16)	0.47793 (17)	0.0280 (4)	
C12	1.4669 (2)	1.21939 (18)	0.48114 (18)	0.0329 (4)	
H12A	1.5031	1.1635	0.5143	0.039*	
C13	1.5432 (2)	1.28651 (19)	0.43436 (18)	0.0303 (4)	
H13A	1.6331	1.2773	0.4384	0.036*	
C14	1.5780 (2)	1.44426 (18)	0.33786 (18)	0.0298 (4)	
C15	0.72279 (18)	0.18861 (15)	0.16263 (14)	0.0198 (3)	
C16	0.84417 (19)	0.18967 (15)	0.13214 (15)	0.0208 (3)	
C17	0.8599 (2)	0.08327 (16)	0.08805 (16)	0.0247 (4)	
H17A	0.9375	0.0866	0.0669	0.030*	
C18	0.65597 (18)	−0.03553 (15)	0.10430 (14)	0.0201 (3)	
C19	0.62933 (18)	0.06987 (15)	0.14683 (14)	0.0195 (3)	
C20	0.51069 (19)	0.06089 (16)	0.17796 (15)	0.0224 (3)	
H20A	0.4918	0.1299	0.2068	0.027*	
C21	0.42376 (19)	−0.04923 (17)	0.16565 (16)	0.0239 (4)	
C22	0.44917 (19)	−0.15747 (15)	0.12569 (15)	0.0216 (3)	
C23	0.56632 (19)	−0.14844 (15)	0.09490 (15)	0.0208 (3)	
H23A	0.5859	−0.2178	0.0677	0.025*	
C24	0.3535 (2)	−0.28055 (17)	0.22389 (17)	0.0278 (4)	
H24A	0.3440	−0.2084	0.2647	0.033*	
H24B	0.4467	−0.2906	0.2713	0.033*	
C25	0.2255 (2)	−0.38815 (17)	0.20169 (19)	0.0303 (4)	
H25A	0.2272	−0.3970	0.2737	0.036*	

H25B	0.1318	−0.3765	0.1578	0.036*	
C26	0.2411 (2)	−0.48454 (17)	0.02785 (17)	0.0314 (4)	
H26A	0.1473	−0.4761	−0.0203	0.038*	
H26B	0.2525	−0.5562	−0.0121	0.038*	
C27	0.3680 (2)	−0.37514 (16)	0.04987 (16)	0.0271 (4)	
H27A	0.4625	−0.3864	0.0925	0.032*	
H27B	0.3646	−0.3653	−0.0223	0.032*	
C28	0.95504 (19)	0.30350 (15)	0.14442 (16)	0.0230 (4)	
C29	0.8106 (2)	−0.13254 (17)	0.02814 (19)	0.0298 (4)	
H29A	0.8568	−0.1147	−0.0216	0.036*	
H29B	0.7203	−0.1998	−0.0167	0.036*	
C30	0.9141 (3)	−0.1668 (2)	0.1229 (2)	0.0460 (6)	
H30A	0.9362	−0.2358	0.0915	0.069*	
H30B	0.8681	−0.1855	0.1718	0.069*	
H30C	1.0044	−0.1010	0.1665	0.069*	
F1	0.30490 (14)	−0.05557 (11)	0.18978 (12)	0.0368 (3)	
N1	0.77241 (17)	−0.02611 (13)	0.07263 (14)	0.0234 (3)	
N2	0.35453 (17)	−0.26761 (13)	0.11516 (13)	0.0232 (3)	
N3	0.23945 (18)	−0.49768 (14)	0.13743 (14)	0.0272 (3)	
H3B	0.1626	−0.5617	0.1228	0.033*	
H3C	0.3240	−0.5105	0.1802	0.033*	
O1	1.01455 (17)	0.61842 (12)	0.38860 (14)	0.0356 (3)	
O2	1.04421 (16)	0.66314 (13)	0.56977 (14)	0.0323 (3)	
O3	1.71509 (15)	1.46076 (13)	0.38222 (13)	0.0342 (3)	
O4	1.51348 (18)	1.48909 (17)	0.26125 (17)	0.0451 (4)	
O5	1.26452 (19)	1.18672 (13)	0.53831 (14)	0.0360 (3)	
O6	0.69325 (14)	0.28045 (11)	0.19922 (12)	0.0260 (3)	
O7	0.96748 (15)	0.40179 (12)	0.20826 (12)	0.0291 (3)	
O8	1.03114 (17)	0.29361 (12)	0.08966 (14)	0.0366 (4)	
O1W	0.7413 (5)	0.5678 (6)	0.2066 (4)	0.0338 (16)	0.50 (2)
H1	0.8224	0.6189	0.2575	0.051*	
H2	0.6698	0.5411	0.2226	0.051*	
O1W'	0.7286 (5)	0.6219 (15)	0.2009 (4)	0.064 (3)	0.50 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02024 (16)	0.01816 (15)	0.02471 (16)	0.00072 (10)	0.01335 (11)	0.00295 (11)
C1	0.0233 (9)	0.0223 (9)	0.0277 (9)	0.0064 (7)	0.0100 (7)	0.0088 (7)
C2	0.0276 (9)	0.0303 (10)	0.0235 (9)	0.0084 (7)	0.0120 (7)	0.0111 (7)
C3	0.0333 (10)	0.0251 (9)	0.0217 (9)	0.0085 (7)	0.0113 (7)	0.0047 (7)
C4	0.0290 (10)	0.0202 (8)	0.0281 (9)	0.0054 (7)	0.0120 (7)	0.0074 (7)
C5	0.0406 (11)	0.0261 (9)	0.0300 (10)	0.0049 (8)	0.0209 (8)	0.0080 (8)
C6	0.0356 (11)	0.0235 (9)	0.0302 (10)	0.0053 (7)	0.0184 (8)	0.0039 (7)
C7	0.0199 (9)	0.0237 (9)	0.0373 (10)	0.0071 (7)	0.0136 (7)	0.0098 (8)
C8	0.0223 (9)	0.0252 (9)	0.0318 (10)	0.0059 (7)	0.0130 (7)	0.0071 (7)
C9	0.0314 (11)	0.0360 (11)	0.0426 (12)	0.0168 (8)	0.0214 (9)	0.0214 (9)
C10	0.0287 (10)	0.0331 (10)	0.0395 (11)	0.0105 (8)	0.0193 (8)	0.0149 (9)

C11	0.0343 (10)	0.0203 (8)	0.0271 (9)	0.0026 (7)	0.0152 (8)	0.0047 (7)
C12	0.0404 (11)	0.0278 (10)	0.0330 (10)	0.0144 (8)	0.0149 (9)	0.0122 (8)
C13	0.0237 (9)	0.0321 (10)	0.0357 (11)	0.0115 (7)	0.0123 (8)	0.0096 (8)
C14	0.0269 (10)	0.0271 (9)	0.0386 (11)	0.0086 (7)	0.0189 (8)	0.0070 (8)
C15	0.0185 (8)	0.0178 (8)	0.0187 (8)	0.0002 (6)	0.0073 (6)	0.0038 (6)
C16	0.0178 (8)	0.0193 (8)	0.0235 (8)	−0.0016 (6)	0.0115 (6)	0.0050 (6)
C17	0.0220 (9)	0.0221 (8)	0.0302 (9)	0.0002 (6)	0.0164 (7)	0.0048 (7)
C18	0.0184 (8)	0.0195 (8)	0.0205 (8)	0.0010 (6)	0.0092 (6)	0.0052 (6)
C19	0.0185 (8)	0.0190 (8)	0.0188 (8)	0.0012 (6)	0.0086 (6)	0.0050 (6)
C20	0.0212 (9)	0.0207 (8)	0.0248 (8)	0.0026 (6)	0.0128 (7)	0.0041 (7)
C21	0.0171 (8)	0.0268 (9)	0.0292 (9)	0.0013 (6)	0.0150 (7)	0.0072 (7)
C22	0.0208 (8)	0.0192 (8)	0.0206 (8)	−0.0018 (6)	0.0085 (6)	0.0067 (6)
C23	0.0186 (8)	0.0170 (8)	0.0247 (8)	0.0009 (6)	0.0103 (6)	0.0048 (6)
C24	0.0331 (10)	0.0230 (9)	0.0271 (9)	0.0009 (7)	0.0165 (8)	0.0084 (7)
C25	0.0330 (11)	0.0257 (9)	0.0395 (11)	0.0051 (8)	0.0238 (9)	0.0133 (8)
C26	0.0347 (11)	0.0220 (9)	0.0281 (10)	−0.0059 (7)	0.0127 (8)	0.0050 (7)
C27	0.0311 (10)	0.0205 (8)	0.0254 (9)	−0.0025 (7)	0.0143 (7)	0.0051 (7)
C28	0.0219 (9)	0.0187 (8)	0.0270 (9)	−0.0015 (6)	0.0141 (7)	0.0052 (7)
C29	0.0315 (10)	0.0193 (8)	0.0406 (11)	0.0031 (7)	0.0237 (8)	0.0011 (7)
C30	0.0532 (15)	0.0436 (13)	0.0495 (14)	0.0252 (11)	0.0262 (12)	0.0118 (11)
F1	0.0323 (7)	0.0301 (6)	0.0591 (8)	0.0045 (5)	0.0345 (6)	0.0122 (6)
N1	0.0222 (7)	0.0173 (7)	0.0319 (8)	0.0020 (5)	0.0167 (6)	0.0039 (6)
N2	0.0238 (8)	0.0188 (7)	0.0248 (8)	−0.0020 (5)	0.0126 (6)	0.0070 (6)
N3	0.0251 (8)	0.0222 (7)	0.0341 (9)	0.0002 (6)	0.0152 (7)	0.0111 (6)
O1	0.0395 (8)	0.0201 (6)	0.0445 (9)	0.0001 (6)	0.0227 (7)	0.0043 (6)
O2	0.0312 (7)	0.0333 (7)	0.0440 (8)	0.0142 (6)	0.0213 (6)	0.0214 (6)
O3	0.0235 (7)	0.0362 (8)	0.0410 (8)	0.0066 (6)	0.0180 (6)	0.0017 (6)
O4	0.0338 (9)	0.0575 (10)	0.0628 (11)	0.0180 (7)	0.0291 (8)	0.0375 (9)
O5	0.0542 (10)	0.0213 (7)	0.0401 (8)	0.0064 (6)	0.0314 (7)	0.0087 (6)
O6	0.0214 (6)	0.0181 (6)	0.0350 (7)	0.0007 (5)	0.0144 (5)	0.0017 (5)
O7	0.0322 (7)	0.0191 (6)	0.0358 (8)	−0.0029 (5)	0.0232 (6)	0.0017 (5)
O8	0.0412 (9)	0.0226 (7)	0.0504 (9)	−0.0047 (6)	0.0370 (7)	0.0003 (6)
O1W	0.0325 (17)	0.036 (2)	0.0339 (17)	0.0081 (9)	0.0168 (11)	0.0111 (9)
O1W'	0.051 (3)	0.092 (8)	0.057 (3)	0.018 (3)	0.028 (2)	0.035 (3)

Geometric parameters (Å, °)

Mn1—O3^{i}	2.0723 (16)	C18—C19	1.401 (2)
Mn1—O2^{ii}	2.0997 (15)	C18—C23	1.411 (2)
Mn1—O1	2.1028 (16)	C19—C20	1.408 (2)
Mn1—O7	2.1170 (15)	C20—C21	1.360 (2)
Mn1—O6	2.1827 (14)	C20—H20A	0.9300
C1—C6	1.390 (3)	C21—F1	1.356 (2)
C1—C2	1.395 (3)	C21—C22	1.414 (3)
C1—C7	1.496 (3)	C22—C23	1.390 (3)
C2—C3	1.379 (3)	C22—N2	1.402 (2)
C2—H2A	0.9300	C23—H23A	0.9300
C3—C4	1.387 (3)	C24—N2	1.476 (2)
C3—H3A	0.9300	C24—C25	1.515 (3)

C4—O5	1.378 (2)	C24—H24A	0.9700
C4—C5	1.385 (3)	C24—H24B	0.9700
C5—C6	1.387 (3)	C25—N3	1.483 (3)
C5—H5A	0.9300	C25—H25A	0.9700
C6—H6A	0.9300	C25—H25B	0.9700
C7—O2	1.256 (3)	C26—N3	1.490 (3)
C7—O1	1.264 (3)	C26—C27	1.523 (2)
C8—C9	1.393 (3)	C26—H26A	0.9700
C8—C13	1.394 (3)	C26—H26B	0.9700
C8—C14	1.498 (3)	C27—N2	1.468 (2)
C9—C10	1.386 (3)	C27—H27A	0.9700
C9—H9A	0.9300	C27—H27B	0.9700
C10—C11	1.380 (3)	C28—O8	1.252 (2)
C10—H10A	0.9300	C28—O7	1.259 (2)
C11—C12	1.387 (3)	C29—N1	1.487 (2)
C11—O5	1.392 (2)	C29—C30	1.494 (3)
C12—C13	1.381 (3)	C29—H29A	0.9700
C12—H12A	0.9300	C29—H29B	0.9700
C13—H13A	0.9300	C30—H30A	0.9600
C14—O3	1.251 (3)	C30—H30B	0.9600
C14—O4	1.263 (3)	C30—H30C	0.9600
C15—O6	1.255 (2)	N3—H3B	0.9000
C15—C16	1.437 (2)	N3—H3C	0.9000
C15—C19	1.456 (2)	O2—Mn1^{ii}	2.0997 (15)
C16—C17	1.361 (3)	O3—Mn1^{iii}	2.0723 (16)
C16—C28	1.507 (2)	O1W—H1	0.8501
C17—N1	1.344 (2)	O1W—H2	0.8500
C17—H17A	0.9300	O1W'—H1	0.9823
C18—N1	1.390 (2)	O1W'—H2	1.1648
O3^{i}—Mn1—O2^{ii}	94.25 (7)	C19—C20—H20A	120.1
O3^{i}—Mn1—O1	99.66 (7)	F1—C21—C20	118.42 (16)
O2^{ii}—Mn1—O1	110.98 (7)	F1—C21—C22	118.55 (15)
O3^{i}—Mn1—O7	159.82 (6)	C20—C21—C22	123.01 (16)
O2^{ii}—Mn1—O7	98.92 (6)	C23—C22—N2	123.11 (16)
O1—Mn1—O7	89.87 (6)	C23—C22—C21	117.17 (15)
O3^{i}—Mn1—O6	83.01 (6)	N2—C22—C21	119.69 (16)
O2^{ii}—Mn1—O6	90.64 (6)	C22—C23—C18	120.92 (16)
O1—Mn1—O6	157.82 (6)	C22—C23—H23A	119.5
O7—Mn1—O6	81.62 (6)	C18—C23—H23A	119.5
C6—C1—C2	118.53 (18)	N2—C24—C25	110.46 (16)
C6—C1—C7	121.02 (17)	N2—C24—H24A	109.6
C2—C1—C7	120.45 (18)	C25—C24—H24A	109.6
C3—C2—C1	120.77 (18)	N2—C24—H24B	109.6
C3—C2—H2A	119.6	C25—C24—H24B	109.6
C1—C2—H2A	119.6	H24A—C24—H24B	108.1
C2—C3—C4	119.57 (18)	N3—C25—C24	109.14 (16)
C2—C3—H3A	120.2	N3—C25—H25A	109.9

C4—C3—H3A	120.2	C24—C25—H25A	109.9
O5—C4—C5	124.49 (18)	N3—C25—H25B	109.9
O5—C4—C3	114.36 (17)	C24—C25—H25B	109.9
C5—C4—C3	121.01 (18)	H25A—C25—H25B	108.3
C4—C5—C6	118.62 (19)	N3—C26—C27	110.69 (15)
C4—C5—H5A	120.7	N3—C26—H26A	109.5
C6—C5—H5A	120.7	C27—C26—H26A	109.5
C5—C6—C1	121.51 (18)	N3—C26—H26B	109.5
C5—C6—H6A	119.2	C27—C26—H26B	109.5
C1—C6—H6A	119.2	H26A—C26—H26B	108.1
O2—C7—O1	125.27 (18)	N2—C27—C26	109.42 (16)
O2—C7—C1	117.92 (18)	N2—C27—H27A	109.8
O1—C7—C1	116.81 (18)	C26—C27—H27A	109.8
C9—C8—C13	118.67 (19)	N2—C27—H27B	109.8
C9—C8—C14	121.97 (18)	C26—C27—H27B	109.8
C13—C8—C14	119.29 (17)	H27A—C27—H27B	108.2
C10—C9—C8	121.04 (19)	O8—C28—O7	123.65 (15)
C10—C9—H9A	119.5	O8—C28—C16	116.83 (16)
C8—C9—H9A	119.5	O7—C28—C16	119.52 (16)
C11—C10—C9	118.86 (19)	N1—C29—C30	111.51 (17)
C11—C10—H10A	120.6	N1—C29—H29A	109.3
C9—C10—H10A	120.6	C30—C29—H29A	109.3
C10—C11—C12	121.40 (19)	N1—C29—H29B	109.3
C10—C11—O5	116.02 (19)	C30—C29—H29B	109.3
C12—C11—O5	122.25 (19)	H29A—C29—H29B	108.0
C13—C12—C11	119.01 (19)	C29—C30—H30A	109.5
C13—C12—H12A	120.5	C29—C30—H30B	109.5
C11—C12—H12A	120.5	H30A—C30—H30B	109.5
C12—C13—C8	120.93 (19)	C29—C30—H30C	109.5
C12—C13—H13A	119.5	H30A—C30—H30C	109.5
C8—C13—H13A	119.5	H30B—C30—H30C	109.5
O3—C14—O4	124.1 (2)	C17—N1—C18	119.41 (15)
O3—C14—C8	116.81 (19)	C17—N1—C29	117.84 (15)
O4—C14—C8	119.05 (18)	C18—N1—C29	122.66 (15)
O6—C15—C16	124.88 (15)	C22—N2—C27	115.72 (15)
O6—C15—C19	119.88 (16)	C22—N2—C24	114.10 (14)
C16—C15—C19	115.23 (15)	C27—N2—C24	111.64 (15)
C17—C16—C15	119.13 (15)	C25—N3—C26	110.69 (15)
C17—C16—C28	117.57 (16)	C25—N3—H3B	109.5
C15—C16—C28	123.30 (16)	C26—N3—H3B	109.5
N1—C17—C16	125.34 (17)	C25—N3—H3C	109.5
N1—C17—H17A	117.3	C26—N3—H3C	109.5
C16—C17—H17A	117.3	H3B—N3—H3C	108.1
N1—C18—C19	118.70 (15)	C7—O1—Mn1	127.16 (13)
N1—C18—C23	121.14 (16)	C7—O2—Mn1^{ii}	139.01 (13)
C19—C18—C23	120.16 (16)	C14—O3—Mn1^{iii}	136.07 (15)
C18—C19—C20	118.98 (16)	C4—O5—C11	120.98 (16)
C18—C19—C15	122.11 (16)	C15—O6—Mn1	119.80 (11)

C20—C19—C15	118.89 (16)	C28—O7—Mn1	131.03 (11)
C21—C20—C19	119.72 (17)	H1—O1W—H2	120.8
C21—C20—H20A	120.1	H1—O1W'—H2	86.6

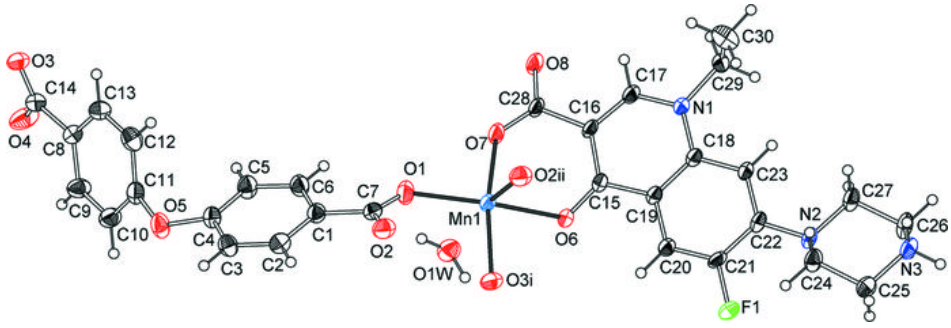
Symmetry codes: (i) *x*−1, *y*−1, *z*; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*+1, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W'—H2···O3^{i}	1.16	2.40	3.359 (14)	138
O1W'—H2···O4^{i}	1.16	1.87	2.874 (12)	142
N3—H3B···O8^{i}	0.90	1.80	2.694 (3)	169
N3—H3C···O4^{iv}	0.90	1.83	2.716 (3)	169

Symmetry codes: (i) *x*−1, *y*−1, *z*; (iv) *x*−1, *y*−2, *z*.

Fig. 1


O3
C14
C13
O4
C8
C12
C11
C9
O5
C10
C5
C6
C4
C1
C3
C2
C7
O1
O2
Mn1
O1W
O3i
O2ii
O6
O7
O8
C28
C16
C17
C30
C29
N1
C18
C23
C15
C19
C22
C20
C21
F1
N2
C27
C26
N3
C24
C25