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Bis(μ-4-carboxybenzene-1,2-dicarboxylato)-1:2κ^3O^3,O^4:O^3;1:2κ^3O^3:O^3,O^4-bis[1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(piperazin-1-yl)quinoline-3-carboxylato-κ^2O,O']dizinc(II) hexahydrate

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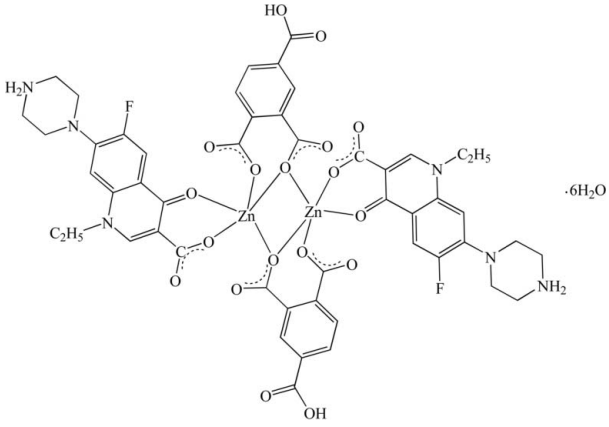
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.035; wR factor = 0.104; data-to-parameter ratio = 15.8.

In the crystal structure of the title compound, $[Zn_2(C_{16}H_{18}FN_3O_3)_2(C_9H_4O_6)_2]\cdot 6H_2O$, the Zn^{II} atoms are each coordinated by five O atoms within a distorted trigonal biyramid. The two Zn^{II} atoms are connected by two symmetry-related carboxylate O atoms into dimers, which are located on centres of inversion. These dimers are linked by N—H···O and O—H···O hydrogen bonding.

Related literature

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



Experimental

Crystal data

$[Zn_2(C_{16}H_{18}FN_3O_3)_2(C_9H_4O_6)_2]\cdot 6H_2O$
M_r = 1293.75
Triclinic, $P\overline{1}$
a = 11.296 (2) Å
b = 11.764 (2) Å
c = 12.398 (3) Å
α = 66.95 (3)°
β = 87.62 (3)°
γ = 61.97 (3)°
V = 1317.3 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 298 (2) K
0.31 × 0.25 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.744, T_{max} = 0.831
13057 measured reflections
5989 independent reflections
5274 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.104
S = 1.01
5989 reflections
379 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1···O4	0.85	1.86	2.711 (5)	174
O3W—H6···O2	0.85	2.03	2.799 (5)	151
O1W—H2···O5^{i}	0.85	2.07	2.789 (5)	142
O2W—H3···O1^{ii}	0.85	1.85	2.688 (5)	167
N3—H3B···O8^{iii}	0.90	1.80	2.696 (5)	177
N3—H3C···O2W^{iii}	0.90	1.93	2.824 (6)	171

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

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: NC2071).

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supplementary materials

Acta Cryst. (2007). E**63**, m2965 [**doi:10.1107/S1600536807055274**]

Bis(μ-4-carboxybenzene-1,2-dicarboxylato)-1:2κ^3O^3,O^4:O^3;1:2κ^3O^3:O^3,O^4-bis[1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(piperazin-1-yl)quinoline-3-carboxylato-κ^2O,O']dizinc(II) hexahydrate

J. Hong

Comment

Norfloxacin [1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(piperazin-1-yl)quinoline-3-carboxylic acid] 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 Zn atoms are coordinated by two oxygen atoms of one 1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7- (piperazin-1-yl)quinoline-3-carboxylato-O,*O*')anion and three oxygen atoms of two 4-carboxybenzene-1,2-dicarboxylato-O,*O*' dianions within a distorted trigonal biyramid geometry (Fig. 1). Two of these octahedra are connected *via* common edges into dimers, which are located on centres of inversion. These dinuclear dimers are connected by N—H···O and O—H···O hydrogen bonding into a three-dimensional network (Table 1).

Experimental

A mixture of $ZnNO_3{\cdot}6H_2O$ (0.5 mmol), norfloxacin (0.5 mmol), benzene-1,2,4-tricarboxylic acid (0.8 mmol) were stirred for 20 min in 10 ml of water) and then transferred into a 23 ml Teflon reactor. The reactor was kept at 433 K for 120 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, N—H = 0.9 Å, and O—H = 0.82 Å and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,*N*), H atoms of water molecule were located in difference maps and refined isotropically with O—H = 0.85 Å and U_{iso}(H) = 1.5U_{eq}(O)

Figures

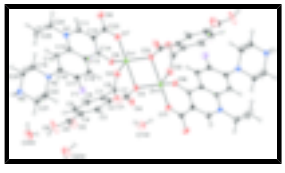


Fig. 1. Crystal structure of (I) with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: i = −*x*,-*y* + 1,-*z*

Bis(μ-4-carboxybenzene-1,2-dicarboxylato)- 1:2κ^3*O*^{3},*O*^{4}:*O*^{3};1:2κ^3*O*^{3}:*O*^{3},*O*^{4}– bis[1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(piperazin-1-yl)quinoline-3- carboxylato-κ^2*O*,*O*'] dizinc(II) hexahydrate

Crystal data

$[Zn_2(C_{16}H_{18}FN_3O_3)_2(C_9H_4O_6)_2]\cdot 6H_2O$	$Z = 1$
$M_r = 1293.75$	$F_{000} = 668$
Triclinic, $P\overline{1}$	$D_x = 1.631$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 11.296$ (2) Å	Cell parameters from 13057 reflections
$b = 11.764$ (2) Å	θ = 3.1–27.5º
$c = 12.398$ (3) Å	μ = 1.01 mm^{-1}
α = 66.95 (3)º	$T = 298$ (2) K
β = 87.62 (3)º	Block, colourless
γ = 61.97 (3)º	0.31 × 0.25 × 0.19 mm
$V = 1317.3$ (5) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	5989 independent reflections
Radiation source: fine-focus sealed tube	5274 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 298$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14\rightarrow14$
$T_{min} = 0.744$, $T_{max} = 0.831$	$k = -13\rightarrow15$
13057 measured reflections	$l = -15\rightarrow16$

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-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.9168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.007$
5989 reflections	$\Delta\rho_{max} = 0.46$ e Å^{-3}
379 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
9 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}
Zn1	−0.11988 (5)	0.52096 (5)	0.08633 (4)	0.01963 (17)
F1	0.3341 (3)	−0.0548 (3)	0.5724 (2)	0.0315 (6)
O1	−0.0390 (4)	0.8105 (4)	0.0927 (3)	0.0382 (9)
O2	−0.1451 (3)	0.6892 (3)	0.1040 (3)	0.0269 (7)
O3	0.0951 (3)	0.4928 (3)	0.0671 (3)	0.0252 (6)
O4	0.2887 (4)	0.2983 (4)	0.1743 (3)	0.0340 (8)
O5	0.4119 (4)	0.1723 (4)	0.5979 (3)	0.0443 (10)
O6	0.3091 (6)	0.3438 (5)	0.6612 (4)	0.0649 (15)
H6B	0.3732	0.2937	0.7171	0.078*
O7	−0.3011 (3)	0.5376 (3)	0.1017 (3)	0.0272 (7)
O8	−0.4599 (3)	0.5006 (4)	0.1932 (3)	0.0307 (7)
O9	−0.0314 (3)	0.3377 (3)	0.2322 (2)	0.0227 (6)
N1	−0.2222 (3)	0.2296 (4)	0.5123 (3)	0.0204 (7)
N2	0.2171 (4)	−0.1024 (4)	0.7755 (3)	0.0209 (7)
N3	0.3583 (4)	−0.2514 (4)	1.0164 (3)	0.0232 (7)
H3B	0.4190	−0.3326	1.0768	0.028*
H3C	0.3249	−0.1821	1.0419	0.028*
C1	0.0529 (4)	0.5859 (4)	0.2505 (4)	0.0212 (8)
C2	0.1611 (4)	0.4548 (4)	0.2613 (3)	0.0195 (8)
C3	0.2508 (4)	0.3620 (4)	0.3700 (4)	0.0221 (8)
H3A	0.3238	0.2758	0.3775	0.027*
C4	0.2330 (5)	0.3960 (5)	0.4663 (4)	0.0246 (9)
C5	0.1253 (5)	0.5263 (5)	0.4544 (4)	0.0291 (10)
H5A	0.1127	0.5501	0.5188	0.035*
C6	0.0375 (5)	0.6198 (5)	0.3478 (4)	0.0273 (9)
H6A	−0.0334	0.7072	0.3404	0.033*
C7	0.1867 (4)	0.4086 (4)	0.1619 (4)	0.0203 (8)
C8	−0.0487 (4)	0.7019 (4)	0.1383 (4)	0.0232 (8)
C9	0.3269 (5)	0.2930 (5)	0.5819 (4)	0.0282 (9)
C10	−0.2389 (4)	0.3663 (4)	0.3046 (3)	0.0187 (8)
C11	−0.2937 (4)	0.3236 (4)	0.4033 (4)	0.0210 (8)
H11A	−0.3879	0.3632	0.3935	0.025*
C12	−0.0811 (4)	0.1636 (4)	0.5312 (3)	0.0174 (7)

C13	−0.0176 (4)	0.1976 (4)	0.4332 (3)	0.0171 (7)
C14	−0.0954 (4)	0.3054 (4)	0.3155 (3)	0.0170 (7)
C15	−0.0041 (4)	0.0677 (4)	0.6455 (3)	0.0189 (8)
H15A	−0.0486	0.0519	0.7101	0.023*
C16	0.1367 (4)	−0.0038 (4)	0.6641 (3)	0.0193 (8)
C17	0.1978 (4)	0.0240 (4)	0.5611 (4)	0.0201 (8)
C18	0.1255 (4)	0.1228 (4)	0.4512 (4)	0.0200 (8)
H18A	0.1706	0.1413	0.3875	0.024*
C19	0.1459 (4)	−0.1380 (5)	0.8740 (4)	0.0233 (9)
H19A	0.0787	−0.1562	0.8492	0.028*
H19B	0.0987	−0.0583	0.8950	0.028*
C20	0.2463 (4)	−0.2687 (5)	0.9821 (4)	0.0247 (9)
H20A	0.1986	−0.2852	1.0485	0.030*
H20B	0.2838	−0.3510	0.9643	0.030*
C21	0.4275 (5)	−0.2153 (5)	0.9146 (4)	0.0287 (10)
H21A	0.4691	−0.2926	0.8903	0.034*
H21B	0.4987	−0.2014	0.9383	0.034*
C22	0.3252 (5)	−0.0811 (5)	0.8118 (4)	0.0278 (10)
H22A	0.2854	−0.0032	0.8354	0.033*
H22B	0.3705	−0.0571	0.7452	0.033*
C23	−0.3403 (4)	0.4758 (4)	0.1921 (3)	0.0201 (8)
C24	−0.3002 (5)	0.2042 (5)	0.6093 (4)	0.0296 (10)
H24A	−0.2451	0.1091	0.6712	0.035*
H24B	−0.3814	0.2101	0.5785	0.035*
C25	−0.3403 (7)	0.3091 (7)	0.6615 (5)	0.0502 (15)
H25A	−0.3902	0.2891	0.7242	0.075*
H25B	−0.3966	0.4032	0.6008	0.075*
H25C	−0.2601	0.3026	0.6931	0.075*
O1W	0.3947 (4)	0.0289 (4)	0.1959 (3)	0.0403 (9)
H1	0.3596	0.1155	0.1839	0.060*
H2	0.4260	−0.0044	0.2692	0.060*
O2W	−0.7730 (4)	0.9659 (4)	0.0955 (3)	0.0421 (9)
H3	−0.8331	1.0442	0.0418	0.063*
H4	−0.7165	0.9879	0.1117	0.063*
O3W	−0.4213 (4)	0.8368 (5)	0.1153 (4)	0.0521 (11)
H6	−0.3461	0.8208	0.0908	0.078*
H5	−0.4603	0.9196	0.1161	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0200 (3)	0.0207 (3)	0.0132 (2)	−0.0084 (2)	0.00266 (17)	−0.00461 (19)
F1	0.0135 (12)	0.0362 (15)	0.0273 (13)	−0.0031 (11)	−0.0007 (10)	−0.0082 (12)
O1	0.036 (2)	0.0218 (17)	0.041 (2)	−0.0139 (15)	−0.0076 (16)	0.0022 (15)
O2	0.0198 (15)	0.0249 (15)	0.0318 (16)	−0.0061 (12)	0.0001 (12)	−0.0137 (14)
O3	0.0205 (15)	0.0325 (17)	0.0163 (13)	−0.0084 (13)	0.0016 (11)	−0.0103 (13)
O4	0.0289 (18)	0.0305 (18)	0.0294 (17)	−0.0016 (14)	0.0006 (14)	−0.0163 (15)
O5	0.042 (2)	0.037 (2)	0.0328 (19)	−0.0095 (17)	−0.0129 (16)	−0.0050 (17)

O6	0.093 (4)	0.056 (3)	0.029 (2)	−0.021 (3)	−0.016 (2)	−0.020 (2)
O7	0.0211 (15)	0.0306 (17)	0.0157 (13)	−0.0104 (13)	−0.0008 (11)	0.0006 (13)
O8	0.0156 (14)	0.0338 (18)	0.0228 (15)	−0.0083 (13)	−0.0024 (12)	0.0022 (14)
O9	0.0174 (14)	0.0249 (15)	0.0166 (13)	−0.0080 (12)	0.0038 (11)	−0.0033 (12)
N1	0.0155 (16)	0.0231 (17)	0.0154 (15)	−0.0083 (14)	0.0021 (12)	−0.0030 (14)
N2	0.0184 (17)	0.0223 (17)	0.0149 (15)	−0.0094 (14)	−0.0032 (13)	−0.0014 (14)
N3	0.0201 (17)	0.0212 (17)	0.0164 (15)	−0.0055 (14)	−0.0045 (13)	−0.0021 (14)
C1	0.020 (2)	0.0194 (19)	0.0216 (19)	−0.0093 (16)	0.0017 (16)	−0.0069 (17)
C2	0.0190 (19)	0.0211 (19)	0.0173 (18)	−0.0092 (16)	0.0021 (15)	−0.0078 (16)
C3	0.0198 (19)	0.021 (2)	0.0211 (19)	−0.0081 (16)	0.0000 (15)	−0.0065 (17)
C4	0.028 (2)	0.025 (2)	0.0188 (19)	−0.0138 (18)	0.0004 (16)	−0.0059 (17)
C5	0.039 (3)	0.031 (2)	0.023 (2)	−0.018 (2)	0.0070 (19)	−0.0163 (19)
C6	0.029 (2)	0.023 (2)	0.030 (2)	−0.0105 (18)	0.0052 (18)	−0.0145 (19)
C7	0.0189 (19)	0.022 (2)	0.0175 (18)	−0.0086 (16)	0.0025 (15)	−0.0077 (16)
C8	0.019 (2)	0.020 (2)	0.024 (2)	−0.0046 (16)	0.0023 (16)	−0.0088 (17)
C9	0.033 (2)	0.033 (2)	0.021 (2)	−0.019 (2)	−0.0004 (18)	−0.0093 (19)
C10	0.0173 (18)	0.0180 (18)	0.0143 (17)	−0.0060 (15)	−0.0013 (14)	−0.0039 (15)
C11	0.0150 (18)	0.021 (2)	0.0184 (18)	−0.0056 (15)	0.0006 (14)	−0.0044 (16)
C12	0.0166 (18)	0.0159 (18)	0.0164 (17)	−0.0067 (15)	0.0000 (14)	−0.0052 (15)
C13	0.0158 (18)	0.0170 (18)	0.0149 (17)	−0.0069 (15)	−0.0001 (14)	−0.0045 (15)
C14	0.0189 (19)	0.0163 (18)	0.0138 (17)	−0.0075 (15)	0.0014 (14)	−0.0059 (15)
C15	0.0179 (19)	0.0188 (19)	0.0148 (17)	−0.0083 (15)	−0.0002 (14)	−0.0030 (16)
C16	0.0190 (19)	0.0171 (18)	0.0169 (18)	−0.0079 (15)	−0.0026 (15)	−0.0033 (16)
C17	0.0137 (18)	0.022 (2)	0.0219 (19)	−0.0067 (15)	0.0010 (15)	−0.0091 (17)
C18	0.0178 (19)	0.021 (2)	0.0178 (18)	−0.0089 (16)	0.0025 (15)	−0.0061 (16)
C19	0.0181 (19)	0.025 (2)	0.0191 (18)	−0.0100 (17)	−0.0027 (15)	−0.0019 (17)
C20	0.024 (2)	0.023 (2)	0.0174 (18)	−0.0107 (17)	−0.0022 (16)	−0.0010 (17)
C21	0.020 (2)	0.038 (3)	0.0194 (19)	−0.0142 (19)	−0.0037 (16)	−0.0041 (19)
C22	0.026 (2)	0.033 (2)	0.0197 (19)	−0.0184 (19)	−0.0054 (17)	−0.0001 (18)
C23	0.0168 (19)	0.0189 (19)	0.0176 (18)	−0.0053 (15)	−0.0012 (15)	−0.0052 (16)
C24	0.019 (2)	0.035 (2)	0.0193 (19)	−0.0109 (18)	0.0050 (16)	−0.0003 (19)
C25	0.049 (3)	0.045 (3)	0.036 (3)	−0.012 (3)	0.023 (3)	−0.013 (3)
O1W	0.041 (2)	0.0298 (18)	0.044 (2)	−0.0130 (16)	−0.0025 (17)	−0.0144 (17)
O2W	0.047 (2)	0.0273 (18)	0.0373 (19)	−0.0107 (16)	−0.0111 (17)	−0.0079 (16)
O3W	0.032 (2)	0.063 (3)	0.049 (2)	−0.0019 (19)	−0.0005 (17)	−0.039 (2)

Geometric parameters (Å, °)

Zn1—O2	1.962 (3)	C5—H5A	0.9300
Zn1—O3^{i}	1.969 (3)	C6—H6A	0.9300
Zn1—O7	1.970 (3)	C10—C11	1.371 (6)
Zn1—O9	1.998 (3)	C10—C14	1.417 (6)
Zn1—O3	2.307 (3)	C10—C23	1.501 (5)
F1—C17	1.351 (5)	C11—H11A	0.9300
O1—C8	1.236 (6)	C12—C15	1.402 (5)
O2—C8	1.277 (5)	C12—C13	1.403 (5)
O3—C7	1.289 (5)	C13—C18	1.406 (6)
O3—Zn1^{i}	1.969 (3)	C13—C14	1.456 (5)
O4—C7	1.219 (5)	C15—C16	1.383 (6)

O5—C9	1.221 (6)	C15—H15A	0.9300
O6—C9	1.302 (6)	C16—C17	1.423 (6)
O6—H6B	0.8200	C17—C18	1.355 (6)
O7—C23	1.267 (5)	C18—H18A	0.9300
O8—C23	1.242 (5)	C19—C20	1.523 (6)
O9—C14	1.274 (5)	C19—H19A	0.9700
N1—C11	1.335 (5)	C19—H19B	0.9700
N1—C12	1.387 (5)	C20—H20A	0.9700
N1—C24	1.480 (5)	C20—H20B	0.9700
N2—C16	1.392 (5)	C21—C22	1.511 (6)
N2—C19	1.466 (5)	C21—H21A	0.9700
N2—C22	1.474 (5)	C21—H21B	0.9700
N3—C20	1.475 (6)	C22—H22A	0.9700
N3—C21	1.481 (6)	C22—H22B	0.9700
N3—H3B	0.9000	C24—C25	1.492 (8)
N3—H3C	0.9000	C24—H24A	0.9700
C1—C6	1.392 (6)	C24—H24B	0.9700
C1—C2	1.404 (6)	C25—H25A	0.9600
C1—C8	1.513 (6)	C25—H25B	0.9600
C2—C3	1.397 (6)	C25—H25C	0.9600
C2—C7	1.498 (6)	O1W—H1	0.8503
C3—C4	1.380 (6)	O1W—H2	0.8500
C3—H3A	0.9300	O2W—H3	0.8500
C4—C5	1.392 (7)	O2W—H4	0.8499
C4—C9	1.485 (6)	O3W—H6	0.8500
C5—C6	1.373 (7)	O3W—H5	0.8643
O2—Zn1—O3^{i}	121.12 (14)	N1—C12—C13	118.1 (3)
O2—Zn1—O7	101.54 (14)	C15—C12—C13	120.9 (4)
O3^{i}—Zn1—O7	101.61 (14)	C12—C13—C18	117.9 (3)
O2—Zn1—O9	116.22 (13)	C12—C13—C14	122.0 (4)
O3^{i}—Zn1—O9	116.25 (13)	C18—C13—C14	120.1 (4)
O7—Zn1—O9	91.84 (13)	O9—C14—C10	125.6 (4)
O2—Zn1—O3	80.92 (13)	O9—C14—C13	118.7 (4)
O3^{i}—Zn1—O3	76.93 (13)	C10—C14—C13	115.7 (3)
O7—Zn1—O3	177.54 (13)	C16—C15—C12	121.2 (4)
O9—Zn1—O3	87.08 (12)	C16—C15—H15A	119.4
C8—O2—Zn1	124.5 (3)	C12—C15—H15A	119.4
C7—O3—Zn1^{i}	123.5 (3)	C15—C16—N2	123.1 (4)
C7—O3—Zn1	116.3 (3)	C15—C16—C17	116.3 (4)
Zn1^{i}—O3—Zn1	103.07 (13)	N2—C16—C17	120.5 (4)
C9—O6—H6B	112.1	F1—C17—C18	118.1 (4)
C23—O7—Zn1	128.9 (3)	F1—C17—C16	118.6 (3)
C14—O9—Zn1	122.5 (3)	C18—C17—C16	123.2 (4)
C11—N1—C12	120.0 (3)	C17—C18—C13	120.0 (4)
C11—N1—C24	117.2 (3)	C17—C18—H18A	120.0
C12—N1—C24	122.9 (3)	C13—C18—H18A	120.0
C16—N2—C19	116.8 (3)	N2—C19—C20	110.6 (3)

C16—N2—C22	116.0 (3)	N2—C19—H19A	109.5
C19—N2—C22	111.1 (3)	C20—C19—H19A	109.5
C20—N3—C21	111.0 (3)	N2—C19—H19B	109.5
C20—N3—H3B	109.4	C20—C19—H19B	109.5
C21—N3—H3B	109.4	H19A—C19—H19B	108.1
C20—N3—H3C	109.4	N3—C20—C19	111.6 (3)
C21—N3—H3C	109.4	N3—C20—H20A	109.3
H3B—N3—H3C	108.0	C19—C20—H20A	109.3
C6—C1—C2	119.4 (4)	N3—C20—H20B	109.3
C6—C1—C8	114.7 (4)	C19—C20—H20B	109.3
C2—C1—C8	125.9 (4)	H20A—C20—H20B	108.0
C3—C2—C1	118.8 (4)	N3—C21—C22	109.6 (4)
C3—C2—C7	117.8 (4)	N3—C21—H21A	109.7
C1—C2—C7	123.4 (4)	C22—C21—H21A	109.7
C4—C3—C2	121.3 (4)	N3—C21—H21B	109.7
C4—C3—H3A	119.3	C22—C21—H21B	109.7
C2—C3—H3A	119.3	H21A—C21—H21B	108.2
C3—C4—C5	119.4 (4)	N2—C22—C21	109.8 (4)
C3—C4—C9	120.1 (4)	N2—C22—H22A	109.7
C5—C4—C9	120.6 (4)	C21—C22—H22A	109.7
C6—C5—C4	120.2 (4)	N2—C22—H22B	109.7
C6—C5—H5A	119.9	C21—C22—H22B	109.7
C4—C5—H5A	119.9	H22A—C22—H22B	108.2
C5—C6—C1	121.0 (4)	O8—C23—O7	123.3 (4)
C5—C6—H6A	119.5	O8—C23—C10	117.3 (4)
C1—C6—H6A	119.5	O7—C23—C10	119.4 (4)
O4—C7—O3	124.8 (4)	N1—C24—C25	111.8 (4)
O4—C7—C2	120.0 (4)	N1—C24—H24A	109.2
O3—C7—C2	115.2 (4)	C25—C24—H24A	109.2
O1—C8—O2	124.3 (4)	N1—C24—H24B	109.2
O1—C8—C1	115.6 (4)	C25—C24—H24B	109.2
O2—C8—C1	119.7 (4)	H24A—C24—H24B	107.9
O5—C9—O6	124.7 (4)	C24—C25—H25A	109.5
O5—C9—C4	121.3 (4)	C24—C25—H25B	109.5
O6—C9—C4	113.9 (4)	H25A—C25—H25B	109.5
C11—C10—C14	119.0 (4)	C24—C25—H25C	109.5
C11—C10—C23	115.3 (4)	H25A—C25—H25C	109.5
C14—C10—C23	125.7 (4)	H25B—C25—H25C	109.5
N1—C11—C10	125.0 (4)	H1—O1W—H2	95.1
N1—C11—H11A	117.5	H3—O2W—H4	102.2
C10—C11—H11A	117.5	H6—O3W—H5	109.3
N1—C12—C15	120.9 (4)		

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

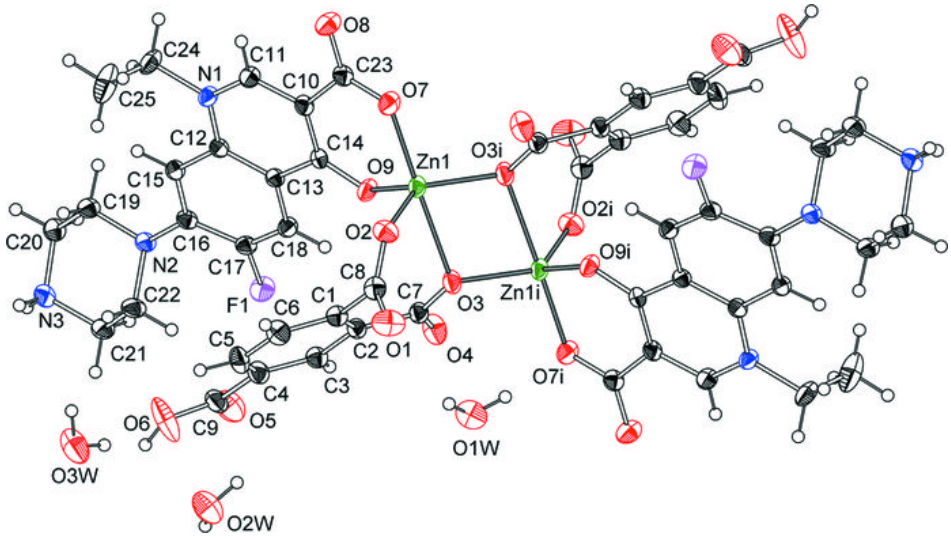
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1···O4	0.85	1.86	2.711 (5)	174
O3W—H6···O2	0.85	2.03	2.799 (5)	151

O1W—H2···O5^{ii}	0.85	2.07	2.789 (5)	142
O2W—H3···O1^{iii}	0.85	1.85	2.688 (5)	167
N3—H3B···O8^{iv}	0.90	1.80	2.696 (5)	177
N3—H3C···O2W^{iv}	0.90	1.93	2.824 (6)	171

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

Fig. 1


O8
C24
C11
N1
C23
C10
O7
C25
C12
C14
Zn1
O3i
C15
C13
O9
C19
O2i
C20
C16
O2
C18
N2
C17
O9i
C8
C22
F1
C6
C1
C7
Zn1i
N3
O3
C5
C2
O1
O4
C21
O7i
C4
C3
O6
C9
O5
O1W
O3W
O2W