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Diaquabis(*N*,*N*-diethylnicotinamide-κ*N*)-bis(4-fluorobenzoato-κ*O*)zinc(II)

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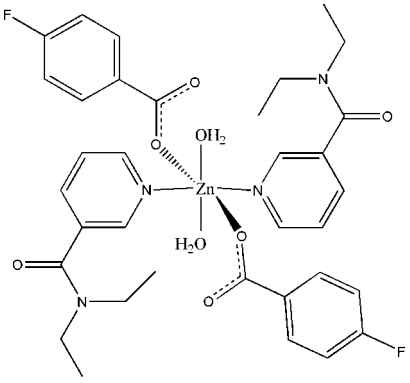
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.140; data-to-parameter ratio = 15.2.

The title Zn^{II} complex, $[Zn(C_7H_4FO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, is centrosymmetric. It contains two 4-fluorobenzoate and two diethylnicotinamide ligands and two water molecules, all ligands being monodentate. The four O atoms in the equatorial plane around the Zn atom form a slightly distorted square-planar arrangement, while the distorted octahedral coordination is completed by the two N atoms in the axial positions. In the crystal structure, O—H···O hydrogen bonds link the molecules into infinite chains.

Related literature

For general background, see: Antolini *et al.* (1982); Nadzhafov *et al.* (1981); Shnulin *et al.* (1981); Antsyshkina *et al.* (1980); Amiraslanov *et al.* (1979); Adiwidjaja *et al.* (1978). For related literature, see: Guseinov *et al.* (1984); Clegg *et al.* (1986*a*,*b*, 1987); Capilla & Aranda (1979); van Niekerk *et al.* (1953); Usubaliev *et al.* (1992); Bigoli *et al.* (1972, 1973*a*,*b*,*c*); Hökelek *et al.* (1995, 1997); Hökelek & Necefoğlu (1996, 1997, 2007*a*,*b*,*c*); Necefoğlu *et al.* (2002); Çaylak, Hökelek & Necefoğlu (2007); Çaylak, Hökelek, Öztürkkan & Necefoğlu (2007).



Experimental

Crystal data

$[Zn(C_7H_4FO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
M_r = 736.10
Triclinic, $P\overline{1}$
a = 7.4261 (2) Å
b = 8.7188 (3) Å
c = 15.0798 (4) Å
α = 98.44 (2)°
β = 95.73 (2)°
γ = 112.94 (3)°
V = 876.1 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.760, T_{max} = 0.891
3830 measured reflections
3547 independent reflections
2934 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.140
S = 1.08
3547 reflections
233 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—O1	2.090 (2)	Zn—N1	2.169 (3)
Zn—O4	2.143 (2)		
O1—Zn—O4	91.98 (10)	O4—Zn—N1	86.54 (10)
O1—Zn—N1	91.17 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H41···O2	0.96 (3)	1.71 (4)	2.654 (4)	167 (4)
O4—H42···O3^{i}	0.93 (4)	1.87 (4)	2.795 (4)	171 (4)

Symmetry code: (i) $-x+1, -y, -z$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2321).

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supporting information

Acta Cryst. (2007). E**63**, m2561–m2562 [https://doi.org/10.1107/S1600536807045382]

Diaquabis(*N*,*N*-diethylnicotinamide-κN)bis(4-fluorobenzoato-κO)zinc(II)

Tuncer Hökelek, Nagihan Çaylak and Hacali Necefoğlu

S1. Comment

Transition metal complexes with biochemical molecules show interesting physical and/or chemical properties, through which they may find applications in biological systems (Antolini *et al.*, 1982). The structure-function-coordination relationships of the arylcarboxylate ion in Zn^{II} complexes of benzoic acid derivatives, depending on the nature and position of the substituted groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of the synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981; Antsyshkina *et al.*, 1980; Amiraslanov *et al.*, 1979; Adiwidjaja *et al.*, 1978).

The solid-state structures of anhydrous zinc(II) carboxylates include one-dimensional (Guseinov *et al.*, 1984; Clegg *et al.*, 1986*a*), two-dimensional (Clegg *et al.*, 1986*b*, 1987) and three-dimensional (Capilla & Aranda, 1979) polymeric motifs of different types, while discerete monomeric complexes with octahedral or tetrahedral coordination geometry are found if water or other donor molecules are coordinated to Zn (van Niekerk *et al.*, 1953; Usubaliev *et al.*, 1992).

N,*N*-Diethylnicotinamide (DENA) is an important respiratory stimulant. The structures of several complexes obtained by reacting divalent transition metal ions with DENA have been determined, including those of $Mn(DENA)_2(NCS)_2$ (Bigoli *et al.*, 1973*b*), $Zn(DENA)_2(NCS)_2(H_2O)_2$ (Bigoli *et al.*, 1973*a*), $Zn_2(DENA)_2(NCS)_4$ (Bigoli *et al.*, 1973*c*), $Cd(DENA)(SCN)_2$ (Bigoli *et al.*, 1972), $Cu_2(DENA)_2(C_6H_5COO)_4$ (Hökelek *et al.*, 1995), $[Zn_2(DENA)_2(C_7H_5O_3)_4].2H_2O$ (Hökelek & Necefoğlu, 1996), $[Co(DENA)_2(C_7H_5O_3)_2(H_2O)_2]$ (Hökelek & Necefoğlu, 1997) and $[Cu(DENA)_2(C_7H_4NO_4)_2(H_2O)_2]$ (Hökelek *et al.*, 1997).

The structure determination of the title compound, (I), a zinc complex with two fluorobenzoate (FB), two diethylnicotinamide (DENA) ligands and two water molecules, was undertaken in order to determine the properties of the FB and DENA ligands and also to compare the results obtained with those reported previously.

Compound (I) is a monomeric complex, with the Zn atom on a centre of symmetry. It contains two FB, two DENA ligands and two water molecules (Fig. 1). All ligands are monodentate. The four O atoms (O1, O4, and the symmetry-related atoms, O1′, O4′) in the equatorial plane around the Zn atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the DENA ligands (N1, N1′) in the axial positions (Table 1 and Fig. 1).

The near equality of the C1—O1 [1.260 (4) Å] and C1—O2 [1.252 (4) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, as in bis(4-hydroxybenzoato-κO)bis(nicotinamide-κN)zinc(II) (Necefoğlu *et al.*, 2002), diaquabis[4-(dimethylamino)benzoato-κO]-(nicotinamide-κN^1)cobalt(II) dihydrate (Hökelek & Necefoğlu, 2007*b*), tetraaquabis[4-(dimethylamino)benzoato-κO]manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*a*), diaquabis[4-(dimethylamino)benzoato-κO]-(nicotinamide-κN^1)manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*c*), diaquabis(4-fluorobenzoato-κO)bis(nicotinamide-κN^1)cobalt(II) (Çaylak, Hökelek & Necefoğlu, 2007) and diaquabis(4-chlorobenzoato-κO)bis(nicotinamide-κN)cobalt(II) (Çaylak, Hökelek, Öztürkkan & Necefoğlu, 2007). This may be due to the intramolecular O—H···O hydrogen bonding of the carboxylate O

atoms (Table 2). The Zn atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by -0.881 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring C2—C7 is 2.80 (33)°, while that between rings C2—C7 and N1/C8—C12 is 78.40 (13)°.

As can be seen from the packing diagram (Fig. 2), the Zn atoms are located at the corners of the unit cell and the molecules of (I) are linked into infinite chains, along the *a* axis, by intermolecular O—H···O hydrogen bonds (Table 2). Dipole-dipole and van der Waals interactions are also effective in the molecular packing.

S2. Experimental

The title compound was prepared by the reaction of $Zn(NO_3)_2$ (1.89 g, 10 mmol) in H_2O (25 ml) and DENA (3.56 g, 20 mmol) in H_2O (25 ml) with sodium *p*-fluorobenzoate (3.24 g, 20 mmol) in H_2O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving colorless single crystals.

S3. Refinement

H atoms of water molecule were located in difference syntheses and refined isotropically [O—H = 0.960 (16) and 0.94 (2) Å and U_{iso}(H) = 0.062 (13) and 0.087 (18) Å^2]. The remaining H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms. The restrains on the O—H bond lengths and H—O—H bond angle of water molecule were applied.

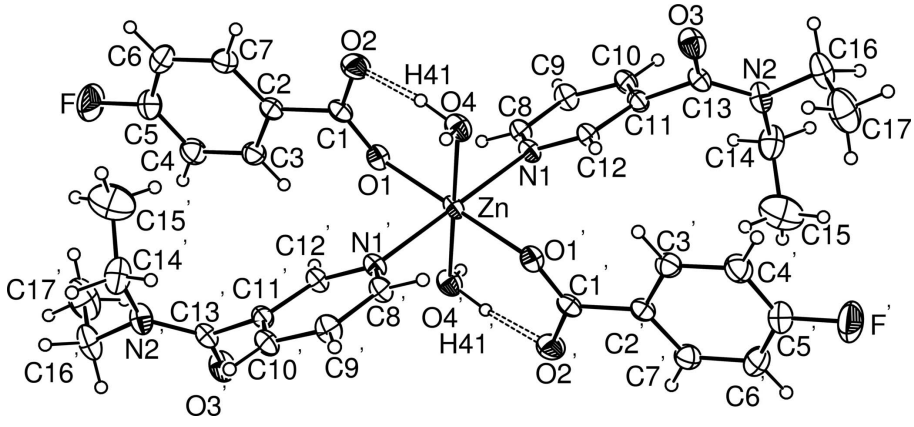

Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Primed atoms are generated by the symmetry operator (-*x*, -*y*, -*z*).

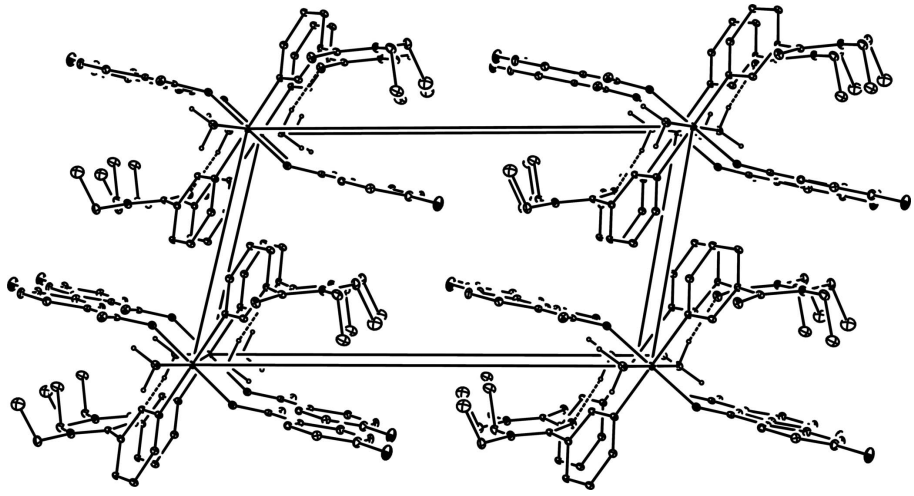

Figure 2

A partial packing diagram of (I), viewed down the *a* axis, showing hydrogen bonds (dashed lines) linking the molecules into chains, where b and c axes are vertical and horizontal, respectively. H atoms not involved in hydrogen bonding are omitted.

Diaquabis(*N*,*N*-diethylnicotinamide-κN)bis(4-fluorobenzoato-κO)zinc(II)

Crystal data

$[Zn(C_7H_4FO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
$M_r = 736.10$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.4261$ (2) Å
$b = 8.7188$ (3) Å
$c = 15.0798$ (4) Å
$\alpha = 98.44$ (2)°
$\beta = 95.73$ (2)°
$\gamma = 112.94$ (3)°
$V = 876.1$ (2) Å^3
$Z = 1$
$F(000) = 384$
$D_x = 1.395$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 3.6$–18.7°
$\mu = 0.77$ mm^{-1}
$T = 298$ K
Rod-shaped, colorless
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Non–profiled ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.760$, $T_{max} = 0.891$
3830 measured reflections
3547 independent reflections
2934 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.6°$
$h = -9 \rightarrow 0$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 18$
3 standard reflections every 120 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.140$
$S = 1.08$
3547 reflections
233 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 0.159P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.0000	0.0000	0.0000	0.0333 (2)
F	−0.3354 (5)	0.3270 (5)	0.4677 (2)	0.0928 (11)
O1	−0.0243 (4)	0.1622 (3)	0.11031 (16)	0.0395 (6)
O2	0.2370 (4)	0.2052 (4)	0.2136 (2)	0.0531 (7)
O3	0.7298 (4)	0.2781 (4)	−0.12884 (19)	0.0521 (7)
O4	0.2728 (4)	0.0115 (4)	0.06928 (18)	0.0435 (6)
H41	0.277 (7)	0.080 (5)	0.1259 (18)	0.062 (13)*
H42	0.274 (9)	−0.089 (4)	0.083 (3)	0.087 (18)*
N1	0.1816 (4)	0.2150 (3)	−0.05431 (19)	0.0344 (6)
N2	0.6281 (5)	0.3228 (4)	−0.2636 (2)	0.0480 (8)
C1	0.0665 (5)	0.1978 (4)	0.1908 (2)	0.0347 (7)
C2	−0.0416 (5)	0.2319 (4)	0.2653 (2)	0.0355 (7)
C3	−0.2285 (5)	0.2311 (4)	0.2447 (2)	0.0398 (8)
H3	−0.2871	0.2087	0.1841	0.048*
C4	−0.3288 (6)	0.2630 (5)	0.3124 (3)	0.0494 (9)
H4	−0.4537	0.2628	0.2984	0.059*
C5	−0.2385 (7)	0.2948 (6)	0.4006 (3)	0.0572 (11)
C6	−0.0556 (7)	0.2952 (6)	0.4250 (3)	0.0577 (11)
H6	0.0004	0.3161	0.4859	0.069*
C7	0.0434 (6)	0.2635 (5)	0.3561 (3)	0.0452 (9)
H7	0.1680	0.2635	0.3709	0.054*
C8	0.1608 (5)	0.3607 (4)	−0.0438 (2)	0.0369 (7)
H8	0.0637	0.3706	−0.0119	0.044*
C9	0.2759 (6)	0.4980 (5)	−0.0779 (3)	0.0416 (8)
H9	0.2578	0.5984	−0.0686	0.050*
C10	0.4202 (5)	0.4829 (4)	−0.1265 (2)	0.0384 (8)
H10	0.4991	0.5727	−0.1511	0.046*
C11	0.4439 (5)	0.3320 (4)	−0.1375 (2)	0.0332 (7)
C12	0.3234 (5)	0.2019 (4)	−0.0995 (2)	0.0342 (7)

H12	0.3414	0.1014	−0.1055	0.041*
C13	0.6110 (5)	0.3076 (4)	−0.1774 (2)	0.0365 (7)
C14	0.4823 (8)	0.3458 (7)	−0.3274 (3)	0.0639 (12)
H14A	0.5514	0.4202	−0.3663	0.077*
H14B	0.4119	0.4005	−0.2933	0.077*
C15	0.3370 (10)	0.1828 (10)	−0.3848 (6)	0.113 (2)
H15A	0.4033	0.1361	−0.4251	0.169*
H15B	0.2355	0.2022	−0.4198	0.169*
H15C	0.2779	0.1045	−0.3467	0.169*
C16	0.8024 (7)	0.3107 (6)	−0.2978 (3)	0.0619 (12)
H16A	0.9172	0.3679	−0.2497	0.074*
H16B	0.8279	0.3705	−0.3477	0.074*
C17	0.7806 (9)	0.1333 (7)	−0.3299 (5)	0.0887 (19)
H17A	0.7677	0.0760	−0.2797	0.133*
H17B	0.8957	0.1359	−0.3547	0.133*
H17C	0.6645	0.0739	−0.3761	0.133*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0261 (3)	0.0353 (3)	0.0398 (3)	0.0099 (2)	0.0119 (2)	0.0154 (2)
F	0.082 (2)	0.142 (3)	0.0599 (17)	0.052 (2)	0.0345 (15)	0.0057 (18)
O1	0.0392 (13)	0.0389 (13)	0.0424 (14)	0.0150 (10)	0.0128 (11)	0.0134 (11)
O2	0.0343 (14)	0.0615 (18)	0.0589 (17)	0.0182 (12)	0.0058 (12)	0.0041 (14)
O3	0.0423 (15)	0.0706 (19)	0.0576 (16)	0.0322 (14)	0.0140 (12)	0.0263 (14)
O4	0.0346 (13)	0.0499 (15)	0.0525 (16)	0.0207 (11)	0.0099 (11)	0.0184 (13)
N1	0.0293 (13)	0.0333 (14)	0.0412 (15)	0.0102 (11)	0.0102 (11)	0.0138 (12)
N2	0.0486 (18)	0.058 (2)	0.0491 (18)	0.0274 (16)	0.0231 (15)	0.0205 (15)
C1	0.0307 (16)	0.0255 (15)	0.0461 (19)	0.0071 (12)	0.0091 (14)	0.0126 (13)
C2	0.0335 (17)	0.0282 (16)	0.0415 (18)	0.0081 (13)	0.0077 (14)	0.0095 (13)
C3	0.0375 (18)	0.0386 (18)	0.0405 (18)	0.0125 (15)	0.0047 (15)	0.0101 (15)
C4	0.041 (2)	0.053 (2)	0.056 (2)	0.0203 (17)	0.0120 (17)	0.0104 (18)
C5	0.056 (2)	0.067 (3)	0.049 (2)	0.024 (2)	0.0216 (19)	0.009 (2)
C6	0.060 (3)	0.074 (3)	0.034 (2)	0.024 (2)	0.0063 (18)	0.0082 (19)
C7	0.0373 (18)	0.049 (2)	0.046 (2)	0.0143 (16)	0.0046 (15)	0.0098 (17)
C8	0.0306 (16)	0.0391 (18)	0.0432 (18)	0.0143 (14)	0.0117 (14)	0.0109 (14)
C9	0.0448 (19)	0.0360 (18)	0.052 (2)	0.0210 (15)	0.0143 (16)	0.0170 (15)
C10	0.0365 (17)	0.0334 (17)	0.0461 (19)	0.0104 (14)	0.0125 (15)	0.0180 (15)
C11	0.0281 (15)	0.0360 (17)	0.0346 (16)	0.0100 (13)	0.0071 (13)	0.0122 (13)
C12	0.0304 (16)	0.0314 (16)	0.0425 (18)	0.0115 (13)	0.0123 (13)	0.0121 (13)
C13	0.0314 (16)	0.0343 (17)	0.0448 (19)	0.0106 (13)	0.0126 (14)	0.0154 (14)
C14	0.077 (3)	0.080 (3)	0.050 (2)	0.042 (3)	0.022 (2)	0.024 (2)
C15	0.072 (4)	0.111 (6)	0.143 (7)	0.028 (4)	0.004 (4)	0.021 (5)
C16	0.061 (3)	0.065 (3)	0.076 (3)	0.029 (2)	0.042 (2)	0.032 (2)
C17	0.095 (4)	0.074 (4)	0.125 (5)	0.049 (3)	0.061 (4)	0.034 (3)

Geometric parameters (Å, º)

Zn—O1	2.090 (2)	C6—H6	0.9300
Zn—O1^{i}	2.090 (2)	C7—C6	1.387 (6)
Zn—O4	2.143 (2)	C7—H7	0.9300
Zn—O4^{i}	2.143 (2)	C8—H8	0.9300
Zn—N1^{i}	2.169 (3)	C9—C8	1.378 (5)
Zn—N1	2.169 (3)	C9—C10	1.393 (5)
F—C5	1.357 (5)	C9—H9	0.9300
O1—C1	1.260 (4)	C10—H10	0.9300
O2—C1	1.252 (4)	C11—C10	1.383 (5)
O3—C13	1.218 (4)	C11—C12	1.385 (4)
O4—H41	0.960 (16)	C11—C13	1.504 (5)
O4—H42	0.94 (2)	C12—H12	0.9300
N1—C8	1.327 (4)	C14—C15	1.480 (8)
N1—C12	1.341 (4)	C14—H14A	0.9700
N2—C13	1.340 (5)	C14—H14B	0.9700
N2—C14	1.468 (6)	C15—H15A	0.9600
N2—C16	1.476 (5)	C15—H15B	0.9600
C2—C1	1.504 (5)	C15—H15C	0.9600
C2—C3	1.388 (5)	C16—C17	1.490 (7)
C3—H3	0.9300	C16—H16A	0.9700
C2—C7	1.390 (5)	C16—H16B	0.9700
C3—C4	1.380 (5)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C4—C5	1.366 (6)	C17—H17C	0.9600
C5—C6	1.370 (7)		
O1—Zn—O1^{i}	180.00 (14)	C6—C7—H7	119.6
O1—Zn—O4	91.98 (10)	C2—C7—H7	119.6
O1^{i}—Zn—O4	88.02 (10)	N1—C8—C9	123.3 (3)
O1—Zn—O4^{i}	88.02 (10)	N1—C8—H8	118.4
O1^{i}—Zn—O4^{i}	91.98 (10)	C9—C8—H8	118.4
O4—Zn—O4^{i}	180.00 (15)	C8—C9—C10	118.5 (3)
O1—Zn—N1^{i}	88.83 (10)	C8—C9—H9	120.7
O1^{i}—Zn—N1^{i}	91.17 (10)	C10—C9—H9	120.7
O4—Zn—N1^{i}	93.46 (10)	C11—C10—C9	118.8 (3)
O4^{i}—Zn—N1^{i}	86.54 (10)	C11—C10—H10	120.6
O1—Zn—N1	91.17 (10)	C9—C10—H10	120.6
O1^{i}—Zn—N1	88.83 (10)	C10—C11—C12	118.6 (3)
O4—Zn—N1	86.54 (10)	C10—C11—C13	123.8 (3)
O4^{i}—Zn—N1	93.46 (10)	C12—C11—C13	117.0 (3)
N1^{i}—Zn—N1	180.00 (15)	N1—C12—C11	122.7 (3)
C1—O1—Zn	126.6 (2)	N1—C12—H12	118.6
Zn—O4—H41	97 (3)	C11—C12—H12	118.6
Zn—O4—H42	118 (4)	O3—C13—N2	122.0 (3)
H41—O4—H42	106 (3)	O3—C13—C11	118.3 (3)
C8—N1—C12	118.1 (3)	N2—C13—C11	119.7 (3)

C8—N1—Zn	122.9 (2)	N2—C14—C15	112.4 (5)
C12—N1—Zn	118.9 (2)	N2—C14—H14A	109.1
C13—N2—C14	124.5 (3)	C15—C14—H14A	109.1
C13—N2—C16	117.9 (3)	N2—C14—H14B	109.1
C14—N2—C16	117.6 (3)	C15—C14—H14B	109.1
O2—C1—O1	125.5 (3)	H14A—C14—H14B	107.8
O2—C1—C2	117.8 (3)	C14—C15—H15A	109.5
O1—C1—C2	116.7 (3)	C14—C15—H15B	109.5
C3—C2—C7	118.8 (3)	H15A—C15—H15B	109.5
C3—C2—C1	120.7 (3)	C14—C15—H15C	109.5
C7—C2—C1	120.5 (3)	H15A—C15—H15C	109.5
C4—C3—C2	121.3 (3)	H15B—C15—H15C	109.5
C4—C3—H3	119.4	N2—C16—C17	114.4 (4)
C2—C3—H3	119.4	N2—C16—H16A	108.7
C5—C4—C3	117.8 (4)	C17—C16—H16A	108.7
C5—C4—H4	121.1	N2—C16—H16B	108.7
C3—C4—H4	121.1	C17—C16—H16B	108.7
F—C5—C4	118.3 (4)	H16A—C16—H16B	107.6
F—C5—C6	118.2 (4)	C16—C17—H17A	109.5
C4—C5—C6	123.6 (4)	C16—C17—H17B	109.5
C5—C6—C7	117.9 (4)	H17A—C17—H17B	109.5
C5—C6—H6	121.1	C16—C17—H17C	109.5
C7—C6—H6	121.1	H17A—C17—H17C	109.5
C6—C7—C2	120.7 (4)	H17B—C17—H17C	109.5

O4—Zn—O1—C1	−17.4 (3)	C14—N2—C16—C17	−95.3 (5)
O4^{i}—Zn—O1—C1	162.6 (3)	C3—C2—C1—O2	177.9 (3)
N1^{i}—Zn—O1—C1	76.0 (3)	C7—C2—C1—O2	−2.5 (5)
N1—Zn—O1—C1	−104.0 (3)	C3—C2—C1—O1	−2.8 (5)
O1—Zn—N1—C8	−31.8 (3)	C7—C2—C1—O1	176.7 (3)
O1^{i}—Zn—N1—C8	148.2 (3)	C7—C2—C3—C4	0.7 (5)
O4—Zn—N1—C8	−123.7 (3)	C1—C2—C3—C4	−179.7 (3)
O4^{i}—Zn—N1—C8	56.3 (3)	C3—C2—C7—C6	−0.5 (6)
O1—Zn—N1—C12	147.2 (3)	C1—C2—C7—C6	179.9 (4)
O1^{i}—Zn—N1—C12	−32.8 (3)	C2—C3—C4—C5	−0.2 (6)
O4—Zn—N1—C12	55.3 (3)	C3—C4—C5—F	179.7 (4)
O4^{i}—Zn—N1—C12	−124.7 (3)	C3—C4—C5—C6	−0.6 (7)
Zn—O1—C1—O2	31.6 (5)	F—C5—C6—C7	−179.5 (4)
Zn—O1—C1—C2	−147.5 (2)	C4—C5—C6—C7	0.8 (7)
C12—N1—C8—C9	0.7 (5)	C2—C7—C6—C5	−0.2 (7)
Zn—N1—C8—C9	179.8 (3)	C10—C9—C8—N1	0.6 (6)
C8—N1—C12—C11	−1.9 (5)	C8—C9—C10—C11	−0.9 (5)
Zn—N1—C12—C11	179.0 (2)	C12—C11—C10—C9	−0.1 (5)
C14—N2—C13—O3	175.3 (4)	C13—C11—C10—C9	−171.5 (3)
C16—N2—C13—O3	−2.8 (6)	C10—C11—C12—N1	1.6 (5)
C14—N2—C13—C11	−6.4 (6)	C13—C11—C12—N1	173.6 (3)
C16—N2—C13—C11	175.5 (3)	C10—C11—C13—O3	115.7 (4)
C13—N2—C14—C15	−94.3 (5)	C12—C11—C13—O3	−55.8 (5)

C16—N2—C14—C15	83.8 (6)	C10—C11—C13—N2	−62.7 (5)
C13—N2—C16—C17	82.9 (6)	C12—C11—C13—N2	125.8 (4)

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41···O2	0.96 (3)	1.71 (4)	2.654 (4)	167 (4)
O4—H42···O3^{ii}	0.93 (4)	1.87 (4)	2.795 (4)	171 (4)

Symmetry code: (ii) −*x*+1, −*y*, −*z*.