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Diaquabis(4-chlorobenzoato-κO)bis(*N*,*N*-diethylnicotinamide-κN^1)-manganese(II)

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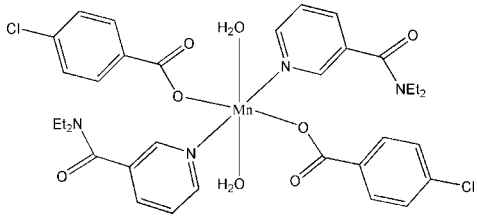
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.009 Å; R factor = 0.081; wR factor = 0.255; data-to-parameter ratio = 16.7.

The title compound, $[Mn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, is a monomeric complex with the Mn^{II} atom lying on an inversion center. It contains two 4-chlorobenzoate and two diethylnicotinamide ligands and two water molecules, all of which are monodentate. The four O atoms in the equatorial plane around the Mn atom form a slightly distorted square-planar arrangement, while the distorted octahedral geometry is completed by two N atoms in the axial positions. In the crystal structure, O—H···O hydrogen bonds link the molecules into an infinite chain.

Related literature

For general background, see: Adiwidjaja *et al.* (1978); Amiraslanov *et al.* (1979); Antolini *et al.* (1982); Antsyshkina *et al.* (1980); Nadzhafov *et al.* (1981); Shnulin *et al.* (1981). For related structures, see: Hökelek *et al.* (1995, 1997); Hökelek *et al.* (2007); Hökelek & Necefoğlu (1996, 1997, 2007).



Experimental

Crystal data

$[Mn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
M_r = 758.54
Triclinic, $P\overline{1}$
a = 7.3552 (1) Å
b = 8.6465 (2) Å
c = 15.9847 (3) Å
α = 84.500 (16)°
β = 78.616 (17)°
γ = 68.154 (17)°
V = 924.73 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 294 (2) K
0.30 × 0.15 × 0.10 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.902, T_{max} = 0.950
4010 measured reflections
3752 independent reflections
2604 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.254
S = 1.04
3752 reflections
225 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn—O1	2.141 (3)	Mn—N1	2.281 (4)
Mn—O4	2.205 (4)		
O1^i—Mn—O4	90.38 (14)	O4—Mn—N1^i	92.72 (14)
O1—Mn—O4	89.62 (14)	O1—Mn—N1	87.77 (14)
O1—Mn—N1^i	92.23 (14)	O4—Mn—N1	87.28 (14)

Symmetry code: (i) $-x, -y+2, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H41···O2^i	0.99 (4)	1.71 (5)	2.670 (6)	162 (7)
O4—H42···O3^{ii}	0.93 (5)	1.85 (5)	2.766 (6)	168 (7)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (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: HY2120).

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Diaquabis(4-chlorobenzoato-κO)bis(*N*,*N*-diethylnicotinamide-κN^1)manganese(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 structural functions and coordination relationships of the arylcarboxylate ions in manganese(II) complexes of benzoic acid derivatives may be changed, 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 (Adiwidjaja *et al.*, 1978; Amiraslanov *et al.*, 1979; Antsyshkina *et al.*, 1980; Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981).

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 in our laboratory, including those of $Cu_2(DENA)_2(C_6H_5COO)_4$, (II), (Hökelek *et al.*, 1995), $[Zn_2(DENA)_2(C_7H_5O_3)_4].2H_2O$, (III), (Hökelek & Necefoğlu, 1996), $[Co(DENA)_2(C_7H_5O_3)_2(H_2O)_2]$, (IV), (Hökelek & Necefoğlu, 1997), $[Cu(DENA)_2(C_7H_4NO_4)_2(H_2O)_2]$, (V), (Hökelek *et al.*, 1997) and $[Zn(DENA)_2(C_7H_4FO_2)_2(H_2O)_2]$, (VI), (Hökelek *et al.*, 2007). The structure determination of the title compound, (I), a manganese(II) complex with two chlorobenzoate (CB), two DENA ligands and two water molecules, was undertaken in order to determine the properties of the CB and DENA ligands and also to compare the results obtained with those reported previously.

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

The near equality of the C1—O1 [1.256 (6) Å] and C1—O2 [1.245 (6) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, and may be compared with the corresponding distances: 1.259 (9) and 1.273 (9) Å in (II), 1.279 (4) and 1.246 (4) Å in (III), 1.251 (6) and 1.254 (7) Å in (IV), 1.278 (3) and 1.246 (3) Å in (V) and 1.265 (6) and 1.275 (6) Å in $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2H_2O$, (VII), (Hökelek & Necefoğlu, 2007). This may be due to the intramolecular O—H···O hydrogen bond involving the carboxylate O atom (Table 2). In (I), the average Mn—O bond length is 2.173 (3) Å. The Mn atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by 0.890 (1) Å; this is reported as 2.185 (4) and 1.365 (3) Å, respectively, in (VII). The dihedral angle between the planar carboxylate group and the benzene ring A (C2 to C7) is 3.0 (4)°, while that between rings A and B (N1/C8 to C12) is 81.0 (4)°.

As can be seen from the packing diagram (Fig. 2), the Mn 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).

S2. Experimental

The title compound was prepared by the reaction of $Mn(NO_3)_2$ (1.79 g, 10 mmol) in H_2O (25 ml) and DENA (3.56 g, 20 mmol) in H_2O (25 ml) with sodium *p*-chlorobenzoate (3.57 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 the water molecule were located in a difference Fourier map and refined isotropically. The remaining H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (methylene) and 0.96 Å (methyl) and with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.0 for H atoms of C15 methyl, 1.5 for H atoms of C17 methyl, and 1.2 for other H atoms. The restrains on the C14—C15 bond length and O—H bond lengths and H—O—H bond angle of water molecule were applied. The highest residual electron density was found 0.92 Å from H15B and the deepest hole 0.14 Å from C15.

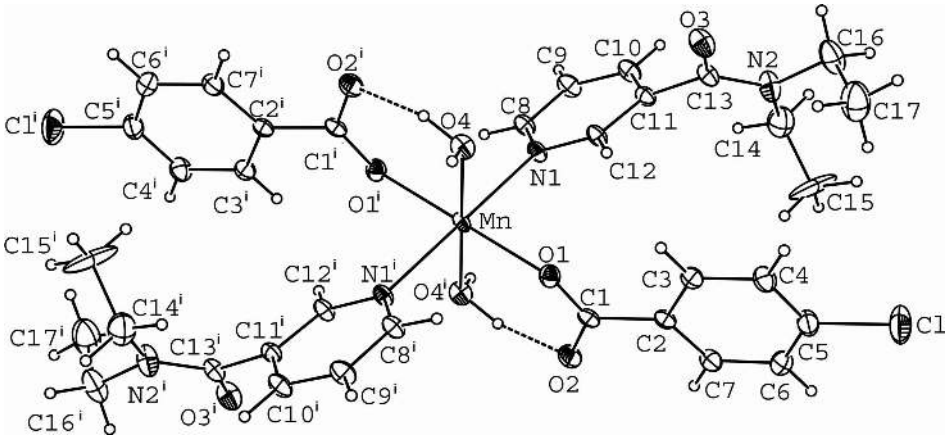

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 20% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) -*x*, 2 - *y*, -*z*.]

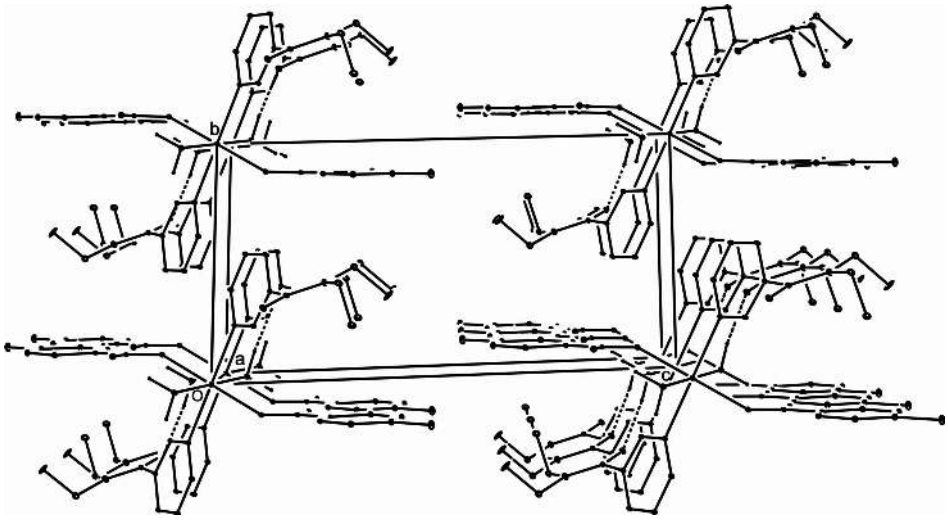

Figure 2

A packing diagram of the title compound, viewed down the *a*-axis, showing hydrogen bonds (dashed lines) linking the molecules into chains. H atoms not involved in hydrogen bonds have been omitted for clarity.

Diaquabis(4-chlorobenzoato-κO)bis(*N*,*N*-diethylnicotinamide-κN^1)manganese(II)

Crystal data

$[Mn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$
$M_r = 758.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3552$ (1) Å
$b = 8.6465$ (2) Å
$c = 15.9847$ (3) Å
$\alpha = 84.500$ (16)°
$\beta = 78.616$ (17)°
$\gamma = 68.154$ (17)°
$V = 924.73$ (12) Å^3
$Z = 1$
$F(000) = 395$
$D_x = 1.362$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 5.2$–11.6°
$\mu = 0.56$ mm^{-1}
$T = 294$ K
Block, colorless
0.30 × 0.15 × 0.10 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.902$, $T_{max} = 0.950$
4010 measured reflections
3752 independent reflections
2604 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 26.3°$, $\theta_{min} = 3.0°$
$h = -8 \rightarrow 9$
$k = 0 \rightarrow 10$
$l = -19 \rightarrow 19$
3 standard reflections every 120 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.080$
$wR(F^2) = 0.254$
$S = 1.04$
3752 reflections
225 parameters
5 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

$w = 1/[\sigma^2(F_o^2) + (0.1471P)^2 + 1.5562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.26$ e Å^{-3}
$\Delta\rho_{min} = -1.31$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn	0.0000	1.0000	0.0000	0.0323 (3)
Cl	−0.7397 (3)	0.8445 (3)	0.46709 (13)	0.0925 (7)
O1	−0.1119 (5)	0.8758 (4)	0.1086 (2)	0.0408 (8)
O2	0.0744 (5)	0.8690 (5)	0.2036 (3)	0.0508 (10)
O3	−0.8388 (6)	1.3270 (5)	0.1267 (3)	0.0576 (11)
O4	−0.2247 (6)	0.9829 (5)	−0.0681 (2)	0.0463 (9)
H41	−0.195 (10)	1.042 (7)	−0.122 (2)	0.07 (2)*
H42	−0.221 (12)	0.880 (5)	−0.083 (4)	0.08 (2)*
N1	−0.2326 (6)	1.2447 (5)	0.0532 (3)	0.0360 (9)
N2	−0.8349 (8)	1.4183 (8)	0.2506 (4)	0.0649 (15)
C1	−0.0808 (7)	0.8688 (6)	0.1836 (3)	0.0366 (11)
C2	−0.2462 (7)	0.8636 (5)	0.2547 (3)	0.0350 (10)
C3	−0.4206 (7)	0.8580 (6)	0.2372 (3)	0.0381 (11)
H3	−0.4358	0.8589	0.1807	0.046*
C4	−0.5733 (8)	0.8509 (7)	0.3024 (4)	0.0487 (13)
H4	−0.6898	0.8463	0.2904	0.058*
C5	−0.5477 (9)	0.8509 (8)	0.3850 (4)	0.0525 (14)
C6	−0.3789 (9)	0.8586 (8)	0.4047 (4)	0.0533 (14)
H6	−0.3655	0.8585	0.4613	0.064*
C7	−0.2282 (8)	0.8665 (7)	0.3392 (3)	0.0434 (12)
H7	−0.1138	0.8739	0.3520	0.052*
C8	−0.2050 (7)	1.3893 (6)	0.0424 (3)	0.0390 (11)
H8	−0.0855	1.3917	0.0107	0.047*
C9	−0.3452 (8)	1.5356 (6)	0.0760 (4)	0.0461 (13)
H9	−0.3203	1.6343	0.0676	0.055*
C10	−0.5227 (8)	1.5332 (6)	0.1223 (4)	0.0442 (13)
H10	−0.6197	1.6304	0.1458	0.053*
C11	−0.5554 (7)	1.3848 (6)	0.1334 (3)	0.0359 (11)
C12	−0.4080 (7)	1.2446 (6)	0.0965 (3)	0.0380 (11)
H12	−0.4315	1.1453	0.1020	0.046*
C13	−0.7519 (7)	1.3715 (6)	0.1710 (3)	0.0413 (12)
C14	−0.7427 (13)	1.4762 (10)	0.3087 (5)	0.080 (2)
H14A	−0.6247	1.4935	0.2770	0.096*
H14B	−0.8350	1.5823	0.3318	0.096*
C15	−0.6883 (17)	1.3572 (14)	0.3785 (7)	0.132
H15A	−0.6290	1.3989	0.4151	0.132*
H15B	−0.5949	1.2527	0.3558	0.132*
H15C	−0.8052	1.3412	0.4106	0.132*
C16	−1.0402 (11)	1.4197 (10)	0.2815 (6)	0.080 (2)

H16A	−1.1031	1.4942	0.3291	0.096*
H16B	−1.1177	1.4616	0.2362	0.096*
C17	−1.0391 (16)	1.2541 (11)	0.3085 (7)	0.107 (3)
H17A	−1.1734	1.2589	0.3272	0.160*
H17B	−0.9659	1.2137	0.3546	0.160*
H17C	−0.9773	1.1802	0.2614	0.160*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn	0.0261 (5)	0.0275 (5)	0.0373 (6)	−0.0030 (4)	−0.0004 (4)	−0.0107 (4)
Cl	0.0696 (12)	0.144 (2)	0.0638 (12)	−0.0517 (13)	0.0190 (9)	−0.0096 (12)
O1	0.043 (2)	0.0384 (19)	0.0390 (19)	−0.0133 (16)	−0.0033 (15)	−0.0072 (14)
O2	0.034 (2)	0.061 (3)	0.057 (2)	−0.0162 (18)	−0.0097 (17)	−0.0010 (19)
O3	0.043 (2)	0.066 (3)	0.070 (3)	−0.022 (2)	−0.0078 (19)	−0.022 (2)
O4	0.043 (2)	0.046 (2)	0.054 (2)	−0.0195 (17)	−0.0090 (17)	−0.0081 (18)
N1	0.030 (2)	0.026 (2)	0.046 (2)	−0.0054 (16)	−0.0002 (17)	−0.0086 (16)
N2	0.052 (3)	0.079 (4)	0.061 (3)	−0.026 (3)	0.011 (2)	−0.024 (3)
C1	0.031 (2)	0.022 (2)	0.049 (3)	−0.0010 (18)	−0.007 (2)	−0.0055 (19)
C2	0.034 (2)	0.022 (2)	0.044 (3)	−0.0032 (18)	−0.006 (2)	−0.0050 (18)
C3	0.037 (3)	0.033 (3)	0.043 (3)	−0.012 (2)	−0.007 (2)	−0.005 (2)
C4	0.036 (3)	0.058 (3)	0.055 (3)	−0.021 (3)	−0.005 (2)	−0.005 (3)
C5	0.044 (3)	0.055 (3)	0.051 (3)	−0.015 (3)	0.005 (3)	−0.005 (3)
C6	0.055 (3)	0.064 (4)	0.038 (3)	−0.018 (3)	−0.006 (2)	−0.001 (3)
C7	0.036 (3)	0.045 (3)	0.047 (3)	−0.010 (2)	−0.008 (2)	−0.008 (2)
C8	0.032 (2)	0.032 (2)	0.051 (3)	−0.009 (2)	−0.005 (2)	−0.009 (2)
C9	0.042 (3)	0.030 (3)	0.066 (4)	−0.012 (2)	−0.007 (3)	−0.009 (2)
C10	0.040 (3)	0.027 (2)	0.059 (3)	−0.003 (2)	−0.005 (2)	−0.018 (2)
C11	0.031 (2)	0.032 (2)	0.040 (3)	−0.0040 (19)	−0.0066 (19)	−0.0103 (19)
C12	0.030 (2)	0.028 (2)	0.050 (3)	−0.0054 (19)	0.000 (2)	−0.010 (2)
C13	0.031 (2)	0.038 (3)	0.051 (3)	−0.007 (2)	−0.003 (2)	−0.013 (2)
C14	0.085 (5)	0.078 (5)	0.072 (5)	−0.029 (4)	−0.002 (4)	−0.009 (4)
C15	0.180	0.156	0.138	−0.130	−0.127	0.126
C16	0.060 (4)	0.067 (5)	0.098 (6)	−0.015 (4)	0.018 (4)	−0.026 (4)
C17	0.116 (8)	0.071 (6)	0.112 (7)	−0.031 (5)	0.030 (6)	−0.014 (5)

Geometric parameters (Å, º)

Mn—O1^{i}	2.141 (3)	C7—C6	1.383 (8)
Mn—O1	2.141 (3)	C7—H7	0.9300
Mn—O4	2.205 (4)	C8—H8	0.9300
Mn—O4^{i}	2.205 (4)	C9—C8	1.376 (7)
Mn—N1^{i}	2.281 (4)	C9—H9	0.9300
Mn—N1	2.281 (4)	C10—C9	1.373 (8)
Cl—C5	1.741 (6)	C10—H10	0.9300
O1—C1	1.256 (6)	C11—C12	1.378 (6)
O2—C1	1.245 (6)	C11—C10	1.380 (7)
O3—C13	1.214 (6)	C12—H12	0.9300

O4—H41	0.99 (4)	C13—N2	1.328 (7)
O4—H42	0.93 (5)	C13—C11	1.494 (7)
N1—C8	1.330 (6)	C14—C15	1.453 (9)
N1—C12	1.339 (6)	C14—H14A	0.9700
N2—C14	1.471 (10)	C14—H14B	0.9700
N2—C16	1.489 (9)	C15—H15A	0.9600
C2—C3	1.384 (7)	C15—H15B	0.9600
C2—C7	1.387 (7)	C15—H15C	0.9600
C2—C1	1.502 (7)	C16—C17	1.453 (11)
C3—H3	0.9300	C16—H16A	0.9700
C4—C5	1.369 (8)	C16—H16B	0.9700
C4—C3	1.388 (7)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—C6	1.366 (9)	C17—H17C	0.9600
C6—H6	0.9300		

O1^{i}—Mn—O1	180.000 (1)	C6—C7—H7	119.7
O1^{i}—Mn—O4	90.38 (14)	C2—C7—H7	119.7
O1—Mn—O4	89.62 (14)	N1—C8—C9	122.9 (5)
O1^{i}—Mn—O4^{i}	89.62 (14)	N1—C8—H8	118.5
O1—Mn—O4^{i}	90.38 (14)	C9—C8—H8	118.5
O4—Mn—O4^{i}	180.00 (16)	C10—C9—C8	118.8 (5)
O1^{i}—Mn—N1^{i}	87.77 (14)	C10—C9—H9	120.6
O1—Mn—N1^{i}	92.23 (14)	C8—C9—H9	120.6
O4—Mn—N1^{i}	92.72 (14)	C9—C10—C11	119.2 (4)
O4^{i}—Mn—N1^{i}	87.28 (14)	C9—C10—H10	120.4
O1^{i}—Mn—N1	92.23 (14)	C11—C10—H10	120.4
O1—Mn—N1	87.77 (14)	C12—C11—C10	118.2 (5)
O4—Mn—N1	87.28 (14)	C12—C11—C13	117.2 (4)
O4^{i}—Mn—N1	92.72 (14)	C10—C11—C13	123.8 (4)
N1^{i}—Mn—N1	180.0	N1—C12—C11	123.0 (5)
C1—O1—Mn	127.5 (3)	N1—C12—H12	118.5
Mn—O4—H41	100 (4)	C11—C12—H12	118.5
Mn—O4—H42	121 (5)	O3—C13—N2	120.8 (5)
H41—O4—H42	107 (4)	O3—C13—C11	119.4 (5)
C8—N1—C12	117.7 (4)	N2—C13—C11	119.7 (5)
C8—N1—Mn	123.5 (3)	C15—C14—N2	111.7 (7)
C12—N1—Mn	118.8 (3)	C15—C14—H14A	109.3
C13—N2—C14	124.8 (6)	N2—C14—H14A	109.3
C13—N2—C16	117.3 (6)	C15—C14—H14B	109.3
C14—N2—C16	117.8 (6)	N2—C14—H14B	109.3
O2—C1—O1	125.2 (5)	H14A—C14—H14B	107.9
O2—C1—C2	117.6 (5)	C14—C15—H15A	109.5
O1—C1—C2	117.1 (4)	C14—C15—H15B	109.5
C3—C2—C7	118.6 (5)	H15A—C15—H15B	109.5
C3—C2—C1	120.8 (5)	C14—C15—H15C	109.5
C7—C2—C1	120.6 (5)	H15A—C15—H15C	109.5
C2—C3—C4	121.2 (5)	H15B—C15—H15C	109.5

C2—C3—H3	119.4	C17—C16—N2	111.5 (7)
C4—C3—H3	119.4	C17—C16—H16A	109.3
C5—C4—C3	118.2 (5)	N2—C16—H16A	109.3
C5—C4—H4	120.9	C17—C16—H16B	109.3
C3—C4—H4	120.9	N2—C16—H16B	109.3
C6—C5—C4	122.2 (5)	H16A—C16—H16B	108.0
C6—C5—Cl	119.3 (5)	C16—C17—H17A	109.5
C4—C5—Cl	118.5 (5)	C16—C17—H17B	109.5
C5—C6—C7	119.1 (5)	H17A—C17—H17B	109.5
C5—C6—H6	120.5	C16—C17—H17C	109.5
C7—C6—H6	120.5	H17A—C17—H17C	109.5
C6—C7—C2	120.6 (5)	H17B—C17—H17C	109.5
O4—Mn—O1—C1	−164.0 (4)	C7—C2—C1—O2	2.8 (7)
O4^{i}—Mn—O1—C1	16.0 (4)	C3—C2—C1—O1	3.3 (6)
N1^{i}—Mn—O1—C1	103.3 (4)	C7—C2—C1—O1	−175.9 (4)
N1—Mn—O1—C1	−76.7 (4)	C7—C2—C3—C4	−1.7 (7)
O1^{i}—Mn—N1—C8	−32.0 (4)	C1—C2—C3—C4	179.1 (5)
O1—Mn—N1—C8	148.0 (4)	C5—C4—C3—C2	0.5 (8)
O4—Mn—N1—C8	−122.3 (4)	C3—C4—C5—C6	0.4 (9)
O4^{i}—Mn—N1—C8	57.7 (4)	C3—C4—C5—Cl	179.2 (4)
O1^{i}—Mn—N1—C12	146.8 (4)	C4—C5—C6—C7	−0.1 (10)
O1—Mn—N1—C12	−33.2 (4)	Cl—C5—C6—C7	−178.9 (5)
O4—Mn—N1—C12	56.6 (4)	C2—C7—C6—C5	−1.2 (9)
O4^{i}—Mn—N1—C12	−123.4 (4)	C10—C9—C8—N1	−0.6 (9)
Mn—O1—C1—O2	−31.6 (7)	C11—C10—C9—C8	−0.2 (8)
Mn—O1—C1—C2	146.9 (3)	C12—C11—C10—C9	−0.7 (8)
Mn—N1—C8—C9	−178.9 (4)	C13—C11—C10—C9	−170.7 (5)
C12—N1—C8—C9	2.2 (8)	C10—C11—C12—N1	2.4 (8)
C8—N1—C12—C11	−3.2 (8)	C13—C11—C12—N1	173.1 (5)
Mn—N1—C12—C11	177.9 (4)	O3—C13—N2—C14	−179.1 (6)
C13—N2—C14—C15	−111.0 (9)	C11—C13—N2—C14	−3.4 (10)
C16—N2—C14—C15	72.0 (10)	O3—C13—N2—C16	−2.2 (9)
C13—N2—C16—C17	81.2 (9)	C11—C13—N2—C16	173.5 (5)
C14—N2—C16—C17	−101.6 (9)	O3—C13—C11—C10	114.1 (6)
C3—C2—C7—C6	2.0 (8)	N2—C13—C11—C10	−61.6 (8)
C1—C2—C7—C6	−178.8 (5)	O3—C13—C11—C12	−55.9 (7)
C3—C2—C1—O2	−178.0 (4)	N2—C13—C11—C12	128.3 (6)

Symmetry code: (i) −*x*, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41···O2^{i}	0.99 (4)	1.71 (5)	2.670 (6)	162 (7)
O4—H42···O3^{ii}	0.93 (5)	1.85 (5)	2.766 (6)	168 (7)

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