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Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl)-picolinato]manganese(II) trihydrate

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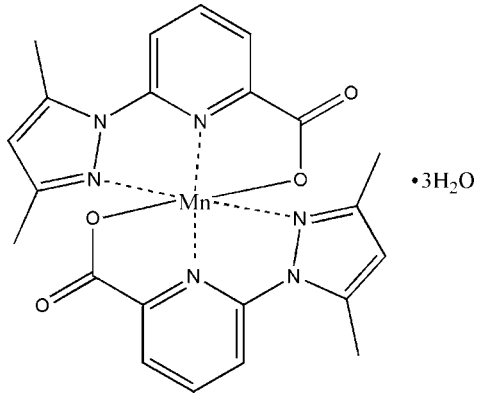
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.048; wR factor = 0.150; data-to-parameter ratio = 12.7.

In the title complex, $[Mn(C_{11}H_{10}N_3O_2)_2]\cdot 3H_2O$, the Mn^{II} atom is coordinated by four N atoms and two O atoms in a distorted octahedral geometry. The molecules are linked together *via* hydrogen bonds involving the water molecules. One of these is disordered equally over two positions.

Related literature

For related literature, see: Zhao *et al.* (2007); Yin *et al.* (2007).



Experimental

Crystal data

$[Mn(C_{11}H_{10}N_3O_2)_2]\cdot 3H_2O$
M_r = 541.43
Triclinic, $P\overline{1}$
a = 9.7950 (10) Å
b = 10.9030 (12) Å
c = 12.8070 (15) Å
α = 70.162 (2)°
β = 74.825 (2)°
γ = 83.760 (3)°
V = 1241.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 293 (2) K
0.53 × 0.49 × 0.47 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.747, T_{max} = 0.770
6455 measured reflections
4308 independent reflections
3050 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.150
S = 1.07
4308 reflections
338 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2^{i}	0.85	1.98	2.830 (4)	178
O5—H5B···O4^{ii}	0.85	1.97	2.819 (5)	178
O6—H6A···O5	0.85	1.89	2.740 (6)	176
O6—H6B···O7^{iii}	0.85	2.00	2.843 (8)	175
O7—H7D···O6	0.85	1.87	2.715 (8)	173
O7—H7E···O8^{iii}	0.85	1.65	2.497 (12)	172
O8—H8A···O4^{ii}	0.85	2.00	2.829 (8)	167
O8—H8B···O4^{iii}	0.85	2.00	2.829 (9)	166

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2211).

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Zhao, K., Yin, X.-H., Feng, Y. & Zhu, J. (2007). *Acta Cryst.* E**63**, m3024.

supporting information

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Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato]manganese(II) trihydrate

Yu Feng, Zhao Kai, Xian-Hong Yin, Jie Zhu and Cui-Wu Lin

S1. Comment

Recently we reported the crystal structures of bis(6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato)zinc(II) trihydrate (Yin *et al.*, 2007) and bis[3-chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato]cobalt(II) 2.5- hydrate (Zhao *et al.*, 2007). As a continuation of these investigations, we report in this paper the crystal structure of Bis(6-(3,5-dimethyl-1*H*-pyrazol-1-yl) picolinato)manganese(II)trihydrate.

The structure consists of the manganese(II) complex and three uncoordinated water molecules. The Mn atom is six-coordinated by four N atoms and two O atoms derived from the tridentate ligands, 6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinate (DPP), that define a distorted octahedral environment; the Mn—O bond lengths are 2.143 (3) and 2.154 (3) Å, The Mn—N distances range from 2.199 (3) to 2.277 (3) Å, *i.e.* normal values, The C1—C2 bond length is 1.522 (5) Å, being in the normal C—C ranges in manganese carboxylate complexes.

In the crystal structure, the oxygen atoms contribute to the formation of intermolecular hydrogen bonds involving the solvate water molecules; three water molecules and two DDP O atoms *via* intermolecular H—O···H hydrogen bonds. A great number of hydrogen contacts link the complex into a three-dimensional network. (Fig. 2; for symmetry codes see Table 1).

S2. Experimental

6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinic acid, and $MnCl_2$. $6H_2O$ were available commercially and were used without further purification. Equimolar 6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinic acid (1 mmol, 217 mg) was dissolved in anhydrous ethyl alcohol (AR,99.9%) (15 ml). The mixture was stirred to give a clear solution, To this solution was added $MnCl_2.6H_2O$ (0.5 mmol, 119 mg) in anhydrous alcohol (10 ml). After keeping the resulting solution in air to evaporate about half of the solvents, yellow blocks of the title compound were formed. The crystals were isolated, washed with alcohol three times(Yield75%). Elemental analysis: found: C, 48.65; H, 5.01; O, 20.87; calc. for $C_{22}H_{26}Mn_N6_O7$: C, 48.80; H, 4.84; O, 20.69.

S3. Refinement

H atoms on C atoms were positoned geometrically and refined using a riding model with C—H = 0.96Å and U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in difference Fourier maps and the O—H distances were constrained 0.85 Å, with U_{iso}(H) = 1.2U_{eq}(O).

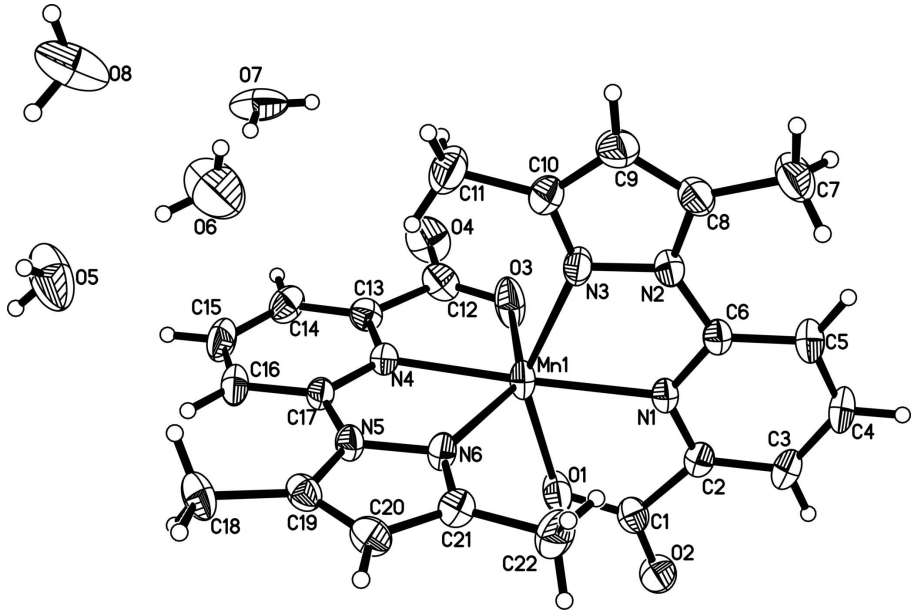

Figure 1

The structure of the title compound (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

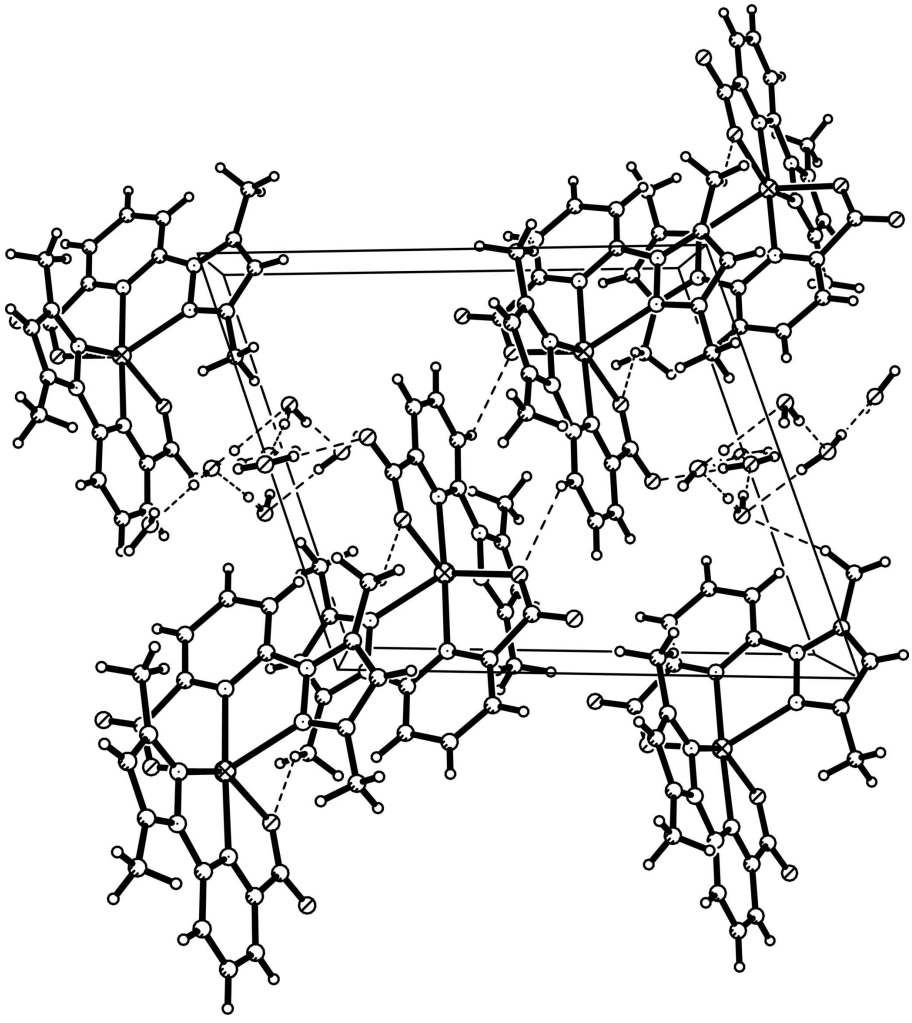

Figure 2

Crystal packing of (I) showing the hydrogen bonded interactions as dashed lines.

Bis[6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato]manganese(II) trihydrate

Crystal data

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$M_r = 541.43$
Triclinic, $P\overline{1}$
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$\beta = 74.825\ (2)°$
$\gamma = 83.760\ (3)°$
$V = 1241.4\ (2)$ Å^3
$Z = 2$
$F(000) = 562$
$D_x = 1.448$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2622 reflections
$\theta = 2.2–24.3°$
$\mu = 0.59$ mm^{-1}
$T = 293$ K
Block, yellow
0.53 × 0.49 × 0.47 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.747, T_{max} = 0.770
6455 measured reflections
4308 independent reflections
3050 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −11→11
k = −12→12
l = −15→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.150
S = 1.07
4308 reflections
338 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 0.3474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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}	Occ. (<1)
Mn1	0.71418 (5)	0.77632 (5)	0.27494 (5)	0.0466 (2)	
N1	0.8241 (3)	0.9608 (2)	0.2282 (2)	0.0393 (6)	
N2	0.7833 (3)	1.0148 (3)	0.0499 (2)	0.0446 (7)	
N3	0.7221 (3)	0.8947 (3)	0.0899 (3)	0.0497 (7)	
N4	0.6120 (3)	0.5904 (2)	0.3154 (2)	0.0392 (6)	
N5	0.3986 (3)	0.6848 (3)	0.3745 (2)	0.0420 (7)	
N6	0.4768 (3)	0.7939 (3)	0.3460 (2)	0.0444 (7)	
O1	0.7731 (3)	0.7770 (3)	0.4245 (2)	0.0640 (8)	
O2	0.8860 (3)	0.8766 (3)	0.5015 (2)	0.0624 (7)	
O3	0.8791 (3)	0.6429 (3)	0.2293 (3)	0.0763 (9)	
O4	0.9341 (3)	0.4450 (3)	0.2160 (3)	0.0884 (10)	
O5	0.1776 (4)	0.3403 (4)	0.2963 (3)	0.1229 (15)	
H5A	0.1559	0.2755	0.3571	0.147*	
H5B	0.1027	0.3702	0.2738	0.147*	
O6	0.4031 (5)	0.4792 (5)	0.1413 (4)	0.1482 (18)	
H6A	0.3308	0.4374	0.1866	0.178*	

H6B	0.3820	0.5237	0.0787	0.178*	
O7	0.6528 (7)	0.3620 (7)	0.0713 (5)	0.091 (2)	0.50
H7D	0.5787	0.4047	0.0917	0.109*	0.50
H7E	0.7237	0.4108	0.0498	0.109*	0.50
O8	0.1259 (9)	0.5103 (8)	−0.0015 (6)	0.126 (3)	0.50
H8A	0.0580	0.4912	0.0579	0.151*	0.50
H8B	0.0936	0.5213	−0.0596	0.151*	0.50
C1	0.8435 (4)	0.8683 (3)	0.4221 (3)	0.0473 (9)	
C2	0.8803 (3)	0.9762 (3)	0.3073 (3)	0.0411 (8)	
C3	0.9641 (4)	1.0799 (3)	0.2834 (3)	0.0519 (9)	
H3	1.0008	1.0911	0.3395	0.062*	
C4	0.9924 (4)	1.1670 (3)	0.1738 (4)	0.0594 (11)	
H4	1.0502	1.2372	0.1555	0.071*	
C5	0.9367 (4)	1.1518 (3)	0.0912 (4)	0.0552 (10)	
H5	0.9565	1.2098	0.0169	0.066*	
C6	0.8496 (3)	1.0464 (3)	0.1233 (3)	0.0405 (8)	
C7	0.8161 (5)	1.2156 (4)	−0.1267 (4)	0.0803 (14)	
H7A	0.7824	1.2723	−0.0816	0.120*	
H7B	0.7791	1.2456	−0.1937	0.120*	
H7C	0.9176	1.2161	−0.1490	0.120*	
C8	0.7683 (4)	1.0808 (4)	−0.0581 (3)	0.0549 (10)	
C9	0.6970 (5)	1.0015 (4)	−0.0857 (4)	0.0656 (11)	
H9	0.6703	1.0198	−0.1541	0.079*	
C10	0.6709 (4)	0.8872 (4)	0.0073 (3)	0.0559 (10)	
C11	0.6005 (5)	0.7670 (4)	0.0192 (4)	0.0819 (14)	
H11A	0.6708	0.7055	−0.0019	0.123*	
H11B	0.5363	0.7889	−0.0299	0.123*	
H11C	0.5492	0.7291	0.0971	0.123*	
C12	0.8506 (4)	0.5290 (4)	0.2427 (4)	0.0606 (10)	
C13	0.6970 (4)	0.4915 (3)	0.2970 (3)	0.0460 (8)	
C14	0.6473 (5)	0.3689 (3)	0.3275 (4)	0.0582 (10)	
H14	0.7075	0.3009	0.3142	0.070*	
C15	0.5062 (5)	0.3488 (4)	0.3784 (4)	0.0665 (12)	
H15	0.4706	0.2655	0.4016	0.080*	
C16	0.4175 (4)	0.4493 (3)	0.3953 (3)	0.0568 (10)	
H16	0.3214	0.4366	0.4283	0.068*	
C17	0.4754 (3)	0.5708 (3)	0.3617 (3)	0.0402 (8)	
C18	0.1427 (4)	0.6136 (4)	0.4516 (4)	0.0638 (11)	
H18A	0.0528	0.6560	0.4699	0.096*	
H18B	0.1554	0.5423	0.5176	0.096*	
H18C	0.1458	0.5812	0.3901	0.096*	
C19	0.2586 (4)	0.7093 (4)	0.4162 (3)	0.0477 (9)	
C20	0.2486 (4)	0.8342 (4)	0.4157 (3)	0.0524 (9)	
H20	0.1664	0.8784	0.4402	0.063*	
C21	0.3839 (4)	0.8842 (3)	0.3718 (3)	0.0479 (9)	
C22	0.4326 (5)	1.0165 (4)	0.3515 (4)	0.0681 (12)	
H22A	0.4185	1.0314	0.4234	0.102*	
H22B	0.3794	1.0806	0.3045	0.102*	

H22C	0.5313	1.0231	0.3136	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0390 (3)	0.0378 (3)	0.0600 (4)	−0.0121 (2)	−0.0096 (3)	−0.0103 (2)
N1	0.0341 (15)	0.0344 (14)	0.0472 (17)	−0.0064 (11)	−0.0079 (13)	−0.0103 (13)
N2	0.0423 (16)	0.0408 (15)	0.0466 (18)	−0.0084 (12)	−0.0089 (13)	−0.0081 (13)
N3	0.0523 (18)	0.0414 (16)	0.0567 (19)	−0.0142 (13)	−0.0139 (15)	−0.0131 (14)
N4	0.0398 (16)	0.0349 (14)	0.0423 (16)	−0.0043 (12)	−0.0094 (13)	−0.0111 (12)
N5	0.0324 (15)	0.0432 (15)	0.0502 (17)	−0.0079 (12)	−0.0081 (13)	−0.0142 (13)
N6	0.0424 (16)	0.0361 (14)	0.0558 (18)	−0.0077 (12)	−0.0109 (14)	−0.0149 (13)
O1	0.0644 (18)	0.0632 (16)	0.0582 (17)	−0.0303 (13)	−0.0210 (14)	0.0016 (13)
O2	0.0605 (17)	0.0727 (18)	0.0581 (17)	−0.0093 (13)	−0.0234 (14)	−0.0170 (14)
O3	0.0387 (15)	0.0537 (17)	0.120 (3)	−0.0087 (12)	0.0034 (16)	−0.0222 (17)
O4	0.071 (2)	0.070 (2)	0.108 (3)	0.0221 (17)	−0.0015 (18)	−0.0313 (19)
O5	0.084 (3)	0.144 (3)	0.108 (3)	−0.040 (2)	−0.045 (2)	0.028 (2)
O6	0.126 (4)	0.177 (5)	0.114 (3)	−0.021 (3)	−0.015 (3)	−0.017 (3)
O7	0.081 (4)	0.142 (6)	0.066 (4)	0.037 (4)	−0.023 (3)	−0.062 (4)
O8	0.145 (7)	0.129 (7)	0.061 (4)	0.021 (6)	0.007 (5)	−0.010 (4)
C1	0.0324 (18)	0.054 (2)	0.054 (2)	−0.0042 (15)	−0.0106 (17)	−0.0144 (18)
C2	0.0322 (17)	0.0385 (17)	0.055 (2)	0.0022 (13)	−0.0122 (16)	−0.0177 (16)
C3	0.050 (2)	0.0410 (19)	0.074 (3)	−0.0029 (16)	−0.023 (2)	−0.0244 (19)
C4	0.063 (3)	0.0334 (18)	0.083 (3)	−0.0141 (17)	−0.024 (2)	−0.0111 (19)
C5	0.056 (2)	0.0367 (19)	0.067 (3)	−0.0109 (16)	−0.017 (2)	−0.0050 (18)
C6	0.0348 (18)	0.0354 (17)	0.049 (2)	−0.0029 (13)	−0.0084 (15)	−0.0116 (15)
C7	0.092 (4)	0.076 (3)	0.058 (3)	−0.033 (3)	−0.023 (3)	0.010 (2)
C8	0.052 (2)	0.057 (2)	0.048 (2)	−0.0097 (18)	−0.0058 (18)	−0.0100 (18)
C9	0.071 (3)	0.079 (3)	0.050 (2)	−0.011 (2)	−0.019 (2)	−0.017 (2)
C10	0.055 (2)	0.059 (2)	0.059 (2)	−0.0113 (18)	−0.017 (2)	−0.021 (2)
C11	0.097 (4)	0.075 (3)	0.089 (3)	−0.025 (3)	−0.037 (3)	−0.027 (3)
C12	0.055 (2)	0.053 (2)	0.061 (3)	0.0065 (19)	−0.005 (2)	−0.011 (2)
C13	0.050 (2)	0.0394 (18)	0.045 (2)	0.0019 (16)	−0.0124 (17)	−0.0092 (15)
C14	0.073 (3)	0.0379 (19)	0.070 (3)	0.0035 (18)	−0.023 (2)	−0.0216 (18)
C15	0.080 (3)	0.040 (2)	0.083 (3)	−0.019 (2)	−0.021 (2)	−0.018 (2)
C16	0.054 (2)	0.048 (2)	0.068 (3)	−0.0198 (18)	−0.012 (2)	−0.0146 (19)
C17	0.0403 (19)	0.0407 (18)	0.0412 (19)	−0.0100 (14)	−0.0101 (15)	−0.0123 (15)
C18	0.036 (2)	0.072 (3)	0.071 (3)	−0.0153 (18)	−0.0052 (19)	−0.010 (2)
C19	0.037 (2)	0.059 (2)	0.043 (2)	−0.0054 (16)	−0.0095 (16)	−0.0101 (17)
C20	0.041 (2)	0.059 (2)	0.053 (2)	0.0059 (17)	−0.0089 (17)	−0.0160 (18)
C21	0.047 (2)	0.0443 (19)	0.053 (2)	0.0033 (16)	−0.0162 (17)	−0.0159 (17)
C22	0.067 (3)	0.048 (2)	0.096 (3)	0.0025 (19)	−0.021 (2)	−0.032 (2)

Geometric parameters (Å, º)

Mn1—O1	2.143 (3)	C4—C5	1.373 (5)
Mn1—O3	2.154 (3)	C4—H4	0.9300
Mn1—N4	2.199 (3)	C5—C6	1.388 (4)

Mn1—N1	2.209 (2)	C5—H5	0.9300
Mn1—N3	2.267 (3)	C7—C8	1.486 (5)
Mn1—N6	2.277 (3)	C7—H7A	0.9600
N1—C6	1.327 (4)	C7—H7B	0.9600
N1—C2	1.336 (4)	C7—H7C	0.9600
N2—C8	1.364 (5)	C8—C9	1.353 (5)
N2—N3	1.375 (4)	C9—C10	1.393 (6)
N2—C6	1.419 (4)	C9—H9	0.9300
N3—C10	1.311 (5)	C10—C11	1.491 (5)
N4—C17	1.322 (4)	C11—H11A	0.9600
N4—C13	1.336 (4)	C11—H11B	0.9600
N5—C19	1.368 (4)	C11—H11C	0.9600
N5—N6	1.375 (3)	C12—C13	1.519 (5)
N5—C17	1.416 (4)	C13—C14	1.365 (5)
N6—C21	1.332 (4)	C14—C15	1.371 (6)
O1—C1	1.259 (4)	C14—H14	0.9300
O2—C1	1.227 (4)	C15—C16	1.364 (5)
O3—C12	1.247 (5)	C15—H15	0.9300
O4—C12	1.235 (5)	C16—C17	1.382 (4)
O5—H5A	0.8500	C16—H16	0.9300
O5—H5B	0.8500	C18—C19	1.500 (5)
O6—H6A	0.8500	C18—H18A	0.9600
O6—H6B	0.8500	C18—H18B	0.9600
O7—H7D	0.8499	C18—H18C	0.9600
O7—H7E	0.8500	C19—C20	1.353 (5)
O8—H8A	0.8500	C20—C21	1.389 (5)
O8—H8B	0.8500	C20—H20	0.9300
C1—C2	1.522 (5)	C21—C22	1.486 (5)
C2—C3	1.372 (5)	C22—H22A	0.9600
C3—C4	1.377 (5)	C22—H22B	0.9600
C3—H3	0.9300	C22—H22C	0.9600

O1—Mn1—O3	96.39 (13)	H7A—C7—H7B	109.5
O1—Mn1—N4	108.16 (10)	C8—C7—H7C	109.5
O3—Mn1—N4	73.44 (10)	H7A—C7—H7C	109.5
O1—Mn1—N1	73.16 (10)	H7B—C7—H7C	109.5
O3—Mn1—N1	104.29 (10)	C9—C8—N2	106.2 (3)
N4—Mn1—N1	177.41 (10)	C9—C8—C7	128.3 (4)
O1—Mn1—N3	143.23 (10)	N2—C8—C7	125.5 (4)
O3—Mn1—N3	92.96 (12)	C8—C9—C10	107.2 (4)
N4—Mn1—N3	108.59 (10)	C8—C9—H9	126.4
N1—Mn1—N3	70.08 (10)	C10—C9—H9	126.4
O1—Mn1—N6	95.74 (11)	N3—C10—C9	110.2 (3)
O3—Mn1—N6	142.92 (10)	N3—C10—C11	121.0 (4)
N4—Mn1—N6	69.49 (10)	C9—C10—C11	128.8 (4)
N1—Mn1—N6	112.76 (9)	C10—C11—H11A	109.5
N3—Mn1—N6	97.89 (11)	C10—C11—H11B	109.5
C6—N1—C2	120.1 (3)	H11A—C11—H11B	109.5

C6—N1—Mn1	122.8 (2)	C10—C11—H11C	109.5
C2—N1—Mn1	116.5 (2)	H11A—C11—H11C	109.5
C8—N2—N3	110.3 (3)	H11B—C11—H11C	109.5
C8—N2—C6	132.4 (3)	O4—C12—O3	126.6 (4)
N3—N2—C6	117.2 (3)	O4—C12—C13	117.5 (4)
C10—N3—N2	106.0 (3)	O3—C12—C13	115.9 (3)
C10—N3—Mn1	137.2 (2)	N4—C13—C14	121.7 (3)
N2—N3—Mn1	116.4 (2)	N4—C13—C12	113.6 (3)
C17—N4—C13	119.7 (3)	C14—C13—C12	124.6 (3)
C17—N4—Mn1	123.7 (2)	C13—C14—C15	118.2 (4)
C13—N4—Mn1	116.5 (2)	C13—C14—H14	120.9
C19—N5—N6	110.6 (3)	C15—C14—H14	120.9
C19—N5—C17	133.0 (3)	C16—C15—C14	120.8 (3)
N6—N5—C17	116.4 (2)	C16—C15—H15	119.6
C21—N6—N5	105.3 (3)	C14—C15—H15	119.6
C21—N6—Mn1	137.7 (2)	C15—C16—C17	117.7 (4)
N5—N6—Mn1	116.96 (19)	C15—C16—H16	121.1
C1—O1—Mn1	121.2 (2)	C17—C16—H16	121.1
C12—O3—Mn1	120.3 (2)	N4—C17—C16	121.9 (3)
H5A—O5—H5B	108.4	N4—C17—N5	113.3 (3)
H6A—O6—H6B	108.5	C16—C17—N5	124.8 (3)
H7D—O7—H7E	108.6	C19—C18—H18A	109.5
H8A—O8—H8B	108.7	C19—C18—H18B	109.5
O2—C1—O1	126.6 (3)	H18A—C18—H18B	109.5
O2—C1—C2	118.3 (3)	C19—C18—H18C	109.5
O1—C1—C2	115.1 (3)	H18A—C18—H18C	109.5
N1—C2—C3	121.5 (3)	H18B—C18—H18C	109.5
N1—C2—C1	113.6 (3)	C20—C19—N5	106.5 (3)
C3—C2—C1	124.9 (3)	C20—C19—C18	128.6 (3)
C2—C3—C4	118.1 (3)	N5—C19—C18	124.9 (3)
C2—C3—H3	121.0	C19—C20—C21	107.2 (3)
C4—C3—H3	121.0	C19—C20—H20	126.4
C5—C4—C3	121.1 (3)	C21—C20—H20	126.4
C5—C4—H4	119.4	N6—C21—C20	110.4 (3)
C3—C4—H4	119.4	N6—C21—C22	119.9 (3)
C4—C5—C6	117.2 (3)	C20—C21—C22	129.6 (3)
C4—C5—H5	121.4	C21—C22—H22A	109.5
C6—C5—H5	121.4	C21—C22—H22B	109.5
N1—C6—C5	121.9 (3)	H22A—C22—H22B	109.5
N1—C6—N2	112.8 (3)	C21—C22—H22C	109.5
C5—C6—N2	125.2 (3)	H22A—C22—H22C	109.5
C8—C7—H7A	109.5	H22B—C22—H22C	109.5
C8—C7—H7B	109.5		

O1—Mn1—N1—C6	177.3 (3)	O1—C1—C2—N1	3.9 (4)
O3—Mn1—N1—C6	84.8 (3)	O2—C1—C2—C3	3.5 (5)
N4—Mn1—N1—C6	56 (2)	O1—C1—C2—C3	−175.3 (3)
N3—Mn1—N1—C6	−3.1 (2)	N1—C2—C3—C4	−1.7 (5)

N6—Mn1—N1—C6	−93.5 (3)	C1—C2—C3—C4	177.4 (3)
O1—Mn1—N1—C2	5.3 (2)	C2—C3—C4—C5	1.0 (6)
O3—Mn1—N1—C2	−87.1 (2)	C3—C4—C5—C6	0.8 (6)
N4—Mn1—N1—C2	−116 (2)	C2—N1—C6—C5	1.5 (5)
N3—Mn1—N1—C2	−175.1 (3)	Mn1—N1—C6—C5	−170.2 (3)
N6—Mn1—N1—C2	94.5 (2)	C2—N1—C6—N2	179.3 (3)
C8—N2—N3—C10	0.3 (4)	Mn1—N1—C6—N2	7.6 (4)
C6—N2—N3—C10	−178.9 (3)	C4—C5—C6—N1	−2.1 (5)
C8—N2—N3—Mn1	−173.8 (2)	C4—C5—C6—N2	−179.7 (3)
C6—N2—N3—Mn1	7.0 (4)	C8—N2—C6—N1	171.8 (3)
O1—Mn1—N3—C10	−173.2 (3)	N3—N2—C6—N1	−9.3 (4)
O3—Mn1—N3—C10	82.0 (4)	C8—N2—C6—C5	−10.5 (6)
N4—Mn1—N3—C10	8.5 (4)	N3—N2—C6—C5	168.5 (3)
N1—Mn1—N3—C10	−173.9 (4)	N3—N2—C8—C9	0.1 (4)
N6—Mn1—N3—C10	−62.5 (4)	C6—N2—C8—C9	179.1 (3)
O1—Mn1—N3—N2	−1.6 (3)	N3—N2—C8—C7	177.4 (4)
O3—Mn1—N3—N2	−106.4 (2)	C6—N2—C8—C7	−3.6 (6)
N4—Mn1—N3—N2	−179.9 (2)	N2—C8—C9—C10	−0.4 (5)
N1—Mn1—N3—N2	−2.3 (2)	C7—C8—C9—C10	−177.6 (4)
N6—Mn1—N3—N2	109.2 (2)	N2—N3—C10—C9	−0.5 (4)
O1—Mn1—N4—C17	87.0 (3)	Mn1—N3—C10—C9	171.7 (3)
O3—Mn1—N4—C17	178.4 (3)	N2—N3—C10—C11	177.8 (4)
N1—Mn1—N4—C17	−153 (2)	Mn1—N3—C10—C11	−10.0 (6)
N3—Mn1—N4—C17	−94.1 (3)	C8—C9—C10—N3	0.6 (5)
N6—Mn1—N4—C17	−2.5 (2)	C8—C9—C10—C11	−177.6 (4)
O1—Mn1—N4—C13	−89.2 (2)	Mn1—O3—C12—O4	177.1 (4)
O3—Mn1—N4—C13	2.2 (2)	Mn1—O3—C12—C13	−2.7 (5)
N1—Mn1—N4—C13	31 (2)	C17—N4—C13—C14	−1.8 (5)
N3—Mn1—N4—C13	89.7 (2)	Mn1—N4—C13—C14	174.6 (3)
N6—Mn1—N4—C13	−178.6 (3)	C17—N4—C13—C12	179.6 (3)
C19—N5—N6—C21	0.7 (4)	Mn1—N4—C13—C12	−4.1 (4)
C17—N5—N6—C21	−176.2 (3)	O4—C12—C13—N4	−175.3 (4)
C19—N5—N6—Mn1	179.8 (2)	O3—C12—C13—N4	4.5 (5)
C17—N5—N6—Mn1	2.9 (3)	O4—C12—C13—C14	6.1 (6)
O1—Mn1—N6—C21	71.0 (4)	O3—C12—C13—C14	−174.1 (4)
O3—Mn1—N6—C21	179.6 (3)	N4—C13—C14—C15	0.0 (6)
N4—Mn1—N6—C21	178.2 (4)	C12—C13—C14—C15	178.4 (4)
N1—Mn1—N6—C21	−3.1 (4)	C13—C14—C15—C16	1.6 (6)
N3—Mn1—N6—C21	−74.8 (4)	C14—C15—C16—C17	−1.3 (6)
O1—Mn1—N6—N5	−107.7 (2)	C13—N4—C17—C16	2.1 (5)
O3—Mn1—N6—N5	0.9 (3)	Mn1—N4—C17—C16	−174.0 (3)
N4—Mn1—N6—N5	−0.4 (2)	C13—N4—C17—N5	−179.2 (3)
N1—Mn1—N6—N5	178.2 (2)	Mn1—N4—C17—N5	4.7 (4)
N3—Mn1—N6—N5	106.6 (2)	C15—C16—C17—N4	−0.5 (6)
O3—Mn1—O1—C1	99.9 (3)	C15—C16—C17—N5	−179.1 (3)
N4—Mn1—O1—C1	174.5 (3)	C19—N5—C17—N4	179.2 (3)
N1—Mn1—O1—C1	−3.2 (3)	N6—N5—C17—N4	−4.7 (4)
N3—Mn1—O1—C1	−3.8 (4)	C19—N5—C17—C16	−2.1 (6)

N6—Mn1—O1—C1	−115.3 (3)	N6—N5—C17—C16	173.9 (3)
O1—Mn1—O3—C12	107.5 (3)	N6—N5—C19—C20	−1.0 (4)
N4—Mn1—O3—C12	0.5 (3)	C17—N5—C19—C20	175.2 (3)
N1—Mn1—O3—C12	−178.3 (3)	N6—N5—C19—C18	177.7 (3)
N3—Mn1—O3—C12	−108.1 (3)	C17—N5—C19—C18	−6.1 (6)
N6—Mn1—O3—C12	−0.8 (5)	N5—C19—C20—C21	0.8 (4)
Mn1—O1—C1—O2	−177.9 (3)	C18—C19—C20—C21	−177.8 (4)
Mn1—O1—C1—C2	0.8 (4)	N5—N6—C21—C20	−0.2 (4)
C6—N1—C2—C3	0.5 (5)	Mn1—N6—C21—C20	−179.0 (3)
Mn1—N1—C2—C3	172.7 (2)	N5—N6—C21—C22	−179.9 (3)
C6—N1—C2—C1	−178.8 (3)	Mn1—N6—C21—C22	1.4 (6)
Mn1—N1—C2—C1	−6.6 (3)	C19—C20—C21—N6	−0.4 (4)
O2—C1—C2—N1	−177.3 (3)	C19—C20—C21—C22	179.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O2^{i}	0.85	1.98	2.830 (4)	178
O5—H5*B*···O4^{ii}	0.85	1.97	2.819 (5)	178
O6—H6*A*···O5	0.85	1.89	2.740 (6)	176
O6—H6*B*···O7^{iii}	0.85	2.00	2.843 (8)	175
O7—H7*D*···O6	0.85	1.87	2.715 (8)	173
O7—H7*E*···O8^{iii}	0.85	1.65	2.497 (12)	172
O8—H8*A*···O4^{ii}	0.85	2.00	2.829 (8)	167
O8—H8*B*···O4^{iii}	0.85	2.00	2.829 (9)	166

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