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Diaquabis{5-carboxy-2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*-imidazole-4-carboxylato}manganese(II)

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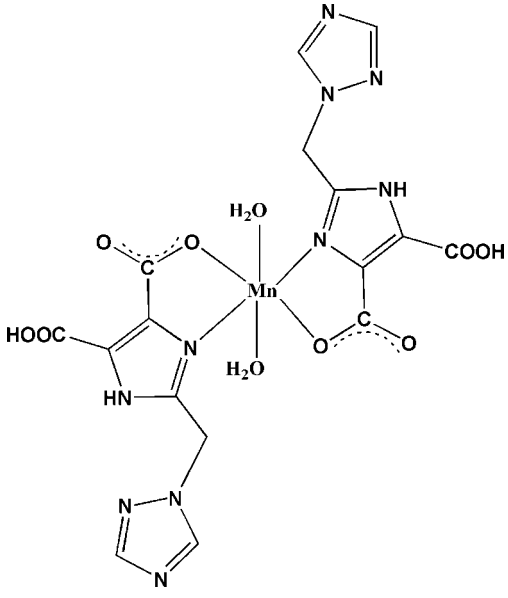
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.077; data-to-parameter ratio = 12.3.

In the title compound, $[Mn(C_8H_6N_5O_4)_2(H_2O)_2]$, the Mn^{II} ion is situated on an inversion center and is six-coordinated by two N and two O atoms from two L ligands (HL = 2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*-imidazole-4,5-dicarboxylic acid) and two water molecules in a distorted octahedral geometry. In ligand L, the imidazole and triazole rings form a dihedral angle of 74.25 (8)°. Molecules are assembled into a three-dimensional structure *via* intermolecular O—H···O, O—H···N and N—H···N hydrogen-bonds, and π–π interactions with a short distance of 3.665 (2) Å between the centroids of the imidazole and triazole rings of neighbouring molecules.

Related literature

For related structures, see: Lee *et al.* (2005); Ouellette *et al.* (2007); Won *et al.* (2007).



Experimental

Crystal data

$[Mn(C_8H_6N_5O_4)_2(H_2O)_2]$
M_r = 563.33
Monoclinic, $P2_1/c$
a = 7.730 (2) Å
b = 14.498 (3) Å
c = 11.588 (4) Å
β = 125.70 (2)°
V = 1054.6 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 293 K
0.20 × 0.15 × 0.10 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.871, T_{max} = 0.933
11281 measured reflections
2074 independent reflections
1974 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
S = 1.05
2074 reflections
169 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 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
O3—H3*C*···O2	0.98	1.50	2.483 (2)	178
O5—H5*B*···N2^{i}	0.78	2.18	2.878 (2)	149
O5—H5*C*···O4^{ii}	0.80	1.98	2.755 (2)	162
N5—H5*A*···N3^{iii}	0.86	1.96	2.811 (2)	169

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: CV2709).

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Ouellette, W., Hudson, B. & Zubieta, J. (2007). *Inorg. Chem.* **46**, 4887–4904.
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supporting information

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Diaquabis{5-carboxy-2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*-imidazole-4-carboxylato}manganese(II)

De-Gang Ding and Yan Tong

S1. Comment

Multidentate ligands containing rich coordination sites (N and/or O donors) are often employed to produce polymeric networks with structural diversity owing to their various coordination modes (Lee *et al.*, 2005; Ouellette *et al.*, 2007; Won *et al.*, 2007). As ligands with multiple coordination sites, 1,2,4-triazole and its derivatives have been shown to be good organic linkers in generation of structurally versatile metal-organic frameworks since it can bridge different metal centers to afford coordination polymers that exhibit extraordinary structural diversity and facile accessibility of functionalized materials. We selected a ligand containing 1,2,4-triazole, imidazole, and carboxylate groups, 2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*-imidazole-4,5-dicarboxylic acid, to study its coordination chemistry. As a result, we report herein the crystal structure of the title compound (I).

In (I), Mn^{II} ion located on an inversion center is six–coordinated by two imidazole nitrogen atoms (N4), two carboxylate group oxygen atoms (O1) from two ligands, and two water oxygen atoms (Fig. 1). The coordination bond lengths Mn—N and Mn—O are 2.248 (1), 2.186 (1) Å and 2.188 (2) Å, respectively. The coordination geometry around Mn^{II} is a distorted octahedron - the Mn^{II} coordination angles are in the range from 75.75 (6)° to 180.00 (1)°. Each *L* acts as a bidentate ligand.

In the crystal structure, the intra- and intermolecular hydrogen bonds (Table 1) and π–π interactions with short distance of 3.665 (2) Å between the centroids of imidazole and triazole rings from the neighbouring molecules consolidate the crystal packing.

S2. Experimental

All solvents and chemicals were of analytical grade and were used without further purification. The compound $[ML_2(H_2O)_2]$ was synthesized as follows: 2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*-imidazole-4,5-dicarboxylic acid (1.0 mmol) was added to 5 cm^3 water and the resulting solution was adjusted pH to 7.0 by NaOH aqueous. Then $MnCl_2$(0.5 mmol) was added to the above solution, and the mixture was stirred for 30 min and filtered. After one days, pink single crystals suitable for X-ray analysis were obtained. Analysis calculated (%) for $C_{16}H_{16}MnN_{10}O_{10}$: C 34.12, H 2.86, N 24.87; found (%): C 34.23, H 2.65, N 24.75.

S3. Refinement

The H atoms were included in calculated positions and treated as riding atoms: C—H = 0.93 Å for the triazole, 0.97 Å for the methylene H atoms, O—H = 0.79 Å for water molecule, 0.98 Å for carboxylic acid, and N—H = 0.86 Å for the imidazole, with $U_{iso}(H) = 1.5U_{eq}$(parent O-atom) and $1.2U_{eq}$(parent N-atom and C-atom).

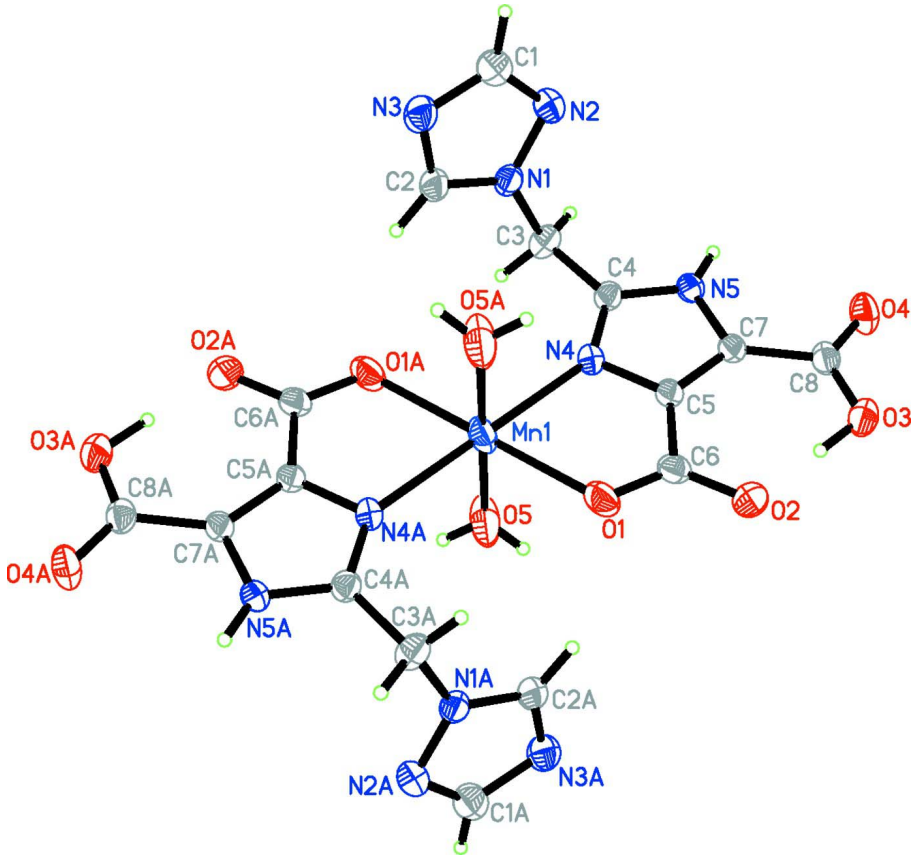

Figure 1

The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering [symmetry code: (A) - *x* - 1, - *y*, - *z*].

Diaquabis{5-carboxy-2-[(1*H*-1,2,4-triazol-1-yl)methyl]-1*H*- imidazole-4-carboxylato}manganese(II)

Crystal data

$[Mn(C_8H_6N_5O_4)_2(H_2O)_2]$
$M_r = 563.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.730$ (2) Å
$b = 14.498$ (3) Å
$c = 11.588$ (4) Å
$\beta = 125.70$ (2)°
$V = 1054.6$ (5) Å^3
$Z = 2$
$F(000) = 574$
$D_x = 1.774$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3276 reflections
$\theta = 2.6$–30.8°
$\mu = 0.71$ mm^{-1}
$T = 293$ K
Prism, pink
0.20 × 0.15 × 0.10 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{min} = 0.871$, $T_{max} = 0.933$
11281 measured reflections
2074 independent reflections
1974 reflections with $I > 2\sigma(I)$

R_{int} = 0.033
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −9→9
k = −17→17
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
S = 1.05
2074 reflections
169 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
$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles.

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}
Mn1	−0.5000	0.0000	0.0000	0.02963 (14)
O1	−0.2806 (2)	0.11091 (10)	0.13249 (15)	0.0333 (4)
O2	−0.0902 (2)	0.17418 (10)	0.34848 (15)	0.0319 (3)
O3	−0.0253 (2)	0.14770 (10)	0.58250 (15)	0.0328 (4)
H3C	−0.0491	0.1596	0.4908	0.049*
O4	−0.1284 (2)	0.04886 (11)	0.67687 (15)	0.0353 (4)
O5	−0.7693 (3)	0.08739 (13)	−0.05545 (17)	0.0516 (5)
H5B	−0.7549	0.1335	−0.0155	0.077*
H5C	−0.8757	0.0886	−0.1346	0.077*
N1	−0.4778 (3)	−0.24271 (11)	0.21460 (17)	0.0247 (4)
N2	−0.3256 (3)	−0.29594 (12)	0.32424 (18)	0.0316 (4)
N3	−0.3707 (3)	−0.33526 (13)	0.12013 (18)	0.0318 (4)
N4	−0.4235 (3)	−0.02708 (11)	0.21633 (16)	0.0229 (4)
N5	−0.3572 (3)	−0.05521 (11)	0.42541 (16)	0.0221 (4)
H5A	−0.3594	−0.0820	0.4907	0.026*
C1	−0.2671 (4)	−0.34974 (16)	0.2612 (2)	0.0337 (5)
H1A	−0.1620	−0.3945	0.3101	0.040*
C2	−0.5007 (4)	−0.26688 (14)	0.0956 (2)	0.0290 (5)
H2A	−0.5952	−0.2394	0.0074	0.035*
C3	−0.5880 (3)	−0.16935 (14)	0.2336 (2)	0.0283 (5)
H3A	−0.6208	−0.1902	0.2984	0.034*
H3B	−0.7215	−0.1559	0.1430	0.034*

C4	−0.4575 (3)	−0.08370 (13)	0.2908 (2)	0.0219 (4)
C5	−0.2913 (3)	0.04042 (13)	0.30983 (19)	0.0208 (4)
C6	−0.2149 (3)	0.11379 (14)	0.2602 (2)	0.0249 (4)
C7	−0.2507 (3)	0.02413 (13)	0.44029 (19)	0.0212 (4)
C8	−0.1284 (3)	0.07527 (14)	0.5765 (2)	0.0252 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0324 (3)	0.0372 (3)	0.0167 (2)	−0.0015 (2)	0.0129 (2)	0.00040 (18)
O1	0.0379 (9)	0.0365 (9)	0.0233 (8)	−0.0041 (7)	0.0166 (7)	0.0066 (6)
O2	0.0335 (8)	0.0273 (8)	0.0316 (8)	−0.0063 (6)	0.0172 (7)	−0.0006 (6)
O3	0.0347 (8)	0.0307 (8)	0.0279 (8)	−0.0076 (7)	0.0153 (7)	−0.0074 (6)
O4	0.0384 (9)	0.0452 (10)	0.0207 (8)	−0.0050 (7)	0.0162 (7)	−0.0059 (7)
O5	0.0416 (10)	0.0684 (13)	0.0262 (9)	0.0132 (9)	0.0093 (8)	−0.0137 (8)
N1	0.0317 (9)	0.0216 (9)	0.0235 (9)	−0.0040 (7)	0.0176 (8)	−0.0033 (7)
N2	0.0376 (10)	0.0316 (10)	0.0224 (9)	−0.0003 (8)	0.0156 (8)	0.0009 (7)
N3	0.0410 (11)	0.0312 (10)	0.0293 (10)	−0.0014 (8)	0.0240 (9)	−0.0032 (8)
N4	0.0250 (8)	0.0240 (9)	0.0175 (8)	−0.0010 (7)	0.0111 (7)	−0.0016 (6)
N5	0.0268 (9)	0.0229 (9)	0.0185 (8)	0.0000 (7)	0.0144 (7)	0.0004 (6)
C1	0.0351 (12)	0.0332 (12)	0.0300 (12)	0.0032 (10)	0.0174 (10)	0.0006 (9)
C2	0.0410 (12)	0.0249 (11)	0.0227 (10)	−0.0040 (9)	0.0196 (10)	−0.0022 (8)
C3	0.0330 (11)	0.0243 (11)	0.0332 (11)	−0.0039 (9)	0.0225 (10)	−0.0057 (9)
C4	0.0230 (10)	0.0213 (10)	0.0217 (10)	0.0002 (8)	0.0133 (8)	−0.0016 (8)
C5	0.0210 (9)	0.0201 (9)	0.0189 (9)	0.0021 (8)	0.0102 (8)	0.0004 (8)
C6	0.0234 (10)	0.0238 (10)	0.0240 (10)	0.0033 (8)	0.0119 (9)	0.0046 (8)
C7	0.0207 (9)	0.0214 (10)	0.0188 (9)	0.0019 (8)	0.0100 (8)	0.0004 (7)
C8	0.0227 (10)	0.0274 (11)	0.0211 (10)	0.0034 (8)	0.0102 (8)	−0.0025 (8)

Geometric parameters (Å, º)

Mn1—O5^{i}	2.1886 (17)	N2—C1	1.316 (3)
Mn1—O5	2.1886 (17)	N3—C2	1.319 (3)
Mn1—O1^{i}	2.1862 (16)	N3—C1	1.353 (3)
Mn1—O1	2.1862 (16)	N4—C4	1.324 (2)
Mn1—N4	2.2489 (18)	N4—C5	1.373 (2)
Mn1—N4^{i}	2.2489 (18)	N5—C4	1.339 (2)
O1—C6	1.254 (2)	N5—C7	1.366 (2)
O2—C6	1.262 (2)	N5—H5A	0.8600
O3—C8	1.296 (3)	C1—H1A	0.9300
O3—H3C	0.9817	C2—H2A	0.9300
O4—C8	1.224 (2)	C3—C4	1.489 (3)
O5—H5B	0.7826	C3—H3A	0.9700
O5—H5C	0.7987	C3—H3B	0.9700
N1—C2	1.331 (3)	C5—C7	1.373 (3)
N1—N2	1.360 (2)	C5—C6	1.486 (3)
N1—C3	1.458 (3)	C7—C8	1.481 (3)

O5^{i}—Mn1—O5	180.00 (12)	C4—N5—H5A	126.2
O5^{i}—Mn1—O1^{i}	89.74 (7)	C7—N5—H5A	126.2
O5—Mn1—O1^{i}	90.26 (7)	N2—C1—N3	115.2 (2)
O5^{i}—Mn1—O1	90.26 (7)	N2—C1—H1A	122.4
O5—Mn1—O1	89.74 (7)	N3—C1—H1A	122.4
O1^{i}—Mn1—O1	180.00 (10)	N3—C2—N1	110.49 (19)
O5^{i}—Mn1—N4	89.15 (6)	N3—C2—H2A	124.8
O5—Mn1—N4	90.85 (6)	N1—C2—H2A	124.8
O1^{i}—Mn1—N4	104.25 (6)	N1—C3—C4	111.81 (16)
O1—Mn1—N4	75.75 (6)	N1—C3—H3A	109.3
O5^{i}—Mn1—N4^{i}	90.85 (6)	C4—C3—H3A	109.3
O5—Mn1—N4^{i}	89.15 (6)	N1—C3—H3B	109.3
O1^{i}—Mn1—N4^{i}	75.75 (6)	C4—C3—H3B	109.3
O1—Mn1—N4^{i}	104.25 (6)	H3A—C3—H3B	107.9
N4—Mn1—N4^{i}	180.00 (11)	N4—C4—N5	111.56 (17)
C6—O1—Mn1	117.87 (13)	N4—C4—C3	124.59 (17)
C8—O3—H3C	111.3	N5—C4—C3	123.85 (18)
Mn1—O5—H5B	122.5	N4—C5—C7	109.45 (17)
Mn1—O5—H5C	121.0	N4—C5—C6	119.06 (16)
H5B—O5—H5C	110.9	C7—C5—C6	131.47 (18)
C2—N1—N2	109.77 (17)	O1—C6—O2	124.89 (19)
C2—N1—C3	127.77 (18)	O1—C6—C5	117.01 (18)
N2—N1—C3	122.43 (16)	O2—C6—C5	118.10 (17)
C1—N2—N1	102.01 (17)	N5—C7—C5	105.79 (16)
C2—N3—C1	102.53 (18)	N5—C7—C8	121.25 (17)
C4—N4—C5	105.50 (15)	C5—C7—C8	132.93 (18)
C4—N4—Mn1	144.26 (13)	O4—C8—O3	122.92 (18)
C5—N4—Mn1	110.24 (12)	O4—C8—C7	120.16 (19)
C4—N5—C7	107.68 (16)	O3—C8—C7	116.91 (18)

O5^{i}—Mn1—O1—C6	−90.63 (15)	C5—N4—C4—C3	−178.15 (18)
O5—Mn1—O1—C6	89.37 (15)	Mn1—N4—C4—C3	2.4 (4)
O1^{i}—Mn1—O1—C6	178 (100)	C7—N5—C4—N4	−0.3 (2)
N4—Mn1—O1—C6	−1.57 (14)	C7—N5—C4—C3	178.78 (18)
N4^{i}—Mn1—O1—C6	178.43 (14)	N1—C3—C4—N4	73.8 (2)
C2—N1—N2—C1	−0.1 (2)	N1—C3—C4—N5	−105.2 (2)
C3—N1—N2—C1	−178.39 (18)	C4—N4—C5—C7	−1.2 (2)
O5^{i}—Mn1—N4—C4	−87.9 (2)	Mn1—N4—C5—C7	178.46 (12)
O5—Mn1—N4—C4	92.1 (2)	C4—N4—C5—C6	177.62 (17)
O1^{i}—Mn1—N4—C4	1.6 (2)	Mn1—N4—C5—C6	−2.7 (2)
O1—Mn1—N4—C4	−178.4 (2)	Mn1—O1—C6—O2	−179.15 (15)
N4^{i}—Mn1—N4—C4	171 (100)	Mn1—O1—C6—C5	0.6 (2)
O5^{i}—Mn1—N4—C5	92.68 (13)	N4—C5—C6—O1	1.6 (3)
O5—Mn1—N4—C5	−87.32 (13)	C7—C5—C6—O1	−179.9 (2)
O1^{i}—Mn1—N4—C5	−177.81 (12)	N4—C5—C6—O2	−178.64 (17)
O1—Mn1—N4—C5	2.19 (12)	C7—C5—C6—O2	−0.1 (3)
N4^{i}—Mn1—N4—C5	−9 (100)	C4—N5—C7—C5	−0.4 (2)
N1—N2—C1—N3	−0.3 (2)	C4—N5—C7—C8	177.95 (17)

C2—N3—C1—N2	0.6 (3)	N4—C5—C7—N5	1.0 (2)
C1—N3—C2—N1	−0.7 (2)	C6—C5—C7—N5	−177.59 (19)
N2—N1—C2—N3	0.6 (2)	N4—C5—C7—C8	−177.1 (2)
C3—N1—C2—N3	178.69 (18)	C6—C5—C7—C8	4.3 (4)
C2—N1—C3—C4	−97.8 (2)	N5—C7—C8—O4	−3.0 (3)
N2—N1—C3—C4	80.2 (2)	C5—C7—C8—O4	174.9 (2)
C5—N4—C4—N5	0.9 (2)	N5—C7—C8—O3	177.23 (17)
Mn1—N4—C4—N5	−178.52 (16)	C5—C7—C8—O3	−4.9 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*C*···O2	0.98	1.50	2.483 (2)	178
O5—H5*B*···N2^{ii}	0.78	2.18	2.878 (2)	149
O5—H5*C*···O4^{iii}	0.80	1.98	2.755 (2)	162
N5—H5*A*···N3^{iv}	0.86	1.96	2.811 (2)	169

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