

Poly[μ_2 -aqua- $[\mu_2$ -1,1'-(butane-1,4-diyl)-diimidazole]bis(μ_4 -naphthalene-1,4-dicarboxylato)dimanganese(II)]

Zhi-Qiang Chen, Wen-Zhi Zhang* and Qun Xu

College of Chemistry and Chemical Engineering, Qiqihar University, Qiqihar 161006, Heilongjiang Province, People's Republic of China
Correspondence e-mail: zhangwenzhi1968@yahoo.com.cn

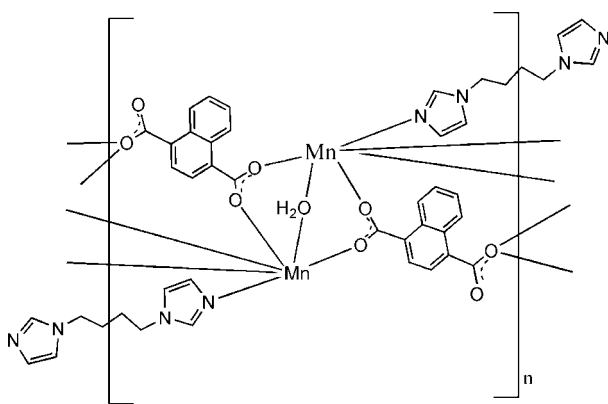
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 13.4.

In the title compound, $[\text{Mn}_2(\text{C}_{12}\text{H}_6\text{O}_4)_2(\text{C}_{10}\text{H}_{14}\text{N}_4)(\text{H}_2\text{O})]_n$ or $[\text{Mn}_2(1,4\text{-ndc})_2(L)(\text{H}_2\text{O})]_n$, where 1,4-ndc is naphthalene-1,4-dicarboxylate and L is 1,1'-(butane-1,4-diyl)diimidazole, the coordination polyhedron around each Mn^{II} atom is distorted octahedral. The water molecule and the L ligand are situated across a twofold rotation axis. The Mn^{II} atoms are bridged by 1,4-ndc and L ligands, forming a three-dimensional network. $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds are observed within the network.

Related literature

For general background, see: Ma *et al.* (2003); Yang *et al.* (2008).



Experimental

Crystal data

$[\text{Mn}_2(\text{C}_{12}\text{H}_6\text{O}_4)_2(\text{C}_{10}\text{H}_{14}\text{N}_4)(\text{H}_2\text{O})]$
 $M_r = 746.48$

Monoclinic, $C2/c$
 $a = 18.386$ (2) Å

$b = 14.8887$ (18) Å
 $c = 13.9121$ (17) Å
 $\beta = 126.319$ (1)°
 $V = 3068.5$ (6) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.89$ mm⁻¹
 $T = 293$ (2) K
 $0.31 \times 0.29 \times 0.23$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
 $T_{\text{min}} = 0.754$, $T_{\text{max}} = 0.814$

8475 measured reflections
3032 independent reflections
2643 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.081$
 $S = 1.06$
3032 reflections
226 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Selected bond lengths (Å).

Mn1—N1	2.2157 (17)	Mn1—O2 ⁱ	2.1535 (14)
Mn1—O1	2.1343 (15)	Mn1—O4 ⁱⁱ	2.2115 (14)
Mn1—O1W	2.2085 (11)	Mn1—O4 ⁱⁱⁱ	2.4148 (13)

Symmetry codes: (i) $-x + 1, y, -z + \frac{3}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H1W1 \cdots O3 ⁱⁱⁱ	0.83 (3)	1.72 (3)	2.5361 (19)	166 (3)

Symmetry code: (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: CI2711).

References

- Bruker (1998). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ma, J.-F., Yang, J., Zheng, G.-L., Li, L. & Liu, J.-F. (2003). *Inorg. Chem.* **42**, 7531–7534.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Yang, J., Ma, J.-F., Batten, S. R. & Su, Z.-M. (2008). *Chem. Commun.* pp. 2233–2235.

supporting information

Acta Cryst. (2008). E64, m1543 [doi:10.1107/S1600536808036787]

Poly[μ_2 -aqua- $[\mu_2$ -1,1'-(butane-1,4-diyl)diimidazole]bis(μ_4 -naphthalene-1,4-dicarboxylato)dimanganese(II)]

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S1. Comment

Some interesting interpenetrated or entangled metal-organic networks with bis(imidazole)-containing ligands have been documented (Yang *et al.*, 2008). But, flexible ligands such as 1,1'-(1,4-butanediyl)bis(imidazole) (*L*) have not been well explored (Ma *et al.*, 2003). In this work, we used 1,4-naphthalenedicarboxylic acid (1,4-H₂ndc) and *L* as linkers to obtain a new coordination polymer, [Mn₂(1,4-ndc)₂(*L*)(H₂O)]. We report here its crystal structure.

In the title compound, each Mn^{II} atom displays a distorted octahedral coordination sphere, completed by one N atom from one *L* ligand, four carboxylate O atoms from 1,4-ndc ligand and the O atom of the water molecule (Fig. 1). Both the water molecule and *L* ligand are situated across a twofold rotation axis. Two adjacent Mn^{II} atoms are bridged by carboxylate groups of 1,4-ndc ligands and water molecules forming a three-dimensional network containing [Mn₂(1,4-ndc)₂(H₂O)] units. The network is further strengthened by the coordination of *L* ligands (Fig. 2).

S2. Experimental

A mixture of 1,4-H₂ndc (0.5 mmol), *L* (0.5 mmol), NaOH (1 mmol) and MnCl₂·2H₂O (0.5 mmol) was suspended in 14 ml of deionized water and sealed in a 20-ml Teflon-lined autoclave. Upon heating at 413 K for 3 d, the autoclave was slowly cooled to room temperature. The crystals formed were collected, washed with deionized water and dried.

S3. Refinement

C-bound H atoms were positioned geometrically (C-H = 0.93–0.97 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The water H atom was located in a difference Fourier map and refined freely.

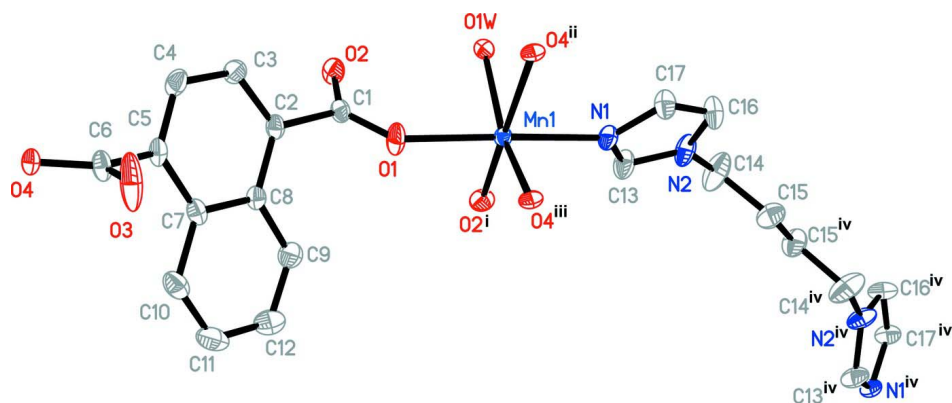


Figure 1

Part of the polymeric structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i) $1-x, y, 3/2-z$; (ii) $3/2-x, 1/2+y, 3/1-z$; (iii) $x-1/2, 1/2-y, z-1/2$; (iv) $-x, y, 1/2-z$.

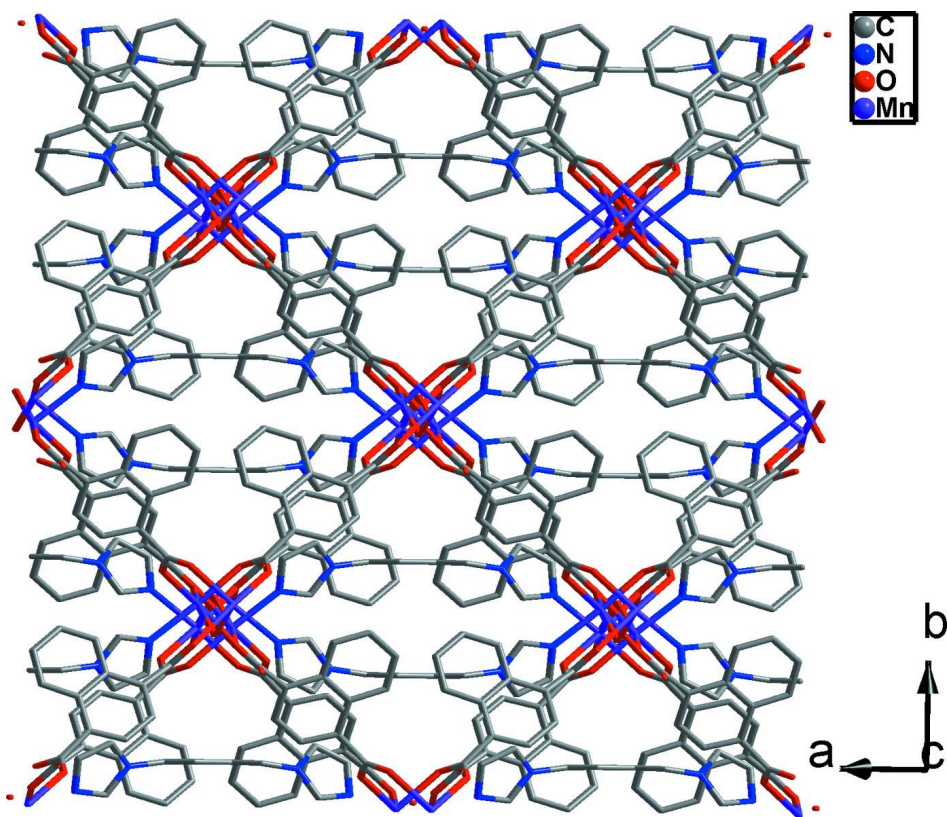


Figure 2

View of the three-dimensional framework of the title compound.

Poly[μ_2 -aqua- μ_2 -1,1'-(butane-1,4-diyl)diimidazole]bis(μ_4 -naphthalene-1,4-dicarboxylato)dimanganese(II)]

Crystal data

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Monoclinic, $C2/c$
Hall symbol: $-C\ 2yc$

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 $c = 13.9121$ (17) Å
 $\beta = 126.319$ (1)°
 $V = 3068.5$ (6) Å³
 $Z = 4$
 $F(000) = 1528$
 $D_x = 1.616$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 3032 reflections
 $\theta = 1.1$ – 26.1 °
 $\mu = 0.89$ mm⁻¹
 $T = 293$ K
 Block, colourless
 $0.31 \times 0.29 \times 0.23$ mm

Data collection

Bruker APEX CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 1998)
 $T_{\min} = 0.754$, $T_{\max} = 0.814$

8475 measured reflections
 3032 independent reflections
 2643 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\max} = 26.1$ °, $\theta_{\min} = 1.9$ °
 $h = -21 \rightarrow 22$
 $k = -17 \rightarrow 18$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.081$
 $S = 1.06$
 3032 reflections
 226 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 3.0197P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.36$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.62201 (13)	0.35715 (13)	0.80331 (19)	0.0292 (4)
C2	0.69094 (14)	0.28719 (14)	0.82714 (18)	0.0284 (4)
C3	0.78080 (14)	0.30737 (15)	0.90435 (19)	0.0365 (5)
H3	0.7985	0.3593	0.9502	0.044*
C4	0.84703 (15)	0.25114 (16)	0.9159 (2)	0.0380 (5)
H4	0.9076	0.2671	0.9671	0.046*
C5	0.82279 (14)	0.17325 (14)	0.85222 (18)	0.0312 (5)
C6	0.89049 (15)	0.12254 (14)	0.84487 (19)	0.0340 (5)

C7	0.73108 (15)	0.14565 (14)	0.77897 (19)	0.0311 (5)
C8	0.66391 (14)	0.20353 (14)	0.76583 (18)	0.0287 (4)
C9	0.57318 (16)	0.17399 (16)	0.6942 (2)	0.0412 (5)
H9	0.5284	0.2108	0.6844	0.049*
C10	0.70427 (18)	0.06162 (16)	0.7191 (2)	0.0433 (6)
H10	0.7475	0.0238	0.7262	0.052*
C11	0.6163 (2)	0.03575 (17)	0.6515 (3)	0.0547 (7)
H11	0.5998	-0.0196	0.6132	0.066*
C12	0.55052 (19)	0.09235 (19)	0.6395 (3)	0.0562 (7)
H12	0.4905	0.0739	0.5934	0.067*
C13	0.26433 (15)	0.55518 (18)	0.4740 (2)	0.0458 (6)
H13	0.2502	0.5058	0.5011	0.055*
C14	0.12054 (17)	0.6389 (3)	0.3926 (3)	0.0710 (10)
H14A	0.1202	0.6951	0.4277	0.085*
H14B	0.1097	0.5909	0.4298	0.085*
C15	0.04623 (15)	0.6403 (2)	0.2644 (2)	0.0521 (7)
H15A	0.0518	0.5883	0.2273	0.062*
H15B	0.0525	0.6934	0.2295	0.062*
C16	0.25299 (18)	0.68327 (19)	0.3927 (2)	0.0509 (7)
H16	0.2318	0.7383	0.3541	0.061*
C17	0.33284 (16)	0.64368 (16)	0.4330 (2)	0.0420 (6)
H17	0.3763	0.6682	0.4265	0.050*
N1	0.34027 (11)	0.56325 (13)	0.48419 (16)	0.0334 (4)
N2	0.21024 (13)	0.62621 (16)	0.42028 (18)	0.0474 (5)
O1	0.56289 (11)	0.37653 (11)	0.69574 (14)	0.0431 (4)
O2	0.63083 (10)	0.39108 (10)	0.89143 (13)	0.0384 (4)
O1W	0.5000	0.54659 (13)	0.7500	0.0258 (4)
O3	0.88390 (16)	0.13596 (16)	0.75292 (18)	0.0801 (8)
O4	0.94753 (9)	0.07087 (9)	0.92823 (12)	0.0271 (3)
Mn1	0.456815 (18)	0.470697 (19)	0.58778 (3)	0.02220 (10)
H1W1	0.542 (2)	0.578 (2)	0.760 (3)	0.080 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0272 (11)	0.0277 (10)	0.0356 (12)	0.0069 (8)	0.0203 (10)	0.0041 (9)
C2	0.0293 (11)	0.0307 (10)	0.0280 (11)	0.0099 (8)	0.0186 (9)	0.0049 (8)
C3	0.0322 (12)	0.0365 (12)	0.0344 (12)	0.0065 (9)	0.0163 (10)	-0.0075 (9)
C4	0.0250 (11)	0.0478 (13)	0.0333 (12)	0.0089 (10)	0.0129 (10)	-0.0012 (10)
C5	0.0329 (11)	0.0359 (11)	0.0272 (10)	0.0153 (9)	0.0192 (10)	0.0098 (9)
C6	0.0373 (12)	0.0355 (11)	0.0365 (12)	0.0165 (9)	0.0259 (11)	0.0104 (10)
C7	0.0389 (12)	0.0284 (10)	0.0319 (11)	0.0095 (9)	0.0243 (10)	0.0061 (9)
C8	0.0303 (11)	0.0304 (10)	0.0269 (10)	0.0062 (8)	0.0177 (9)	0.0048 (8)
C9	0.0331 (12)	0.0437 (13)	0.0441 (13)	0.0018 (10)	0.0214 (11)	-0.0002 (11)
C10	0.0604 (17)	0.0318 (12)	0.0464 (14)	0.0081 (11)	0.0363 (14)	0.0011 (10)
C11	0.0689 (19)	0.0365 (13)	0.0581 (17)	-0.0120 (13)	0.0373 (16)	-0.0132 (12)
C12	0.0455 (15)	0.0541 (16)	0.0578 (17)	-0.0147 (13)	0.0245 (14)	-0.0098 (14)
C13	0.0282 (12)	0.0585 (15)	0.0465 (14)	0.0064 (11)	0.0197 (11)	0.0183 (12)

C14	0.0301 (14)	0.129 (3)	0.0529 (17)	0.0267 (16)	0.0241 (13)	0.0157 (18)
C15	0.0276 (13)	0.0674 (18)	0.0541 (16)	-0.0057 (12)	0.0204 (12)	-0.0056 (14)
C16	0.0488 (15)	0.0516 (15)	0.0530 (15)	0.0214 (12)	0.0306 (13)	0.0239 (13)
C17	0.0376 (13)	0.0472 (14)	0.0455 (14)	0.0088 (11)	0.0270 (12)	0.0150 (11)
N1	0.0242 (9)	0.0398 (10)	0.0318 (10)	0.0062 (8)	0.0141 (8)	0.0070 (8)
N2	0.0266 (10)	0.0719 (15)	0.0412 (11)	0.0179 (10)	0.0188 (9)	0.0174 (11)
O1	0.0433 (9)	0.0510 (10)	0.0346 (9)	0.0273 (8)	0.0228 (8)	0.0121 (7)
O2	0.0373 (9)	0.0419 (9)	0.0358 (8)	0.0138 (7)	0.0216 (8)	-0.0021 (7)
O1W	0.0245 (11)	0.0252 (10)	0.0319 (11)	0.000	0.0190 (10)	0.000
O3	0.1034 (17)	0.1078 (18)	0.0677 (13)	0.0817 (15)	0.0718 (14)	0.0575 (13)
O4	0.0232 (7)	0.0305 (7)	0.0271 (7)	0.0091 (6)	0.0146 (6)	0.0064 (6)
Mn1	0.01989 (17)	0.02365 (16)	0.02283 (17)	0.00100 (11)	0.01253 (13)	0.00210 (11)

Geometric parameters (Å, °)

C1—O2	1.245 (2)	C13—H13	0.93
C1—O1	1.256 (2)	C14—N2	1.467 (3)
C1—C2	1.518 (3)	C14—C15	1.470 (4)
C2—C3	1.368 (3)	C14—H14A	0.97
C2—C8	1.423 (3)	C14—H14B	0.97
C3—C4	1.406 (3)	C15—C15 ⁱ	1.497 (4)
C3—H3	0.93	C15—H15A	0.97
C4—C5	1.364 (3)	C15—H15B	0.97
C4—H4	0.93	C16—C17	1.357 (3)
C5—C7	1.420 (3)	C16—N2	1.358 (3)
C5—C6	1.510 (3)	C16—H16	0.93
C6—O3	1.228 (3)	C17—N1	1.358 (3)
C6—O4	1.263 (2)	C17—H17	0.93
C7—C10	1.420 (3)	Mn1—N1	2.2157 (17)
C7—C8	1.426 (3)	Mn1—O1	2.1343 (15)
C8—C9	1.414 (3)	Mn1—O2 ⁱⁱ	2.1535 (14)
C9—C12	1.362 (4)	Mn1—O1W	2.2085 (11)
C9—H9	0.93	O1W—Mn1 ⁱⁱ	2.2085 (11)
C10—C11	1.359 (4)	O1W—H1W1	0.83 (3)
C10—H10	0.93	O4—Mn1 ⁱⁱⁱ	2.2115 (14)
C11—C12	1.401 (4)	O4—Mn1 ^{iv}	2.4148 (13)
C11—H11	0.93	Mn1—O2 ⁱⁱ	2.1535 (14)
C12—H12	0.93	Mn1—O4 ^v	2.2115 (14)
C13—N1	1.323 (3)	Mn1—O4 ^{vi}	2.4148 (13)
C13—N2	1.336 (3)		
O2—C1—O1	126.60 (18)	C15—C14—H14B	108.7
O2—C1—C2	117.30 (18)	H14A—C14—H14B	107.6
O1—C1—C2	116.07 (18)	C14—C15—C15 ⁱ	114.7 (3)
C3—C2—C8	119.57 (18)	C14—C15—H15A	108.6
C3—C2—C1	119.00 (19)	C15 ⁱ —C15—H15A	108.6
C8—C2—C1	121.33 (18)	C14—C15—H15B	108.6
C2—C3—C4	121.3 (2)	C15 ⁱ —C15—H15B	108.6

C2—C3—H3	119.3	H15A—C15—H15B	107.6
C4—C3—H3	119.3	C17—C16—N2	106.1 (2)
C5—C4—C3	120.3 (2)	C17—C16—H16	127.0
C5—C4—H4	119.9	N2—C16—H16	127.0
C3—C4—H4	119.9	C16—C17—N1	110.4 (2)
C4—C5—C7	120.31 (18)	C16—C17—H17	124.8
C4—C5—C6	120.2 (2)	N1—C17—H17	124.8
C7—C5—C6	118.88 (19)	C13—N1—C17	104.58 (19)
O3—C6—O4	124.86 (19)	C13—N1—Mn1	124.47 (16)
O3—C6—C5	114.36 (18)	C17—N1—Mn1	130.37 (15)
O4—C6—C5	120.78 (18)	C13—N2—C16	106.84 (19)
C5—C7—C10	121.9 (2)	C13—N2—C14	126.7 (2)
C5—C7—C8	119.17 (19)	C16—N2—C14	126.5 (2)
C10—C7—C8	119.0 (2)	C1—O1—Mn1	140.78 (13)
C9—C8—C2	122.82 (19)	C1—O2—Mn1 ⁱⁱ	133.19 (13)
C9—C8—C7	118.2 (2)	Mn1—O1W—Mn1 ⁱⁱ	118.46 (9)
C2—C8—C7	118.94 (19)	Mn1—O1W—H1W1	101 (2)
C12—C9—C8	120.9 (2)	Mn1 ⁱⁱ —O1W—H1W1	112 (2)
C12—C9—H9	119.5	C6—O4—Mn1 ⁱⁱⁱ	128.35 (12)
C8—C9—H9	119.5	C6—O4—Mn1 ^{iv}	123.05 (12)
C11—C10—C7	120.9 (2)	Mn1 ⁱⁱⁱ —O4—Mn1 ^{iv}	106.99 (5)
C11—C10—H10	119.6	O1—Mn1—O2 ⁱⁱ	89.34 (6)
C7—C10—H10	119.6	O1—Mn1—O1W	89.50 (6)
C10—C11—C12	120.1 (2)	O2 ⁱⁱ —Mn1—O1W	89.38 (5)
C10—C11—H11	119.9	O1—Mn1—O4 ^v	91.01 (6)
C12—C11—H11	119.9	O2 ⁱⁱ —Mn1—O4 ^v	111.20 (5)
C9—C12—C11	120.9 (2)	O1W—Mn1—O4 ^v	159.42 (5)
C9—C12—H12	119.5	O1—Mn1—N1	174.19 (6)
C11—C12—H12	119.5	O2 ⁱⁱ —Mn1—N1	85.26 (6)
N1—C13—N2	112.1 (2)	O1W—Mn1—N1	88.30 (6)
N1—C13—H13	123.9	O4 ^v —Mn1—N1	92.93 (6)
N2—C13—H13	123.9	O1—Mn1—O4 ^{vi}	93.37 (6)
N2—C14—C15	114.4 (2)	O2 ⁱⁱ —Mn1—O4 ^{vi}	174.98 (6)
N2—C14—H14A	108.7	O1W—Mn1—O4 ^{vi}	86.42 (4)
C15—C14—H14A	108.7	O4 ^v —Mn1—O4 ^{vi}	73.01 (5)
N2—C14—H14B	108.7	N1—Mn1—O4 ^{vi}	91.86 (6)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $-x+1, y, -z+3/2$; (iii) $x+1/2, -y+1/2, z+1/2$; (iv) $-x+3/2, y-1/2, -z+3/2$; (v) $x-1/2, -y+1/2, z-1/2$; (vi) $-x+3/2, y+1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W1 \cdots O3 ^{vi}	0.83 (3)	1.72 (3)	2.5361 (19)	166 (3)

Symmetry code: (vi) $-x+3/2, y+1/2, -z+3/2$.