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Crystal structure of *trans*-diaquabis(nicotinamide-κN^1)bis(4-nitrobenzoato-κO)manganese(II)

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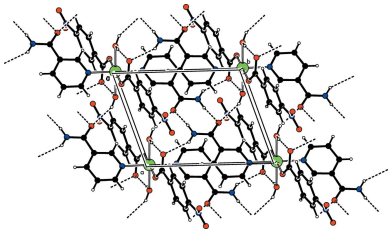
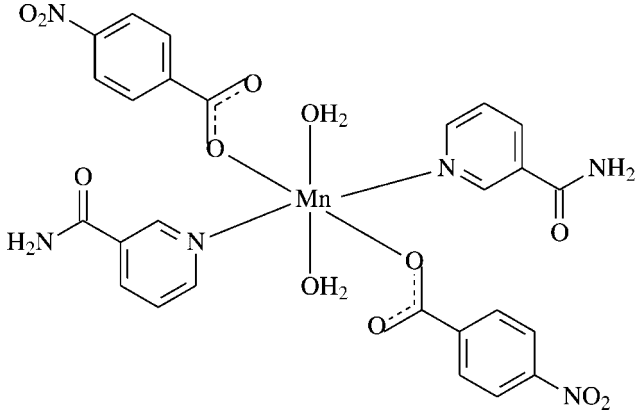
The asymmetric unit of the title compound, $[Mn(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$, contains one Mn^{II} atom, one 4-nitrobenzoate (NB) anion, one nicotinamide (NA) ligand and one water molecule; NA and NB each act as a monodentate ligand. The Mn^{II} atom, lying on an inversion centre, is coordinated by four O atoms and two pyridine N atoms in a distorted octahedral geometry. The water molecules are hydrogen bonded to the carboxylate O atoms. The dihedral angle between the carboxylate group and the adjacent benzene ring is 24.4 (3)°, while the benzene and pyridine rings are oriented at a dihedral angle of 86.63 (11)°. In the crystal, O—H···O and N—H···O hydrogen bonds link the molecules, forming a layer parallel to the *ab* plane. The layers are further linked *via* weak C—H···O hydrogen bonds, a π–π stacking interaction [centroid–centroid distance = 3.868 (2) Å] and a weak C—H···π interaction, resulting in a three-dimensional network.

1. Chemical context

Nicotinamide (NA) is one form of niacin. A deficiency of this vitamin leads to loss of copper from the body, known as pellagra disease. The NA ring is the reactive part of nicotinamide adenine dinucleotide (NAD) and its phosphate (NADP), which are the major electron carriers in many biological oxidation–reduction reactions (You *et al.*, 1978). The nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli *et al.*, 1972). Transition metal complexes with biochemical molecules show interesting physical and/or chemical properties with potential applications in biological systems (Antolini *et al.*, 1982).





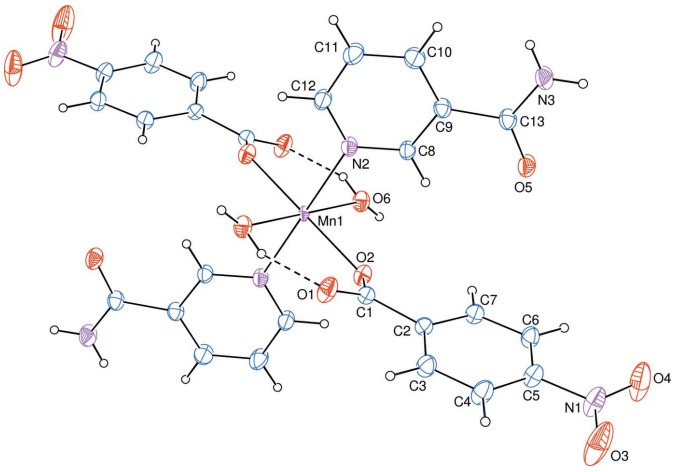


Figure 1
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Intramolecular O—H···O hydrogen bonds are shown as dashed lines. Unlabelled atoms are symmetry-related to labelled atoms by ($-x$, $-y$, $-z$).

Crystal structures of metal complexes with benzoic acid derivatives have been reported extensively because of the varieties of their coordination modes. For example, Co and Cd complexes with 4-aminobenzoic acid (Chen & Chen, 2002; Amiraslanov *et al.*, 1979; Hauptmann *et al.*, 2000), Co complexes with benzoic acid (Catterick *et al.*, 1974), 4-nitrobenzoic acid (Nadzhafov *et al.*, 1981) and phthalic acid (Adiwidjaja *et al.*, 1978), and Cu with 4-hydroxybenzoic acid (Shnulin *et al.*, 1981) have been described. Mn complexes closely related to the title compound, diaquabis(4-nitrobenzoato)bis(1*H*-1,2,4-triazol-3-amine)manganese (Zhang *et al.*, 2013) and diaquabis(1*H*-imidazole)bis(4-nitrobenzoato)-manganese (Xu & Xu, 2004), have also been reported.

2. Structural commentary

The asymmetric unit of the title mononuclear complex contains one Mn^{II} atom (site symmetry $\overline{1}$), one 4-nitrobenzoate (NB) anion, one nicotinamide (NA) ligand and one water molecule, all ligands coordinating in a monodentate manner. In the complex, the two carboxylate O atoms (O2 and $O2^{iii}$) of the two symmetry-related monodentate NB anions and the two symmetry-related water O atoms (O6 and $O6^{iii}$) around the Mn^{II} atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination sphere is completed by the two pyridine N atoms (N2 and $N2^{iii}$) of the two symmetry-related monodentate NA ligands in the axial positions [symmetry code: (iii) $-x$, $-y$, $-z$; Fig. 1].

The near equality of C—O bond lengths [C1—O1 = 1.253 (4) and C1—O2 = 1.248 (4) Å] in the carboxylate group indicates delocalized bonds rather than localized single and double bonds. The Mn—O bond lengths [2.156 (2) and 2.115 (2) Å] and the Mn—N bond length [2.134 (3) Å] are close to the standard values. Atom Mn1 lies 0.4172 (1) Å above the O1/O2/C1 plane of the carboxylate group. The O—Mn—O and O—Mn—N bond angles deviate slightly from the ideal value of 90°. The dihedral angle between the carboxylate group (O1/O2/C1) and the adjacent benzene (C2–C7) ring is 24.4 (3)°, while the benzene ring and the pyridine (N2/C8–C12) ring are oriented at a dihedral angle of 86.63 (11)°.

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

*Cg*2 is the centroid of the N2/C8–C12 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O5^{i}	0.90 (5)	2.07 (6)	2.898 (6)	152 (4)
N3—H3B···O1^{ii}	0.90 (4)	2.19 (5)	2.923 (4)	138 (4)
O6—H61···O1^{iii}	0.90 (4)	1.78 (5)	2.646 (5)	161 (4)
O6—H62···O5^{iv}	0.89 (3)	2.10 (4)	2.897 (3)	148 (4)
C3—H3···O4^{v}	0.93	2.59	3.456 (6)	156
C6—H6···O1^{vi}	0.93	2.40	3.319 (4)	170
C12—H12···O3^{vii}	0.93	2.54	3.416 (7)	157
C4—H4···*Cg*2^{viii}	0.93	2.91	3.827 (4)	172

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

3. Supramolecular features

In the crystal, intermolecular N—H_{na}···O_{na} (na = nicotinamide), N—H_{na}···O_c (c = carboxylate group) and O—H_w···O_{na} (w = water) hydrogen bonds (Table 1) link the molecules, forming a layer parallel to the *ab* plane (Fig. 2). In the layer, $R_2^2(8)$ and $R_4^2(8)$ ring motifs are observed. The layers are further linked *via* weak C—H···O hydrogen bonds, a weak C—H···π interaction (Table 1) and a π–π interaction between the benzene rings [$Cg1\cdots Cg1^{ix}$ = 3.868 (2) Å; symmetry code: (ix) $1-x, -y, 1-z$, where *Cg*1 is the centroid of the C2–C7 ring].

4. Synthesis and crystallization

The title compound was prepared by the reaction of $MnSO_4\cdot H_2O$ (0.85 g, 25 mmol) in H_2O (25 ml) and nicotina-

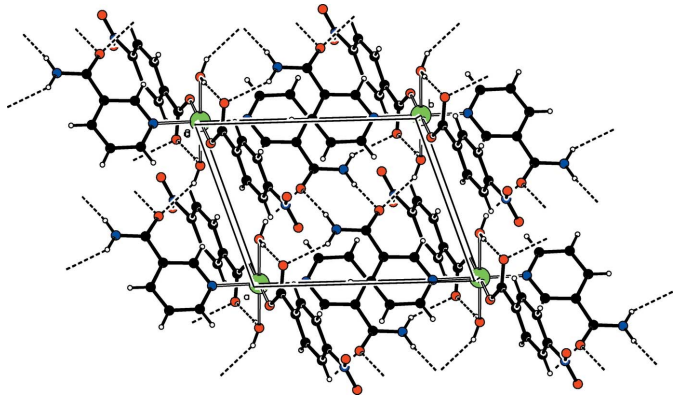


Figure 2
A packing diagram of the title compound, viewed down the *c* axis. Intermolecular O—H···O and N—H···O hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Mn(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r	667.45
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.6051 (3), 10.0027 (4), 10.2152 (4)
α, β, γ (°)	78.067 (3), 88.430 (4), 71.746 (3)
V (Å^3)	721.45 (5)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.53
Crystal size (mm)	0.45 × 0.35 × 0.32
Data collection	
Diffractometer	Bruker SMART BREEZE CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.765, 0.815
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17255, 3595, 3475
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.178, 1.17
No. of reflections	3595
No. of parameters	217
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.00, −0.50

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

mide (1.22 g, 10 mmol) in H_2O (25 ml) with sodium 4-nitrobenzoate (1.90 g, 10 mmol) in H_2O (150 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving colourless single crystals.

5. Refinement

The experimental details including the crystal data, data collection and refinement are summarized in Table 2. Atoms H61 and H62 of the water molecule and atoms H3*A* and H3*B* of the NH_2 group were located in a difference Fourier map, and their coordinates were refined with distance restraints of O—H = 0.85 (2) Å and N—H = 0.86 (2) Å, and with U_{iso}(H) = 1.5U_{eq}(O,N). The C-bound H atoms were positioned geometrically with C—H = 0.93 Å and were constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

trans-Diaquabis(nicotinamide-κN^1)bis(4-nitrobenzoato-κO)manganese(II)

Crystal data

$[Mn(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r = 667.45
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.6051 (3) Å
b = 10.0027 (4) Å
c = 10.2152 (4) Å
α = 78.067 (3)°
β = 88.430 (4)°
γ = 71.746 (3)°
V = 721.45 (5) Å^3
Z = 1
$F(000)$ = 343
D_x = 1.536 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9891 reflections
θ = 2.2–28.4°
μ = 0.53 mm^{-1}
T = 296 K
Prism, colourless
0.45 × 0.35 × 0.32 mm

Data collection

Bruker SMART BREEZE CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.765, T_{max} = 0.815
17255 measured reflections
3595 independent reflections
3475 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.4°, θ_{min} = 2.0°
h = −10→9
k = −12→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.178
S = 1.17
3595 reflections
217 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

$w = 1/[\sigma^2(F_o^2) + (0.0908P)^2 + 0.7889P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.00$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.0000	0.0000	0.0000	0.02437 (17)
O1	−0.1121 (4)	0.1452 (4)	0.2673 (3)	0.0638 (7)
O2	0.1322 (3)	0.0165 (3)	0.1728 (2)	0.0479 (5)
O3	0.4619 (6)	0.2860 (8)	0.6872 (5)	0.147 (3)
O4	0.6545 (6)	0.2824 (7)	0.5355 (5)	0.124 (2)
O5	0.4269 (4)	0.3417 (3)	−0.0003 (3)	0.0598 (7)
O6	0.2722 (3)	−0.0746 (3)	−0.0769 (3)	0.0506 (6)
H61	0.227 (7)	−0.084 (6)	−0.154 (3)	0.076*
H62	0.377 (4)	−0.135 (4)	−0.034 (5)	0.076*
N1	0.5113 (5)	0.2645 (5)	0.5801 (4)	0.0736 (11)
N2	−0.0042 (4)	0.2124 (3)	−0.0942 (3)	0.0427 (6)
N3	0.3202 (5)	0.5611 (4)	−0.1340 (4)	0.0645 (9)
H3A	0.424 (5)	0.579 (6)	−0.113 (6)	0.097*
H3B	0.227 (6)	0.623 (5)	−0.189 (5)	0.097*
C1	0.0585 (4)	0.0898 (3)	0.2563 (3)	0.0409 (6)
C2	0.1853 (4)	0.1239 (3)	0.3472 (3)	0.0406 (6)
C3	0.1181 (5)	0.1682 (5)	0.4643 (4)	0.0533 (8)
H3	−0.0002	0.1685	0.4902	0.064*
C4	0.2265 (5)	0.2118 (5)	0.5428 (4)	0.0605 (10)
H4	0.1835	0.2402	0.6220	0.073*
C5	0.3994 (5)	0.2121 (4)	0.5000 (4)	0.0516 (8)
C6	0.4712 (5)	0.1680 (4)	0.3862 (3)	0.0489 (7)
H6	0.5888	0.1696	0.3601	0.059*
C7	0.3619 (5)	0.1205 (4)	0.3104 (3)	0.0455 (7)
H7	0.4088	0.0863	0.2344	0.055*
C8	0.1370 (4)	0.2581 (3)	−0.0689 (3)	0.0417 (6)
H8	0.2343	0.1949	−0.0119	0.050*
C9	0.1454 (4)	0.3939 (3)	−0.1231 (3)	0.0428 (6)
C10	−0.0002 (6)	0.4870 (4)	−0.2088 (4)	0.0617 (10)
H10	0.0003	0.5796	−0.2475	0.074*
C11	−0.1449 (6)	0.4407 (4)	−0.2358 (5)	0.0666 (11)
H11	−0.2433	0.5015	−0.2932	0.080*

C12	−0.1424 (5)	0.3030 (4)	−0.1765 (4)	0.0501 (7)
H12	−0.2409	0.2724	−0.1948	0.060*
C13	0.3087 (5)	0.4309 (3)	−0.0821 (4)	0.0464 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0212 (3)	0.0226 (3)	0.0332 (3)	−0.01052 (18)	−0.00068 (17)	−0.00816 (18)
O1	0.0382 (12)	0.091 (2)	0.0654 (16)	−0.0140 (13)	−0.0016 (11)	−0.0323 (15)
O2	0.0433 (12)	0.0484 (12)	0.0548 (13)	−0.0132 (9)	−0.0050 (9)	−0.0175 (10)
O3	0.081 (3)	0.287 (7)	0.131 (4)	−0.070 (4)	0.026 (3)	−0.155 (5)
O4	0.087 (3)	0.220 (6)	0.126 (4)	−0.093 (3)	0.027 (3)	−0.102 (4)
O5	0.0565 (15)	0.0446 (12)	0.0814 (18)	−0.0224 (11)	−0.0182 (13)	−0.0067 (12)
O6	0.0376 (11)	0.0527 (13)	0.0614 (14)	−0.0119 (10)	0.0006 (10)	−0.0152 (11)
N1	0.0497 (18)	0.104 (3)	0.079 (2)	−0.0200 (19)	−0.0025 (16)	−0.052 (2)
N2	0.0390 (12)	0.0402 (12)	0.0517 (14)	−0.0156 (10)	−0.0025 (10)	−0.0104 (11)
N3	0.067 (2)	0.0450 (16)	0.087 (2)	−0.0305 (15)	−0.0144 (18)	−0.0052 (15)
C1	0.0398 (14)	0.0415 (14)	0.0414 (14)	−0.0142 (12)	−0.0017 (11)	−0.0062 (11)
C2	0.0383 (14)	0.0410 (14)	0.0411 (14)	−0.0117 (11)	−0.0015 (11)	−0.0066 (11)
C3	0.0396 (15)	0.074 (2)	0.0493 (17)	−0.0174 (15)	0.0056 (13)	−0.0201 (16)
C4	0.0453 (18)	0.092 (3)	0.0505 (18)	−0.0181 (18)	0.0062 (14)	−0.0341 (19)
C5	0.0430 (16)	0.061 (2)	0.0534 (18)	−0.0133 (14)	−0.0036 (13)	−0.0231 (15)
C6	0.0385 (15)	0.0613 (19)	0.0509 (17)	−0.0173 (14)	0.0034 (13)	−0.0179 (15)
C7	0.0420 (15)	0.0530 (17)	0.0441 (15)	−0.0149 (13)	0.0043 (12)	−0.0162 (13)
C8	0.0394 (14)	0.0385 (14)	0.0499 (16)	−0.0154 (11)	−0.0037 (12)	−0.0091 (12)
C9	0.0440 (15)	0.0358 (13)	0.0514 (16)	−0.0144 (12)	0.0007 (12)	−0.0124 (12)
C10	0.065 (2)	0.0387 (16)	0.078 (3)	−0.0181 (16)	−0.0145 (19)	0.0012 (16)
C11	0.057 (2)	0.0495 (19)	0.085 (3)	−0.0138 (16)	−0.027 (2)	0.0046 (18)
C12	0.0424 (16)	0.0481 (17)	0.0606 (19)	−0.0155 (13)	−0.0095 (14)	−0.0097 (14)
C13	0.0467 (16)	0.0386 (14)	0.0586 (18)	−0.0171 (12)	0.0001 (13)	−0.0144 (13)

Geometric parameters (Å, º)

Mn1—O2	2.115 (2)	C2—C7	1.377 (4)
Mn1—O2^{i}	2.115 (2)	C3—C4	1.385 (5)
Mn1—O6	2.156 (2)	C3—H3	0.9300
Mn1—O6^{i}	2.156 (2)	C4—H4	0.9300
Mn1—N2	2.134 (3)	C5—N1	1.471 (5)
Mn1—N2^{i}	2.134 (3)	C5—C4	1.375 (5)
O1—C1	1.253 (4)	C6—C5	1.368 (5)
O2—C1	1.248 (4)	C6—C7	1.397 (5)
O3—N1	1.187 (5)	C6—H6	0.9300
O4—N1	1.219 (5)	C7—H7	0.9300
O5—C13	1.238 (4)	C8—C9	1.377 (4)
O6—H61	0.903 (19)	C8—H8	0.9300
O6—H62	0.892 (19)	C9—C10	1.389 (5)
N2—C8	1.342 (4)	C9—C13	1.495 (4)
N2—C12	1.330 (4)	C10—C11	1.375 (6)

N3—C13	1.330 (4)	C10—H10	0.9300
N3—H3A	0.90 (2)	C11—H11	0.9300
N3—H3B	0.90 (2)	C12—C11	1.380 (5)
C2—C1	1.515 (4)	C12—H12	0.9300
C2—C3	1.390 (4)		

O2^{i}—Mn1—O2	180.00 (7)	C2—C3—H3	119.8
O2—Mn1—O6	87.19 (10)	C4—C3—C2	120.3 (3)
O2^{i}—Mn1—O6	92.81 (10)	C4—C3—H3	119.8
O2—Mn1—O6^{i}	92.81 (10)	C3—C4—H4	121.0
O2^{i}—Mn1—O6^{i}	87.19 (10)	C5—C4—C3	118.1 (3)
O2—Mn1—N2	89.98 (10)	C5—C4—H4	121.0
O2^{i}—Mn1—N2	90.02 (10)	C4—C5—N1	118.1 (3)
O2—Mn1—N2^{i}	90.02 (10)	C6—C5—N1	118.5 (3)
O2^{i}—Mn1—N2^{i}	89.98 (10)	C6—C5—C4	123.4 (3)
O6—Mn1—O6^{i}	180.00 (13)	C5—C6—C7	117.7 (3)
N2—Mn1—O6	87.00 (10)	C5—C6—H6	121.1
N2^{i}—Mn1—O6	93.00 (10)	C7—C6—H6	121.1
N2—Mn1—O6^{i}	93.00 (10)	C2—C7—C6	120.6 (3)
N2^{i}—Mn1—O6^{i}	87.00 (10)	C2—C7—H7	119.7
N2^{i}—Mn1—N2	180.00 (7)	C6—C7—H7	119.7
C1—O2—Mn1	126.2 (2)	N2—C8—C9	123.4 (3)
Mn1—O6—H61	93 (3)	N2—C8—H8	118.3
Mn1—O6—H62	129 (3)	C9—C8—H8	118.3
H61—O6—H62	124 (5)	C8—C9—C10	117.7 (3)
O3—N1—O4	121.7 (4)	C8—C9—C13	117.2 (3)
O3—N1—C5	119.3 (4)	C10—C9—C13	125.1 (3)
O4—N1—C5	119.0 (4)	C9—C10—H10	120.4
C8—N2—Mn1	119.1 (2)	C11—C10—C9	119.3 (3)
C12—N2—Mn1	122.8 (2)	C11—C10—H10	120.4
C12—N2—C8	118.1 (3)	C10—C11—C12	119.1 (3)
C13—N3—H3A	117 (4)	C10—C11—H11	120.4
C13—N3—H3B	118 (4)	C12—C11—H11	120.4
H3A—N3—H3B	125 (5)	N2—C12—C11	122.4 (3)
O1—C1—C2	116.4 (3)	N2—C12—H12	118.8
O2—C1—O1	126.0 (3)	C11—C12—H12	118.8
O2—C1—C2	117.5 (3)	O5—C13—N3	122.0 (3)
C3—C2—C1	119.5 (3)	O5—C13—C9	119.8 (3)
C7—C2—C1	120.5 (3)	N3—C13—C9	118.2 (3)
C7—C2—C3	119.9 (3)		

O6—Mn1—O2—C1	160.3 (3)	C7—C2—C3—C4	1.4 (6)
O6^{i}—Mn1—O2—C1	−19.7 (3)	C1—C2—C7—C6	172.5 (3)
N2—Mn1—O2—C1	73.3 (3)	C3—C2—C7—C6	−3.2 (5)
N2^{i}—Mn1—O2—C1	−106.7 (3)	C2—C3—C4—C5	1.0 (6)
O2—Mn1—N2—C8	34.5 (2)	C4—C5—N1—O3	10.2 (8)
O2^{i}—Mn1—N2—C8	−145.5 (2)	C4—C5—N1—O4	−171.0 (5)
O2—Mn1—N2—C12	−144.8 (3)	C6—C5—N1—O3	−170.6 (6)

O2^{i}—Mn1—N2—C12	35.2 (3)	C6—C5—N1—O4	8.1 (7)
O6—Mn1—N2—C8	−52.7 (2)	N1—C5—C4—C3	177.4 (4)
O6^{i}—Mn1—N2—C8	127.3 (2)	C6—C5—C4—C3	−1.8 (7)
O6—Mn1—N2—C12	128.0 (3)	C7—C6—C5—N1	−179.1 (4)
O6^{i}—Mn1—N2—C12	−52.0 (3)	C7—C6—C5—C4	0.0 (6)
Mn1—O2—C1—O1	14.1 (5)	C5—C6—C7—C2	2.5 (5)
Mn1—O2—C1—C2	−161.6 (2)	N2—C8—C9—C10	−0.4 (5)
Mn1—N2—C8—C9	−178.9 (2)	N2—C8—C9—C13	178.0 (3)
C12—N2—C8—C9	0.4 (5)	C8—C9—C10—C11	0.1 (6)
Mn1—N2—C12—C11	179.2 (3)	C13—C9—C10—C11	−178.3 (4)
C8—N2—C12—C11	−0.1 (6)	C8—C9—C13—O5	−1.5 (5)
C3—C2—C1—O1	22.0 (5)	C8—C9—C13—N3	179.5 (3)
C3—C2—C1—O2	−161.8 (3)	C10—C9—C13—O5	176.8 (4)
C7—C2—C1—O1	−153.7 (3)	C10—C9—C13—N3	−2.2 (6)
C7—C2—C1—O2	22.4 (4)	C9—C10—C11—C12	0.3 (7)
C1—C2—C3—C4	−174.4 (4)	N2—C12—C11—C10	−0.3 (7)

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the N2/C8–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O5^{ii}	0.90 (5)	2.07 (6)	2.898 (6)	152 (4)
N3—H3*B*···O1^{iii}	0.90 (4)	2.19 (5)	2.923 (4)	138 (4)
O6—H61···O1^{i}	0.90 (4)	1.78 (5)	2.646 (5)	161 (4)
O6—H62···O5^{iv}	0.89 (3)	2.10 (4)	2.897 (3)	148 (4)
C3—H3···O4^{v}	0.93	2.59	3.456 (6)	156
C6—H6···O1^{vi}	0.93	2.40	3.319 (4)	170
C12—H12···O3^{vii}	0.93	2.54	3.416 (7)	157
C4—H4···*Cg*2^{viii}	0.93	2.91	3.827 (4)	172

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) −*x*+1, −*y*, −*z*; (v) *x*−1, *y*, *z*; (vi) *x*+1, *y*, *z*; (vii) *x*−1, *y*, *z*−1; (viii) *x*, *y*, *z*+1.