metal-organic compounds

Bis[N^3-(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato-κ^3N^1,N^2,O]-manganese(II)

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In the title compound, [Mn(C$_{13}$H$_{11}$N$_4$O$_2$)$_2$], the Mn atom is coordinated in a distorted octahedral manner by pyridyl N atoms, amidrazonato N atoms and carbamoy O atoms from two tridentate N^3-salicyloylpyridine-2-carboxamidrazonato ligands. N—H⋯O hydrogen bonds result in the formation of two chains, one parallel to the b axis and the other parallel to the c axis. These two chains are cross-linked, building up layers parallel to the (100) plane.

Related literature

For related structures, see: Van Koningsbruggen *et al.* (1993, 1995); Li (2007).
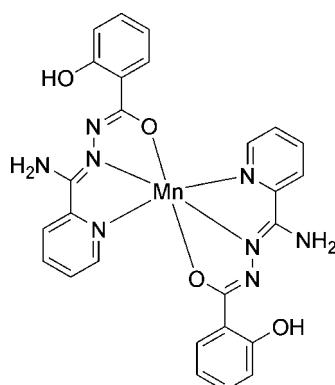
Experimental

Crystal data

[Mn(C$_{13}$H$_{11}$N$_4$O$_2$)$_2$]
M_r = 565.46
Monoclinic, $P2/c$
a = 10.7661 (16) Å
b = 13.049 (2) Å
c = 19.998 (3) Å
β = 116.192 (7)°

V = 2521.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 173 (2) K
0.35 × 0.32 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.816, T_{max} = 0.850

13210 measured reflections
4676 independent reflections
4155 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.110
S = 1.07
4676 reflections

352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2A⋯N4	0.84	1.82	2.564 (2)	146
O4—H4A⋯N8	0.84	1.80	2.541 (2)	147
N3—H3A⋯O2^i	0.88	2.37	3.072 (3)	137
N3—H3B⋯O3^{ii}	0.88	2.20	2.847 (3)	130
N6—H6A⋯O4^{iii}	0.88	2.44	3.065 (3)	129
N6—H6B⋯O1^{iv}	0.88	2.19	2.907 (3)	138

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL* ; molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *XP* (in *SHELXTL*); software used to prepare material for publication: *SHELXTL*.

References

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supporting information

Bis[N^3-(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato-κ^3N^1,N^2,O]manganese(II)

Yong Li

S1. Comment

The N^3-salicyloylpyridine-2-carboxamidrazonato ligand (abbreviated as Hspa) has several potential donor atoms and can occur in different chemical and structural conformations. In the Copper(II) coordination compound containing the de-hydrogenated spa ligand (Van Koningsbruggen *et al.*, 1995), this spa ligand is fairly planar, whereas in the title complex it is slighted bent around the central Mn—N bonds, with a dihedral angle of 20.53 (7)° between the two aromatic rings (Fig. 1).

Hydrogen bonds N6—H6A···O4 and N3—H3B···O3 forms chain parallel to the *b* axis (Table 1) whereas hydrogen bonds of N6—H6A···O4 and N3—H3A···O2 result in a chain parallels to *c* axis. These two chains are crosslinked to build up layers parallel to the (1 0 0) plane. There are also intramolecular O—H···N hydrogen bonds which do not participate to the packing (Table 1).

S2. Experimental

The ligand N^3-salicyloylpyridine-2-carboxamidrazonato (Hspa) was synthesized according to literature (Van Koningsbruggen *et al.*, 1995). [Mn(C$_{13}$H$_{11}$N$_4$O$_2$)$_2$] was synthesized by adding ligand (0.0256 g, 0.10 mmol) and Et$_3$N (0.010 g, 0.1 mmol) in 1 ml DMSO to a solution of Mn(acac)$_2$ (0.0253 g, 0.10 mmol) in CH$_2$Cl$_2$ (4 ml). The compound crystallized upon evaporation of the solvent at room temperature after a few days.

S3. Refinement

H atoms bonded to N and O atoms were located in a difference map and refined with distance restraints, and with U_{iso}(H) = 1.2U_{eq}(N,O). Other H atoms were positioned geometrically and refined using a riding model with U_{iso}(H) = 1.2 times U_{eq}(C).
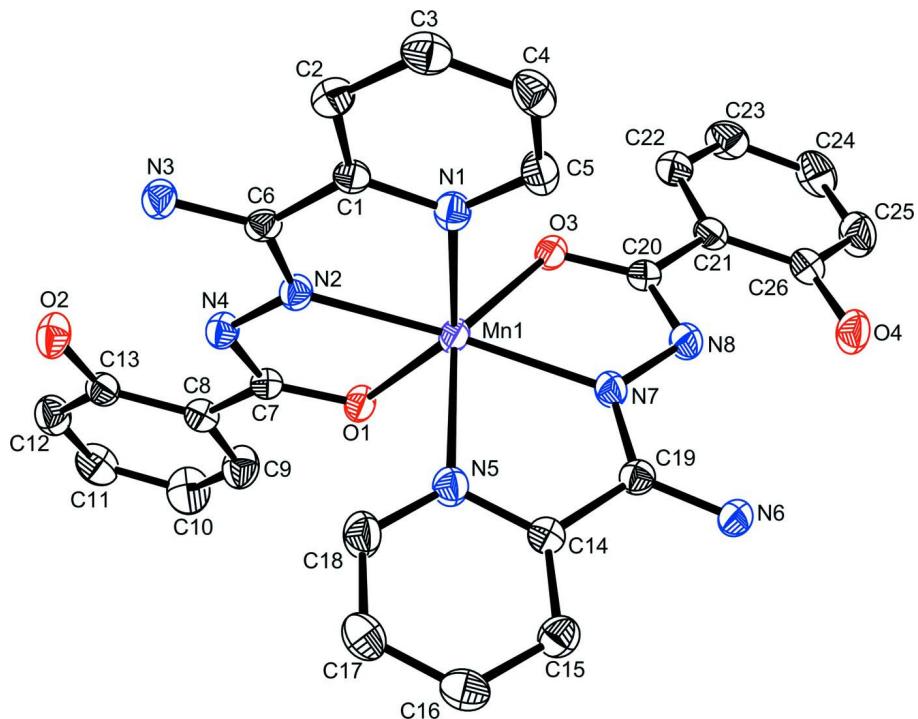
Figure 1

A view of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.
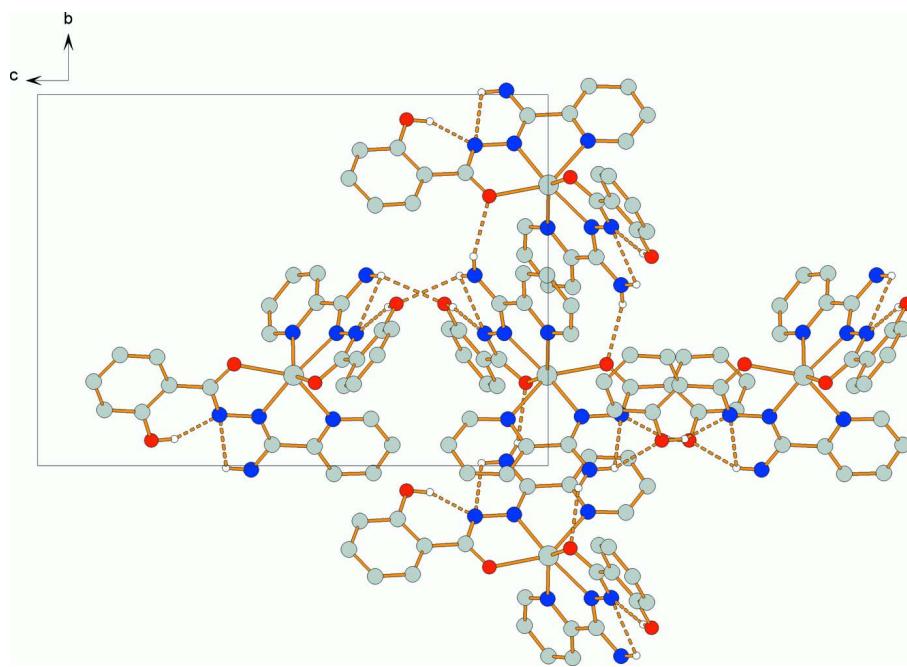
Figure 2

View down *a*, showing the crosslinking chains by hydrogen bonds. The *c* axis is horizontal. H atoms not involved in H bondings are removed for purpose of clarity.

Bis[N^3-(2-hydroxybenzoyl)pyridine-2-carboxamidrazonato- $\kappa^3 N^1,N^2,O$]manganese(II)

Crystal data

[Mn(C$_{13}$H$_{11}$N$_4$O$_2$)$_2$]	$F(000) = 1164$
$M_r = 565.46$	$D_x = 1.490$ Mg m^{-3}
Monoclinic, $P2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yc	Cell parameters from 9514 reflections
$a = 10.7661$ (16) Å	$\theta = 2.5–28.3°$
$b = 13.049$ (2) Å	$\mu = 0.57$ mm^{-1}
$c = 19.998$ (3) Å	$T = 173$ K
$\beta = 116.192$ (7)°	Block, red
$V = 2521.0$ (7) Å^3	$0.35 \times 0.32 \times 0.28$ mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	13210 measured reflections
Radiation source: fine-focus sealed tube	4676 independent reflections
Graphite monochromator	4155 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.051$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{max} = 25.5°$, $\theta_{min} = 1.6°$
	$h = -13 \rightarrow 12$
$T_{min} = 0.816$, $T_{max} = 0.850$	$k = -15 \rightarrow 15$
	$l = -24 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.110$	
$S = 1.07$	H-atom parameters constrained
4676 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 2.5739P]$ where $P = (F_o^2 + 2F_c^2)/3$
352 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.71$ e Å^{-3}
	$\Delta\rho_{min} = -0.46$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.48496 (3)	0.24317 (2)	0.001305 (18)	0.01994 (12)
O1	0.34073 (16)	0.27345 (12)	−0.11489 (9)	0.0227 (3)
O2	0.34502 (18)	0.06726 (13)	−0.27699 (9)	0.0303 (4)
H2A	0.4017	0.0720	−0.2318	0.045*

O3	0.33067 (16)	0.22300 (12)	0.04389 (9)	0.0230 (3)
O4	0.33727 (19)	0.43655 (13)	0.20316 (10)	0.0327 (4)
H4A	0.3958	0.4277	0.1866	0.049*
N1	0.64892 (19)	0.12437 (15)	0.07874 (10)	0.0229 (4)
N2	0.52421 (19)	0.13187 (14)	−0.06626 (10)	0.0210 (4)
N3	0.6414 (2)	−0.01103 (14)	−0.08148 (11)	0.0243 (4)
H3A	0.6011	−0.0063	−0.1304	0.029*
H3B	0.7018	−0.0602	−0.0596	0.029*
N4	0.44572 (19)	0.13650 (14)	−0.14337 (10)	0.0218 (4)
N5	0.64734 (19)	0.35892 (15)	−0.00045 (11)	0.0242 (4)
N6	0.6224 (2)	0.51303 (15)	0.14364 (11)	0.0287 (5)
H6A	0.5814	0.5115	0.1731	0.034*
H6B	0.6772	0.5645	0.1462	0.034*
N7	0.52385 (19)	0.35738 (14)	0.08584 (10)	0.0218 (4)
N8	0.4424 (2)	0.35657 (15)	0.12401 (11)	0.0238 (4)
C1	0.6845 (2)	0.05120 (16)	0.04260 (12)	0.0194 (4)
C2	0.7836 (2)	−0.02275 (18)	0.08055 (13)	0.0249 (5)
H2	0.8065	−0.0739	0.0540	0.030*
C3	0.8486 (2)	−0.02049 (19)	0.15777 (14)	0.0289 (5)
H3	0.9160	−0.0707	0.1849	0.035*
C4	0.8145 (2)	0.0552 (2)	0.19479 (13)	0.0291 (5)
H4	0.8589	0.0588	0.2477	0.035*
C5	0.7136 (2)	0.12593 (19)	0.15304 (13)	0.0270 (5)
H5	0.6895	0.1778	0.1786	0.032*
C6	0.6109 (2)	0.05651 (16)	−0.04034 (12)	0.0195 (4)
C7	0.3522 (2)	0.21080 (16)	−0.16168 (12)	0.0202 (4)
C8	0.2524 (2)	0.21631 (18)	−0.24186 (13)	0.0228 (5)
C9	0.1513 (3)	0.2926 (2)	−0.26567 (14)	0.0327 (6)
H9	0.1509	0.3419	−0.2308	0.039*
C10	0.0521 (3)	0.2982 (2)	−0.33867 (15)	0.0391 (6)
H10	−0.0147	0.3516	−0.3538	0.047*
C11	0.0499 (3)	0.2261 (2)	−0.38990 (14)	0.0345 (6)
H11	−0.0199	0.2290	−0.4399	0.041*
C12	0.1491 (3)	0.1499 (2)	−0.36856 (14)	0.0309 (5)
H12	0.1480	0.1011	−0.4041	0.037*
C13	0.2511 (2)	0.14416 (17)	−0.29498 (12)	0.0235 (5)
C14	0.6746 (2)	0.43915 (17)	0.04641 (12)	0.0202 (4)
C15	0.7624 (2)	0.51802 (18)	0.04861 (13)	0.0264 (5)
H15	0.7787	0.5742	0.0817	0.032*
C16	0.8263 (3)	0.51342 (19)	0.00135 (14)	0.0297 (5)
H16	0.8870	0.5665	0.0017	0.036*
C17	0.8001 (3)	0.4310 (2)	−0.04579 (14)	0.0319 (6)
H17	0.8427	0.4259	−0.0783	0.038*
C18	0.7105 (3)	0.3555 (2)	−0.04503 (14)	0.0306 (5)
H18	0.6930	0.2986	−0.0776	0.037*
C19	0.6018 (2)	0.43734 (16)	0.09498 (12)	0.0208 (5)
C20	0.3441 (2)	0.28614 (17)	0.09614 (12)	0.0218 (5)
C21	0.2390 (2)	0.28714 (18)	0.12565 (12)	0.0236 (5)

C22	0.1321 (3)	0.21487 (19)	0.09977 (14)	0.0285 (5)
H22	0.1339	0.1612	0.0681	0.034*
C23	0.0237 (3)	0.2198 (2)	0.11919 (15)	0.0348 (6)
H23	−0.0481	0.1701	0.1010	0.042*
C24	0.0211 (3)	0.2983 (2)	0.16550 (15)	0.0389 (6)
H24	−0.0544	0.3033	0.1779	0.047*
C25	0.1270 (3)	0.3689 (2)	0.19368 (15)	0.0361 (6)
H25	0.1250	0.4212	0.2263	0.043*
C26	0.2376 (3)	0.36451 (18)	0.17467 (13)	0.0267 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.02221 (19)	0.01706 (19)	0.0222 (2)	−0.00067 (13)	0.01128 (15)	−0.00370 (13)
O1	0.0249 (8)	0.0214 (8)	0.0214 (8)	0.0025 (6)	0.0099 (7)	−0.0026 (6)
O2	0.0325 (9)	0.0330 (9)	0.0216 (8)	0.0076 (7)	0.0085 (7)	−0.0036 (7)
O3	0.0269 (8)	0.0200 (8)	0.0253 (8)	−0.0025 (6)	0.0144 (7)	−0.0038 (6)
O4	0.0392 (10)	0.0340 (10)	0.0344 (10)	−0.0081 (8)	0.0250 (8)	−0.0119 (8)
N1	0.0224 (9)	0.0242 (10)	0.0232 (10)	−0.0024 (8)	0.0112 (8)	−0.0025 (8)
N2	0.0223 (9)	0.0209 (9)	0.0184 (9)	0.0006 (8)	0.0078 (8)	−0.0013 (7)
N3	0.0295 (10)	0.0225 (10)	0.0210 (10)	0.0074 (8)	0.0113 (8)	0.0012 (7)
N4	0.0224 (9)	0.0219 (10)	0.0197 (9)	0.0015 (8)	0.0079 (8)	−0.0015 (7)
N5	0.0248 (10)	0.0253 (10)	0.0249 (10)	−0.0018 (8)	0.0132 (8)	−0.0031 (8)
N6	0.0400 (12)	0.0236 (10)	0.0303 (11)	−0.0106 (9)	0.0227 (10)	−0.0082 (8)
N7	0.0241 (9)	0.0236 (10)	0.0217 (9)	−0.0030 (8)	0.0138 (8)	−0.0028 (8)
N8	0.0273 (10)	0.0243 (10)	0.0255 (10)	−0.0026 (8)	0.0169 (8)	−0.0030 (8)
C1	0.0187 (10)	0.0188 (11)	0.0226 (11)	−0.0041 (8)	0.0108 (9)	−0.0006 (8)
C2	0.0239 (11)	0.0218 (11)	0.0284 (12)	−0.0010 (9)	0.0112 (10)	−0.0004 (9)
C3	0.0248 (12)	0.0300 (13)	0.0270 (12)	−0.0007 (10)	0.0071 (10)	0.0053 (10)
C4	0.0263 (12)	0.0387 (14)	0.0186 (11)	−0.0060 (10)	0.0066 (10)	0.0001 (10)
C5	0.0282 (12)	0.0318 (13)	0.0230 (12)	−0.0036 (10)	0.0133 (10)	−0.0033 (10)
C6	0.0185 (10)	0.0171 (11)	0.0249 (11)	−0.0041 (8)	0.0114 (9)	−0.0010 (8)
C7	0.0227 (11)	0.0183 (10)	0.0212 (11)	−0.0014 (9)	0.0111 (9)	−0.0003 (8)
C8	0.0229 (11)	0.0234 (11)	0.0225 (11)	−0.0004 (9)	0.0103 (10)	0.0012 (9)
C9	0.0323 (13)	0.0338 (14)	0.0302 (13)	0.0082 (11)	0.0122 (11)	−0.0003 (11)
C10	0.0320 (14)	0.0450 (16)	0.0336 (14)	0.0164 (12)	0.0084 (12)	0.0074 (12)
C11	0.0276 (13)	0.0460 (16)	0.0215 (12)	0.0006 (11)	0.0032 (10)	0.0059 (11)
C12	0.0313 (13)	0.0358 (14)	0.0257 (12)	−0.0037 (11)	0.0128 (11)	−0.0031 (10)
C13	0.0249 (11)	0.0243 (12)	0.0226 (11)	−0.0023 (9)	0.0117 (10)	0.0000 (9)
C14	0.0170 (10)	0.0221 (11)	0.0190 (10)	0.0017 (8)	0.0057 (9)	0.0018 (9)
C15	0.0236 (12)	0.0262 (12)	0.0281 (12)	−0.0028 (9)	0.0102 (10)	−0.0025 (10)
C16	0.0226 (11)	0.0334 (14)	0.0360 (14)	−0.0040 (10)	0.0155 (11)	0.0029 (11)
C17	0.0291 (13)	0.0392 (15)	0.0351 (14)	0.0000 (11)	0.0212 (11)	0.0006 (11)
C18	0.0324 (13)	0.0333 (13)	0.0318 (13)	−0.0012 (10)	0.0195 (11)	−0.0059 (10)
C19	0.0207 (11)	0.0197 (11)	0.0210 (11)	0.0017 (8)	0.0085 (9)	0.0011 (9)
C20	0.0266 (11)	0.0183 (11)	0.0216 (11)	0.0008 (9)	0.0116 (9)	0.0019 (9)
C21	0.0274 (12)	0.0242 (12)	0.0219 (11)	0.0004 (9)	0.0133 (10)	0.0029 (9)
C22	0.0322 (13)	0.0276 (12)	0.0284 (13)	−0.0035 (10)	0.0157 (11)	0.0004 (10)

C23	0.0302 (13)	0.0389 (15)	0.0383 (15)	−0.0085 (11)	0.0180 (12)	0.0019 (12)
C24	0.0351 (14)	0.0535 (17)	0.0394 (15)	−0.0013 (13)	0.0267 (13)	0.0005 (13)
C25	0.0392 (15)	0.0420 (15)	0.0364 (14)	−0.0009 (12)	0.0251 (12)	−0.0050 (12)
C26	0.0313 (12)	0.0286 (12)	0.0233 (12)	−0.0005 (10)	0.0149 (10)	0.0010 (10)

Geometric parameters (Å, º)

Mn1—N2	2.1488 (18)	C4—C5	1.389 (3)
Mn1—N7	2.1517 (18)	C4—H4	0.9500
Mn1—O1	2.1868 (16)	C5—H5	0.9500
Mn1—O3	2.1915 (16)	C7—C8	1.487 (3)
Mn1—N5	2.3223 (19)	C8—C9	1.394 (3)
Mn1—N1	2.3461 (19)	C8—C13	1.415 (3)
O1—C7	1.289 (3)	C9—C10	1.379 (4)
O2—C13	1.356 (3)	C9—H9	0.9500
O2—H2A	0.8410	C10—C11	1.384 (4)
O3—C20	1.288 (3)	C10—H10	0.9500
O4—C26	1.349 (3)	C11—C12	1.382 (4)
O4—H4A	0.8398	C11—H11	0.9500
N1—C5	1.334 (3)	C12—C13	1.396 (3)
N1—C1	1.351 (3)	C12—H12	0.9500
N2—C6	1.296 (3)	C14—C15	1.385 (3)
N2—N4	1.395 (3)	C14—C19	1.493 (3)
N3—C6	1.342 (3)	C15—C16	1.394 (3)
N3—H3A	0.8795	C15—H15	0.9500
N3—H3B	0.8798	C16—C17	1.375 (4)
N4—C7	1.328 (3)	C16—H16	0.9500
N5—C18	1.340 (3)	C17—C18	1.383 (4)
N5—C14	1.348 (3)	C17—H17	0.9500
N6—C19	1.335 (3)	C18—H18	0.9500
N6—H6A	0.8795	C20—C21	1.490 (3)
N6—H6B	0.8797	C21—C22	1.398 (3)
N7—C19	1.301 (3)	C21—C26	1.412 (3)
N7—N8	1.394 (2)	C22—C23	1.384 (4)
N8—C20	1.324 (3)	C22—H22	0.9500
C1—C2	1.390 (3)	C23—C24	1.389 (4)
C1—C6	1.491 (3)	C23—H23	0.9500
C2—C3	1.386 (3)	C24—C25	1.379 (4)
C2—H2	0.9500	C24—H24	0.9500
C3—C4	1.377 (4)	C25—C26	1.402 (3)
C3—H3	0.9500	C25—H25	0.9500
N2—Mn1—N7	159.74 (7)	N4—C7—C8	115.58 (19)
N2—Mn1—O1	72.45 (6)	C9—C8—C13	118.1 (2)
N7—Mn1—O1	120.69 (7)	C9—C8—C7	119.1 (2)
N2—Mn1—O3	123.80 (7)	C13—C8—C7	122.7 (2)
N7—Mn1—O3	72.29 (6)	C10—C9—C8	121.5 (2)
O1—Mn1—O3	97.47 (6)	C10—C9—H9	119.2

N2—Mn1—N5	94.12 (7)	C8—C9—H9	119.2
N7—Mn1—N5	71.01 (7)	C9—C10—C11	120.0 (2)
O1—Mn1—N5	93.02 (6)	C9—C10—H10	120.0
O3—Mn1—N5	142.07 (6)	C11—C10—H10	120.0
N2—Mn1—N1	70.67 (7)	C12—C11—C10	120.2 (2)
N7—Mn1—N1	96.34 (7)	C12—C11—H11	119.9
O1—Mn1—N1	142.69 (6)	C10—C11—H11	119.9
O3—Mn1—N1	98.21 (6)	C11—C12—C13	120.3 (2)
N5—Mn1—N1	95.03 (7)	C11—C12—H12	119.8
C7—O1—Mn1	113.97 (14)	C13—C12—H12	119.8
C13—O2—H2A	109.5	O2—C13—C12	117.8 (2)
C20—O3—Mn1	113.91 (14)	O2—C13—C8	122.3 (2)
C26—O4—H4A	109.5	C12—C13—C8	119.9 (2)
C5—N1—C1	118.4 (2)	N5—C14—C15	122.3 (2)
C5—N1—Mn1	126.56 (16)	N5—C14—C19	115.11 (19)
C1—N1—Mn1	114.98 (14)	C15—C14—C19	122.5 (2)
C6—N2—N4	116.92 (18)	C14—C15—C16	118.7 (2)
C6—N2—Mn1	124.63 (15)	C14—C15—H15	120.6
N4—N2—Mn1	118.34 (13)	C16—C15—H15	120.6
C6—N3—H3A	120.1	C17—C16—C15	119.0 (2)
C6—N3—H3B	120.0	C17—C16—H16	120.5
H3A—N3—H3B	119.9	C15—C16—H16	120.5
C7—N4—N2	110.61 (17)	C16—C17—C18	118.9 (2)
C18—N5—C14	118.0 (2)	C16—C17—H17	120.6
C18—N5—Mn1	126.52 (16)	C18—C17—H17	120.6
C14—N5—Mn1	115.39 (14)	N5—C18—C17	123.0 (2)
C19—N6—H6A	120.1	N5—C18—H18	118.5
C19—N6—H6B	119.9	C17—C18—H18	118.5
H6A—N6—H6B	120.0	N7—C19—N6	125.8 (2)
C19—N7—N8	116.90 (18)	N7—C19—C14	114.38 (19)
C19—N7—Mn1	123.76 (14)	N6—C19—C14	119.8 (2)
N8—N7—Mn1	118.28 (13)	O3—C20—N8	124.7 (2)
C20—N8—N7	110.70 (18)	O3—C20—C21	119.6 (2)
N1—C1—C2	122.0 (2)	N8—C20—C21	115.63 (19)
N1—C1—C6	115.17 (19)	C22—C21—C26	118.7 (2)
C2—C1—C6	122.9 (2)	C22—C21—C20	119.5 (2)
C3—C2—C1	118.8 (2)	C26—C21—C20	121.6 (2)
C3—C2—H2	120.6	C23—C22—C21	121.5 (2)
C1—C2—H2	120.6	C23—C22—H22	119.2
C4—C3—C2	119.4 (2)	C21—C22—H22	119.2
C4—C3—H3	120.3	C22—C23—C24	119.3 (2)
C2—C3—H3	120.3	C22—C23—H23	120.4
C3—C4—C5	118.5 (2)	C24—C23—H23	120.4
C3—C4—H4	120.8	C25—C24—C23	120.6 (2)
C5—C4—H4	120.8	C25—C24—H24	119.7
N1—C5—C4	123.0 (2)	C23—C24—H24	119.7
N1—C5—H5	118.5	C24—C25—C26	120.7 (2)
C4—C5—H5	118.5	C24—C25—H25	119.7

N2—C6—N3	125.5 (2)	C26—C25—H25	119.7
N2—C6—C1	114.53 (19)	O4—C26—C25	118.0 (2)
N3—C6—C1	119.87 (19)	O4—C26—C21	122.8 (2)
O1—C7—N4	124.5 (2)	C25—C26—C21	119.2 (2)
O1—C7—C8	119.82 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N4	0.84	1.82	2.564 (2)	146
O4—H4*A*···N8	0.84	1.80	2.541 (2)	147
N3—H3*A*···O2[i]	0.88	2.37	3.072 (3)	137
N3—H3*B*···O3[ii]	0.88	2.20	2.847 (2)	130
N6—H6*A*···O4[iii]	0.88	2.44	3.065 (3)	129
N6—H6*B*···O1[iv]	0.88	2.19	2.907 (3)	138

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