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μ-4,4′-Diazenediyldiphthalato-κ^2O^2:$O^{2'}$-bis[pentaaquamanganese(II)] tetrahydrate

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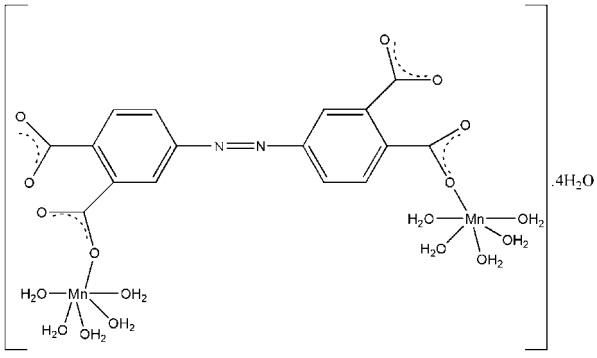
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 14.4.

The dinuclear complex in the title compound, $[Mn_2(C_{16}H_6N_2O_8)(H_2O)_{10}]\cdot 4H_2O$, lies on an inversion center. Two delocalized carboxylate groups are each connected in a monodentate fashion to two similar pentaaquamanganese units, whereas the other two localized carboxylate groups are uncoordinated. The metal ion has octahedral coordination, with the O atom of a carboxylate group and three coordinated water molecules forming the equatorial plane [Mn—O_{COO} = 2.143 (4) Å] and two water molecules occupying the axial positions. The architecture is further consolidated by extensive hydrogen bonds for which coordinated water molecules serve as donors or acceptors.

Related literature

For related literature, see: Gokel *et al.* (2004); Lassahn *et al.* (2004); Liu & Xu (2005); Shan *et al.* (2001); Wang *et al.* (2007).



Experimental

Crystal data

$[Mn_2(C_{16}H_6N_2O_8)(H_2O)_{10}]\cdot 4H_2O$
M_r = 716.33
Monoclinic, $P2_1/c$
a = 6.9674 (10) Å
b = 15.186 (2) Å
c = 13.5576 (19) Å
β = 98.812 (2)°
V = 1417.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 298 (2) K
0.29 × 0.25 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.763, T_{max} = 0.842
7535 measured reflections
2649 independent reflections
2349 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.06
2649 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O7W	0.82	1.95	2.760 (3)	170
O1W—H1WB···O4	0.82	1.85	2.675 (2)	176
O2W—H2WA···O4W^{i}	0.81	2.16	2.948 (2)	163
O2W—H2WA···O1^{i}	0.81	2.64	3.061 (2)	114
O2W—H2WB···O1W^{ii}	0.80	2.63	3.293 (3)	142
O3W—H3WB···O6W	0.83	2.00	2.818 (2)	171
O3W—H3WA···O3^{iii}	0.81	1.89	2.696 (2)	172
O4W—H4WA···O2^{i}	0.81	2.00	2.8162 (19)	174
O4W—H4WB···O3^{iv}	0.82	1.94	2.758 (2)	178
O5W—H5WA···O2^{iv}	0.82	1.95	2.759 (2)	169
O5W—H5WB···O7W^{v}	0.82	1.93	2.744 (2)	173
O6W—H6WA···O4^{ii}	0.87	1.81	2.677 (2)	174
O6W—H6WB···O2^{i}	0.87	2.03	2.894 (2)	175
O7W—H7WB···N1^{vi}	0.91	1.96	2.859 (3)	174
O7W—H7WA···O6W^{vii}	0.87	1.92	2.780 (3)	169

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2281).

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μ-4,4′-Diazenediyldiphthalato-κ^2O^2:$O^{2'}$-bis[pentaaquamanganese(II)] tetrahydrate

Jian-Wei Bai, Jun Wang, Yang Hou, Bao-Zhong Zhao and Qiang Fu

S1. Comment

Transition metal complexes with bipyridine derivatives are suitable models for the study of excited state dynamics. In addition, they are of interest for the development of light-energy conversion devices and optical sensors (Gokel *et al.*, 2004; Shan *et al.*, 2001; Lassahn *et al.*, 2004). Although a great number of metal carboxylate have been obtained to date, the rational design and synthesis of novel metal carboxylates by employing new synthetic tools or by varying the natures of the reactants and synthetic conditions are currently under active investigation (Liu & Xu, 2005). In this context, *L* ligand which can exhibit a variety of coordination abilities and has a tendency to form architectures with multi-dimensional frameworks (Wang *et al.*, 2007). In this paper, we report the synthesis and crystal structure of the title complex,(I).

The title complex (I) is arranged around a crystallographic inversion center located in the middle of the N=N bond. The metal ion is octahedrally coordinated by the oxygen atom of the carboxylate group [Mn-Ocarboxylate =2.143 (4)° A]and five coordinated water molecules. Two delocalized carboxyl $–CO_2$ groups are each connected *via* monodentate fashion to two similar pentaaquamanganese units whereas the other two localized carboxyl $–CO_2$ are free. The architecture is further consolidated by extensive hydrogen bonds for which the water molecules serves as donors or acceptors (Table 1).

S2. Experimental

MnSO4(0.032 g, 0.017 mmol), *L*(0.029 g, 0.014 mmol) and NaOH(0.048 mmol,0.12 mmol), were added in a mixed solvent of acetonitrile, the mixture was heated for six hours under reflux. During the process stirring and influx were required. The resultant was then filtered to give a pure solution which was infiltrated by diethyl ether freely in a closed vessel, a weeks later some single crystals of the size suitable for X-Ray diffraction analysis.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.84 (1)Å and H···H= 1.38 (2) Å) with U_{iso}(H) = 1.5U_{eq}(O). In the last stage of refinement, they were treated as riding on their parent O atoms.

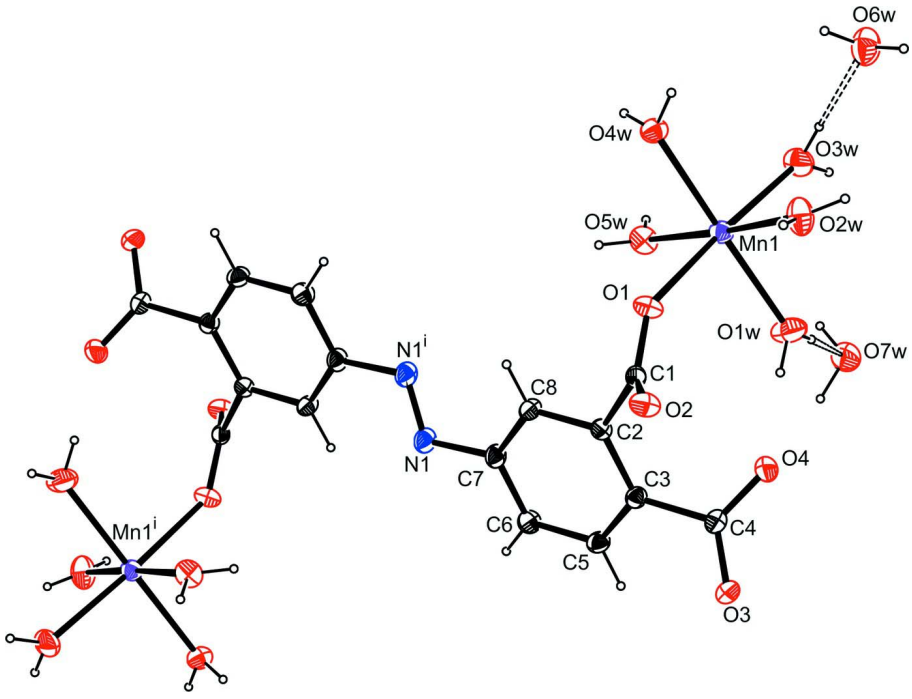

Figure 1

View of complex (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. H atoms are represented as small spheres of arbitrary radii. [Symmetry code (i): 1 - *x*,1 - *y*,1 - *z*].

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Crystal data

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Hall symbol: -P 2ybc
$a = 6.9674\ (10)$ Å
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$c = 13.5576\ (19)$ Å
$\beta = 98.812\ (2)°$
$V = 1417.5\ (3)$ Å^3
$Z = 2$
$F(000) = 740$
$D_x = 1.678$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2649 reflections
$\theta = 2.0–25.5°$
$\mu = 0.99$ mm^{-1}
$T = 298$ K
Block, yellow
0.29 × 0.25 × 0.18 mm

Data collection

Bruker APEX-II area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.763$, $T_{max} = 0.842$
7535 measured reflections
2649 independent reflections
2349 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.0°$
$h = -8\rightarrow7$
$k = -18\rightarrow17$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.090$
$S = 1.06$
2649 reflections
184 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
$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.4924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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}
Mn1	1.15210 (4)	0.59508 (2)	0.87665 (2)	0.02864 (12)
O1	0.9887 (2)	0.47791 (9)	0.83401 (10)	0.0337 (3)
O2	0.9981 (2)	0.33199 (9)	0.83063 (10)	0.0333 (3)
O3	1.3292 (2)	0.26635 (10)	0.62459 (11)	0.0367 (4)
O4	1.3672 (2)	0.37832 (10)	0.73190 (12)	0.0388 (4)
O1W	1.3818 (3)	0.54312 (11)	0.80243 (14)	0.0528 (5)
H1WA	1.4600	0.5680	0.7730	0.079*
H1WB	1.3730	0.4930	0.7790	0.079*
O2W	1.2906 (2)	0.52547 (12)	1.01240 (12)	0.0484 (4)
H2WA	1.2359	0.4830	1.0320	0.073*
H2WB	1.3829	0.5350	1.0540	0.073*
O3W	1.3327 (2)	0.70714 (11)	0.92397 (13)	0.0479 (4)
H3WB	1.3530	0.7149	0.9850	0.072*
H3WA	1.4280	0.7279	0.9050	0.072*
O4W	0.9230 (2)	0.63843 (10)	0.96205 (10)	0.033
H4WA	0.9370	0.6470	1.0220	0.050*
H4WB	0.8500	0.6770	0.9370	0.050*
O5W	0.9978 (2)	0.66502 (10)	0.74917 (10)	0.0379 (4)
H5WA	1.0061	0.7170	0.7330	0.057*
H5WB	0.8841	0.6530	0.7280	0.057*
O6W	1.3892 (3)	0.71325 (14)	1.13418 (13)	0.0563 (5)
H6WA	1.4620	0.6809	1.1780	0.085*
H6WB	1.2720	0.7029	1.1450	0.085*
O7W	1.6084 (3)	0.63676 (12)	0.68914 (14)	0.0547 (5)
H7WB	1.5680	0.6040	0.6340	0.082*

H7WA	1.5380	0.6840	0.6800	0.082*
N1	0.5413 (2)	0.47199 (12)	0.47708 (12)	0.0319 (4)
C1	0.9867 (3)	0.40586 (12)	0.78879 (14)	0.0235 (4)
C2	0.9492 (3)	0.40791 (12)	0.67589 (14)	0.0225 (4)
C4	1.2725 (3)	0.33562 (13)	0.66100 (14)	0.0266 (4)
C7	0.7227 (3)	0.44018 (14)	0.52778 (14)	0.0275 (4)
C6	0.8475 (3)	0.40308 (13)	0.46864 (15)	0.0299 (5)
H6	0.8129	0.4012	0.3996	0.036*
C5	1.0234 (3)	0.36904 (13)	0.51324 (14)	0.0284 (4)
H5	1.1074	0.3444	0.4737	0.034*
C3	1.0769 (3)	0.37103 (13)	0.61650 (14)	0.0240 (4)
C8	0.7726 (3)	0.44200 (13)	0.63154 (14)	0.0259 (4)
H8	0.6874	0.4661	0.6707	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0314 (2)	0.02601 (19)	0.02938 (19)	−0.00248 (12)	0.00726 (14)	−0.00193 (12)
O1	0.0456 (9)	0.0266 (8)	0.0288 (7)	−0.0029 (6)	0.0055 (6)	−0.0064 (6)
O2	0.0488 (9)	0.0263 (8)	0.0237 (7)	0.0037 (6)	0.0023 (6)	0.0022 (6)
O3	0.0288 (8)	0.0391 (9)	0.0409 (9)	0.0106 (6)	0.0014 (7)	−0.0095 (7)
O4	0.0311 (8)	0.0381 (9)	0.0432 (9)	0.0052 (7)	−0.0073 (7)	−0.0100 (7)
O1W	0.0564 (11)	0.0408 (10)	0.0688 (12)	−0.0066 (8)	0.0341 (9)	−0.0147 (8)
O2W	0.0398 (9)	0.0596 (11)	0.0423 (9)	−0.0040 (8)	−0.0046 (7)	0.0144 (8)
O3W	0.0429 (10)	0.0472 (10)	0.0571 (11)	−0.0201 (8)	0.0179 (8)	−0.0139 (8)
O4W	0.039	0.036	0.025	0.007	0.005	0.002
O5W	0.0456 (9)	0.0326 (8)	0.0347 (8)	−0.0026 (7)	0.0037 (7)	0.0072 (7)
O6W	0.0440 (10)	0.0748 (13)	0.0481 (10)	0.0035 (9)	0.0002 (8)	0.0117 (9)
O7W	0.0524 (11)	0.0463 (11)	0.0631 (12)	−0.0002 (8)	0.0013 (9)	−0.0084 (9)
N1	0.0277 (9)	0.0406 (10)	0.0261 (8)	0.0068 (7)	−0.0006 (7)	0.0023 (7)
C1	0.0198 (9)	0.0282 (11)	0.0222 (9)	−0.0003 (7)	0.0024 (8)	−0.0009 (8)
C2	0.0238 (10)	0.0211 (9)	0.0220 (9)	0.0001 (7)	0.0019 (7)	0.0007 (7)
C4	0.0232 (10)	0.0298 (11)	0.0272 (10)	0.0027 (8)	0.0051 (8)	0.0024 (8)
C7	0.0243 (10)	0.0309 (11)	0.0256 (10)	0.0041 (8)	−0.0010 (8)	0.0030 (8)
C6	0.0320 (11)	0.0356 (12)	0.0211 (9)	0.0039 (9)	0.0008 (8)	0.0007 (8)
C5	0.0287 (11)	0.0336 (11)	0.0237 (10)	0.0043 (9)	0.0065 (8)	−0.0023 (8)
C3	0.0236 (10)	0.0219 (10)	0.0262 (10)	0.0022 (7)	0.0033 (8)	0.0017 (8)
C8	0.0243 (10)	0.0282 (10)	0.0258 (9)	0.0057 (8)	0.0055 (8)	0.0005 (8)

Geometric parameters (Å, º)

Mn1—O1	2.1435 (15)	O5W—H5WB	0.8207
Mn1—O3W	2.1548 (16)	O6W—H6WA	0.8708
Mn1—O1W	2.1657 (17)	O6W—H6WB	0.8656
Mn1—O5W	2.1683 (15)	O7W—H7WB	0.9061
Mn1—O4W	2.2108 (14)	O7W—H7WA	0.8666
Mn1—O2W	2.2119 (16)	N1—N1^{i}	1.245 (3)
O1—C1	1.253 (2)	N1—C7	1.427 (3)

O2—C1	1.254 (2)	C1—C2	1.513 (3)
O3—C4	1.251 (2)	C2—C8	1.385 (3)
O4—C4	1.259 (2)	C2—C3	1.405 (3)
O1W—H1WA	0.8156	C4—C3	1.503 (3)
O1W—H1WB	0.8230	C7—C6	1.389 (3)
O2W—H2WA	0.8145	C7—C8	1.397 (3)
O2W—H2WB	0.8008	C6—C5	1.382 (3)
O3W—H3WB	0.8259	C6—H6	0.9300
O3W—H3WA	0.8120	C5—C3	1.393 (3)
O4W—H4WA	0.8148	C5—H5	0.9300
O4W—H4WB	0.8151	C8—H8	0.9300
O5W—H5WA	0.8240		

O1—Mn1—O3W	176.04 (7)	Mn1—O5W—H5WB	120.3
O1—Mn1—O1W	88.39 (6)	H5WA—O5W—H5WB	102.9
O3W—Mn1—O1W	89.24 (7)	H6WA—O6W—H6WB	104.4
O1—Mn1—O5W	90.78 (6)	H7WB—O7W—H7WA	103.9
O3W—Mn1—O5W	92.65 (7)	N1^{i}—N1—C7	115.7 (2)
O1W—Mn1—O5W	96.88 (7)	O1—C1—O2	124.37 (18)
O1—Mn1—O4W	89.55 (6)	O1—C1—C2	117.65 (16)
O3W—Mn1—O4W	92.55 (6)	O2—C1—C2	117.72 (16)
O1W—Mn1—O4W	174.90 (6)	C8—C2—C3	119.93 (17)
O5W—Mn1—O4W	87.82 (6)	C8—C2—C1	116.82 (17)
O1—Mn1—O2W	88.49 (6)	C3—C2—C1	123.04 (17)
O3W—Mn1—O2W	88.24 (7)	O3—C4—O4	125.04 (18)
O1W—Mn1—O2W	87.31 (7)	O3—C4—C3	117.63 (17)
O5W—Mn1—O2W	175.73 (6)	O4—C4—C3	117.32 (18)
O4W—Mn1—O2W	87.97 (6)	C6—C7—C8	120.53 (18)
C1—O1—Mn1	145.33 (14)	C6—C7—N1	116.47 (17)
Mn1—O1W—H1WA	130.9	C8—C7—N1	122.95 (17)
Mn1—O1W—H1WB	120.0	C5—C6—C7	119.41 (18)
H1WA—O1W—H1WB	104.8	C5—C6—H6	120.3
Mn1—O2W—H2WA	118.9	C7—C6—H6	120.3
Mn1—O2W—H2WB	134.5	C6—C5—C3	120.97 (18)
H2WA—O2W—H2WB	106.2	C6—C5—H5	119.5
Mn1—O3W—H3WB	114.5	C3—C5—H5	119.5
Mn1—O3W—H3WA	132.9	C5—C3—C2	119.30 (18)
H3WB—O3W—H3WA	103.8	C5—C3—C4	118.84 (17)
Mn1—O4W—H4WA	125.8	C2—C3—C4	121.84 (17)
Mn1—O4W—H4WB	116.8	C2—C8—C7	119.84 (18)
H4WA—O4W—H4WB	105.8	C2—C8—H8	120.1
Mn1—O5W—H5WA	129.4	C7—C8—H8	120.1

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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O2*W*—H2*WA*···O4*W*^{i}	0.81	2.16	2.948 (2)	163
O2*W*—H2*WA*···O1^{ii}	0.81	2.64	3.061 (2)	114
O2*W*—H2*WB*···O1*W*^{iii}	0.80	2.63	3.293 (3)	142
O3*W*—H3*WB*···O6*W*	0.83	2.00	2.818 (2)	171
O3*W*—H3*WA*···O3^{iv}	0.81	1.89	2.696 (2)	172
O4*W*—H4*WA*···O2^{ii}	0.81	2.00	2.8162 (19)	174
O4*W*—H4*WB*···O3^{v}	0.82	1.94	2.758 (2)	178
O5*W*—H5*WA*···O2^{v}	0.82	1.95	2.759 (2)	169
O5*W*—H5*WB*···O7*W*^{vi}	0.82	1.93	2.744 (2)	173
O6*W*—H6*WA*···O4^{iii}	0.87	1.81	2.677 (2)	174
O6*W*—H6*WB*···O2^{ii}	0.87	2.03	2.894 (2)	175
O7*W*—H7*WB*···N1^{vii}	0.91	1.96	2.859 (3)	174
O7*W*—H7*WA*···O6*W*^{viii}	0.87	1.92	2.780 (3)	169

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+2; (iii) −*x*+3, −*y*+1, −*z*+2; (iv) −*x*+3, *y*+1/2, −*z*+3/2; (v) −*x*+2, *y*+1/2, −*z*+3/2; (vi) *x*−1, *y*, *z*; (vii) −*x*+2, −*y*+1, −*z*+1; (viii) *x*, −*y*+3/2, *z*−1/2.