

Tetraaquabis[2-[4-(3-pyridyl)pyrimidin-2-ylsulfanyl]acetato]manganese(II) dihydrate

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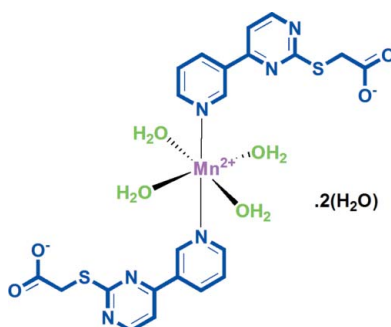
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 17.0.

In the title compound, $[\text{Mn}(\text{C}_{11}\text{H}_8\text{N}_3\text{O}_2\text{S})_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$, the Mn^{II} ion lies on an inversion centre and is coordinated by four water molecules in equatorial positions and two N atoms from two 2-[4-(3-pyridyl)pyrimidin-2-ylsulfanyl]acetate ligands in the axial positions. The water molecules, including the uncoordinated water molecules, and the acetate O atoms are involved in $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen-bonding interactions, which link the components into layers parallel to the a ($b + c$) plane.

Related literature

For hydro(solvo)thermal reactions between (heterocyclic-thio)acetic acid and metal ions, see: Zhu *et al.* (2009); Hao *et al.* (2008); He *et al.* (2007). For a Cu(II) coordination compound with 4-(pyridin-4-yl)pyrimidine-2-sulfonate, see Li *et al.* (2009).



Experimental

Crystal data

 $[\text{Mn}(\text{C}_{11}\text{H}_8\text{N}_3\text{O}_2\text{S})_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$
 $M_r = 655.58$

 Triclinic, $P\bar{1}$
 $a = 8.459$ (3) Å
 $b = 9.240$ (3) Å
 $c = 9.360$ (4) Å
 $\alpha = 87.396$ (6)°
 $\beta = 75.862$ (5)°
 $\gamma = 79.872$ (5)°

 $V = 698.4$ (4) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.69$ mm⁻¹
 $T = 298$ K
 $0.14 \times 0.12 \times 0.10$ mm

Data collection

 Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\text{min}} = 0.884$, $T_{\text{max}} = 0.920$

 4518 measured reflections
 3181 independent reflections
 2443 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.094$
 $S = 0.98$
 3181 reflections

 187 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O}2-\text{H}1 \cdots \text{O}3^{\text{i}}$	0.85	1.82	2.655 (2)	168
$\text{O}1-\text{H}2 \cdots \text{O}4$	0.85	1.88	2.709 (2)	165
$\text{O}2-\text{H}3 \cdots \text{O}4$	0.85	1.97	2.743 (2)	150
$\text{O}1-\text{H}4 \cdots \text{O}5^{\text{ii}}$	0.85	1.81	2.642 (3)	167
$\text{O}5-\text{H}5 \cdots \text{N}1^{\text{iii}}$	0.85	2.09	2.888 (3)	155
$\text{O}5-\text{H}6 \cdots \text{O}3$	0.85	2.01	2.775 (3)	149

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); data reduction: SAINT-Plus; 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: CV2600).

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supplementary materials

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Tetraaquabis{2-[4-(3-pyridyl)pyrimidin-2-ylsulfanyl]acetato}manganese(II) dihydrate

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Comment

Hydro(solvo)thermal reactions of (heterocyclicthio)acetic acid with both transition metal ions and lanthanide ions have been investigated in several reports (Zhu *et al.*, 2009; Hao *et al.*, 2008; He *et al.*, 2007), wherein *in situ* C—S cleavage has taken place under these situations. Herein, we report a manganese (II) coordination complex with a newly synthesized (heterocyclicthio)acetic acid, namely 2-(4-(pyridine-3-yl)pyrimidin-2-ylthio)acetic acid.

As shown in **Fig. 1**, the coordination arrangement around Mn(II) center is similar to our previously reported Cu(II) compound with the ligand of 4-(pyridin-4-yl)pyrimidine-2-sulfonate (Li *et al.*, 2009). The Mn(II) center also adopts an octahedral coordination geometry completed by four water O atoms in equatorial positions and two N atoms in apical positions. In the title complex, the Mn^{II} atom sits on an inversion centre with the asymmetric unit containing half of the complex and one free water molecule. The Mn—O bond lengths vary from 2.189 (2) to 2.192 (2) Å and the Mn—N bond distance is 2.276 (2) Å. Intra- and intermolecular hydrogen bonding interactions, such as O—H···O and O—H···N are observed in the crystal structure (**Table 1**).

Experimental

The mixture of Mn(OAc)₂ (0.1 mmol), 2-(4-(pyridine-3-yl)pyrimidin-2-ylthio)acetic acid (0.2 mmol) and NaOH (0.2 mmol) in 6 ml of H₂O was stirred for 20 min at room temperature. After filtration, the mother liquid was stood for one week to give the colorless crystals suitable for X-raydiffraction analysis.

Refinement

C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The positions of the water H atoms were found from a difference Fourier map, but placed in idealized positions (O—H = 0.85 Å), and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{O5})$.

Figures

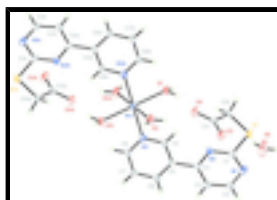


Fig. 1. The coordination environment around Mn(II) in the title complex with the atom-labeling scheme [symmetry code: (A) $-x, 2-y, 1-z$]. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

Tetraaquabis{2-[4-(3-pyridyl)pyrimidin-2-ylsulfanyl]acetato}manganese(II) dihydrate

Crystal data

$[\text{Mn}(\text{C}_{11}\text{H}_8\text{N}_3\text{O}_2\text{S})_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$	$Z = 1$
$M_r = 655.58$	$F_{000} = 339$
Triclinic, $P\bar{1}$	$D_x = 1.559 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.459 (3) \text{ \AA}$	Cell parameters from 3181 reflections
$b = 9.240 (3) \text{ \AA}$	$\theta = 2.2\text{--}28.1^\circ$
$c = 9.360 (4) \text{ \AA}$	$\mu = 0.69 \text{ mm}^{-1}$
$\alpha = 87.396 (6)^\circ$	$T = 298 \text{ K}$
$\beta = 75.862 (5)^\circ$	Block, colourless
$\gamma = 79.872 (5)^\circ$	$0.14 \times 0.12 \times 0.10 \text{ mm}$
$V = 698.4 (4) \text{ \AA}^3$	

Data collection

Bruker APEXII CCD area-detector diffractometer	3181 independent reflections
Radiation source: fine-focus sealed tube	2443 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.031$
$T = 298 \text{ K}$	$\theta_{\text{max}} = 28.1^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.884$, $T_{\text{max}} = 0.920$	$k = -6 \rightarrow 12$
4518 measured reflections	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$
$S = 0.98$	where $P = (F_o^2 + 2F_c^2)/3$
3181 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
187 parameters	$\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.55 \text{ e \AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.0000	1.0000	0.5000	0.02786 (13)
S1	0.71353 (7)	0.62719 (6)	0.00440 (6)	0.03937 (16)
O1	0.12141 (17)	0.98576 (16)	0.26485 (16)	0.0383 (4)
O2	0.24139 (17)	1.03191 (17)	0.52792 (17)	0.0447 (4)
N2	0.49123 (19)	0.56249 (17)	0.24128 (18)	0.0291 (4)
O4	0.44775 (17)	0.95387 (16)	0.25780 (16)	0.0412 (4)
N1	0.6987 (2)	0.36606 (19)	0.1238 (2)	0.0379 (4)
C1	0.6227 (2)	0.5074 (2)	0.1385 (2)	0.0310 (4)
O3	0.71010 (18)	0.85073 (17)	0.23595 (17)	0.0455 (4)
C5	0.2749 (2)	0.5349 (2)	0.4544 (2)	0.0279 (4)
N3	0.0768 (2)	0.75451 (18)	0.53326 (19)	0.0335 (4)
C11	0.5782 (2)	0.8717 (2)	0.1953 (2)	0.0302 (4)
C4	0.4233 (2)	0.4687 (2)	0.3417 (2)	0.0295 (4)
C9	0.2097 (2)	0.6826 (2)	0.4396 (2)	0.0323 (5)
H9A	0.2621	0.7342	0.3595	0.039*
C10	0.5730 (3)	0.7975 (2)	0.0536 (2)	0.0342 (5)
H10A	0.5956	0.8662	-0.0272	0.041*
H10B	0.4614	0.7793	0.0633	0.041*
C6	0.1962 (3)	0.4588 (2)	0.5742 (2)	0.0354 (5)
H6A	0.2354	0.3600	0.5882	0.042*
C8	0.0031 (3)	0.6779 (2)	0.6484 (2)	0.0364 (5)
H8A	-0.0899	0.7256	0.7149	0.044*
C7	0.0596 (3)	0.5315 (2)	0.6721 (2)	0.0394 (5)
H7A	0.0058	0.4824	0.7534	0.047*
C2	0.6305 (3)	0.2757 (2)	0.2252 (3)	0.0415 (5)
H2C	0.6786	0.1769	0.2209	0.050*
C3	0.4920 (3)	0.3206 (2)	0.3369 (3)	0.0402 (5)
H3A	0.4466	0.2544	0.4060	0.048*
O5	1.0477 (2)	0.7838 (2)	0.1129 (2)	0.0871 (8)
H1	0.2712	1.0656	0.5985	0.105*
H2	0.2259	0.9808	0.2469	0.105*
H3	0.3309	1.0079	0.4625	0.105*
H4	0.0999	0.9300	0.2053	0.105*

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H5	1.0980	0.7268	0.0413	0.105*
H6	0.9449	0.7871	0.1208	0.105*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0239 (2)	0.0266 (2)	0.0312 (3)	-0.00261 (17)	-0.00359 (17)	-0.00345 (17)
S1	0.0421 (3)	0.0381 (3)	0.0316 (3)	-0.0063 (2)	0.0042 (2)	-0.0080 (2)
O1	0.0354 (8)	0.0416 (9)	0.0347 (8)	-0.0006 (7)	-0.0053 (6)	-0.0082 (6)
O2	0.0289 (8)	0.0619 (11)	0.0447 (10)	-0.0092 (7)	-0.0080 (7)	-0.0149 (8)
N2	0.0291 (9)	0.0264 (9)	0.0310 (9)	-0.0038 (7)	-0.0055 (7)	-0.0033 (7)
O4	0.0305 (8)	0.0442 (9)	0.0447 (9)	-0.0013 (7)	-0.0023 (7)	-0.0141 (7)
N1	0.0360 (10)	0.0308 (10)	0.0452 (11)	0.0008 (8)	-0.0091 (8)	-0.0125 (8)
C1	0.0313 (11)	0.0301 (11)	0.0339 (12)	-0.0060 (8)	-0.0105 (9)	-0.0066 (8)
O3	0.0342 (8)	0.0558 (10)	0.0482 (10)	-0.0005 (7)	-0.0147 (7)	-0.0200 (8)
C5	0.0274 (10)	0.0260 (10)	0.0319 (11)	-0.0056 (8)	-0.0095 (8)	0.0004 (8)
N3	0.0293 (9)	0.0303 (9)	0.0371 (10)	-0.0036 (7)	-0.0019 (7)	-0.0008 (7)
C11	0.0309 (11)	0.0293 (11)	0.0301 (11)	-0.0086 (8)	-0.0039 (8)	-0.0006 (8)
C4	0.0304 (10)	0.0259 (10)	0.0344 (11)	-0.0039 (8)	-0.0125 (9)	-0.0017 (8)
C9	0.0314 (11)	0.0267 (10)	0.0361 (12)	-0.0048 (8)	-0.0035 (9)	0.0027 (8)
C10	0.0415 (12)	0.0325 (11)	0.0283 (11)	-0.0068 (9)	-0.0075 (9)	0.0003 (8)
C6	0.0428 (12)	0.0274 (11)	0.0374 (12)	-0.0076 (9)	-0.0121 (10)	0.0045 (9)
C8	0.0324 (11)	0.0390 (12)	0.0342 (12)	-0.0070 (9)	-0.0003 (9)	-0.0015 (9)
C7	0.0427 (13)	0.0403 (13)	0.0335 (12)	-0.0119 (10)	-0.0036 (10)	0.0084 (9)
C2	0.0462 (13)	0.0246 (11)	0.0512 (14)	0.0041 (10)	-0.0130 (11)	-0.0077 (10)
C3	0.0456 (13)	0.0253 (11)	0.0470 (14)	-0.0031 (9)	-0.0081 (11)	0.0008 (9)
O5	0.0420 (10)	0.1175 (19)	0.0989 (17)	-0.0176 (11)	0.0041 (11)	-0.0692 (14)

Geometric parameters (\AA , $^\circ$)

Mn1—O1	2.1889 (16)	C5—C9	1.393 (3)
Mn1—O1 ⁱ	2.1889 (16)	C5—C4	1.485 (3)
Mn1—O2 ⁱ	2.1919 (15)	N3—C9	1.335 (2)
Mn1—O2	2.1919 (15)	N3—C8	1.345 (3)
Mn1—N3 ⁱ	2.2761 (18)	C11—C10	1.534 (3)
Mn1—N3	2.2761 (18)	C4—C3	1.388 (3)
S1—C1	1.759 (2)	C9—H9A	0.9300
S1—C10	1.800 (2)	C10—H10A	0.9700
O1—H2	0.8520	C10—H10B	0.9700
O1—H4	0.8477	C6—C7	1.375 (3)
O2—H1	0.8510	C6—H6A	0.9300
O2—H3	0.8511	C8—C7	1.380 (3)
N2—C1	1.320 (2)	C8—H8A	0.9300
N2—C4	1.342 (3)	C7—H7A	0.9300
O4—C11	1.252 (2)	C2—C3	1.382 (3)
N1—C2	1.327 (3)	C2—H2C	0.9300
N1—C1	1.347 (2)	C3—H3A	0.9300
O3—C11	1.246 (2)	O5—H5	0.8500

C5—C6	1.386 (3)	O5—H6	0.8501
O1—Mn1—O1 ⁱ	180.000 (1)	C8—N3—Mn1	123.89 (14)
O1—Mn1—O2 ⁱ	95.09 (6)	O3—C11—O4	125.43 (18)
O1 ⁱ —Mn1—O2 ⁱ	84.91 (6)	O3—C11—C10	118.76 (18)
O1—Mn1—O2	84.91 (6)	O4—C11—C10	115.76 (18)
O1 ⁱ —Mn1—O2	95.09 (6)	N2—C4—C3	120.38 (18)
O2 ⁱ —Mn1—O2	180.00 (8)	N2—C4—C5	115.60 (16)
O1—Mn1—N3 ⁱ	87.81 (6)	C3—C4—C5	124.02 (18)
O1 ⁱ —Mn1—N3 ⁱ	92.19 (6)	N3—C9—C5	124.01 (18)
O2 ⁱ —Mn1—N3 ⁱ	88.48 (6)	N3—C9—H9A	118.0
O2—Mn1—N3 ⁱ	91.52 (6)	C5—C9—H9A	118.0
O1—Mn1—N3	92.19 (6)	C11—C10—S1	116.57 (14)
O1 ⁱ —Mn1—N3	87.81 (6)	C11—C10—H10A	108.1
O2 ⁱ —Mn1—N3	91.52 (6)	S1—C10—H10A	108.1
O2—Mn1—N3	88.48 (6)	C11—C10—H10B	108.1
N3 ⁱ —Mn1—N3	180.000 (1)	S1—C10—H10B	108.1
C1—S1—C10	101.21 (10)	H10A—C10—H10B	107.3
Mn1—O1—H2	113.5	C7—C6—C5	119.14 (19)
Mn1—O1—H4	123.8	C7—C6—H6A	120.4
H2—O1—H4	108.6	C5—C6—H6A	120.4
Mn1—O2—H1	132.6	N3—C8—C7	122.84 (19)
Mn1—O2—H3	122.8	N3—C8—H8A	118.6
H1—O2—H3	104.6	C7—C8—H8A	118.6
C1—N2—C4	117.31 (17)	C6—C7—C8	119.36 (19)
C2—N1—C1	114.58 (18)	C6—C7—H7A	120.3
N2—C1—N1	127.05 (19)	C8—C7—H7A	120.3
N2—C1—S1	118.41 (15)	N1—C2—C3	123.44 (19)
N1—C1—S1	114.55 (15)	N1—C2—H2C	118.3
C6—C5—C9	117.58 (18)	C3—C2—H2C	118.3
C6—C5—C4	124.11 (18)	C2—C3—C4	117.2 (2)
C9—C5—C4	118.31 (17)	C2—C3—H3A	121.4
C9—N3—C8	117.06 (18)	C4—C3—H3A	121.4
C9—N3—Mn1	118.88 (13)	H5—O5—H6	106.5
C4—N2—C1—N1	-0.9 (3)	C9—C5—C4—C3	-174.50 (19)
C4—N2—C1—S1	179.48 (14)	C8—N3—C9—C5	0.1 (3)
C2—N1—C1—N2	0.1 (3)	Mn1—N3—C9—C5	175.57 (15)
C2—N1—C1—S1	179.79 (15)	C6—C5—C9—N3	-0.1 (3)
C10—S1—C1—N2	-3.72 (17)	C4—C5—C9—N3	179.86 (18)
C10—S1—C1—N1	176.59 (14)	O3—C11—C10—S1	28.1 (3)
O1—Mn1—N3—C9	24.51 (15)	O4—C11—C10—S1	-154.45 (16)
O1 ⁱ —Mn1—N3—C9	-155.49 (15)	C1—S1—C10—C11	71.70 (17)
O2 ⁱ —Mn1—N3—C9	119.67 (15)	C9—C5—C6—C7	-0.2 (3)
O2—Mn1—N3—C9	-60.33 (15)	C4—C5—C6—C7	179.86 (19)
O1—Mn1—N3—C8	-160.35 (16)	C9—N3—C8—C7	0.2 (3)
O1 ⁱ —Mn1—N3—C8	19.65 (16)	Mn1—N3—C8—C7	-175.02 (15)

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O2 ⁱ —Mn1—N3—C8	-65.20 (17)	C5—C6—C7—C8	0.5 (3)
O2—Mn1—N3—C8	114.80 (17)	N3—C8—C7—C6	-0.5 (3)
C1—N2—C4—C3	0.9 (3)	C1—N1—C2—C3	0.6 (3)
C1—N2—C4—C5	-179.45 (16)	N1—C2—C3—C4	-0.5 (3)
C6—C5—C4—N2	-174.15 (19)	N2—C4—C3—C2	-0.3 (3)
C9—C5—C4—N2	5.9 (3)	C5—C4—C3—C2	-179.9 (2)
C6—C5—C4—C3	5.5 (3)		

Symmetry codes: (i) $-x, -y+2, -z+1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H1 \cdots O3 ⁱⁱ	0.85	1.82	2.655 (2)	168
O1—H2 \cdots O4	0.85	1.88	2.709 (2)	165
O2—H3 \cdots O4	0.85	1.97	2.743 (2)	150
O1—H4 \cdots O5 ⁱⁱⁱ	0.85	1.81	2.642 (3)	167
O5—H5 \cdots N1 ^{iv}	0.85	2.09	2.888 (3)	155
O5—H6 \cdots O3	0.85	2.01	2.775 (3)	149

Symmetry codes: (ii) $-x+1, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $-x+2, -y+1, -z$.

Fig. 1

