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## Key indicators

Single-crystal X-ray study  
 $T = 120\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.030  
 $wR$  factor = 0.068  
Data-to-parameter ratio = 19.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Propane-1,2-diaminium selenite monohydrate

The title compound,  $\text{C}_3\text{H}_{12}\text{N}_2^{2+}\cdot\text{SeO}_3^{2-}\cdot\text{H}_2\text{O}$ , contains a network of propane-1,2-diaminium ( $\text{C}_3\text{H}_{12}\text{N}_2^{2+}$ ) cations, selenite ( $\text{SeO}_3^{2-}$ ) anions and water molecules. The crystal packing involves  $\text{N}-\text{H}\cdots\text{O}$  [average  $\text{H}\cdots\text{O} = 1.89\text{ \AA}$ ,  $\text{N}-\text{H}\cdots\text{O} = 165^\circ$  and  $\text{N}\cdots\text{O} = 2.777(3)\text{ \AA}$ ] and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, resulting in a layered structure.

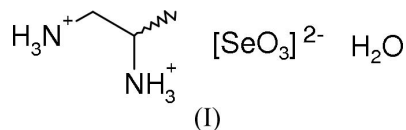
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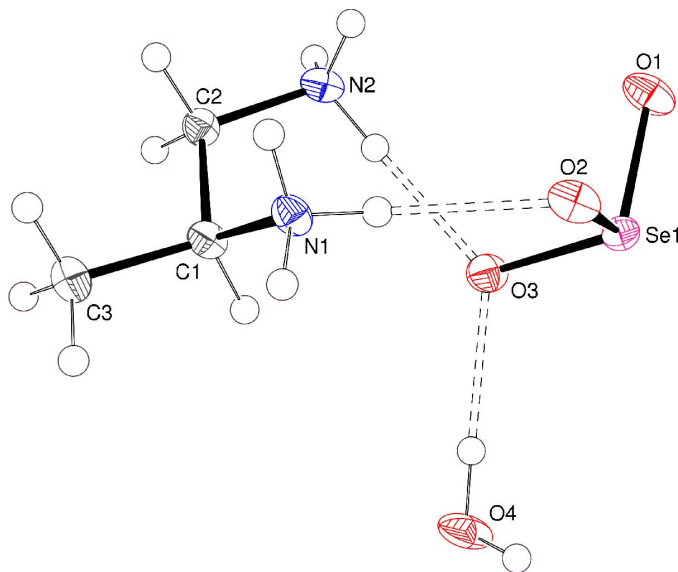
Online 7 May 2005

## Comment

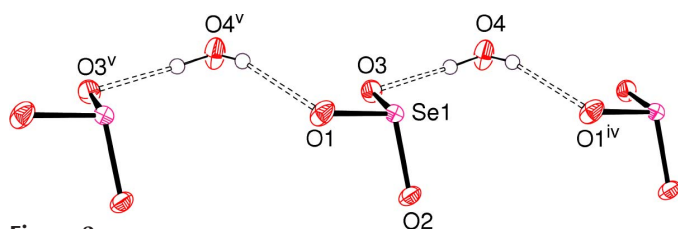
The title compound, (I), was prepared as part of our ongoing studies of hydrogen-bonding interactions in the crystal structures of (protonated) amine phosphates (Demir *et al.*, 2003), phosphites (Harrison, 2003), selenites (Ritchie & Harrison, 2003) and arsenates (Lee & Harrison, 2003*a,b,c*; Wilkinson & Harrison, 2004).



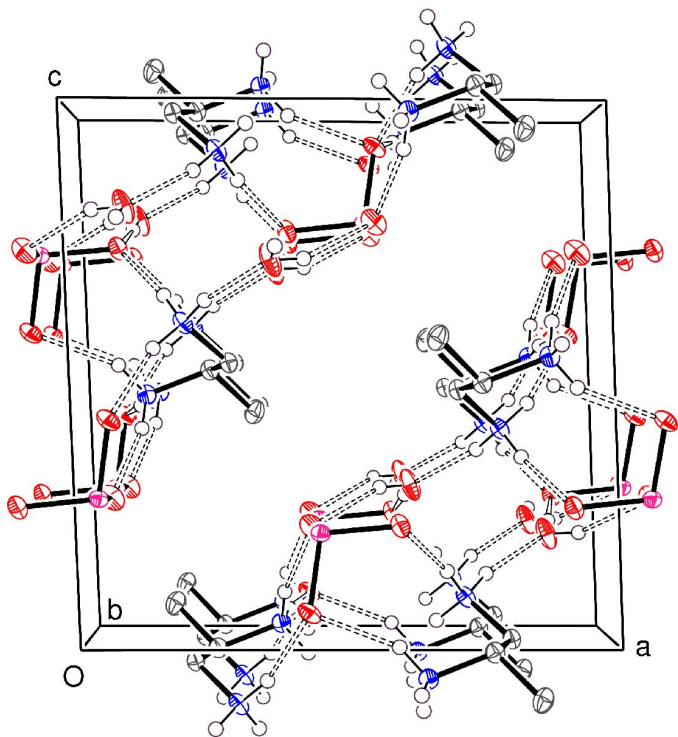
The asymmetric unit of (I) contains one  $\text{C}_3\text{H}_{12}\text{N}_2^{2+}$  cation, one  $\text{SeO}_3^{2-}$  anion and a water molecule (Fig. 1). The geometric parameters for the organic cation are unexceptional (Lee & Harrison, 2003*a*). This species is chiral (C1 has *S* configuration in the selected asymmetric unit), but crystal symmetry generates a 50:50 mix of enantiomers, consistent



**Figure 1**  
Asymmetric unit of (I), showing 50% displacement ellipsoids (arbitrary spheres for H atoms). Hydrogen bonds are indicated by dashed lines.



**Figure 2**  
Detail of a hydrogen-bonded selenite/water chain in (I). Symmetry codes are as in Table 2 [additionally: (v)  $x, 1 + y, z$ ]. Hydrogen bonds are indicated by dashed lines.



**Figure 3**  
[010] projection of the packing for (I). C-bound H atoms have been omitted for clarity and hydrogen bonds are indicated by dashed lines.

with the racemic starting material. The selenite group in (I) shows its standard (Lee & Harrison, 2003) pyramidal geometry (Table 1) [average Se—O = 1.687 (2) Å], with the Se atom displaced from the plane of its three attached O atoms by 0.7213 (12) Å.

As well as electrostatic attractions, the component species in (I) interact by means of a network of N—H...O and O—H...O hydrogen bonds (Table 2). The selenite anions and water molecules are linked into a polymeric chain in the [010] direction by hydrogen bonds (Fig. 2). The organic species interacts with the selenite/water chains by way of N—H...O hydrogen bonds (Table 2). All six of the  $-\text{NH}_3^+$  H atoms are involved in these links [mean H...O = 1.89 Å, N—H...O = 165° and N...O = 2.777 (3) Å]. These interactions result in (101) selenite/water/aminium layers sandwiched between the carbon backbones of the organic groups (Fig. 3), which themselves interact by way of van der Waals forces.

Propane-1,2-diaminium hydrogenarsenate monohydrate,  $\text{C}_3\text{H}_{12}\text{N}_2^{2+} \cdot \text{HAsO}_4^{2-} \cdot \text{H}_2\text{O}$  (Lee & Harrison, 2003a), has an

equivalent stoichiometry to (I). As might be expected, where the oxo anion has hydrogen-bonding capability (*i.e.* as As—OH...O links), a quite different overall structure arises. An interesting difference also arises for the organic cation; in (I), the  $-\text{NH}_3^+$  and  $-\text{CH}_3$  groups are *trans* about their linking C—C bond (Table 1), whereas in the hydrogenarsenate, they are *gauche* [C—C—N =  $-54.09$  (18)°].

## Experimental

An aqueous 0.5 M propane-1,2-diamine solution (10 ml) was added to aqueous 0.5 M  $\text{H}_2\text{SeO}_3$  solution (10 ml, dissolved  $\text{SeO}_2$ ) to result in a clear solution. A mass of colourless platy crystals of (I), with a pale-pink tinge arising from a surface coating, grew as the water evaporated over the course of a few days.

### Crystal data

$\text{C}_3\text{H}_{12}\text{N}_2^{2+} \cdot \text{SeO}_3^{2-} \cdot \text{H}_2\text{O}$   
 $M_r = 221.12$   
 Monoclinic,  $P2_1/n$   
 $a = 11.5494$  (7) Å  
 $b = 6.1399$  (4) Å  
 $c = 11.6601$  (6) Å  
 $\beta = 92.213$  (3)°  
 $V = 826.23$  (8) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.778$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1941 reflections  
 $\theta = 2.9$ – $27.5$ °  
 $\mu = 4.51$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
 Plate, colourless  
 $0.12 \times 0.10 \times 0.02$  mm

### Data collection

Nonius KappaCCD diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2003)  
 $T_{\min} = 0.613$ ,  $T_{\max} = 0.915$   
 8108 measured reflections  
 1882 independent reflections

1617 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$   
 $\theta_{\max} = 27.5$ °  
 $h = -12 \rightarrow 15$   
 $k = -7 \rightarrow 7$   
 $l = -15 \rightarrow 15$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.068$   
 $S = 1.07$   
 1882 reflections  
 95 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.5437P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.98$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.51$  e Å<sup>-3</sup>  
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0026 (7)

**Table 1**

Selected geometric parameters (Å, °).

Se1—O1	1.673 (2)	Se1—O2	1.7052 (18)
Se1—O3	1.6826 (19)		
N1—C1—C2—N2	55.2 (3)	C3—C1—C2—N2	176.9 (2)

**Table 2**

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O2 <sup>i</sup>	0.91	1.88	2.779 (3)	171
N1—H2...O1 <sup>ii</sup>	0.91	1.81	2.701 (3)	165
N1—H3...O2	0.91	2.00	2.835 (3)	152
N2—H4...O4 <sup>iii</sup>	0.91	1.91	2.802 (3)	165
N2—H5...O3	0.91	1.87	2.777 (3)	173
N2—H6...O2 <sup>ii</sup>	0.91	1.88	2.766 (3)	164
O4—H13...O3	0.88	1.96	2.840 (3)	178
O4—H14...O1 <sup>iv</sup>	0.76	2.04	2.747 (3)	157

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

The non-standard  $P2/n$  setting of the space group was chosen in preference to  $P2/c$  to avoid a unit cell with a very obtuse  $\beta$  angle of  $133.6^\circ$ . The water H atoms were found in a difference map and refined as riding in their as-found relative positions (Table 2). H atoms bonded to C and N atoms were placed in idealized positions (C–H = 0.98–1.00 Å and N–H = 0.91 Å) and refined as riding, allowing for free rotation of the rigid  $-XH_3$  ( $X = C3, N1$  and  $N2$ ) groups. The constraint  $U_{iso}(H) = 1.2U_{eq}(\text{carrier})$  or  $U_{iso}(H) = 1.2U_{eq}(\text{methyl carrier})$  was applied as appropriate.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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## References

- Bruker (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Demir, S., Yilmaz, V. T. & Harrison, W. T. A. (2003). *Acta Cryst.* **E59**, o907–o909.
- Farrugia, L. J. (1997). *J. App. Cryst.* **30**, 565.
- Harrison, W. T. A. (2003). *Acta Cryst.* **E59**, o1267–o1269.
- Lee, C. & Harrison, W. T. A. (2003a). *Acta Cryst.* **E59**, m739–m741.
- Lee, C. & Harrison, W. T. A. (2003b). *Acta Cryst.* **E59**, m959–m960.
- Lee, C. & Harrison, W. T. A. (2003c). *Acta Cryst.* **E59**, m1151–m1153.
- Nonius (1999). *COLLECT*. Nonius, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter & R. M. Sweet, pp. 307–326. London: Academic Press.
- Ritchie, L. K. & Harrison, W. T. A. (2003). *Acta Cryst.* **E59**, o1296–o1298.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wilkinson, H. S. & Harrison, W. T. A. (2004). *Acta Cryst.* **E60**, m1359–m1361.

## supporting information

*Acta Cryst.* (2005). E61, o1538–o1540 [https://doi.org/10.1107/S160053680501278X]

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*Crystal data*

$C_3H_{12}N_2^{2+} \cdot SeO_3^{2-} \cdot H_2O$

$M_r = 221.12$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1\ yac$

$a = 11.5494$  (7) Å

$b = 6.1399$  (4) Å

$c = 11.6601$  (6) Å

$\beta = 92.213$  (3)°

$V = 826.23$  (8) Å<sup>3</sup>

$Z = 4$

$F(000) = 448$

$D_x = 1.778$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1941 reflections

$\theta = 2.9$ – $27.5$ °

$\mu = 4.51$  mm<sup>-1</sup>

$T = 120$  K

Plate, colourless

$0.12 \times 0.10 \times 0.02$  mm

*Data collection*

Nonius KappaCCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2003)

$T_{\min} = 0.613$ ,  $T_{\max} = 0.915$

8108 measured reflections

1882 independent reflections

1617 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.3$ °

$h = -12 \rightarrow 15$

$k = -7 \rightarrow 7$

$l = -15 \rightarrow 15$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.068$

$S = 1.07$

1882 reflections

95 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: difmap (O-H) and geom  
(C-N and N-H)

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 0.5437P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.98$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.51$  e Å<sup>-3</sup>

Extinction correction: SHELXL97,

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0026 (7)

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.44873 (2)	0.81651 (4)	0.21940 (2)	0.01546 (12)
O1	0.43374 (17)	1.0875 (3)	0.22349 (16)	0.0253 (5)
O2	0.42321 (16)	0.7560 (3)	0.07795 (16)	0.0204 (4)
O3	0.59257 (16)	0.7750 (3)	0.23366 (16)	0.0209 (4)
C1	0.7531 (2)	0.6926 (4)	0.0105 (2)	0.0180 (6)
H7	0.7578	0.6212	0.0876	0.022*
C2	0.7916 (2)	0.9266 (4)	0.0239 (2)	0.0169 (5)
H8	0.8708	0.9299	0.0595	0.020*
H9	0.7947	0.9943	-0.0529	0.020*
C3	0.8323 (2)	0.5718 (5)	-0.0684 (2)	0.0240 (6)
H10	0.8072	0.4198	-0.0755	0.036*
H11	0.9120	0.5769	-0.0364	0.036*
H12	0.8290	0.6407	-0.1443	0.036*
N1	0.63165 (19)	0.6781 (3)	-0.03598 (19)	0.0169 (5)
H1	0.6158	0.5383	-0.0573	0.020*
H2	0.6225	0.7671	-0.0981	0.020*
H3	0.5824	0.7199	0.0189	0.020*
N2	0.71339 (19)	1.0567 (4)	0.09542 (19)	0.0180 (5)
H4	0.7554	1.1595	0.1349	0.022*
H5	0.6784	0.9673	0.1458	0.022*
H6	0.6586	1.1229	0.0494	0.022*
O4	0.62226 (18)	0.3308 (3)	0.29602 (19)	0.0283 (5)
H13	0.6129	0.4666	0.2746	0.034*
H14	0.5633	0.2771	0.2923	0.034*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Se1	0.01747 (18)	0.01530 (16)	0.01357 (16)	-0.00069 (11)	0.00008 (11)	0.00103 (10)
O1	0.0291 (11)	0.0169 (10)	0.0293 (11)	0.0055 (9)	-0.0071 (9)	-0.0067 (9)
O2	0.0239 (11)	0.0173 (9)	0.0194 (10)	0.0011 (8)	-0.0077 (8)	-0.0037 (8)
O3	0.0166 (10)	0.0209 (10)	0.0248 (10)	-0.0008 (8)	-0.0037 (8)	0.0036 (8)
C1	0.0180 (14)	0.0158 (13)	0.0203 (14)	0.0017 (11)	-0.0001 (11)	-0.0008 (11)
C2	0.0144 (13)	0.0173 (13)	0.0191 (13)	-0.0005 (11)	-0.0008 (10)	-0.0007 (11)

C3	0.0198 (15)	0.0236 (15)	0.0288 (15)	0.0048 (12)	0.0049 (12)	0.0005 (13)
N1	0.0175 (12)	0.0137 (11)	0.0195 (12)	0.0007 (9)	-0.0002 (9)	-0.0049 (9)
N2	0.0178 (12)	0.0142 (11)	0.0216 (11)	-0.0006 (9)	-0.0060 (9)	0.0000 (9)
O4	0.0199 (11)	0.0156 (10)	0.0482 (13)	0.0024 (8)	-0.0131 (10)	0.0040 (9)

*Geometric parameters (Å, °)*

Se1—O1	1.673 (2)	C3—H11	0.9800
Se1—O3	1.6826 (19)	C3—H12	0.9800
Se1—O2	1.7052 (18)	N1—H1	0.9100
C1—N1	1.487 (3)	N1—H2	0.9100
C1—C2	1.510 (4)	N1—H3	0.9100
C1—C3	1.516 (4)	N2—H4	0.9100
C1—H7	1.0000	N2—H5	0.9100
C2—N2	1.485 (3)	N2—H6	0.9100
C2—H8	0.9900	O4—H13	0.8761
C2—H9	0.9900	O4—H14	0.7566
C3—H10	0.9800		
O1—Se1—O3	104.52 (9)	H10—C3—H11	109.5
O1—Se1—O2	103.29 (9)	C1—C3—H12	109.5
O3—Se1—O2	101.28 (9)	H10—C3—H12	109.5
N1—C1—C2	111.4 (2)	H11—C3—H12	109.5
N1—C1—C3	109.4 (2)	C1—N1—H1	109.5
C2—C1—C3	110.3 (2)	C1—N1—H2	109.5
N1—C1—H7	108.6	H1—N1—H2	109.5
C2—C1—H7	108.6	C1—N1—H3	109.5
C3—C1—H7	108.6	H1—N1—H3	109.5
N2—C2—C1	112.8 (2)	H2—N1—H3	109.5
N2—C2—H8	109.0	C2—N2—H4	109.5
C1—C2—H8	109.0	C2—N2—H5	109.5
N2—C2—H9	109.0	H4—N2—H5	109.5
C1—C2—H9	109.0	C2—N2—H6	109.5
H8—C2—H9	107.8	H4—N2—H6	109.5
C1—C3—H10	109.5	H5—N2—H6	109.5
C1—C3—H11	109.5	H13—O4—H14	107.3
N1—C1—C2—N2	55.2 (3)	C3—C1—C2—N2	176.9 (2)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O2 <sup>i</sup>	0.91	1.88	2.779 (3)	171
N1—H2 $\cdots$ O1 <sup>ii</sup>	0.91	1.81	2.701 (3)	165
N1—H3 $\cdots$ O2	0.91	2.00	2.835 (3)	152
N2—H4 $\cdots$ O4 <sup>iii</sup>	0.91	1.91	2.802 (3)	165
N2—H5 $\cdots$ O3	0.91	1.87	2.777 (3)	173
N2—H6 $\cdots$ O2 <sup>ii</sup>	0.91	1.88	2.766 (3)	164

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O4—H13···O3	0.88	1.96	2.840 (3)	178
O4—H14···O1 <sup>iv</sup>	0.76	2.04	2.747 (3)	157

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