Synthesis and crystal structure of diaqua(1,4,8,11-tetraazacyclotetradecane)zinc(II) bis(hydrogen 4-phosphonatobiphenyl-4'-carboxylato)(1,4,8,11-tetraazacyclotetradecane)zinc(II)

Liudmyla V. Tsymbal, Irina L. Andriichuk, Vasile Lozan, Sergiu Shova and Yaroslav D. Lampeka

In the asymmetric unit of the title compound, trans-diaqua(1,4,8,11-tetraazacyclotetradecane-κ^4N_1,N_4,N_8,N_11)zinc(II) trans-bis(hydrogen 4-phosphonatobiphenyl-4'-carboxylato-κO)(1,4,8,11-tetraazacyclotetradecane-κ^4N_1,N_4,N_8,N_11)-zinc(II), [Zn(C_{10}H_{24}N_4)(H_2O)_2][Zn(C_{13}H_9O_5P)_2(C_{10}H_{24}N_4)], both Zn atoms lie on crystallographic inversion centres and the atoms of the macrocycle in the cation are disordered over two sets of sites. In both macrocyclic units, the metal ions possess a tetragonally elongated ZnN_4O_2 octahedral environment formed by the four secondary N atoms of the macrocyclic ligand in the equatorial plane and the two trans O atoms of the water molecules or anions in the axial positions, with the macrocyclic ligands adopting the most energetically favourable trans-III conformation. The average Zn—N bond lengths in both macrocyclic units do not differ significantly [2.112 (12) Å for the anion and 2.101 (3) Å for the cation] and are shorter than the average axial Zn—O bond lengths [2.189 (4) Å for phosphonate and 2.295 (4) Å for aqua ligands]. In the crystal, the complex cations and anions are connected via hydrogen-bonding interactions between the N—H groups of the macrocycles, the O—H groups of coordinated water molecules and the P—O—H groups of the acids as proton donors, and the O atoms of the phosphonate and carboxylate groups as acceptors, resulting in the formation of layers lying parallel to the (110) plane.

1. Chemical context

Metal–organic frameworks (MOFs) – crystalline coordination polymers with permanent porosity – attract much current attention due to the possibilities of their applications in different areas, including gas storage, separation, sensing, catalysis, etc. (MacGillivray & Lukehart, 2014; Kaska1, 2016). Metal complexes of the tetraaza-macrocycle, in particular cyclam (cyclam = 1,4,8,11-tetraazacyclotetradecane, C_{10}H_{24}N_4, L), possessing high thermodynamic stability and kinetic inertness (Yatsimirskii & Lampeka, 1985), are popular metal-containing building units for the construction of MOFs (Lampeka & Tsymbal, 2004; Suh & Moon, 2007; Suh et al., 2012; Stackhouse & Ma, 2018). The overwhelming majority of these materials are built up using oligocarboxylates as the bridging units (Rao et al., 2004), though linkers with other coordinating groups, in particular oligophosphonates, are also used for the construction of MOFs (Gagnon et al., 2012). At the same time, hybrid bridging molecules containing both phosphonate and carboxylate functional groups have been

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studied to a much lesser extent (see, for example, Heering et al., 2016b), though one can expect that the combination of different acidic donor groups in one ligand molecule could open new possibilities for the creation of MOFs with specific chemical and structural features different from those inherent for MOFs formed by pure ligand classes.

We report here the synthesis and crystal structure of the product of the reaction of \([\text{Zn}(\text{L})]\)(\text{ClO}_4)_2 with 4-phosphonatobiphenyl-4’-carboxylic acid (H_3A) – the closest structural analogue of the ligand 4,4’-diphenyldicarboxylate that is actively used for the preparation of different MOFs – namely, trans-diaqua(1,4,8,11-tetraazacyclotetradecane-\(\kappa^2N^0,N^0,N^0,N^0\))zinc(II) trans-bis(hydrogen 4-phosphonatobiphenyl-4’-carboxylato-\(\kappa^2O\))(1,4,8,11-tetraazacyclotetradecane-\(\kappa^2N^1,N^1,N^1,N^1\))zinc(II), \([\text{Zn}(\text{L})(\text{H}_2\text{O})_2][\text{Zn}(\text{L})(\text{HA})_2]\). Though several ionic compounds and coordination polymers with this ligand have been reported (Heering et al., 2016a,b), none of its complexes with macrocyclic cations have been described up to now.

2. Structural commentary

The molecular structure of the title compound, I, is shown in Fig. 1. Atom Zn1 (site symmetry \(\bar{1}\)) is coordinated by two monodentate doubly deprotonated acidic ligands HA\(^2^-\) via their phosphonate O-donor atoms, resulting in the formation of the \([\text{Zn1}(\text{L})(\text{HA})_2]^{2-}\) divalent anion, which is charge-balanced by the \([\text{Zn2}(\text{L})(\text{H}_2\text{O})_2]^{2+}\) divalent cation (Zn2 site symmetry \(\bar{1}\)). In the latter case, the macrocyclic ligand L is disordered over two orientations, with site occupancies of 50%, which are rotated around the O–Zn2–O axis by approximately 23°. The ligand L in both \([\text{Zn}(\text{L})]\) fragments adopts its energetically favoured trans-III conjugation, with the five- and six-membered chelate rings in gauche and chair conformations, respectively (Bosnich et al., 1965).

Both metal ions possess a tetragonally elongated trans-ZnN_4O_2 octahedral environment formed by the four secondary N atoms of the macrocyclic ligand in the equatorial plane and the two O atoms of the anions or water molecules in the axial positions (Table 1). The location of the metal ions on inversion centres enforces strict planarity of the ZnN_4 coordination moieties. The directivity of the axial Zn–O bonds is nearly orthogonal to the ZnN_4 plane.

The average Zn–N bond lengths in both macrocyclic units do not differ significantly [2.112 (12) Å for Zn1 and 2.101 (3) Å for Zn2] and are shorter than the average axial Zn–O bond lengths. The Zn–O distance for the phosphonate group [2.189 (4) Å] is shorter than that for the aqua ligand [2.295 (4) Å], reflecting the stronger donating properties of the anion. Thus, analogous to the situation for caboxylate groups coordinated to aza-macroyclic cations (Tsymbal et al., 2021), the Zn–O interactions are reinforced by intra-molecular hydrogen bonding between the secondary amino

Table 1
Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond Length (Å)</th>
<th>Symmetry Code</th>
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<tr>
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</tr>
<tr>
<td>Zn1–N1</td>
<td></td>
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<tr>
<td>Zn1–N2</td>
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<tr>
<td>N1–Zn1–N2'</td>
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<td>N1–Zn1–N2</td>
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Table 2
Hydrogen-bond geometry (Å, °).

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<th>D–H⋅⋅⋅A</th>
<th>D–H</th>
<th>H⋅⋅⋅A</th>
<th>D⋅⋅⋅A</th>
<th>D–H⋅⋅⋅A</th>
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<td>1.98</td>
<td>2.923</td>
<td>(6)</td>
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<tr>
<td>N2–H2⋅⋅⋅O4ii</td>
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<td>2.26</td>
<td>3.220</td>
<td>(6)</td>
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<tr>
<td>N3–H3⋅⋅⋅O3</td>
<td>0.98</td>
<td>2.11</td>
<td>3.076</td>
<td>(10)</td>
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<td>N4–H4⋅⋅⋅O5iii</td>
<td>0.98</td>
<td>1.84</td>
<td>2.815</td>
<td>(11)</td>
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<tr>
<td>O3–H3C⋅⋅⋅O4iv</td>
<td>0.86</td>
<td>1.75</td>
<td>2.597</td>
<td>(6)</td>
</tr>
<tr>
<td>O1W–H1WA⋅⋅⋅O2iv</td>
<td>0.87</td>
<td>2.08</td>
<td>2.735</td>
<td>(5)</td>
</tr>
<tr>
<td>O1W–H1WB⋅⋅⋅O5iv</td>
<td>0.86</td>
<td>1.82</td>
<td>2.668</td>
<td>(6)</td>
</tr>
</tbody>
</table>

Symmetry codes: (ii) \(-x+2, y, -z+2\); (iii) \(x+1, y-1, z\); (iv) \(-x+1, -y+1, -z+1\).
group (N1—H1) of ligand L and the O2 atom of the phosphonate fragment (Table 2).

The benzene rings in the HA\(^{2-}\) anion in I are tilted with respect to each other [the angle between their mean planes is 40.4 (2)°], while the uncoordinated carboxylate group is close to being coplanar with the corresponding aromatic fragment [12.3 (2)°]. This carboxylate group displays a high degree of electronic delocalization [the C23—O4 and C23—O5 bond lengths are 1.251 (8) and 1.258 (8) Å, respectively]. The protonated P—O3H bond [1.583 (4) Å] is not involved in delocalization.

3. Supramolecular features

The crystals of I are composed of [Zn1(L)(HA)\(_2\)]\(^{2+}\) anions and [Zn2(L)(H\(_2\)O)\(_2\)]\(^{2+}\) cations that are connected by numerous hydrogen bonds (Table 2). In particular, due to hydrogen bonding between the protonated phosphonate P1—O3—H fragments and the secondary amino N2—H2 groups of the macrocycle L as proton donors, and carboxylate atoms O4 [at (x + 1, y — 1, z)] as acceptors, the complex anions are arranged into one-dimensional tapes running along the [1\(\bar{1}0\)] direction (Fig. 2). These tapes are further connected into two-dimensional arrays lying parallel to the (110) plane by virtue of O—H···O and N—H···O hydrogen bonding between the O1W coordinated water molecule and the amino N3—H3 and N4—H4 groups as donors, and the phosphate and carboxylate atoms O2 [at (−x + 2, −y, −z + 1)], O3 and O5 [at (x + 1, y − 1, z) and (−x + 1, −y + 1, −z + 1)] as acceptors (Fig. 2). The distances Zn1···Zn1(x + 1, y − 1, z) and Zn2···Zn2(x + 1, y − 1, z) in the [1\(\bar{1}0\)] direction are 14.179 (2) Å, while the Zn1···Zn2 distance is 8.131 (1) Å. There are no hydrogen-bonding contacts between the layers and the three-dimensional coherence of the crystal is provided by van der Waals interactions.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update March 2022; Groom et al., 2016) indicated that several ionic compounds including ammonium and hexaamine cobalt(III) cations (refcodes SEDDUD and SEDFEP, respectively; Heering et al., 2016a) and coordination polymers formed by zinc(II) (UNISOB and UNISUH), cadmium(II) (UNITES) and mercury(II) ions (UNIWEV; Heering et al., 2016b) have been structurally characterized to date. In the polymeric complexes, the phosphonate groups of the ligands display a \(\mu_2\)-bridging function and form two-dimensional metal–oxo layers. The complexation behaviour of the carboxylate groups determines the dimensionality of the polymeric systems formed. If, like in I, they are not coordinated, the metal–oxo layers are simply decorated with ligand molecules (UNISOB and UNIWEV). At the same time, the \(\mu_2\) or \(\mu_3\)-bridging function of the carboxylate groups results in the formation of another kind of metal–oxo layer, thus producing three-dimensional coordination polymers (UNISUH and UNITES), in which the ligand molecules act as pillars. Interestingly, the tilting of the benzene rings in the ligand in polymeric complexes is much smaller that in I and does not exceed 7° (UNITES).
Table 3
Experimental details.

Crystal data
Chemical formula [Zn(C_{10}H_{9}N_{4})(H_{2}O)_{2}]-
[Zn(C_{13}H_{24}O_{5}P)_{2}(C_{10}H_{24}N_{4})]

M_{r} 1119.78

Crystal system, space group Triclinic, P\overline{T}

Temperature (K) 296
a, b, c (Å) 8.8781 (15), 9.3224 (14), 16.2627 (14)
\alpha, \beta, \gamma (°) 102.759 (10), 90.777 (11), 102.315 (14)
V (Å³) 1279.9 (3)
Z 1

Radiation type Mo Kα
Absorption correction Multi-scan (CrysAlis PRO; Rigaku OD, 2019)

No. of reflections 4514
No. of restraints 41
No. of parameters 317

\( |F|^2 > 2\sigma(F) \) reflections
\( \sin \theta/\lambda_{\text{max}} (\text{Å}^{-1}) \)
0.866, 1.000

Max. \( |F|^2 \) 9378, 4514, 3242
\( \sin \theta/\lambda_{\text{max}} (\text{Å}^{-1}) \)
0.081

0.69

\( \Delta f_{\text{max}} \), \( \Delta f_{\text{max}} \) (e Å\(^{-3}\))
0.91, −0.69

Computer programs: CrysAlis PRO (Rigaku OD, 2019), SHELXT2018 (Sheldrick, 2015a), SHELXL2018 (Sheldrick, 2015b), Mercury (Macrae et al., 2020) and publCIF (Westrip, 2010).

6. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms in I were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 (ring H atoms) and 0.97 Å (methylene H atoms), and N—H distances of 0.98 Å, with \( U_{iso}(H) \) values of 1.2\( U_{eq} \) of the parent atoms.

Acknowledgements
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References


5. Synthesis and crystallization

All chemicals and solvents used in this work were purchased from Sigma–Aldrich and were used without further purification. The acid H₄A was synthesized according to a procedure described previously (Heering et al., 2016b). The complex [Zn(L₁)][ClO₄]₂ was prepared by mixing equimolar amounts of L and zinc perchlorate hexahydrate in ethanol.

For the preparation of the title compound, I, a solution of [Zn(L₁)][ClO₄]₂ (23 mg, 0.06 mmol) in water (2 ml) was added to a dimethylformamide (DMF) solution (3 ml) of H₄A (11 mg, 0.04 mmol) containing triethylamine (0.05 ml). A white precipitate, which had formed over several days, was filtered off, washed with small amounts of dimethylformamide (DMF) and diethyl ether, and dried in air (yield: 6.7 mg, 15% based on the acid). Analysis calculated (%) for C₈₀H₇₀N₈O₂P₂Zn₂: C 49.34, H 6.30, N 10.01; found: C 49.45, H 6.41, N 10.21. Single crystals of I suitable for X-ray diffraction analysis were selected from the sample resulting from the synthesis. Caution! Perchlorate salts of metal complexes are potentially explosive and should be handled with care.
Synthesis and crystal structure of diaqua(1,4,8,11-tetraazacyclotetradecane)-zinc(II) bis(hydrogen 4-phosphonatobiphenyl-4′-carboxylato)(1,4,8,11-tetraazacyclotetradecane)zinc(II)

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2019); cell refinement: *CrysAlis PRO* (Rigaku OD, 2019); data reduction: *CrysAlis PRO* (Rigaku OD, 2019); program(s) used to solve structure: *SHELXT2018* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae et al., 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

*trans*-Diaqua(1,4,8,11-tetraazacyclotetradecane-κ⁴N₁,N₄,N₈,N₁₁)zinc(II) *trans*-bis(hydrogen 4-phosphonatobiphenyl-4′-carboxylato-κO)(1,4,8,11-tetraazacyclotetradecane-κ⁴N₁,N₄,N₈,N₁₁)zinc(II)

**Crystal data**

\[
\left[\text{Zn(C}_{10}\text{H}_{24}\text{N}_{4})\left(\text{H}_{2}\text{O}\right)_{2}\right] \\
\left[\text{Zn(C}_{10}\text{H}_{24}\text{O}_{5}\text{P}_{2}(\text{C}_{10}\text{H}_{24}\text{N}_{4})\right]
\]

\[
M_r = 1119.78 \\
\text{Triclinic, } P\overline{1} \\
a = 8.8781 (15) \text{ Å} \\
b = 9.3224 (14) \text{ Å} \\
c = 16.2627 (14) \text{ Å} \\
α = 102.759 (10)^\circ \\
β = 90.777 (11)^\circ \\
γ = 102.315 (14)^\circ \\
V = 1279.9 (3) \text{ Å}^3
\]

\[
Z = 1 \\
F(000) = 588 \\
D_r = 1.453 \text{ Mg m}^{-3} \\
\text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
\text{Cell parameters from 1677 reflections} \\
\theta = 2.3–25.6^\circ \\
\mu = 1.07 \text{ mm}^{-1} \\
T = 296 \text{ K} \\
\text{Block, clear light colourless} \\
0.3 \times 0.1 \times 0.05 \text{ mm}
\]

**Data collection**

Rigaku Xcalibur Eos diffractometer

Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 8.0797 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(CrysAlis PRO; Rigaku OD, 2019)

\[
T_{\min} = 0.866, \ T_{\max} = 1.000 \\
9378 \text{ measured reflections} \\
4514 \text{ independent reflections} \\
3242 \text{ reflections with } I > 2\sigma(I) \\
R_{int} = 0.081 \\
\theta_{\text{max}} = 25.0^\circ, \ \theta_{\text{min}} = 2.3^\circ \\
h = -10→10 \\
k = -10→11 \\
l = -19→19
\]
Refinement

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.080$
$wR(F^2) = 0.203$
$S = 1.06$

4514 reflections
317 parameters
41 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/\left[\sigma^2(F_o^2) + (0.084P)^2 + 0.5432P\right]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.91$ e Å$^{-3}$
$\Delta\rho_{\text{min}} = -0.69$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

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<thead>
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<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>$U_{eq}^*/U_{eq}$</th>
<th>Occ. (&lt;1)</th>
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<td>0.00000</td>
<td>1.00000</td>
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<td>0.02758 (16)</td>
<td>0.80359 (8)</td>
<td>0.0265 (4)</td>
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<td>-0.0163 (4)</td>
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<td>0.0323 (9)</td>
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<td>O2</td>
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Zn1—N1—C1—C2             | 54.5 (6)     | C17—C14—C15—C16         | −179.5 (5)   |
Zn1—N1—C5—C4i            | −40.5 (5)    | C17—C18—C19—C20         | 2.4 (9)      |
Zn1—N2—C3—C2             | −58.8 (5)    | C18—C17—C22—C21         | −1.9 (9)     |
Zn1—N2—C4—C5i            | 41.9 (5)     | C18—C19—C20—C21         | −2.6 (9)     |
P1—C11—C12—C13           | 179.7 (4)    | C18—C19—C20—C23         | 174.7 (5)    |
P1—C11—C16—C15           | 179.5 (4)    | C19—C20—C21—C22         | 0.5 (9)      |
O1—P1—C11—C12            | −73.1 (5)    | C19—C20—C23—O4          | 13.2 (8)     |
O1—P1—C11—C16            | 107.0 (4)    | C19—C20—C23—O5          | −167.7 (6)   |
O2—P1—O1—Zn1             | −6.4 (4)     | C20—C21—C22—C17         | 1.7 (9)      |
O2—P1—C11—C12            | 160.4 (4)    | C21—C20—C23—O4          | −169.6 (6)   |
O2—P1—C11—C16            | −19.5 (5)    | C21—C20—C23—O5          | 9.5 (8)      |
O3—P1—O1—Zn1             | 120.7 (3)    | C22—C17—C18—C19         | −0.1 (8)     |
O3—P1—C11—C12            | 43.6 (5)     | C23—C20—C21—C22         | −176.8 (5)   |
O3—P1—C11—C16            | −136.3 (4)   | Zn2—N3—C6—C7            | 41.4 (15)    |
N1—C1—C2—C3              | −72.0 (7)    | Zn2—N3—C10—C9ii         | −42.7 (14)   |
C1—N1—C5—C4i −167.7 (5) Zn2—N4—C8—C7 −48.3 (14)
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C3—N2—C4—C5i 165.2 (5) Zn2—N3X—C6X—C7X 56.2 (14)
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C11—P1—O1—Zn1 −127.4 (3) Zn2—N4X—C9X—C10X ii 43.1 (13)
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C12—C11—C16—C15 −0.4 (8) C6—N3—C10—C9 ii −172.2 (12)
C12—C13—C14—C15 0.2 (8) C6—C7—C8—N4 58 (2)
C12—C13—C14—C17 178.7 (5) C8—N4—C9—C10 ii 168.5 (14)
C13—C14—C15—C16 −1.0 (8) C9—N4—C8—C7 −172.0 (13)
C13—C14—C17—C18 40.4 (8) C10—N3—C6—C7 165.1 (12)
C13—C14—C17—C22 −139.4 (6) N3X—C6X—C7X—C8X −73.0 (16)
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C15—C14—C17—C22 39.0 (8) C10X—N3X—C6X—C7X −177.9 (14)
C16—C11—C12—C13 −0.4 (8)

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

Hydrogen-bond geometry (Å, °)

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

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