

Poly[[dodecaqua-hexakis(μ_2 -pyridine-2,5-dicarboxylato)tricopper(II)-diytterbium(III)] dihydrate]

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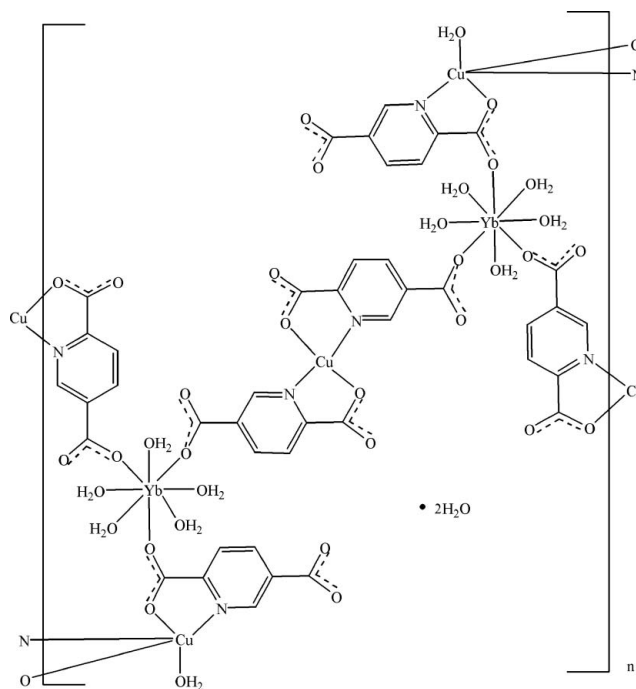
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.049; wR factor = 0.083; data-to-parameter ratio = 15.7.

The asymmetric unit of the title heterometallic coordination polymer, $\{[\text{Cu}_3\text{Yb}_2(\text{C}_7\text{H}_3\text{NO}_4)_6(\text{H}_2\text{O})_{12}] \cdot 2\text{H}_2\text{O}\}_n$, contains one Yb^{III} and two Cu^{II} atoms. The Cu^{II} atom that is located on an inversion center is N,O -chelated by two pyridine-2,5-dicarboxylate (pdc) anions in a square-planar geometry; the Cu atom located on a general position is N,O -chelated by two pdc anions in the basal plane and is further coordinated by a water O atom at the apical position in a distorted square-pyramidal geometry. The $\text{Yb}(\text{III})$ atom is eight coordinated in a distorted square-antiprismatic geometry formed by three carboxylate O atoms from three pdc anions and five water molecules. The pdc anions bridge adjacent $\text{Yb}(\text{III})$ and $\text{Cu}(\text{III})$ atoms, forming a three-dimensional polymeric structure. The crystal structure contains extensive $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. $\pi-\pi$ stacking is present in the crystal structure, the shortest centroid-centroid distance between parallel pyridine rings of adjacent molecules being 3.646 (3) Å.

Related literature

For general background to the use of pdc as a ligand in rare earth transition metal complexes, see: Huang *et al.* (2008). For related structures, see: Wei *et al.* (2005); Wen *et al.* (2007).



Experimental

Crystal data

$[\text{Cu}_3\text{Yb}_2(\text{C}_7\text{H}_3\text{NO}_4)_6(\text{H}_2\text{O})_{12}] \cdot 2\text{H}_2\text{O}$
 $M_r = 1815.58$
 Triclinic, $P\bar{1}$
 $a = 7.3486$ (4) Å
 $b = 13.5417$ (7) Å
 $c = 15.1244$ (8) Å
 $\alpha = 72.534$ (1)°
 $\beta = 76.330$ (1)°

$\gamma = 80.166$ (1)°
 $V = 1386.89$ (13) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 4.59$ mm⁻¹
 $T = 295$ K
 $0.13 \times 0.08 \times 0.05$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\text{min}} = 0.739$, $T_{\text{max}} = 0.973$

14910 measured reflections
 6624 independent reflections
 6010 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.083$
 $S = 1.23$
 6624 reflections

421 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.01$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.68$ e Å⁻³

Table 1

Selected bond lengths (Å).

Yb1—O2	2.299 (5)	Cu1—N1	1.975 (4)
Yb1—O3	2.272 (4)	Cu1—N2 ⁱ	1.955 (4)
Yb1—O4	2.411 (4)	Cu1—O1	2.372 (4)
Yb1—O5	2.278 (4)	Cu1—O8	1.964 (3)
Yb1—O6	2.364 (4)	Cu1—O11 ⁱ	1.943 (3)
Yb1—O7	2.447 (3)	Cu2—N3	1.967 (4)
Yb1—O13	2.364 (4)	Cu2—O17	1.931 (4)
Yb1—O15	2.281 (4)		

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

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1A···O17 ⁱⁱ	0.82	2.50	3.072 (5)	128
O1—H1A···O18 ⁱⁱ	0.82	2.06	2.865 (6)	166
O1—H1B···O9 ⁱⁱⁱ	0.82	2.02	2.840 (6)	173
O2—H2A···O10 ^{iv}	0.82	2.48	2.988 (7)	121
O2—H2B···O19	0.82	1.83	2.644 (8)	173
O3—H3A···O16	0.82	1.91	2.572 (6)	137
O3—H3B···O10 ⁱⁱⁱ	0.82	1.91	2.695 (6)	159
O4—H4A···O9 ⁱⁱⁱ	0.82	1.87	2.670 (6)	165
O4—H4B···O14 ^v	0.82	1.98	2.774 (6)	163
O5—H5A···O14	0.82	1.85	2.586 (6)	148
O5—H5B···O8	0.82	2.06	2.717 (6)	137
O6—H6A···O1 ^{vi}	0.82	2.09	2.826 (6)	149
O6—H6B···O4 ^{vi}	0.82	2.15	2.936 (6)	160
O19—H19A···O20 ^{vii}	0.82	2.06	2.816 (8)	152
O19—H19B···O12 ^{viii}	0.82	2.15	2.965 (7)	171
O20—H20A···O13 ^v	0.82	2.55	3.174 (7)	134
O20—H20B···O16	0.82	2.15	2.957 (9)	166

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve

structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

This work was supported financially by Yuanpei University, Taiwan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5166).

References

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 Huang, Y., Song, Y. S., Yan, B. & Shao, M. (2008). *J. Solid State Chem.* **181**, 1731–1737.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
 Wei, Y.-L., Hou, H.-W., Li, H.-K., Fan, Y.-T. & Zhu, Y. (2005). *Cryst. Growth Des.* **5**, 1405–1413.
 Wen, L.-L., Lu, Z.-D., Lin, J.-G., Tian, Z.-F., Zhu, H.-Z. & Meng, Q.-J. (2007). *Cryst. Growth Des.* **7**, 93–99.

supporting information

Acta Cryst. (2011). E67, m406–m407 [doi:10.1107/S1600536811007446]

Poly[[dodecaqua-hexakis(μ_2 -pyridine-2,5-dicarboxylato)tricopper(II)ytterbium(III)] dihydrate]

Fwu Ming Shen and Shie Fu Lush

S1. Comment

Many studies concerning the use of pdc as a ligand toward transition metal (Wen *et al.*, 2007) and /or rare earth transition metal (Wei *et al.*, 2005; Huang *et al.*, 2008) have shown that a great variety of polymeric structures can be obtained as a result of the different coordination modes of the pdc ligands.

The asymmetric unit of the title heterometallic coordination polymer, $[\text{Cu}_3\text{Yb}_2(\text{C}_7\text{H}_3\text{NO}_4)_6(\text{H}_2\text{O})_{12}\cdot 4\text{H}_2\text{O}]_n$, contains one Yb^{III} and two Cu^{II} atoms, three pyridine-2,5-dicarboxylate (pdc) anions and six water molecules. One Cu^{II} atom is located on an inversion center and is N,O-chelated by two pdc anions in the equatorial plane with square-planar geometry; the other Cu atom is N,O-chelated by two pdc anions in the coordination basal plane and coordinated by a carboxyl O atom at the apical position with a distorted square-pyramidal geometry [Cu—O = 2.374 (4) Å in the apical direction]. The Yb atom is eight coordinated with a distorted square-antiprismatic geometry formed by three carboxylate O atoms from three pdc anions and five water molecules (selected bond lengths are given in Table 1). The pdc anions bridge adjacent Yb and Cu atoms to form the three dimensional polymeric structure (Fig. 1).

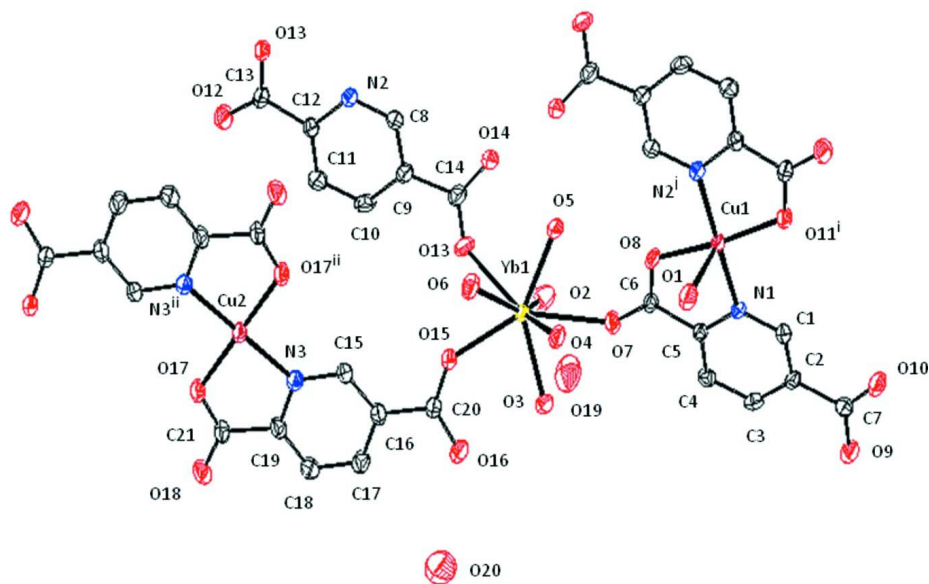
The crystal structure contains the extensive O—H \cdots O and weak C—H \cdots O hydrogen bonds (Fig. 2 and Table 2). π - π stackings are present in the crystal structure, the shortest centroids distance between parallel pyridine rings is 3.646 (3) Å [Cg6ⁱⁱⁱ \cdots Cg6 (N1/C1—C5)] [symmetry code: (iiv) $-x, 2 - y, -z$].

S2. Experimental

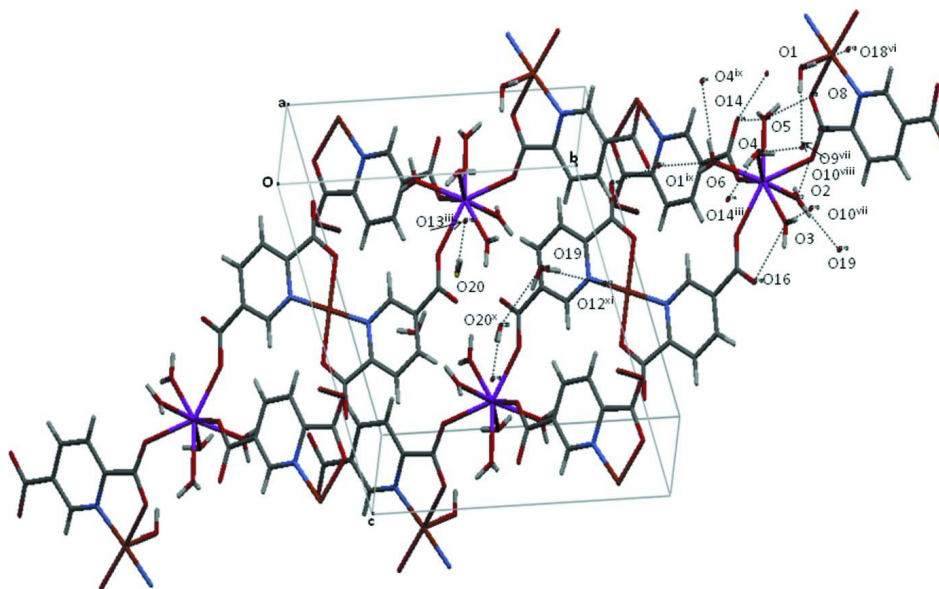
A mixture of ytterbium chloride hexahydrate (0.2438 g, 0.25 mmol), copper acetate hydrate (0.050 g, 0.25 mmol), pyridine-2,5-dicarboxylic acid (0.0418 g, 0.25 mmol,) and 10 ml H_2O were put in a 23-ml Teflon liner reactor and heated at 418 K in oven for 48 h. The resulting solution was slowly cooled to room temperature. The blue transparent single crystals of the title complex were obtained in 34.26% yield (based on Yb).

S3. Refinement

Water H atoms were placed in calculated positions and refined with the distances constraints of O—H = 0.82, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically with C—H = 0.93 Å and refined using a riding model, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.


Figure 1

View of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $2 - x, 1 - y, -z$; (ii) $1 - x, -y, 1 - z$].


Figure 2

The molecular packing for the title compound. Hydrogen bonds are shown as dashed lines.

Poly[[dodecaquaheptakis(μ_2 -pyridine-2,5-dicarboxylato)tricopper(II)diytterbium(III)] dihydrate]

Crystal data

$[\text{Cu}_3\text{Yb}_2(\text{C}_7\text{H}_3\text{NO}_4)_6(\text{H}_2\text{O})_{12}] \cdot 2\text{H}_2\text{O}$
 $M_r = 1815.58$

Triclinic, $P\bar{1}$
 Hall symbol: -P 1

$a = 7.3486$ (4) Å
 $b = 13.5417$ (7) Å
 $c = 15.1244$ (8) Å
 $\alpha = 72.534$ (1)°
 $\beta = 76.330$ (1)°
 $\gamma = 80.166$ (1)°
 $V = 1386.89$ (13) Å³
 $Z = 1$
 $F(000) = 891$

$D_x = 2.174$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 7576 reflections
 $\theta = 2.5$ – 25.0 °
 $\mu = 4.59$ mm⁻¹
 $T = 295$ K
 Columnar, blue
 $0.13 \times 0.08 \times 0.05$ mm

Data collection

Bruker SMART 1000 CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 9 pixels mm⁻¹
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2001)
 $T_{\min} = 0.739$, $T_{\max} = 0.973$

14910 measured reflections
 6624 independent reflections
 6010 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\max} = 28.3$ °, $\theta_{\min} = 1.4$ °
 $h = -9 \rightarrow 9$
 $k = -18 \rightarrow 18$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.083$
 $S = 1.23$
 6624 reflections
 421 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
 $w = 1/[\sigma^2(F_o^2) + (0.019P)^2 + 3.1503P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.01$ e Å⁻³
 $\Delta\rho_{\min} = -1.68$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Yb1	0.46140 (3)	0.553608 (18)	0.188850 (15)	0.01980 (7)
Cu1	0.55405 (9)	0.88959 (5)	-0.15334 (4)	0.02228 (15)
Cu2	0.5000	0.0000	0.5000	0.0251 (2)
O1	0.3238 (6)	0.7999 (3)	-0.1743 (3)	0.0346 (10)
H1A	0.2626	0.8487	-0.2052	0.052*
H1B	0.2574	0.7825	-0.1215	0.052*
O2	0.5782 (7)	0.6367 (4)	0.2722 (3)	0.0489 (12)
H2A	0.6913	0.6273	0.2718	0.073*

H2B	0.5274	0.6672	0.3126	0.073*
O3	0.1694 (6)	0.6205 (3)	0.2490 (3)	0.0416 (12)
H3A	0.1014	0.6001	0.3008	0.062*
H3B	0.1087	0.6689	0.2174	0.062*
O4	0.2936 (5)	0.5798 (3)	0.0631 (3)	0.0280 (9)
H4A	0.2306	0.6367	0.0528	0.042*
H4B	0.2172	0.5369	0.0803	0.042*
O5	0.6992 (5)	0.5902 (3)	0.0603 (3)	0.0322 (10)
H5A	0.8033	0.5564	0.0583	0.048*
H5B	0.7171	0.6486	0.0256	0.048*
O6	0.4981 (6)	0.4061 (3)	0.1308 (3)	0.0329 (9)
H6A	0.5319	0.3489	0.1639	0.049*
H6B	0.5320	0.4054	0.0754	0.049*
O7	0.4094 (5)	0.7414 (3)	0.1179 (2)	0.0276 (9)
O8	0.5572 (5)	0.7817 (3)	−0.0331 (2)	0.0249 (8)
O9	−0.0731 (6)	1.2456 (3)	−0.0036 (3)	0.0334 (10)
O10	0.0874 (6)	1.2581 (3)	−0.1509 (3)	0.0387 (11)
O15	0.3506 (6)	0.4262 (3)	0.3191 (3)	0.0395 (11)
O16	0.0621 (7)	0.4704 (4)	0.3939 (3)	0.0575 (15)
O19	0.3979 (9)	0.7458 (4)	0.3914 (4)	0.0710 (18)
H19A	0.3762	0.7083	0.4458	0.107*
H19B	0.3669	0.8059	0.3945	0.107*
O20	−0.3399 (9)	0.4351 (5)	0.4577 (4)	0.085 (2)
H20A	−0.3755	0.4648	0.4079	0.128*
H20B	−0.2285	0.4429	0.4499	0.128*
N1	0.3689 (6)	0.9653 (3)	−0.0721 (3)	0.0181 (9)
N3	0.3478 (6)	0.1321 (3)	0.5096 (3)	0.0227 (9)
C1	0.2791 (7)	1.0610 (4)	−0.0974 (4)	0.0222 (11)
H1C	0.2999	1.0985	−0.1608	0.027*
C2	0.1559 (7)	1.1059 (4)	−0.0317 (4)	0.0197 (10)
C3	0.1278 (7)	1.0499 (4)	0.0627 (4)	0.0233 (11)
H3C	0.0490	1.0791	0.1083	0.028*
C4	0.2181 (7)	0.9499 (4)	0.0887 (3)	0.0218 (11)
H4C	0.1987	0.9106	0.1515	0.026*
C5	0.3377 (7)	0.9099 (4)	0.0192 (3)	0.0177 (10)
C6	0.4413 (7)	0.8016 (4)	0.0383 (3)	0.0186 (10)
C7	0.0495 (7)	1.2123 (4)	−0.0651 (4)	0.0249 (12)
C15	0.3497 (8)	0.2265 (4)	0.4463 (4)	0.0238 (11)
H15A	0.4393	0.2362	0.3904	0.029*
C16	0.2210 (8)	0.3089 (4)	0.4630 (4)	0.0272 (12)
C17	0.0938 (9)	0.2969 (5)	0.5474 (4)	0.0359 (15)
H17A	0.0073	0.3523	0.5596	0.043*
C18	0.0968 (9)	0.2009 (5)	0.6140 (4)	0.0349 (14)
H18A	0.0148	0.1912	0.6723	0.042*
C19	0.2225 (8)	0.1209 (4)	0.5924 (4)	0.0256 (12)
C20	0.2115 (8)	0.4112 (4)	0.3869 (4)	0.0306 (13)
C21	0.2323 (8)	0.0112 (4)	0.6572 (4)	0.0254 (12)
O17	0.3522 (6)	−0.0560 (3)	0.6238 (2)	0.0290 (9)

O18	0.1287 (6)	-0.0081 (3)	0.7352 (3)	0.0364 (10)
O13	0.7259 (5)	0.4452 (3)	0.2402 (3)	0.0305 (9)
C14	0.8891 (8)	0.4189 (4)	0.2009 (4)	0.0257 (12)
O14	0.9801 (6)	0.4704 (3)	0.1242 (3)	0.0385 (11)
C9	0.9846 (7)	0.3138 (4)	0.2468 (4)	0.0226 (11)
C8	1.1424 (8)	0.2750 (4)	0.1928 (4)	0.0255 (12)
H8A	1.1890	0.3162	0.1329	0.031*
C10	0.9196 (8)	0.2533 (5)	0.3365 (4)	0.0281 (12)
H10A	0.8130	0.2777	0.3744	0.034*
N2	1.2312 (6)	0.1808 (3)	0.2233 (3)	0.0234 (10)
C11	1.0135 (8)	0.1559 (4)	0.3702 (4)	0.0259 (12)
H11A	0.9733	0.1152	0.4312	0.031*
C12	1.1666 (7)	0.1212 (4)	0.3115 (3)	0.0212 (11)
C13	1.2777 (8)	0.0148 (4)	0.3346 (4)	0.0255 (12)
O11	1.4056 (5)	-0.0058 (3)	0.2658 (2)	0.0277 (9)
O12	1.2456 (6)	-0.0441 (3)	0.4144 (3)	0.0398 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb1	0.01978 (12)	0.01595 (11)	0.01753 (11)	0.00351 (8)	-0.00040 (8)	-0.00100 (8)
Cu1	0.0237 (3)	0.0165 (3)	0.0195 (3)	0.0044 (3)	0.0007 (2)	-0.0018 (2)
Cu2	0.0298 (5)	0.0168 (4)	0.0217 (4)	0.0030 (4)	-0.0021 (4)	-0.0002 (4)
O1	0.038 (2)	0.026 (2)	0.038 (2)	0.0019 (18)	-0.0167 (19)	-0.0017 (18)
O2	0.046 (3)	0.059 (3)	0.051 (3)	0.016 (2)	-0.021 (2)	-0.033 (2)
O3	0.033 (2)	0.033 (2)	0.033 (2)	0.0115 (19)	0.0083 (18)	0.0084 (18)
O4	0.029 (2)	0.0157 (18)	0.037 (2)	0.0018 (16)	-0.0095 (17)	-0.0048 (16)
O5	0.026 (2)	0.024 (2)	0.031 (2)	0.0091 (17)	0.0019 (16)	0.0034 (17)
O6	0.044 (3)	0.020 (2)	0.031 (2)	0.0068 (18)	-0.0084 (18)	-0.0072 (17)
O7	0.033 (2)	0.0200 (19)	0.0212 (18)	0.0013 (16)	-0.0008 (16)	0.0003 (15)
O8	0.028 (2)	0.0149 (18)	0.0239 (18)	0.0081 (15)	-0.0009 (15)	-0.0035 (15)
O9	0.035 (2)	0.023 (2)	0.035 (2)	0.0063 (18)	-0.0026 (18)	-0.0064 (17)
O10	0.039 (3)	0.029 (2)	0.033 (2)	0.0116 (19)	-0.0024 (19)	0.0016 (18)
O15	0.033 (2)	0.024 (2)	0.037 (2)	0.0072 (18)	0.0082 (19)	0.0093 (18)
O16	0.048 (3)	0.035 (3)	0.053 (3)	0.018 (2)	0.016 (2)	0.011 (2)
O19	0.100 (5)	0.042 (3)	0.059 (3)	0.010 (3)	0.002 (3)	-0.021 (3)
O20	0.080 (5)	0.083 (5)	0.069 (4)	0.009 (4)	-0.001 (3)	-0.005 (3)
N1	0.017 (2)	0.014 (2)	0.022 (2)	0.0012 (17)	-0.0024 (16)	-0.0055 (16)
N3	0.024 (2)	0.020 (2)	0.022 (2)	0.0002 (19)	-0.0041 (18)	-0.0038 (18)
C1	0.023 (3)	0.019 (3)	0.020 (2)	-0.001 (2)	-0.004 (2)	0.000 (2)
C2	0.015 (2)	0.017 (2)	0.029 (3)	0.000 (2)	-0.008 (2)	-0.007 (2)
C3	0.018 (3)	0.026 (3)	0.027 (3)	0.001 (2)	-0.002 (2)	-0.012 (2)
C4	0.021 (3)	0.025 (3)	0.018 (2)	-0.003 (2)	-0.002 (2)	-0.005 (2)
C5	0.016 (2)	0.016 (2)	0.021 (2)	-0.0014 (19)	-0.0055 (19)	-0.0034 (19)
C6	0.018 (3)	0.016 (2)	0.023 (2)	-0.001 (2)	-0.009 (2)	-0.0022 (19)
C7	0.020 (3)	0.021 (3)	0.033 (3)	-0.004 (2)	-0.006 (2)	-0.004 (2)
C15	0.026 (3)	0.022 (3)	0.018 (2)	-0.002 (2)	-0.002 (2)	0.001 (2)
C16	0.034 (3)	0.017 (3)	0.024 (3)	-0.003 (2)	0.000 (2)	-0.002 (2)

C17	0.042 (4)	0.023 (3)	0.030 (3)	0.008 (3)	0.004 (3)	-0.005 (2)
C18	0.039 (4)	0.030 (3)	0.023 (3)	0.001 (3)	0.009 (2)	-0.002 (2)
C19	0.032 (3)	0.021 (3)	0.018 (2)	-0.002 (2)	-0.001 (2)	-0.001 (2)
C20	0.031 (3)	0.021 (3)	0.029 (3)	0.004 (2)	0.001 (2)	0.001 (2)
C21	0.031 (3)	0.020 (3)	0.022 (3)	-0.003 (2)	-0.006 (2)	0.000 (2)
O17	0.037 (2)	0.0181 (19)	0.0229 (19)	0.0017 (17)	-0.0011 (16)	0.0010 (15)
O18	0.045 (3)	0.029 (2)	0.023 (2)	-0.0034 (19)	0.0053 (18)	0.0012 (17)
O13	0.022 (2)	0.034 (2)	0.027 (2)	0.0098 (17)	-0.0028 (16)	-0.0050 (17)
C14	0.026 (3)	0.022 (3)	0.029 (3)	0.003 (2)	-0.005 (2)	-0.009 (2)
O14	0.025 (2)	0.030 (2)	0.039 (2)	0.0053 (18)	0.0023 (18)	0.0106 (18)
C9	0.020 (3)	0.019 (3)	0.030 (3)	0.000 (2)	-0.006 (2)	-0.008 (2)
C8	0.024 (3)	0.024 (3)	0.021 (3)	0.000 (2)	0.002 (2)	-0.002 (2)
C10	0.022 (3)	0.035 (3)	0.024 (3)	0.004 (2)	0.001 (2)	-0.011 (2)
N2	0.023 (2)	0.019 (2)	0.023 (2)	0.0028 (18)	-0.0005 (18)	-0.0028 (18)
C11	0.026 (3)	0.028 (3)	0.021 (3)	-0.003 (2)	-0.002 (2)	-0.006 (2)
C12	0.024 (3)	0.021 (3)	0.017 (2)	-0.001 (2)	-0.004 (2)	-0.001 (2)
C13	0.027 (3)	0.020 (3)	0.025 (3)	0.002 (2)	-0.006 (2)	-0.002 (2)
O11	0.031 (2)	0.0202 (19)	0.0208 (18)	0.0051 (16)	0.0036 (16)	-0.0004 (15)
O12	0.044 (3)	0.035 (2)	0.023 (2)	0.007 (2)	0.0023 (18)	0.0049 (18)

Geometric parameters (Å, °)

Yb1—O2	2.299 (5)	N1—C5	1.345 (6)
Yb1—O3	2.272 (4)	N3—C15	1.347 (6)
Yb1—O4	2.411 (4)	N3—C19	1.351 (7)
Yb1—O5	2.278 (4)	C1—C2	1.388 (7)
Yb1—O6	2.364 (4)	C1—H1C	0.9300
Yb1—O7	2.447 (3)	C2—C3	1.386 (7)
Yb1—O13	2.364 (4)	C2—C7	1.518 (7)
Yb1—O15	2.281 (4)	C3—C4	1.388 (7)
Cu1—N1	1.975 (4)	C3—H3C	0.9300
Cu1—N2 ⁱ	1.955 (4)	C4—C5	1.384 (7)
Cu1—O1	2.372 (4)	C4—H4C	0.9300
Cu1—O8	1.964 (3)	C5—C6	1.510 (7)
Cu1—O11 ⁱ	1.943 (3)	C15—C16	1.379 (7)
Cu2—N3 ⁱⁱ	1.967 (4)	C15—H15A	0.9300
Cu2—N3	1.967 (4)	C16—C17	1.376 (7)
Cu2—O17	1.931 (4)	C16—C20	1.515 (7)
Cu2—O17 ⁱⁱ	1.931 (4)	C17—C18	1.386 (8)
O1—H1A	0.8187	C17—H17A	0.9300
O1—H1B	0.8198	C18—C19	1.365 (8)
O2—H2A	0.8178	C18—H18A	0.9300
O2—H2B	0.8205	C19—C21	1.516 (7)
O3—H3A	0.8205	C21—O18	1.224 (6)
O3—H3B	0.8178	C21—O17	1.285 (6)
O4—H4A	0.8202	O13—C14	1.250 (6)
O4—H4B	0.8200	C14—O14	1.259 (6)
O5—H5A	0.8202	C14—C9	1.516 (7)

O5—H5B	0.8202	C9—C8	1.374 (7)
O6—H6A	0.8201	C9—C10	1.378 (7)
O6—H6B	0.8196	C8—N2	1.331 (7)
O7—C6	1.230 (6)	C8—H8A	0.9300
O8—C6	1.275 (6)	C10—C11	1.388 (8)
O9—C7	1.264 (6)	C10—H10A	0.9300
O10—C7	1.245 (6)	N2—C12	1.356 (6)
O15—C20	1.260 (6)	N2—Cu1 ⁱ	1.955 (4)
O16—C20	1.247 (7)	C11—C12	1.369 (7)
O19—H19A	0.8211	C11—H11A	0.9300
O19—H19B	0.8196	C12—C13	1.514 (7)
O20—H20A	0.8200	C13—O12	1.225 (6)
O20—H20B	0.8196	C13—O11	1.291 (6)
N1—C1	1.338 (6)	O11—Cu1 ⁱ	1.943 (3)
O3—Yb1—O5	140.82 (13)	C15—N3—Cu2	129.5 (4)
O3—Yb1—O15	74.65 (14)	C19—N3—Cu2	111.9 (3)
O5—Yb1—O15	143.99 (14)	N1—C1—C2	121.8 (5)
O3—Yb1—O2	87.37 (17)	N1—C1—H1C	119.1
O5—Yb1—O2	93.59 (17)	C2—C1—H1C	119.1
O15—Yb1—O2	94.33 (18)	C3—C2—C1	118.6 (5)
O3—Yb1—O6	120.10 (16)	C3—C2—C7	121.8 (5)
O5—Yb1—O6	77.53 (15)	C1—C2—C7	119.6 (4)
O15—Yb1—O6	76.43 (15)	C2—C3—C4	119.6 (5)
O2—Yb1—O6	146.13 (15)	C2—C3—H3C	120.2
O3—Yb1—O13	140.12 (13)	C4—C3—H3C	120.2
O5—Yb1—O13	76.19 (13)	C5—C4—C3	118.6 (5)
O15—Yb1—O13	72.76 (14)	C5—C4—H4C	120.7
O2—Yb1—O13	72.90 (15)	C3—C4—H4C	120.7
O6—Yb1—O13	73.24 (14)	N1—C5—C4	121.8 (4)
O3—Yb1—O4	77.38 (15)	N1—C5—C6	114.6 (4)
O5—Yb1—O4	79.41 (14)	C4—C5—C6	123.5 (4)
O15—Yb1—O4	111.93 (15)	O7—C6—O8	125.8 (5)
O2—Yb1—O4	144.31 (15)	O7—C6—C5	119.7 (5)
O6—Yb1—O4	66.81 (13)	O8—C6—C5	114.5 (4)
O13—Yb1—O4	136.66 (13)	O10—C7—O9	125.6 (5)
O3—Yb1—O7	68.67 (13)	O10—C7—C2	117.4 (5)
O5—Yb1—O7	74.46 (13)	O9—C7—C2	117.0 (5)
O15—Yb1—O7	141.10 (13)	N3—C15—C16	121.1 (5)
O2—Yb1—O7	71.91 (15)	N3—C15—H15A	119.5
O6—Yb1—O7	133.87 (13)	C16—C15—H15A	119.5
O13—Yb1—O7	131.94 (14)	C17—C16—C15	120.0 (5)
O4—Yb1—O7	72.50 (13)	C17—C16—C20	119.6 (5)
O11 ⁱ —Cu1—N2 ⁱ	83.59 (16)	C15—C16—C20	120.4 (5)
O11 ⁱ —Cu1—O8	168.02 (17)	C16—C17—C18	118.8 (5)
N2 ⁱ —Cu1—O8	94.15 (16)	C16—C17—H17A	120.6
O11 ⁱ —Cu1—N1	97.55 (16)	C18—C17—H17A	120.6
N2 ⁱ —Cu1—N1	170.26 (18)	C19—C18—C17	118.7 (5)

O8—Cu1—N1	82.73 (15)	C19—C18—H18A	120.6
O11 ⁱ —Cu1—O1	105.91 (15)	C17—C18—H18A	120.6
N2 ⁱ —Cu1—O1	95.56 (17)	N3—C19—C18	122.7 (5)
O8—Cu1—O1	86.00 (15)	N3—C19—C21	113.7 (5)
N1—Cu1—O1	93.43 (16)	C18—C19—C21	123.6 (5)
O17—Cu2—O17 ⁱⁱ	180.0	O16—C20—O15	125.6 (5)
O17—Cu2—N3 ⁱⁱ	95.81 (16)	O16—C20—C16	117.0 (5)
O17 ⁱⁱ —Cu2—N3 ⁱⁱ	84.19 (16)	O15—C20—C16	117.2 (5)
O17—Cu2—N3	84.19 (16)	O18—C21—O17	124.7 (5)
O17 ⁱⁱ —Cu2—N3	95.81 (16)	O18—C21—C19	119.8 (5)
N3 ⁱⁱ —Cu2—N3	180.0 (3)	O17—C21—C19	115.5 (4)
Cu1—O1—H1A	100.1	C21—O17—Cu2	114.7 (3)
Cu1—O1—H1B	104.2	C14—O13—Yb1	135.2 (3)
H1A—O1—H1B	106.2	O13—C14—O14	125.9 (5)
Yb1—O2—H2A	118.6	O13—C14—C9	117.7 (5)
Yb1—O2—H2B	132.6	O14—C14—C9	116.4 (5)
H2A—O2—H2B	107.7	C8—C9—C10	118.3 (5)
Yb1—O3—H3A	129.8	C8—C9—C14	117.0 (5)
Yb1—O3—H3B	122.7	C10—C9—C14	124.6 (5)
H3A—O3—H3B	107.3	N2—C8—C9	122.4 (5)
Yb1—O4—H4A	112.3	N2—C8—H8A	118.8
Yb1—O4—H4B	108.2	C9—C8—H8A	118.8
H4A—O4—H4B	105.2	C9—C10—C11	119.9 (5)
Yb1—O5—H5A	122.2	C9—C10—H10A	120.0
Yb1—O5—H5B	125.1	C11—C10—H10A	120.0
H5A—O5—H5B	105.8	C8—N2—C12	119.2 (4)
Yb1—O6—H6A	119.0	C8—N2—Cu1 ⁱ	127.6 (4)
Yb1—O6—H6B	126.0	C12—N2—Cu1 ⁱ	113.1 (3)
H6A—O6—H6B	108.2	C12—C11—C10	118.5 (5)
C6—O7—Yb1	136.8 (3)	C12—C11—H11A	120.8
C6—O8—Cu1	115.5 (3)	C10—C11—H11A	120.8
C20—O15—Yb1	140.2 (4)	N2—C12—C11	121.6 (5)
H19A—O19—H19B	106.7	N2—C12—C13	113.0 (4)
H20A—O20—H20B	108.0	C11—C12—C13	125.3 (5)
C1—N1—C5	119.6 (4)	O12—C13—O11	124.6 (5)
C1—N1—Cu1	128.1 (3)	O12—C13—C12	120.2 (5)
C5—N1—Cu1	112.3 (3)	O11—C13—C12	115.2 (4)
C15—N3—C19	118.6 (5)	C13—O11—Cu1 ⁱ	114.7 (3)
O2—Yb1—O7—C6	128.6 (5)	C5—N1—C1—C2	1.0 (8)
O3—Yb1—O7—C6	-137.1 (5)	Cu1—N1—C5—C4	177.6 (4)
O4—Yb1—O7—C6	-54.1 (5)	Cu1—N1—C5—C6	-3.1 (6)
O5—Yb1—O7—C6	29.4 (5)	C1—N1—C5—C4	-1.5 (8)
O6—Yb1—O7—C6	-25.3 (6)	C1—N1—C5—C6	177.7 (5)
O13—Yb1—O7—C6	83.7 (5)	C12—N2—C8—C9	-1.3 (8)
O15—Yb1—O7—C6	-157.6 (5)	Cu1 ⁱ —N2—C8—C9	175.7 (4)
O2—Yb1—O13—C14	-109.4 (5)	C8—N2—C12—C11	-0.6 (8)
O3—Yb1—O13—C14	-173.1 (5)	C8—N2—C12—C13	177.9 (5)

O4—Yb1—O13—C14	46.4 (6)	Cu1 ⁱ —N2—C12—C11	-178.0 (4)
O5—Yb1—O13—C14	-11.1 (5)	Cu1 ⁱ —N2—C12—C13	0.5 (6)
O6—Yb1—O13—C14	69.8 (5)	Cu2—N3—C15—C16	174.8 (4)
O7—Yb1—O13—C14	-64.9 (6)	C19—N3—C15—C16	-3.2 (8)
O15—Yb1—O13—C14	150.4 (6)	Cu2—N3—C19—C18	-177.7 (5)
O2—Yb1—O15—C20	80.6 (6)	Cu2—N3—C19—C21	1.0 (6)
O3—Yb1—O15—C20	-5.5 (6)	C15—N3—C19—C18	0.7 (9)
O4—Yb1—O15—C20	-74.7 (6)	C15—N3—C19—C21	179.4 (5)
O5—Yb1—O15—C20	-177.2 (5)	N1—C1—C2—C3	0.8 (8)
O6—Yb1—O15—C20	-132.4 (6)	N1—C1—C2—C7	-176.6 (5)
O7—Yb1—O15—C20	14.3 (7)	C1—C2—C3—C4	-2.0 (8)
O13—Yb1—O15—C20	151.2 (6)	C7—C2—C3—C4	175.3 (5)
O1—Cu1—O8—C6	-90.2 (4)	C1—C2—C7—O9	173.9 (5)
N1—Cu1—O8—C6	3.8 (4)	C1—C2—C7—O10	-4.5 (8)
N2 ⁱ —Cu1—O8—C6	174.6 (4)	C3—C2—C7—O9	-3.4 (8)
O1—Cu1—N1—C1	-95.5 (5)	C3—C2—C7—O10	178.2 (5)
O1—Cu1—N1—C5	85.5 (4)	C2—C3—C4—C5	1.5 (8)
O8—Cu1—N1—C1	179.0 (5)	C3—C4—C5—N1	0.3 (8)
O8—Cu1—N1—C5	-0.1 (4)	C3—C4—C5—C6	-178.9 (5)
O11 ⁱ —Cu1—N1—C1	11.1 (5)	N1—C5—C6—O7	-173.5 (5)
O11 ⁱ —Cu1—N1—C5	-168.0 (4)	N1—C5—C6—O8	6.4 (7)
O1—Cu1—O11 ⁱ —C13 ⁱ	-88.6 (4)	C4—C5—C6—O7	5.7 (8)
N1—Cu1—O11 ⁱ —C13 ⁱ	175.6 (4)	C4—C5—C6—O8	-174.4 (5)
O1—Cu1—N2 ⁱ —C8 ⁱ	-79.9 (5)	N2—C8—C9—C10	1.5 (9)
O1—Cu1—N2 ⁱ —C12 ⁱ	103.0 (4)	N2—C8—C9—C14	-175.7 (5)
O8—Cu1—N2 ⁱ —C8 ⁱ	6.6 (5)	C8—C9—C10—C11	0.1 (9)
O8—Cu1—N2 ⁱ —C12 ⁱ	-170.6 (4)	C14—C9—C10—C11	177.1 (6)
N3—Cu2—O17—C21	-1.5 (4)	C8—C9—C14—O13	165.0 (5)
O12 ⁱⁱⁱ —Cu2—O17—C21	-92.1 (4)	C8—C9—C14—O14	-12.6 (8)
N3 ⁱⁱ —Cu2—O17—C21	178.5 (4)	C10—C9—C14—O13	-12.0 (9)
O12 ^{iv} —Cu2—O17—C21	88.0 (4)	C10—C9—C14—O14	170.4 (6)
O17—Cu2—N3—C15	-178.0 (5)	C9—C10—C11—C12	-1.9 (9)
O17—Cu2—N3—C19	0.2 (4)	C10—C11—C12—N2	2.2 (8)
O12 ⁱⁱⁱ —Cu2—N3—C15	-86.7 (5)	C10—C11—C12—C13	-176.1 (5)
O12 ⁱⁱⁱ —Cu2—N3—C19	91.5 (4)	N2—C12—C13—O11	-4.9 (7)
O17 ⁱⁱ —Cu2—N3—C15	2.0 (5)	N2—C12—C13—O12	173.9 (5)
O17 ⁱⁱ —Cu2—N3—C19	-179.8 (4)	C11—C12—C13—O11	173.5 (5)
O12 ^{iv} —Cu2—N3—C15	93.3 (5)	C11—C12—C13—O12	-7.7 (9)
O12 ^{iv} —Cu2—N3—C19	-88.6 (4)	N3—C15—C16—C17	3.2 (9)
Yb1—O7—C6—O8	-17.4 (9)	N3—C15—C16—C20	-173.5 (5)
Yb1—O7—C6—C5	162.5 (4)	C15—C16—C17—C18	-0.7 (9)
Cu1—O8—C6—O7	173.5 (4)	C20—C16—C17—C18	176.1 (6)
Cu1—O8—C6—C5	-6.4 (6)	C15—C16—C20—O15	-16.8 (8)
Cu1 ⁱ —O11—C13—O12	-171.8 (5)	C15—C16—C20—O16	159.0 (6)
Cu1 ⁱ —O11—C13—C12	7.0 (6)	C17—C16—C20—O15	166.5 (6)
Cu2 ^v —O12—C13—O11	85.5 (6)	C17—C16—C20—O16	-17.7 (9)
Cu2 ^v —O12—C13—C12	-93.1 (5)	C16—C17—C18—C19	-1.8 (10)
Yb1—O13—C14—O14	25.3 (9)	C17—C18—C19—N3	1.8 (10)

Yb1—O13—C14—C9	-152.0 (4)	C17—C18—C19—C21	-176.7 (6)
Yb1—O15—C20—O16	11.1 (10)	N3—C19—C21—O17	-2.2 (8)
Yb1—O15—C20—C16	-173.6 (4)	N3—C19—C21—O18	178.3 (5)
Cu2—O17—C21—O18	-178.2 (5)	C18—C19—C21—O17	176.4 (6)
Cu2—O17—C21—C19	2.4 (6)	C18—C19—C21—O18	-3.1 (9)
Cu1—N1—C1—C2	-178.0 (4)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O17 ^{vi}	0.82	2.50	3.072 (5)	128
O1—H1A \cdots O18 ^{vi}	0.82	2.06	2.865 (6)	166
O1—H1B \cdots O9 ^{vii}	0.82	2.02	2.840 (6)	173
O2—H2A \cdots O10 ^{viii}	0.82	2.48	2.988 (7)	121
O2—H2B \cdots O19	0.82	1.83	2.644 (8)	173
O3—H3A \cdots O16	0.82	1.91	2.572 (6)	137
O3—H3B \cdots O10 ^{vii}	0.82	1.91	2.695 (6)	159
O4—H4A \cdots O9 ^{vii}	0.82	1.87	2.670 (6)	165
O4—H4B \cdots O14 ⁱⁱⁱ	0.82	1.98	2.774 (6)	163
O5—H5A \cdots O14	0.82	1.85	2.586 (6)	148
O5—H5B \cdots O8	0.82	2.06	2.717 (6)	137
O6—H6A \cdots O1 ^{ix}	0.82	2.09	2.826 (6)	149
O6—H6B \cdots O4 ^{ix}	0.82	2.15	2.936 (6)	160
O19—H19A \cdots O20 ^x	0.82	2.06	2.816 (8)	152
O19—H19B \cdots O12 ^{xi}	0.82	2.15	2.965 (7)	171
O20—H20A \cdots O13 ⁱⁱⁱ	0.82	2.55	3.174 (7)	134
O20—H20B \cdots O16	0.82	2.15	2.957 (9)	166
C3—H3C \cdots O18 ^x	0.93	2.42	3.134 (7)	134
C11—H11A \cdots O12 ^{iv}	0.93	2.52	3.409 (7)	159

Symmetry codes: (iii) $x-1, y, z$; (iv) $-x+2, -y, -z+1$; (vi) $x, y+1, z-1$; (vii) $-x, -y+2, -z$; (viii) $-x+1, -y+2, -z$; (ix) $-x+1, -y+1, -z$; (x) $-x, -y+1, -z+1$; (xi) $x-1, y+1, z$.