

**Electronic Supplementary information (ESI)**

**Table S1.** Strong and medium strength hydrogen bond geometric parameters for compound **1**.

D–H⋯A	D–H (Å)	H⋯A (Å)	D⋯A (Å)	D–H⋯A (°)
O3–H3A⋯O4 <sup>i</sup>	0.85(2)	1.92(2)	2.7613(9)	175(2)
O3–H3B⋯N2 <sup>ii</sup>	0.83(2)	2.08(2)	2.855(1)	155(2)
O4–H4A⋯O5 <sup>iii</sup>	0.90(2)	1.87(2)	2.7718(9)	178(2)
O4–H4B⋯N4 <sup>iv</sup>	0.83(2)	1.98(2)	2.789(1)	166(2)
O5–H5A⋯N3 <sup>iv</sup>	0.83(2)	2.15(2)	2.905(1)	152(2)
O5–H5B⋯O3 <sup>ii</sup>	0.92(2)	1.87(2)	2.7478(9)	160(2)
O5–H5B⋯O1 <sup>v</sup>	0.92(2)	2.59(2)	3.0422(9)	111(2)

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

**Table S2.** Strong hydrogen bond geometric parameters for compound **2**.

D–H⋯A	D–H (Å)	H⋯A (Å)	D⋯A (Å)	D–H⋯A (°)
O3–H31⋯N3 <sup>i</sup>	0.85(2)	2.06(2)	2.872(2)	159(2)
O4–H41⋯N4 <sup>ii</sup>	0.78(2)	2.14(2)	2.923(2)	175(2)
O3–H32⋯O3 <sup>iii</sup>	0.81(3)	2.02(3)	2.833(2)	176(4)
O4–H42⋯O4 <sup>iv</sup>	0.82(3)	1.94(3)	2.764(2)	176(4)
O3–H33⋯O4 <sup>v</sup>	0.91(5)	1.95(5)	2.799(2)	153(3)
O4–H43⋯O3 <sup>vi</sup>	0.79(5)	2.07(5)	2.799(2)	154(3)

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

**Table S3.** Graph-set matrix for strong hydrogen bonding in compound **1**. First level motifs on-diagonal and second level graph-sets off-diagonal (for numbering scheme see Figure 2).

D–H⋯A	A	B	C	D	E	F
O3–H3A⋯O4 <sup>i</sup> (A)	D1,1(2)					
O4–H4A⋯O5 <sup>iii</sup> (B)	D2,2(4)	D1,1(2)				
O5–H5B⋯O3 <sup>ii</sup> (C)	D2,2(4)	D2,2(4)	D1,1(2)			
O3–H3B⋯N2 <sup>ii</sup> (D)	D2,2(5)		D2,2(4)	D1,1(2)		
O4–H4B⋯N4 <sup>iv</sup> (E)	D2,2(4)	D2,2(5)		D2,2(5)	D1,1(2)	
O5–H5A⋯N3 <sup>iv</sup> (F)		D2,2(4)	D2,2(5)	D2,2(4)	D2,2(4)	D1,1(2)

Symmetry codes for **1**: See Table 1.