organic compounds

4-Hydroxy-3,5-dimethoxybenzaldehyde isonicotinoylhydrazone monohydrate

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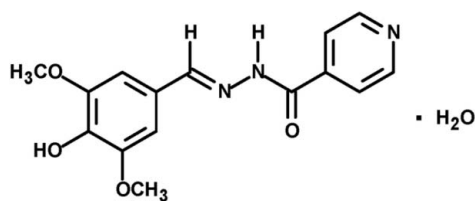Correspondence e-mail: sunyf50@hotmail.com

In the title compound, $C_{15}H_{15}N_3O_4 \cdot H_2O$, the organic molecule exists in the keto–imine tautomeric form. The benzene ring makes a dihedral angle of 49.9 (2)° with the pyridine ring. The molecules pack in a three-dimensional framework structure by a combination of O—H···O, O—H···N, N—H···O and N—H···N hydrogen bonds. The water molecule of hydration is disordered [ratio of components 0.758 (7):0.242 (7)].

Related literature

For background literature, see: Ganjali *et al.* (2006); Getautis *et al.* (2006); Gup & Kirkan (2005); Kuriakose *et al.* (2007). Similar structures have also been observed in related hydrazone analogues (Peralta *et al.*, 2007; Raj & Kurup, 2007; Sun *et al.*, 2007). Other reported compounds exist in the enamine–keto tautomeric form (Liu *et al.*, 2004; Sun *et al.*, 2006).

Experimental

Crystal data

$C_{15}H_{15}N_3O_4 \cdot H_2O$	V = 1523.9 (4) Å^3
M_r = 319.32	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 9.0139 (13) Å	μ = 0.11 mm^{-1}
b = 21.663 (3) Å	T = 273 (2) K
c = 7.8198 (11) Å	$0.18 \times 0.16 \times 0.15$ mm
β = 93.653 (5)°	

Data collection

Bruker SMART CCD area-detector diffractometer	17241 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2687 independent reflections
	2258 reflections with $I > 2\sigma(I)$
T_{min} = 0.981, T_{max} = 0.984	R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	217 parameters
$wR(F^2)$ = 0.112	H-atom parameters constrained
S = 1.05	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
2687 reflections	$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O5^i	0.82	1.99	2.732 (2)	151
O1—H1···O3	0.82	2.24	2.6690 (18)	113
N3—H2···O4^{ii}	0.86	2.17	3.0214 (17)	171
N3—H2···N2^{ii}	0.86	2.69	3.1923 (18)	119
O5—H5E···N1^{iii}	0.89	2.00	2.874 (2)	166
O5—H5F···O5^{iv}	0.85	2.61	3.449 (5)	174

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2036).

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supplementary materials

4-Hydroxy-3,5-dimethoxybenzaldehyde isonicotinoylhydrazone monohydrate

Y.-F. Sun, X.-L. Wang, J.-K. Li, X.-L. Cheng and R.-T. Wu

Comment

Molecules containing hydrazone moieties have attracted great attention not only due to their broad spectrum of biological activities (Gup & Kirkan, 2005) but also to their potential applications in the areas of magnetism, electronics, sensor (Ganjali *et al.*, 2006), nonlinear optics, fluorescent materials and optoelectronic devices (Getautis *et al.*, 2006). Moreover, many of hydrazones have also been employed as ligands for complexation of metal ions (Kuriakose *et al.*, 2007). In continuation of our studies on hydrazone derivatives (Sun *et al.*, 2006; 2007), we herein report the synthesis and crystal structure of the title compound, (I).

The molecule of (I) is not planar and possesses normal geometric parameters. The central spacer unit of the hydrazone component, between atoms C4 and C11 (Fig. 1), is effectively planar with an all-*trans*. extended-chain conformation, as shown by the relevant torsion angles On the other hand, the pyridine and the phenyl rings form an angle of 49.9 (2)° with respect to each other; the pyridine ring is rotated significantly out of the plane of the central spacer unit with torsion angle N3—C10—C11—C12 of −46.3 (2)°. The existence of (I) in the usual keto-imine form in the crystalline state is evident from the O4–C1O and N2—C9 bond lengths of 1.232 (2) and 1.272 (2) Å. The two methoxy groups are almost coplanar with the benzene ring. Similar structures have been observed in the related hydrazone analogues (Peralta *et al.*, 2007; Raj & Kurup, 2007; Sun *et al.*, 2007). In contrast, the enamine–keto tautomeric form is exhibited by compound PMBP-INTH (Liu *et al.*, 2004), in which the molecule is a prototropic isomeric, and the pyridinium formed with the deproton of enol hydroxyl group. The molecules are linked by intermolecular N3–H2···O4 hydrogen bonding into a one-dimensional chain structure along the c direction (Fig. 2), and these chains are cross-linked into a two-dimensional framework by intermolecular O1—H1···O5 and O5—H5E···N1 hydrogen bonds. Therefore, the complete three-dimensional framework structure is achieved by a nearly linear hydrogen bond between water molecules; details have been provided in the Table.

Experimental

A mixture of isonicotinoyl hydrazide (1 mmol) and syringaldehyde (4-hydroxy-3,5-dimethoxy-benzaldehyde) (1 mmol) in anhydrous ethanol (35 ml) were heated under reflux for 3 h. After cooling, the solvent was removed under reduced pressure and the resulting solid residues were recrystallized from ethanol to yield the pure products. Crystals suitable for an X-ray structural analysis were obtained by slowly evaporating an ethanol solution at room temperature. Yield: 74%.

Refinement

The H atoms were located in a difference Fourier map and were treated as riding atoms, with C—H = 0.93 (aromatic and –CH=N–), 0.96 (methyl), N—H = 0.86 and O—H = 0.82 Å, and with U_{iso} = 1.5 times U_{eq}(parent atoms), for the methyl and the hydroxyl groups and x1.2 for all other H atoms. The water of hydration was disordered over two sites with site occupancy factors for O5 and O6 being 0.758 (7) and 0.242 (7), respectively. O6 fraction of the water of hydration was allowed isotropic U_{iso} and disorder in the H-atoms was ignored.
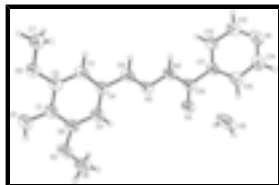
supplementary materials

Figures

Fig. 1. View of the molecule of (I) showing the atom-labelling scheme; displacement ellipsoids are drawn at the 50% probability level. O6 representing the smaller fraction of disordered water of hydration has been ignored.

Fig. 2. The chain structure formed *via* hydrogen bonds in (I); H atoms have been omitted for clarity. The dashed lines indicate H-bonds.

4-Hydroxy-3,5-dimethoxybenzaldehyde isonicotinoylhydrazone monohydrate

Crystal data

$C_{15}H_{15}N_3O_4{\cdot}H_2O$	$F_{000} = 672$
$M_r = 319.32$	$D_x = 1.392$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6268 reflections
$a = 9.0139$ (13) Å	$\theta = 2.5$–27.2°
$b = 21.663$ (3) Å	$\mu = 0.11$ mm^{-1}
$c = 7.8198$ (11) Å	$T = 273$ (2) K
$\beta = 93.653$ (5)°	Block, yellow
$V = 1523.9$ (4) Å^3	$0.18 \times 0.16 \times 0.15$ mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2687 independent reflections
Radiation source: fine-focus sealed tube	2258 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 273(2)$ K	$\theta_{max} = 25.0$°
φ and ω scans	$\theta_{min} = 1.9$°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10{\rightarrow}10$
$T_{min} = 0.981$, $T_{max} = 0.984$	$k = -25{\rightarrow}25$
17241 measured reflections	$l = -8{\rightarrow}9$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.4857P]$

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

$wR(F^2) = 0.112$

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

$S = 1.05$

$\Delta\rho_{max} = 0.33$ e Å^{-3}

2687 reflections

$\Delta\rho_{min} = -0.38$ e Å^{-3}

217 parameters

Extinction correction: SHELXL97 (Sheldrick, 1997)

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.067 (4)

Secondary atom site location: difference Fourier map

Special details

Experimental. Spectroscopic analysis: IR(KBr, ν cm^{-1}): 3494, 3197, 3060, 2933, 2839, 1635, 1585, 1518, 1460, 1408, 1333, 1217, 1120, 1063, 1001, 958, 837, 687. Anal. Calcd. (%) for $C_{15}H_{17}N_3O_5$: C, 56.42; H, 5.37; N, 13.16. Found (%): C, 56.29; H, 5.46; N, 13.07.

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 $F^2 > 2sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	−0.26392 (15)	0.46890 (6)	0.35782 (16)	0.0616 (4)	
H1	−0.2922	0.4499	0.2710	0.092*	
O2	−0.18690 (16)	0.50673 (6)	0.66825 (16)	0.0620 (4)	
O3	−0.15502 (16)	0.36614 (7)	0.22525 (16)	0.0705 (4)	
O4	0.34468 (14)	0.17268 (6)	0.67074 (14)	0.0544 (4)	
N1	0.59210 (17)	0.11847 (8)	1.25173 (19)	0.0571 (4)	
N2	0.20424 (14)	0.28062 (6)	0.72122 (16)	0.0413 (3)	
N3	0.29801 (14)	0.25269 (6)	0.84535 (15)	0.0411 (3)	
H2	0.3163	0.2701	0.9432	0.049*	
C1	−0.16440 (18)	0.43429 (8)	0.4518 (2)	0.0465 (4)	
C2	−0.12051 (19)	0.45386 (8)	0.6169 (2)	0.0461 (4)	
C3	−0.01778 (19)	0.41989 (8)	0.7162 (2)	0.0468 (4)	
H3	0.0121	0.4334	0.8260	0.056*	
C4	0.04127 (18)	0.36573 (7)	0.6537 (2)	0.0428 (4)	
C5	−0.00257 (19)	0.34559 (8)	0.4888 (2)	0.0466 (4)	
H5	0.0360	0.3093	0.4462	0.056*	
C6	−0.10406 (19)	0.38015 (8)	0.3895 (2)	0.0474 (4)	
C7	−0.1517 (3)	0.52670 (10)	0.8388 (3)	0.0784 (7)	
H7A	−0.1776	0.4950	0.9173	0.118*	
H7B	−0.2065	0.5636	0.8606	0.118*	

H7C	−0.0471	0.5351	0.8540	0.118*	
C8	−0.0938 (3)	0.31532 (10)	0.1449 (3)	0.0714 (6)	
H8A	0.0124	0.3195	0.1485	0.107*	
H8B	−0.1325	0.3134	0.0278	0.107*	
H8C	−0.1192	0.2782	0.2032	0.107*	
C9	0.14731 (18)	0.33143 (8)	0.7657 (2)	0.0433 (4)	
H9	0.1744	0.3473	0.8737	0.052*	
C10	0.35979 (17)	0.19835 (8)	0.81136 (19)	0.0413 (4)	
C11	0.44799 (17)	0.17032 (7)	0.96018 (19)	0.0414 (4)	
C12	0.54908 (19)	0.20423 (8)	1.0627 (2)	0.0480 (4)	
H12	0.5697	0.2451	1.0366	0.058*	
C13	0.6184 (2)	0.17607 (9)	1.2039 (2)	0.0543 (5)	
H13	0.6881	0.1988	1.2701	0.065*	
C14	0.4974 (2)	0.08606 (9)	1.1495 (2)	0.0595 (5)	
H14	0.4794	0.0453	1.1786	0.071*	
C15	0.4246 (2)	0.10932 (8)	1.0031 (2)	0.0530 (5)	
H15	0.3610	0.0845	0.9346	0.064*	
O5	0.5522 (3)	0.07028 (13)	0.5882 (3)	0.0748 (11)	0.758 (7)
H5E	0.5759	0.0897	0.4930	0.112*	
H5F	0.5194	0.0367	0.5458	0.112*	
O6	0.6179 (8)	0.0378 (3)	0.5492 (8)	0.059 (2)*	0.242 (7)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0694 (8)	0.0629 (8)	0.0495 (8)	0.0163 (6)	−0.0199 (6)	−0.0031 (6)
O2	0.0795 (9)	0.0538 (7)	0.0501 (8)	0.0187 (6)	−0.0178 (6)	−0.0111 (6)
O3	0.0814 (10)	0.0850 (10)	0.0418 (7)	0.0287 (8)	−0.0211 (6)	−0.0152 (6)
O4	0.0737 (8)	0.0566 (7)	0.0315 (6)	0.0070 (6)	−0.0069 (5)	−0.0061 (5)
N1	0.0581 (9)	0.0684 (10)	0.0436 (8)	0.0094 (8)	−0.0049 (7)	0.0095 (7)
N2	0.0448 (7)	0.0511 (8)	0.0273 (7)	0.0011 (6)	−0.0033 (5)	0.0053 (5)
N3	0.0488 (8)	0.0505 (8)	0.0231 (6)	0.0042 (6)	−0.0055 (5)	0.0008 (5)
C1	0.0469 (9)	0.0520 (9)	0.0394 (9)	0.0022 (7)	−0.0070 (7)	0.0042 (7)
C2	0.0515 (9)	0.0447 (9)	0.0414 (9)	0.0020 (7)	−0.0031 (7)	−0.0007 (7)
C3	0.0542 (10)	0.0511 (10)	0.0340 (8)	0.0003 (7)	−0.0067 (7)	−0.0013 (7)
C4	0.0444 (9)	0.0495 (9)	0.0339 (8)	−0.0004 (7)	−0.0023 (7)	0.0036 (7)
C5	0.0510 (9)	0.0513 (9)	0.0371 (8)	0.0056 (7)	−0.0010 (7)	−0.0010 (7)
C6	0.0509 (9)	0.0578 (10)	0.0322 (8)	0.0028 (8)	−0.0064 (7)	−0.0027 (7)
C7	0.1088 (18)	0.0681 (13)	0.0548 (12)	0.0288 (12)	−0.0214 (12)	−0.0201 (10)
C8	0.0867 (15)	0.0782 (14)	0.0472 (11)	0.0088 (11)	−0.0120 (10)	−0.0186 (10)
C9	0.0482 (9)	0.0519 (10)	0.0291 (8)	0.0010 (7)	−0.0018 (6)	0.0006 (7)
C10	0.0454 (9)	0.0491 (9)	0.0289 (8)	−0.0009 (7)	0.0000 (6)	0.0010 (7)
C11	0.0430 (9)	0.0517 (9)	0.0295 (8)	0.0066 (7)	0.0015 (6)	−0.0008 (7)
C12	0.0498 (10)	0.0536 (10)	0.0398 (9)	−0.0005 (7)	−0.0033 (7)	0.0023 (7)
C13	0.0508 (10)	0.0692 (12)	0.0414 (9)	0.0003 (8)	−0.0086 (8)	−0.0010 (8)
C14	0.0664 (12)	0.0541 (11)	0.0568 (11)	0.0044 (9)	−0.0065 (9)	0.0100 (9)
C15	0.0597 (11)	0.0520 (10)	0.0458 (10)	0.0029 (8)	−0.0079 (8)	−0.0023 (8)
O5	0.0741 (15)	0.098 (2)	0.0510 (12)	−0.0110 (14)	−0.0109 (10)	0.0169 (11)

Geometric parameters (Å, °)

O1—C1	1.3501 (19)	C7—H7A	0.9600
O1—H1	0.8200	C7—H7B	0.9600
O2—C2	1.364 (2)	C7—H7C	0.9600
O2—C7	1.419 (2)	C8—H8A	0.9600
O3—C6	1.3702 (19)	C8—H8B	0.9600
O3—C8	1.399 (2)	C8—H8C	0.9600
O4—C10	1.2320 (18)	C9—H9	0.9300
N1—C13	1.328 (2)	C10—C11	1.496 (2)
N1—C14	1.332 (2)	C11—C15	1.383 (2)
N2—C9	1.272 (2)	C11—C12	1.385 (2)
N2—N3	1.3850 (17)	C12—C13	1.376 (2)
N3—C10	1.336 (2)	C12—H12	0.9300
N3—H2	0.8600	C13—H13	0.9300
C1—C2	1.393 (2)	C14—C15	1.378 (2)
C1—C6	1.394 (2)	C14—H14	0.9300
C2—C3	1.382 (2)	C15—H15	0.9300
C3—C4	1.390 (2)	O5—O6	0.980 (7)
C3—H3	0.9300	O5—H5E	0.8928
C4—C5	1.395 (2)	O5—H5F	0.8450
C4—C9	1.458 (2)	O6—H5E	1.2560
C5—C6	1.382 (2)	O6—H5F	0.8864
C5—H5	0.9300		
C1—O1—H1	109.5	O3—C8—H8B	109.5
C2—O2—C7	117.15 (14)	H8A—C8—H8B	109.5
C6—O3—C8	118.51 (14)	O3—C8—H8C	109.5
C13—N1—C14	116.41 (15)	H8A—C8—H8C	109.5
C9—N2—N3	115.16 (13)	H8B—C8—H8C	109.5
C10—N3—N2	119.27 (12)	N2—C9—C4	122.51 (14)
C10—N3—H2	120.4	N2—C9—H9	118.7
N2—N3—H2	120.4	C4—C9—H9	118.7
O1—C1—C2	118.38 (15)	O4—C10—N3	123.46 (14)
O1—C1—C6	122.54 (15)	O4—C10—C11	122.29 (15)
C2—C1—C6	119.09 (14)	N3—C10—C11	114.24 (13)
O2—C2—C3	124.92 (15)	C15—C11—C12	118.12 (15)
O2—C2—C1	115.11 (14)	C15—C11—C10	119.67 (14)
C3—C2—C1	119.97 (15)	C12—C11—C10	122.16 (15)
C2—C3—C4	120.64 (15)	C13—C12—C11	118.50 (16)
C2—C3—H3	119.7	C13—C12—H12	120.7
C4—C3—H3	119.7	C11—C12—H12	120.7
C3—C4—C5	119.80 (15)	N1—C13—C12	124.24 (17)
C3—C4—C9	118.05 (14)	N1—C13—H13	117.9
C5—C4—C9	122.14 (15)	C12—C13—H13	117.9
C6—C5—C4	119.26 (16)	N1—C14—C15	124.00 (18)
C6—C5—H5	120.4	N1—C14—H14	118.0
C4—C5—H5	120.4	C15—C14—H14	118.0
O3—C6—C5	125.26 (16)	C14—C15—C11	118.61 (16)

O3—C6—C1	113.51 (14)	C14—C15—H15	120.7
C5—C6—C1	121.23 (15)	C11—C15—H15	120.7
O2—C7—H7A	109.5	O6—O5—H5E	84.1
O2—C7—H7B	109.5	O6—O5—H5F	57.6
H7A—C7—H7B	109.5	H5E—O5—H5F	100.1
O2—C7—H7C	109.5	O5—O6—H5E	45.0
H7A—C7—H7C	109.5	O5—O6—H5F	53.6
H7B—C7—H7C	109.5	H5E—O6—H5F	74.7
O3—C8—H8A	109.5		
C9—N2—N3—C10	178.29 (14)	O1—C1—C6—C5	−179.87 (16)
C7—O2—C2—C3	−2.6 (3)	C2—C1—C6—C5	0.4 (3)
C7—O2—C2—C1	176.74 (18)	N3—N2—C9—C4	−177.34 (14)
O1—C1—C2—O2	1.2 (2)	C3—C4—C9—N2	178.17 (16)
C6—C1—C2—O2	−179.01 (16)	C5—C4—C9—N2	−1.3 (3)
O1—C1—C2—C3	−179.40 (16)	N2—N3—C10—O4	4.2 (2)
C6—C1—C2—C3	0.4 (3)	N2—N3—C10—C11	−174.95 (13)
O2—C2—C3—C4	178.54 (16)	O4—C10—C11—C15	−48.3 (2)
C1—C2—C3—C4	−0.8 (3)	N3—C10—C11—C15	130.87 (16)
C2—C3—C4—C5	0.5 (3)	O4—C10—C11—C12	134.61 (18)
C2—C3—C4—C9	−179.00 (15)	N3—C10—C11—C12	−46.3 (2)
C3—C4—C5—C6	0.3 (3)	C15—C11—C12—C13	−1.5 (2)
C9—C4—C5—C6	179.72 (16)	C10—C11—C12—C13	175.68 (15)
C8—O3—C6—C5	−4.5 (3)	C14—N1—C13—C12	3.3 (3)
C8—O3—C6—C1	175.31 (18)	C11—C12—C13—N1	−1.8 (3)
C4—C5—C6—O3	179.13 (17)	C13—N1—C14—C15	−1.7 (3)
C4—C5—C6—C1	−0.7 (3)	N1—C14—C15—C11	−1.3 (3)
O1—C1—C6—O3	0.3 (3)	C12—C11—C15—C14	2.9 (3)
C2—C1—C6—O3	−179.48 (16)	C10—C11—C15—C14	−174.33 (16)

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯O6[i]	0.82	1.89	2.579 (6)	142
O1—H1⋯O5[i]	0.82	1.99	2.732 (2)	151
O1—H1⋯O3	0.82	2.24	2.6690 (18)	113
N3—H2⋯O4[ii]	0.86	2.17	3.0214 (17)	171
N3—H2⋯N2[ii]	0.86	2.69	3.1923 (18)	119
O5—H5E⋯N1[iii]	0.89	2.00	2.874 (2)	166
O5—H5F⋯O6[iv]	0.85	2.14	2.963 (6)	165
O5—H5F⋯O5[iv]	0.85	2.61	3.449 (5)	174

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

Fig. 1

Fig. 2