

4-(4-Nitrobenzenesulfonamido)-pyridinium trifluoroacetate

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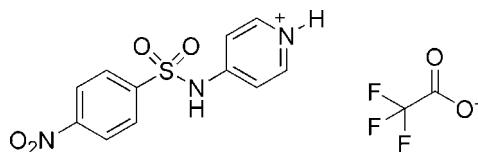
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Key indicators: single-crystal X-ray study; $T = 294\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$; disorder in solvent or counterion; R factor = 0.065; wR factor = 0.151; data-to-parameter ratio = 10.3.

In the title compound, $\text{C}_{11}\text{H}_{10}\text{N}_3\text{O}_4\text{S}^+\cdot\text{C}_2\text{F}_3\text{O}_2^-$, the benzene ring makes an angle of $87.3(2)^\circ$ with the pyridinium ring. The nitro group is essentially coplanar with the benzene ring. The F atoms of the CF_3 group are disordered over two positions with almost equal occupancy [0.531(12)/0.469(12)]. The crystal structure is stabilized by $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For studies of supramolecular chemistry involving pyridinium rings, see: Li *et al.* (2007). For 4-nitro-*N*-(4-pyridyl)benzenesulfonamide, see: Yu & Li (2007). For its salt form, see: Zhou *et al.* (2008).



Experimental

Crystal data

$\text{C}_{11}\text{H}_{10}\text{N}_3\text{O}_4\text{S}^+\cdot\text{C}_2\text{F}_3\text{O}_2^-$

$M_r = 393.30$

Monoclinic, $P2_1/c$
 $a = 5.662(2)\text{ \AA}$
 $b = 17.497(7)\text{ \AA}$
 $c = 16.173(6)\text{ \AA}$
 $\beta = 96.595(7)^\circ$
 $V = 1591.5(11)\text{ \AA}^3$

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.28\text{ mm}^{-1}$
 $T = 294(2)\text{ K}$
 $0.10 \times 0.04 \times 0.04\text{ mm}$

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.973$, $T_{\max} = 0.989$

7696 measured reflections
2763 independent reflections
1596 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.067$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.150$
 $S = 1.05$
2763 reflections
269 parameters
43 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.40\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.33\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1A \cdots O6	0.899 (11)	1.812 (14)	2.706 (5)	173 (5)
N2—H2A \cdots O6 ⁱ	0.86 (5)	2.00 (5)	2.858 (5)	176 (5)
C2—H2 \cdots O5 ⁱ	0.93	2.52	3.343 (6)	148
C3—H3 \cdots O1 ⁱⁱ	0.93	2.56	3.406 (6)	151
C8—H8 \cdots O5 ⁱⁱⁱ	0.93	2.48	3.204 (6)	135
C10—H10 \cdots O3 ^{iv}	0.93	2.39	3.184 (6)	143

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2740).

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supplementary materials

Acta Cryst. (2008). E64, o1513 [doi:10.1107/S1600536808021405]

4-(4-Nitrobenzenesulfonamido)pyridinium trifluoroacetate

J.-S. Li, M.-L. Fan, W.-S. Li and W.-D. Liu

Comment

Organic pyridinium salts have been widely used in the construction of supramolecular architectures. As part of our ongoing studies of supramolecular chemistry involving the pyridinium rings (Li *et al.*, 2007), the structure of the title compound was determined by X-ray diffraction.

In the cations of the title compound the short C—N distance is indicative of the slight conjugation of the sulphonamide N with the pyridinium ring. The benzene ring forms an angle of 87.3 (2) $^{\circ}$ with the pyridinium ring. The nitro group is essentially coplanar with the benzene ring

The crystal packing is stabilized by N—H \cdots O and C—H \cdots O hydrogen bonds.

Experimental

4-Nitro-(*N*-pyridyl)benzenesulfonamide was prepared by the method of Yu & Li (2007). Crystals were obtained by evaporation of a trifluoroacetic acid solution of the amide.

Refinement

The N-bound H atoms were located in a difference map and their coordinates were refined. The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms. The constraint $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C and N})$ was applied. The N1—H1A distance was restrained at 0.90 (1) Å and C—F distances to 1.36 (1) Å. The instruction ISOR (tolerance 0.01) was applied to restrain the displacement ellipsoids of all F atoms to an isotropic behaviour. The CF₃ group was disordered with the occupancy of 0.531 (12):0.469 (12).

Figures

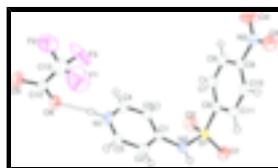
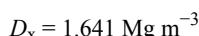
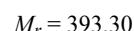
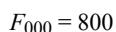


Fig. 1. A view of the title compound with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms). The dashed line indicates a hydrogen bond. Only the major component of the disordered CF₃ group is shown.

4-(4-Nitrobenzenesulfonamido)pyridinium trifluoroacetate

Crystal data



supplementary materials

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 5.662 (2) \text{ \AA}$	Cell parameters from 1671 reflections
$b = 17.497 (7) \text{ \AA}$	$\theta = 2.5\text{--}24.6^\circ$
$c = 16.173 (6) \text{ \AA}$	$\mu = 0.28 \text{ mm}^{-1}$
$\beta = 96.595 (7)^\circ$	$T = 294 (2) \text{ K}$
$V = 1591.5 (11) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.10 \times 0.04 \times 0.04 \text{ mm}$

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2763 independent reflections
Radiation source: fine-focus sealed tube	1596 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.067$
$T = 294(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
ω scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 6$
$T_{\text{min}} = 0.973, T_{\text{max}} = 0.989$	$k = -12 \rightarrow 20$
7696 measured reflections	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.065$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.150$	$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 1.2648P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2763 reflections	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
269 parameters	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$
43 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	1.1485 (2)	0.29446 (8)	0.83034 (7)	0.0340 (4)	
O1	1.1501 (6)	0.2461 (2)	0.90245 (19)	0.0469 (10)	
O2	1.3599 (5)	0.3060 (2)	0.7915 (2)	0.0466 (10)	
O3	0.6073 (7)	0.6017 (2)	0.9593 (2)	0.0536 (11)	
O4	0.8837 (7)	0.6574 (2)	0.9023 (3)	0.0648 (12)	
N1	0.7475 (8)	0.3207 (3)	0.5179 (2)	0.0418 (11)	
H1A	0.723 (8)	0.333 (3)	0.4637 (11)	0.050*	
N2	0.9372 (7)	0.2588 (3)	0.7627 (2)	0.0321 (10)	
H2A	0.853 (8)	0.229 (3)	0.790 (3)	0.039*	
N3	0.7809 (8)	0.6001 (3)	0.9208 (2)	0.0376 (11)	
C1	0.8800 (8)	0.2833 (3)	0.6816 (3)	0.0302 (12)	
C2	0.6688 (8)	0.2553 (3)	0.6379 (3)	0.0343 (12)	
H2	0.5692	0.2240	0.6648	0.041*	
C3	0.6093 (9)	0.2737 (3)	0.5565 (3)	0.0365 (13)	
H3	0.4718	0.2536	0.5276	0.044*	
C4	0.9464 (10)	0.3510 (3)	0.5585 (3)	0.0440 (14)	
H4	1.0385	0.3839	0.5304	0.053*	
C5	1.0155 (9)	0.3343 (3)	0.6397 (3)	0.0388 (13)	
H5	1.1515	0.3566	0.6673	0.047*	
C6	1.0399 (8)	0.3856 (3)	0.8545 (3)	0.0290 (11)	
C7	1.1511 (9)	0.4521 (3)	0.8325 (3)	0.0392 (13)	
H7	1.2837	0.4490	0.8036	0.047*	
C8	1.0671 (9)	0.5226 (3)	0.8528 (3)	0.0392 (13)	
H8	1.1409	0.5673	0.8382	0.047*	
C9	0.8688 (8)	0.5251 (3)	0.8959 (3)	0.0297 (11)	
C10	0.7523 (8)	0.4602 (3)	0.9186 (3)	0.0358 (12)	
H10	0.6186	0.4639	0.9468	0.043*	
C11	0.8397 (8)	0.3893 (3)	0.8981 (3)	0.0366 (13)	
H11	0.7663	0.3447	0.9132	0.044*	
C12	0.5532 (9)	0.3961 (3)	0.3109 (3)	0.0337 (12)	
O5	0.5106 (7)	0.4020 (2)	0.2352 (2)	0.0588 (12)	
O6	0.6749 (6)	0.3465 (2)	0.35187 (18)	0.0418 (9)	
C13	0.4492 (13)	0.4576 (4)	0.3613 (4)	0.075 (2)	
F1	0.320 (2)	0.4376 (10)	0.4198 (8)	0.117 (6)	0.531 (12)
F2	0.367 (2)	0.5185 (5)	0.3176 (6)	0.101 (4)	0.531 (12)
F3	0.6434 (17)	0.4927 (6)	0.4089 (7)	0.115 (5)	0.531 (12)
F1'	0.2000 (16)	0.4600 (8)	0.3372 (7)	0.110 (5)	0.469 (12)
F2'	0.512 (3)	0.5285 (6)	0.3520 (10)	0.116 (5)	0.469 (12)
F3'	0.430 (2)	0.4372 (9)	0.4392 (5)	0.080 (4)	0.469 (12)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0332 (7)	0.0405 (8)	0.0257 (6)	0.0051 (7)	-0.0073 (5)	0.0002 (6)
O1	0.059 (2)	0.046 (2)	0.0306 (19)	0.0025 (19)	-0.0152 (17)	0.0062 (17)
O2	0.0287 (18)	0.058 (3)	0.052 (2)	0.0050 (18)	0.0021 (16)	-0.010 (2)
O3	0.060 (2)	0.050 (3)	0.055 (2)	0.007 (2)	0.023 (2)	0.002 (2)
O4	0.073 (3)	0.033 (2)	0.091 (3)	-0.016 (2)	0.020 (2)	0.006 (2)
N1	0.058 (3)	0.047 (3)	0.020 (2)	0.004 (2)	0.001 (2)	0.004 (2)
N2	0.037 (2)	0.037 (3)	0.022 (2)	-0.006 (2)	0.0007 (17)	0.0050 (18)
N3	0.044 (3)	0.038 (3)	0.030 (2)	0.000 (2)	0.004 (2)	0.002 (2)
C1	0.040 (3)	0.029 (3)	0.021 (2)	0.002 (2)	0.003 (2)	-0.004 (2)
C2	0.037 (3)	0.038 (3)	0.027 (2)	-0.004 (3)	0.004 (2)	-0.002 (2)
C3	0.044 (3)	0.041 (3)	0.024 (2)	-0.003 (3)	-0.001 (2)	-0.001 (2)
C4	0.055 (3)	0.044 (4)	0.035 (3)	-0.006 (3)	0.012 (3)	0.007 (3)
C5	0.044 (3)	0.047 (4)	0.025 (3)	-0.005 (3)	0.000 (2)	-0.002 (2)
C6	0.028 (3)	0.033 (3)	0.024 (2)	-0.001 (2)	-0.005 (2)	0.001 (2)
C7	0.033 (3)	0.048 (4)	0.037 (3)	-0.004 (3)	0.009 (2)	-0.005 (3)
C8	0.044 (3)	0.042 (4)	0.033 (3)	-0.015 (3)	0.011 (2)	0.002 (3)
C9	0.033 (3)	0.033 (3)	0.023 (2)	-0.002 (2)	-0.002 (2)	0.000 (2)
C10	0.028 (3)	0.042 (4)	0.037 (3)	-0.005 (3)	0.007 (2)	-0.001 (3)
C11	0.039 (3)	0.033 (3)	0.038 (3)	-0.010 (3)	0.003 (2)	0.005 (3)
C12	0.044 (3)	0.034 (3)	0.024 (3)	-0.004 (3)	0.006 (2)	0.000 (2)
O5	0.083 (3)	0.067 (3)	0.026 (2)	0.015 (2)	0.0016 (19)	0.0039 (19)
O6	0.056 (2)	0.045 (2)	0.0227 (18)	0.0032 (19)	-0.0004 (16)	-0.0023 (17)
C13	0.107 (6)	0.071 (6)	0.045 (4)	0.018 (5)	0.006 (4)	0.001 (4)
F1	0.110 (9)	0.136 (9)	0.117 (9)	0.002 (7)	0.059 (7)	-0.026 (7)
F2	0.142 (8)	0.060 (6)	0.098 (6)	0.050 (6)	0.005 (6)	-0.013 (5)
F3	0.138 (8)	0.092 (7)	0.114 (7)	-0.003 (6)	0.008 (6)	-0.076 (6)
F1'	0.090 (7)	0.138 (9)	0.105 (7)	0.044 (6)	0.022 (5)	-0.024 (6)
F2'	0.131 (9)	0.079 (8)	0.142 (9)	-0.010 (7)	0.031 (7)	-0.018 (7)
F3'	0.093 (8)	0.097 (7)	0.053 (5)	0.027 (7)	0.023 (5)	-0.026 (5)

Geometric parameters (\AA , $^\circ$)

S1—O2	1.428 (3)	C6—C7	1.388 (7)
S1—O1	1.440 (3)	C6—C11	1.404 (6)
S1—N2	1.648 (4)	C7—C8	1.376 (7)
S1—C6	1.769 (5)	C7—H7	0.9300
O3—N3	1.222 (5)	C8—C9	1.388 (6)
O4—N3	1.213 (5)	C8—H8	0.9300
N1—C3	1.338 (6)	C9—C10	1.384 (6)
N1—C4	1.345 (6)	C10—C11	1.389 (7)
N1—H1A	0.899 (11)	C10—H10	0.9300
N2—C1	1.382 (5)	C11—H11	0.9300
N2—H2A	0.86 (5)	C12—O5	1.225 (5)
N3—C9	1.476 (6)	C12—O6	1.250 (5)
C1—C5	1.401 (7)	C12—C13	1.511 (8)

C1—C2	1.405 (6)	C13—F2'	1.303 (9)
C2—C3	1.359 (6)	C13—F1	1.309 (9)
C2—H2	0.9300	C13—F3'	1.326 (9)
C3—H3	0.9300	C13—F2	1.333 (8)
C4—C5	1.359 (7)	C13—F3	1.408 (8)
C4—H4	0.9300	C13—F1'	1.420 (8)
C5—H5	0.9300		
O2—S1—O1	120.8 (2)	C7—C8—C9	118.0 (5)
O2—S1—N2	110.0 (2)	C7—C8—H8	121.0
O1—S1—N2	104.6 (2)	C9—C8—H8	121.0
O2—S1—C6	107.4 (2)	C10—C9—C8	123.0 (5)
O1—S1—C6	108.7 (2)	C10—C9—N3	118.1 (4)
N2—S1—C6	104.1 (2)	C8—C9—N3	118.8 (5)
C3—N1—C4	121.0 (4)	C9—C10—C11	118.4 (4)
C3—N1—H1A	125 (3)	C9—C10—H10	120.8
C4—N1—H1A	114 (3)	C11—C10—H10	120.8
C1—N2—S1	125.8 (4)	C10—C11—C6	119.4 (5)
C1—N2—H2A	126 (3)	C10—C11—H11	120.3
S1—N2—H2A	107 (3)	C6—C11—H11	120.3
O4—N3—O3	122.9 (5)	O5—C12—O6	128.5 (5)
O4—N3—C9	118.7 (4)	O5—C12—C13	115.8 (5)
O3—N3—C9	118.4 (4)	O6—C12—C13	115.7 (4)
N2—C1—C5	125.1 (4)	F2'—C13—F1	121.4 (11)
N2—C1—C2	117.6 (4)	F2'—C13—F3'	114.8 (11)
C5—C1—C2	117.4 (4)	F1—C13—F3'	29.3 (8)
C3—C2—C1	120.5 (5)	F2'—C13—F2	42.4 (7)
C3—C2—H2	119.8	F1—C13—F2	114.0 (10)
C1—C2—H2	119.8	F3'—C13—F2	131.1 (9)
N1—C3—C2	120.3 (5)	F2'—C13—F3	56.1 (8)
N1—C3—H3	119.9	F1—C13—F3	100.8 (9)
C2—C3—H3	119.9	F3'—C13—F3	75.0 (8)
N1—C4—C5	121.3 (5)	F2—C13—F3	98.4 (9)
N1—C4—H4	119.4	F2'—C13—F1'	102.5 (10)
C5—C4—H4	119.4	F1—C13—F1'	65.5 (8)
C4—C5—C1	119.4 (5)	F3'—C13—F1'	94.7 (9)
C4—C5—H5	120.3	F2—C13—F1'	63.6 (7)
C1—C5—H5	120.3	F3—C13—F1'	145.7 (8)
C7—C6—C11	120.5 (5)	F2'—C13—C12	119.2 (8)
C7—C6—S1	121.3 (4)	F1—C13—C12	119.0 (9)
C11—C6—S1	118.2 (4)	F3'—C13—C12	113.6 (8)
C8—C7—C6	120.7 (5)	F2—C13—C12	114.7 (6)
C8—C7—H7	119.7	F3—C13—C12	106.1 (6)
C6—C7—H7	119.7	F1'—C13—C12	108.0 (6)
O2—S1—N2—C1	-44.4 (5)	C7—C8—C9—N3	178.0 (4)
O1—S1—N2—C1	-175.5 (4)	O4—N3—C9—C10	178.9 (4)
C6—S1—N2—C1	70.4 (4)	O3—N3—C9—C10	-1.0 (6)
S1—N2—C1—C5	10.6 (7)	O4—N3—C9—C8	0.5 (6)
S1—N2—C1—C2	-169.1 (4)	O3—N3—C9—C8	-179.4 (4)

supplementary materials

N2—C1—C2—C3	−176.2 (5)	C8—C9—C10—C11	0.8 (7)
C5—C1—C2—C3	4.1 (7)	N3—C9—C10—C11	−177.6 (4)
C4—N1—C3—C2	−0.4 (8)	C9—C10—C11—C6	−0.8 (7)
C1—C2—C3—N1	−2.1 (8)	C7—C6—C11—C10	0.5 (7)
C3—N1—C4—C5	0.7 (8)	S1—C6—C11—C10	179.4 (4)
N1—C4—C5—C1	1.5 (8)	O5—C12—C13—F2'	−60.9 (12)
N2—C1—C5—C4	176.6 (5)	O6—C12—C13—F2'	118.0 (11)
C2—C1—C5—C4	−3.8 (7)	O5—C12—C13—F1	126.9 (10)
O2—S1—C6—C7	2.8 (4)	O6—C12—C13—F1	−54.3 (12)
O1—S1—C6—C7	135.0 (4)	O5—C12—C13—F3'	159.0 (9)
N2—S1—C6—C7	−113.9 (4)	O6—C12—C13—F3'	−22.1 (11)
O2—S1—C6—C11	−176.1 (3)	O5—C12—C13—F2	−13.2 (11)
O1—S1—C6—C11	−43.8 (4)	O6—C12—C13—F2	165.7 (9)
N2—S1—C6—C11	67.2 (4)	O5—C12—C13—F3	−120.7 (7)
C11—C6—C7—C8	−0.1 (7)	O6—C12—C13—F3	58.2 (8)
S1—C6—C7—C8	−178.9 (4)	O5—C12—C13—F1'	55.4 (9)
C6—C7—C8—C9	0.0 (7)	O6—C12—C13—F1'	−125.8 (8)
C7—C8—C9—C10	−0.4 (7)		

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>
N1—H1A···O6	0.899 (11)	1.812 (14)	2.706 (5)	173 (5)
N2—H2A···O6 ⁱ	0.86 (5)	2.00 (5)	2.858 (5)	176 (5)
C2—H2···O5 ⁱ	0.93	2.52	3.343 (6)	148
C3—H3···O1 ⁱⁱ	0.93	2.56	3.406 (6)	151
C8—H8···O5 ⁱⁱⁱ	0.93	2.48	3.204 (6)	135
C10—H10···O3 ^{iv}	0.93	2.39	3.184 (6)	143

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

Fig. 1

