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4-(4-Nitrobenzenesulfonamido)-pyridinium trifluoroacetate

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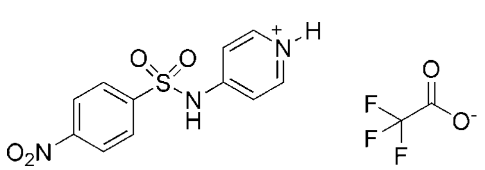
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in solvent or counterion; R factor = 0.065; wR factor = 0.151; data-to-parameter ratio = 10.3.

In the title compound, $C_{11}H_{10}N_3O_4S^+\cdot C_2F_3O_2^-$, the benzene ring makes an angle of 87.3 (2)° 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 N—H···O and C—H···O hydrogen bonds.

Related literature

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



Experimental

Crystal data

$C_{11}H_{10}N_3O_4S^+\cdot C_2F_3O_2^-$
M_r = 393.30
Monoclinic, $P2_1/c$
a = 5.662 (2) Å
b = 17.497 (7) Å
c = 16.173 (6) Å
β = 96.595 (7)°
V = 1591.5 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 294 (2) K
0.10 × 0.04 × 0.04 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_{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 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
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) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (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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4-(4-Nitrobenzenesulfonamido)pyridinium trifluoroacetate

Jiang-Sheng Li, Mei-Lian Fan, Wen-Sheng Li and Wei-Dong Liu

S1. 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)° with the pyridinium ring. The nitro group is essentially coplanar with the benzene ring

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

S2. 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.

S3. 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_{iso}(H) = 1.2 U_{eq}(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 bahaviour. The CF_3 group was disordered with the occupancy of 0.531 (12):0.469 (12).

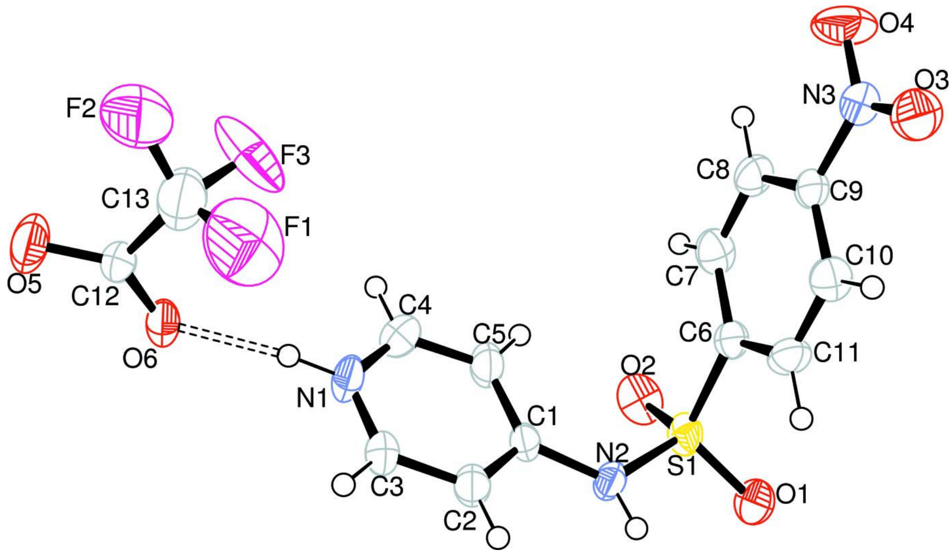

Figure 1

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 CF_3 group is shown.

4-(4-Nitrobenzenesulfonamido)pyridinium trifluoroacetate

Crystal data

$C_{11}H_{10}N_3O_4S^+ \cdot C_2F_3O_2^-$	$F(000) = 800$
$M_r = 393.30$	$D_x = 1.641$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1671 reflections
$a = 5.662$ (2) Å	$\theta = 2.5$–$24.6°$
$b = 17.497$ (7) Å	$\mu = 0.28$ mm^{-1}
$c = 16.173$ (6) Å	$T = 294$ K
$\beta = 96.595$ (7)°	Block, colourless
$V = 1591.5$ (11) Å^3	0.10 × 0.04 × 0.04 mm
$Z = 4$	

Data collection

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

Refinement

Refinement on F^2	43 restraints
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.065$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.150$	Hydrogen site location: inferred from neighbouring sites
$S = 1.05$	
2763 reflections	
269 parameters	

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 1.2648P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{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)

Atomic displacement parameters (Å^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 (Å, º)

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)
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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O6	0.90 (1)	1.81 (1)	2.706 (5)	173 (5)
N2—H2*A*···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.