



IUCrData

ISSN 2414-3146

2-Methyl-*N*-(pyrazin-2-yl)propanamide–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1)

Błażej Dziuk,^{a*} Borys Ośmiałowski,^b Bartosz Zarychta^a and Krzysztof Ejsmont^a

^aFaculty of Chemistry, University of Opole, Oleska 48, 45-052 Opole, Poland, and ^bFaculty of Chemical Technology and Engineering, University of Technology and Life Sciences, Seminaryjna 3, 85-326 Bydgoszcz, Poland. *Correspondence e-mail: bdziuk@uni.opole.pl

Received 16 September 2016

Accepted 16 September 2016

Edited by M. Bolte, Goethe-Universität Frankfurt Germany

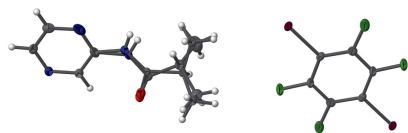
Keywords: 2-aminopyrazine; halogen bonds; disorder; crystal structure.

CCDC reference: 1504625

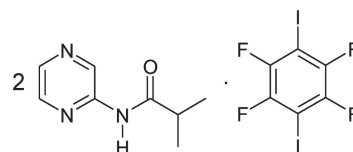
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_8H_{11}N_3O \cdot 0.5C_6F_4I_2$, molecules of ⁱPr-substituted pyrazine are co-crystallized with 1,4-diiodo-2,3,5,6-tetrafluorobenzene. The complete molecule of 1,4-diiodo-2,3,5,6-tetrafluorobenzene is generated by an inversion centre at the middle of the aromatic ring. Both molecules have normal geometry and the ⁱPr acylamine group is disordered over two sets of sites with an occupancy ratio of 0.51:0.49. In the crystal, the components are linked by $I \cdots N$ halogen bonds [2.830 (2) Å] and $C-H \cdots F$ interactions are observed.

3D view



Chemical scheme



Structure description

The aim of our study was to obtain a series of crystals in which halogen bonding is one of the stabilizing forces. It is known that steric effects can be a factor that tunes the type of doubly hydrogen-bonded dimers both in solution and in the solid state. This has previously been shown for 2-acylaminopyridines (Ośmiałowski *et al.*, 2010). Since steric effects may control the stability of the dimer, our intention was to check if the dimer carrying a middle-size group (ⁱPr) would be disturbed in the solid state. The same ⁱPr group in 2-acylaminopyridine allowed efficient dimerization, while adamantyl did not either in 2-acylaminopyridine (Ośmiałowski *et al.*, 2010) or in the analogous pyrazine (Dziuk *et al.*, 2016). In the present work, the ⁱPr substituted-pyrazine was co-crystallized with 1,4-diiodo-2,3,5,6-tetrafluorobenzene (Fig. 1).

The asymmetric unit comprises partially disordered 2-methyl-*N*-(pyrazin-2-yl)propanamide and a half-molecule of 1,2,4,5-tetrafluoro-3,6-diiodobenzene. The geometry of 2-methyl-*N*-(pyrazin-2-yl)propanamide is normal, and corresponds well with similar compounds (Ośmiałowski *et al.*, 2010; Aakeröy *et al.*, 2006; Dziuk *et al.*, 2016). The ⁱPr acylamine group is disordered. The atoms are split between two positions with occupancy factors of 0.49 and 0.51.

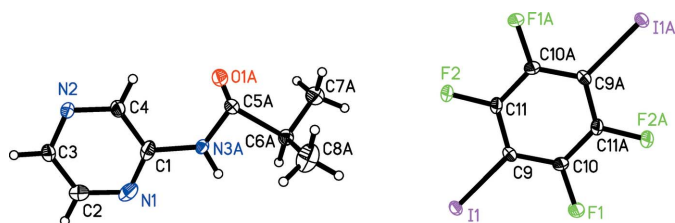


Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. For clarity, only one component of the disordered isopropylacetylamine group is shown.

In the crystal, $I1 \cdots N2^i$ [2.830 (2) Å; symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$] halogen-bonding interactions connect the molecules into two $C_8H_{11}N_3OC_6F_4I_2$ units arranged in a herringbone packing agreement (Fig. 2). The units are connected through $C-H \cdots F$ contacts (Table 1), forming infinite layers. The estimated distance between adjacent layers is 3.636 Å. The 2,2-dimethyl-*N*-(pyrazin-2-yl)acetamide molecules are connected by $N-H \cdots O$ hydrogen bonds (Table 1).

Synthesis and crystallization

The parent pyrazine was obtained using a reported procedure by reaction of 2-aminopyrazine with isobutyryl chloride (Dziuk *et al.*, 2016) in the presence of triethylamine. The co-crystallization was performed by mixing a 1:1 molar ratio of the studied compounds in chloroform followed by slow evaporation of the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The isopropylacetylamine group is disordered over two positions. Refinement of the site-occupation factors lead to a ratio of 0.509 (7)/0.491 (7). Since they correlate with the displacement parameters, they were fixed at 0.51 and 0.49. The displacement parameters of the disordered atoms were restrained to be equal to those of the atoms to

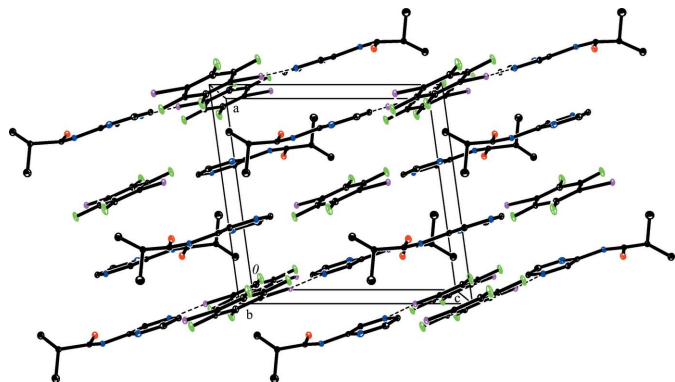


Figure 2

The crystal packing of the title compound, viewed along the *b* axis.

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C2—H2A $\cdots$ F2 ⁱ	0.93	2.46	3.388 (3)	178
C4—H4A $\cdots$ O1A	0.93	2.29	2.831 (5)	116
C4—H4A $\cdots$ O1B	0.93	2.21	2.867 (5)	127
C6A—H6AA $\cdots$ I1 ⁱⁱ	0.98	3.24	4.035 (5)	140
N3A—H3AA $\cdots$ O1A ⁱ	0.86	2.85	3.681 (6)	164
N3B—H3BA $\cdots$ O1B ⁱ	0.86	2.13	2.976 (6)	170

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Table 2

Experimental details.

Crystal data	
Chemical formula	$C_8H_{11}N_3O \cdot 0.5C_6F_4I_2$
M_r	366.13
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.6503 (2), 10.6112 (2), 11.2086 (2)
β (°)	97.857 (2)
<i>V</i> (Å ³)	1254.82 (4)
<i>Z</i>	4
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	2.57
Crystal size (mm)	0.03 × 0.02 × 0.01
Data collection	
Diffractometer	Oxford Diffraction Xcalibur
Absorption correction	Multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2008)
T_{min} , T_{max}	0.912, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7645, 2209, 2073
R_{int}	0.011
$(\sin \theta/\lambda)_{max}$ (Å ^{−1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.015, 0.036, 1.02
No. of reflections	2209
No. of parameters	217
No. of restraints	256
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ^{−3})	0.63, −0.34

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2008), *SHELXS2013* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2013* (Sheldrick, 2015).

which they are bonded and they were restrained to an isotropic behaviour.

References

- Aakeröy, C. B., Hussain, I. & Desper, J. (2006). *Cryst. Growth Des.* **6**, 474–480.
- Dziuk, B., Ośmiałowski, B., Ejsmont, K. & Zarychta, B. (2016). *IUCrData*, **1**, x161258.
- Ośmiałowski, B., Kolehmainen, E., Dobosz, R., Gawinecki, R., Kauppinen, R., Valkonen, A., Koivukorpi, J. & Rissanen, K. (2010). *J. Phys. Chem. A*, **114**, 10421–10426.
- Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst. C* **71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x161466 [doi:10.1107/S2414314616014668]

2-Methyl-*N*-(pyrazin-2-yl)propanamide–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1)

Błażej Dziuk, Borys Ośmiałowski, Bartosz Zarychta and Krzysztof Ejsmont

2-Methyl-*N*-(pyrazin-2-yl)propanamide–1,2,4,5-tetrafluoro-3,6-diiodobenzene (2/1)

Crystal data

$\text{C}_8\text{H}_{11}\text{N}_3\text{O} \cdot 0.5\text{C}_6\text{F}_4\text{I}_2$

$M_r = 366.13$

Monoclinic, $P2_1/n$

$a = 10.6503$ (2) Å

$b = 10.6112$ (2) Å

$c = 11.2086$ (2) Å

$\beta = 97.857$ (2)°

$V = 1254.82$ (4) Å³

$Z = 4$

$F(000) = 708$

$D_x = 1.938$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7645 reflections

$\theta = 3.1\text{--}25.0^\circ$

$\mu = 2.57$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.03 \times 0.02 \times 0.01$ mm

Data collection

Oxford Diffraction Xcalibur
diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 1024 x 1024 with blocks 2
x 2 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(CrysAlis RED; Oxford Diffraction, 2008)

$T_{\min} = 0.912$, $T_{\max} = 1.000$

7645 measured reflections

2209 independent reflections

2073 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.011$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -12 \rightarrow 9$

$k = -12 \rightarrow 12$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.015$

$wR(F^2) = 0.036$

$S = 1.02$

2209 reflections

217 parameters

256 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0188P)^2 + 1.2735P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.63$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
I1	0.94381 (2)	0.23915 (2)	0.78247 (2)	0.01620 (6)	
F1	1.07201 (16)	0.23859 (11)	1.06151 (12)	0.0363 (4)	
F2	0.89029 (14)	−0.05718 (12)	0.77398 (11)	0.0293 (3)	
N1	0.66750 (18)	0.17037 (18)	−0.00151 (18)	0.0265 (4)	
N2	0.61307 (16)	−0.05394 (16)	−0.12506 (15)	0.0179 (4)	
C1	0.6789 (2)	0.0598 (2)	0.05489 (19)	0.0227 (5)	
C2	0.6296 (2)	0.1675 (2)	−0.1196 (2)	0.0240 (5)	
H2A	0.6214	0.2432	−0.1618	0.029*	
C3	0.60207 (19)	0.05664 (19)	−0.18178 (19)	0.0190 (4)	
H3A	0.5755	0.0591	−0.2643	0.023*	
C4	0.6516 (2)	−0.0536 (2)	−0.00667 (18)	0.0204 (4)	
H4A	0.6604	−0.1294	0.0352	0.024*	
N3A	0.7268 (4)	0.0522 (4)	0.1841 (4)	0.0145 (10)	0.51
H3AA	0.7500	0.1233	0.2169	0.017*	0.51
O1A	0.7017 (4)	−0.1154 (5)	0.2410 (4)	0.0215 (10)	0.51
C5A	0.7410 (5)	−0.0491 (6)	0.2620 (4)	0.0156 (10)	0.51
C6A	0.7550 (4)	0.0511 (4)	0.3894 (4)	0.0182 (8)	0.51
H6AA	0.7166	0.1344	0.3734	0.022*	0.51
C7A	0.6945 (8)	−0.0258 (8)	0.4767 (9)	0.028 (2)	0.51
H7AA	0.6988	0.0188	0.5517	0.042*	0.51
H7AB	0.7383	−0.1047	0.4897	0.042*	0.51
H7AC	0.6074	−0.0410	0.4452	0.042*	0.51
C8A	0.8965 (5)	0.0535 (6)	0.4199 (5)	0.0451 (13)	0.51
H8AA	0.9196	0.1040	0.4905	0.068*	0.51
H8AB	0.9332	0.0888	0.3538	0.068*	0.51
H8AC	0.9274	−0.0308	0.4349	0.068*	0.51
N3B	0.7097 (4)	0.0885 (4)	0.1731 (4)	0.0140 (11)	0.49
H3BA	0.7229	0.1661	0.1934	0.017*	0.49
O1B	0.7231 (4)	−0.1556 (4)	0.2297 (4)	0.0187 (10)	0.49
C5B	0.7207 (4)	−0.0021 (5)	0.2620 (4)	0.0121 (10)	0.49
C6B	0.7841 (4)	−0.0153 (4)	0.3948 (4)	0.0140 (8)	0.49
H6BA	0.8511	−0.0793	0.4058	0.017*	0.49
C7B	0.6716 (7)	−0.0435 (8)	0.4675 (8)	0.0176 (16)	0.49
H7BA	0.7041	−0.0554	0.5510	0.026*	0.49
H7BB	0.6284	−0.1184	0.4366	0.026*	0.49
H7BC	0.6136	0.0262	0.4596	0.026*	0.49
C8B	0.8330 (4)	0.1179 (4)	0.4183 (4)	0.0203 (9)	0.49
H8BA	0.8771	0.1234	0.4988	0.030*	0.49
H8BB	0.7629	0.1756	0.4094	0.030*	0.49
H8BC	0.8898	0.1389	0.3618	0.030*	0.49
C9	0.97972 (18)	0.09653 (18)	0.91234 (17)	0.0146 (4)	
C10	1.0348 (2)	0.12112 (18)	1.02892 (18)	0.0188 (4)	
C11	0.94546 (19)	−0.02697 (19)	0.88570 (18)	0.0168 (4)	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02291 (8)	0.01364 (8)	0.01189 (8)	0.00054 (5)	0.00183 (5)	0.00207 (5)
F1	0.0709 (11)	0.0135 (6)	0.0202 (7)	−0.0117 (6)	−0.0093 (7)	0.0003 (5)
F2	0.0500 (8)	0.0209 (6)	0.0134 (6)	−0.0078 (6)	−0.0085 (6)	−0.0003 (5)
N1	0.0237 (10)	0.0266 (10)	0.0299 (11)	−0.0054 (8)	0.0066 (8)	−0.0123 (8)
N2	0.0209 (9)	0.0187 (9)	0.0141 (9)	−0.0022 (7)	0.0026 (7)	−0.0027 (7)
C1	0.0160 (10)	0.0363 (13)	0.0169 (11)	−0.0085 (9)	0.0063 (9)	−0.0085 (9)
C2	0.0229 (11)	0.0191 (11)	0.0303 (13)	−0.0013 (9)	0.0053 (9)	0.0004 (9)
C3	0.0201 (11)	0.0228 (11)	0.0145 (10)	0.0002 (8)	0.0044 (8)	0.0000 (8)
C4	0.0215 (11)	0.0249 (11)	0.0148 (11)	−0.0055 (9)	0.0028 (9)	0.0010 (8)
N3A	0.0159 (13)	0.0136 (13)	0.0136 (13)	0.0007 (9)	0.0003 (9)	−0.0022 (9)
O1A	0.0263 (17)	0.0198 (17)	0.0177 (15)	0.0012 (15)	0.0009 (13)	0.0009 (14)
C5A	0.0153 (13)	0.0164 (13)	0.0154 (13)	0.0006 (10)	0.0026 (9)	0.0017 (9)
C6A	0.0192 (12)	0.0183 (12)	0.0171 (11)	0.0010 (9)	0.0021 (9)	−0.0007 (9)
C7A	0.032 (3)	0.027 (3)	0.026 (3)	−0.0028 (18)	0.0053 (18)	0.0005 (16)
C8A	0.0382 (19)	0.057 (2)	0.039 (2)	−0.0001 (17)	0.0031 (16)	−0.0132 (16)
N3B	0.0150 (13)	0.0136 (13)	0.0131 (13)	0.0009 (9)	0.0005 (9)	−0.0006 (9)
O1B	0.0217 (16)	0.0184 (17)	0.0157 (15)	0.0061 (14)	0.0018 (12)	−0.0010 (13)
C5B	0.0118 (13)	0.0119 (13)	0.0127 (13)	−0.0011 (9)	0.0023 (9)	−0.0007 (9)
C6B	0.0146 (11)	0.0141 (11)	0.0129 (11)	−0.0001 (9)	0.0008 (9)	0.0002 (9)
C7B	0.018 (2)	0.023 (2)	0.013 (2)	−0.0051 (16)	0.0037 (16)	0.0014 (15)
C8B	0.0250 (16)	0.0171 (15)	0.0173 (16)	−0.0028 (14)	−0.0019 (14)	0.0003 (13)
C9	0.0166 (10)	0.0144 (10)	0.0131 (10)	0.0022 (8)	0.0034 (8)	0.0028 (7)
C10	0.0263 (11)	0.0118 (9)	0.0180 (11)	−0.0025 (8)	0.0014 (9)	−0.0015 (8)
C11	0.0204 (11)	0.0187 (10)	0.0106 (10)	−0.0004 (8)	−0.0006 (8)	−0.0013 (8)

Geometric parameters ($\text{\AA}$, $^\circ$)

I1—C9	2.0983 (19)	C7A—H7AB	0.9600
F1—C10	1.343 (2)	C7A—H7AC	0.9600
F2—C11	1.347 (2)	C8A—H8AA	0.9600
N1—C2	1.330 (3)	C8A—H8AB	0.9600
N1—C1	1.330 (3)	C8A—H8AC	0.9600
N2—C3	1.332 (3)	N3B—C5B	1.378 (7)
N2—C4	1.334 (3)	N3B—H3BA	0.8600
C1—N3B	1.356 (5)	O1B—C5B	1.670 (6)
C1—C4	1.398 (3)	C5B—C6B	1.554 (6)
C1—N3A	1.471 (5)	C6B—C8B	1.517 (6)
C2—C3	1.379 (3)	C6B—C7B	1.567 (9)
C2—H2A	0.9300	C6B—H6BA	0.9800
C3—H3A	0.9300	C7B—H7BA	0.9600
C4—H4A	0.9300	C7B—H7BB	0.9600
N3A—C5A	1.380 (7)	C7B—H7BC	0.9600
N3A—H3AA	0.8600	C8B—H8BA	0.9600
O1A—C5A	0.836 (6)	C8B—H8BB	0.9600
C5A—C6A	1.770 (7)	C8B—H8BC	0.9600

C6A—C7A	1.487 (10)	C9—C11	1.382 (3)
C6A—C8A	1.500 (7)	C9—C10	1.382 (3)
C6A—H6AA	0.9800	C10—C11 ⁱ	1.379 (3)
C7A—H7AA	0.9600	C11—C10 ⁱ	1.379 (3)
C2—N1—C1	116.62 (19)	C6A—C8A—H8AC	109.5
C3—N2—C4	117.87 (18)	H8AA—C8A—H8AC	109.5
N1—C1—N3B	105.1 (3)	H8AB—C8A—H8AC	109.5
N1—C1—C4	121.70 (19)	C1—N3B—C5B	122.3 (4)
N3B—C1—C4	133.0 (3)	C1—N3B—H3BA	118.8
N1—C1—N3A	120.9 (2)	C5B—N3B—H3BA	118.8
C4—C1—N3A	117.4 (3)	N3B—C5B—C6B	137.6 (4)
N1—C2—C3	122.5 (2)	N3B—C5B—O1B	121.8 (4)
N1—C2—H2A	118.7	C6B—C5B—O1B	95.8 (4)
C3—C2—H2A	118.7	C8B—C6B—C5B	100.2 (3)
N2—C3—C2	120.77 (19)	C8B—C6B—C7B	110.8 (5)
N2—C3—H3A	119.6	C5B—C6B—C7B	104.6 (4)
C2—C3—H3A	119.6	C8B—C6B—H6BA	113.4
N2—C4—C1	120.5 (2)	C5B—C6B—H6BA	113.4
N2—C4—H4A	119.7	C7B—C6B—H6BA	113.4
C1—C4—H4A	119.7	C6B—C7B—H7BA	109.5
C5A—N3A—C1	131.2 (4)	C6B—C7B—H7BB	109.5
C5A—N3A—H3AA	114.4	H7BA—C7B—H7BB	109.5
C1—N3A—H3AA	114.4	C6B—C7B—H7BC	109.5
O1A—C5A—N3A	118.0 (6)	H7BA—C7B—H7BC	109.5
O1A—C5A—C6A	135.7 (6)	H7BB—C7B—H7BC	109.5
N3A—C5A—C6A	91.8 (4)	C6B—C8B—H8BA	109.5
C7A—C6A—C8A	111.8 (5)	C6B—C8B—H8BB	109.5
C7A—C6A—C5A	101.9 (5)	H8BA—C8B—H8BB	109.5
C8A—C6A—C5A	99.5 (4)	C6B—C8B—H8BC	109.5
C7A—C6A—H6AA	114.1	H8BA—C8B—H8BC	109.5
C8A—C6A—H6AA	114.1	H8BB—C8B—H8BC	109.5
C5A—C6A—H6AA	114.1	C11—C9—C10	116.65 (18)
C6A—C7A—H7AA	109.5	C11—C9—I1	121.09 (14)
C6A—C7A—H7AB	109.5	C10—C9—I1	122.23 (15)
H7AA—C7A—H7AB	109.5	F1—C10—C11 ⁱ	118.16 (18)
C6A—C7A—H7AC	109.5	F1—C10—C9	120.23 (18)
H7AA—C7A—H7AC	109.5	C11 ⁱ —C10—C9	121.60 (19)
H7AB—C7A—H7AC	109.5	F2—C11—C10 ⁱ	118.57 (18)
C6A—C8A—H8AA	109.5	F2—C11—C9	119.68 (17)
C6A—C8A—H8AB	109.5	C10 ⁱ —C11—C9	121.75 (18)
H8AA—C8A—H8AB	109.5		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2A $\cdots$ F2 ⁱⁱ	0.93	2.46	3.388 (3)	178

C4—H4 <i>A</i> ...O1 <i>A</i>	0.93	2.29	2.831 (5)	116
C4—H4 <i>A</i> ...O1 <i>B</i>	0.93	2.21	2.867 (5)	127
C6 <i>A</i> —H6 <i>AA</i> ...I1 ⁱⁱⁱ	0.98	3.24	4.035 (5)	140
N3 <i>A</i> —H3 <i>AA</i> ...O1 <i>A</i> ⁱⁱ	0.86	2.85	3.681 (6)	164
N3 <i>B</i> —H3 <i>BA</i> ...O1 <i>B</i> ⁱⁱ	0.86	2.13	2.976 (6)	170

Symmetry codes: (ii) $-x+3/2, y+1/2, -z+1/2$; (iii) $x-1/2, -y+1/2, z-1/2$.