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1,2,4,5-Tetrafluoro-3,6-diiodobenzene–2,3-bis(pyridin-2-yl)pyrazine (1/1)

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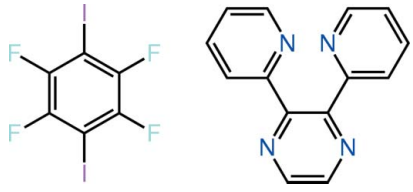
Key indicators: single-crystal X-ray study; T = 98 K; mean σ(C–C) = 0.007 Å; R factor = 0.039; wR factor = 0.109; data-to-parameter ratio = 13.9.

The components of the title 1:1 co-crystal, $C_{14}H_{10}N_4{\cdot}C_6F_4I_2$, are connected *via* an N$\cdots$I [2.959 (4) Å] halogen bond, in which the N atom is part of the relatively electron-rich pyrazine ring. The $C_6F_4I_2$ molecule is almost planar [r.m.s. deviation = 0.038 Å] but there are significant twists in the pyrazine derivative, as seen in the dihedral angles [31.3 (2) and 54.6 (2)°] formed between the pendant pyridyl rings and the central pyrazine ring. The bimolecular aggregates are sustained in the crystal by C—H$\cdots$F and π–π interactions [ring centroid(pyridyl)–ring centroid(benzene) = 3.678 (3) Å].

Related literature

For related studies on co-crystal formation, see: Broker & Tiekink (2007); Broker *et al.* (2008); Arman *et al.* (2010). For background to halogen bonding, see: Metrangolo *et al.* (2008); Pennington *et al.* (2008).



Experimental

Crystal data

$C_{14}H_{10}N_4{\cdot}C_6F_4I_2$ M_r = 636.04
Triclinic, $P\overline{1}$
a = 6.3997 (15) Å
b = 10.737 (2) Å
c = 15.092 (4) Å
α = 74.237 (10)°
β = 85.877 (11)°
γ = 80.283 (12)°
V = 983.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.25 mm^{-1}
T = 98 K
0.40 × 0.13 × 0.07 mm

Data collection

Rigaku AFC12/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.504, T_{max} = 1.000
5074 measured reflections
3775 independent reflections
3550 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.09
3775 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −1.20 e Å^{-3}

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots$F4	0.95	2.54	3.145 (6)	121
C9—H9$\cdots$F4	0.95	2.46	3.100 (6)	125
C18—H18$\cdots$F2^{i}	0.95	2.52	3.341 (7)	144

Symmetry code: (i) $x+1, y+1, z-1$.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5683).

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supporting information

Acta Cryst. (2010). E**66**, o2885 [https://doi.org/10.1107/S1600536810041668]

1,2,4,5-Tetrafluoro-3,6-diiodobenzene–2,3-bis(pyridin-2-yl)pyrazine (1/1)

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S1. Comment

The title co-crystal was prepared during on-going studies investigating co-crystals with pyridine-type molecules (Broker & Tiekink, 2007; Broker *et al.*, 2008) including halogen bonding (Arman *et al.*, 2010). The co-crystallization experiment whereby equimolar amounts of 1,2,4,5-tetrafluoro-3,6-diiodobenzene and 2,3-bis(pyridin-2-yl)pyrazine were dissolved in methylene chloride resulted in the isolation of the title 1/1 co-crystal, (I).

The molecule of 1,2,4,5-tetrafluoro-3,6-diiodobenzene, Fig. 1, is flat with the r.m.s. deviation of the 12 constituent atoms being 0.038 Å [maximum deviation = 0.084 (1) Å for atom I2]. In the molecule of 2,3-bis(pyridin-2-yl)pyrazine, Fig. 2, the N3- and N4-pyridyl rings form dihedral angles of 31.3 (2) and 54.6 (2) ° with the pyrazine ring; the dihedral angle formed between the pyridyl rings = 60.2 (2) °.

The primary connection between the constituent molecules of (I) is a N2···I2 contact of 2.959 (4) Å, representing an halogen bond (Metrangolo *et al.*, 2008; Pennington *et al.*, 2008). Of note is the observation that the interaction involves a pyrazine-N rather than a pyridine-N, consistent with the N in the pyrazine ring being more electron rich. The molecules are stabilized in the crystal packing *via* a combination of C—H···F [the F4 atom is bifurcated], Table 1, and π···π interactions [ring centroid(N3,C11–C15)···ring centroid(C1–C6)^{i} = 3.678 (3) Å for *i*: 1 - *x*, 1 - *y*, 1 - *z*], Fig. 3.

S2. Experimental

Initially 1,2,4,5-tetrafluoro-3,6-diiodobenzene (Aldrich, 0.09 mmol) and 2,3-bis(pyridin-2-yl)pyrazine (Aldrich, 0.04 mmol) were dissolved in chloroform and after evaporation of the solvent, the powder was then dissolved in tetrahydrafuran (THF). Upon evaporation of THF, methylene chloride was added to the powder. Colourless prisms of (I) were formed after three days through slow evaporation of solvent, m. pt. 409–411 K.

S3. Refinement

C-bound H-atoms were placed in calculated positions (C–H 0.95 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{eq}(C). The maximum and minimum residual electron density peaks of 1.32 and 1.20 e Å^{-3}, respectively, were located 0.62 Å and 0.86 Å from the H13 and I1 atoms, respectively.

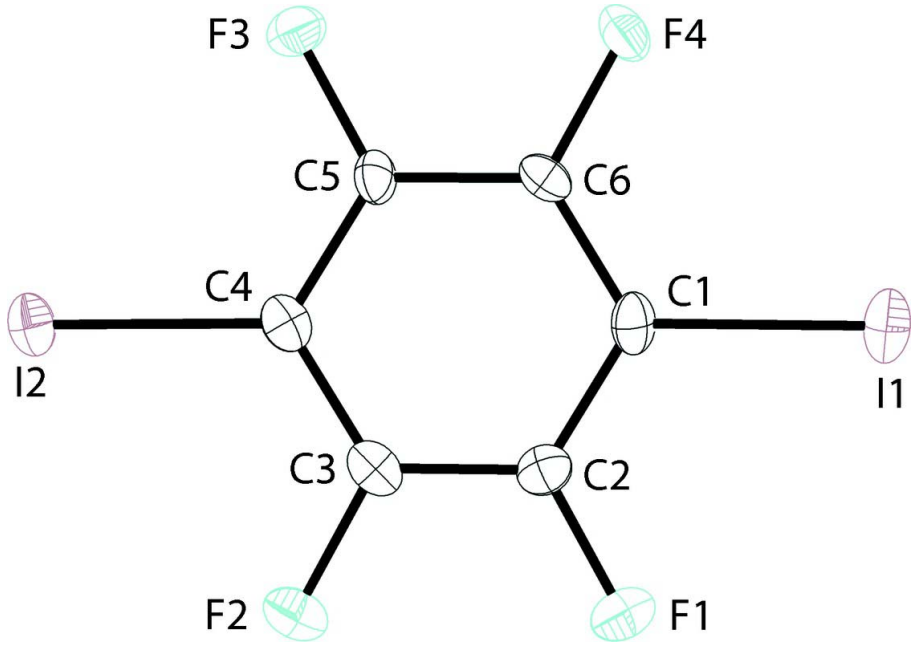

Figure 1

Molecular structure of 1,2,4,5-tetrafluoro-3,6-diiodobenzene found in the structure of (I) showing displacement ellipsoids at the 50% probability level

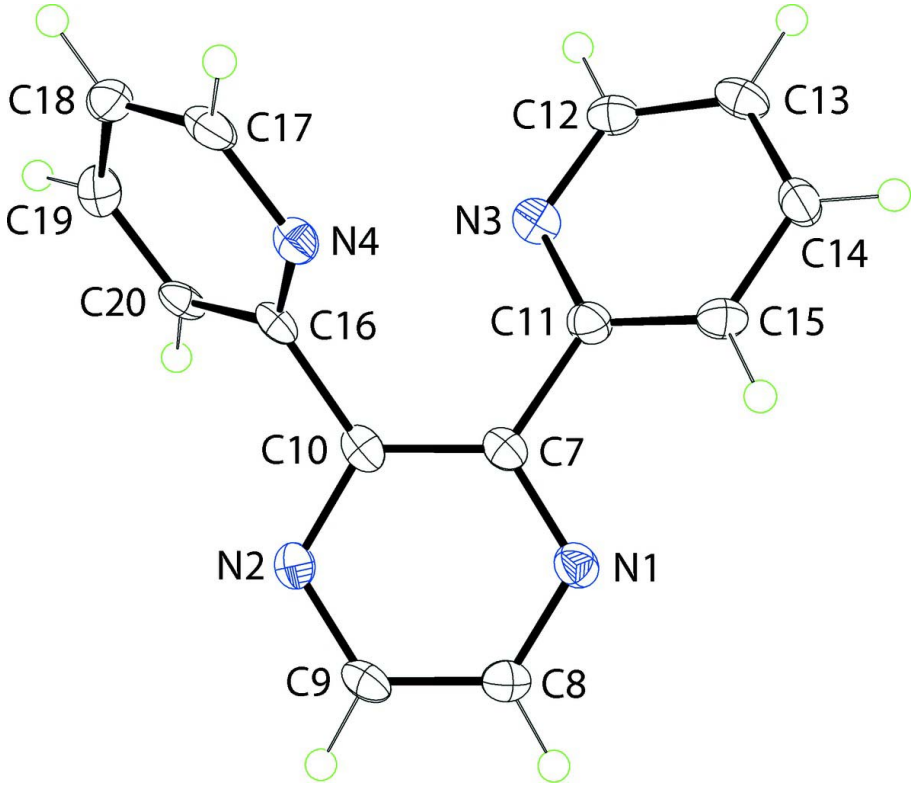

Figure 2

Molecular structure of 2,3-bis(pyridin-2-yl)pyrazine found in the structure of (I) showing displacement ellipsoids at the 50% probability level.

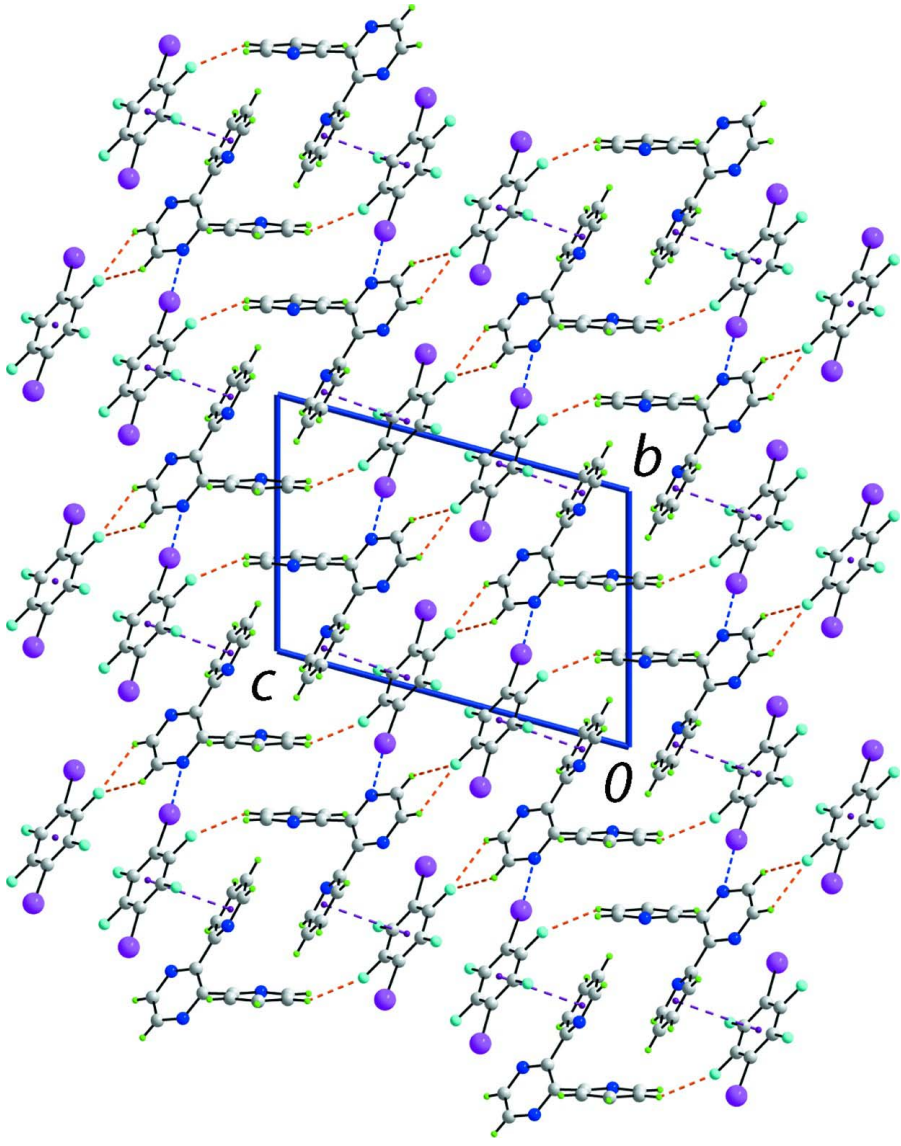

Figure 3

A view in projection down the *a* axis showing the unit-cell contents. The N···I, C—H···F and $\pi\cdots\pi$ interactions are shown as blue, orange and purple dashed lines, respectively.

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Hall symbol: -P 1
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$c = 15.092\ (4)$ Å
$\alpha = 74.237\ (10)°$
$\beta = 85.877\ (11)°$
$\gamma = 80.283\ (12)°$
$V = 983.3\ (4)$ Å^3
$Z = 2$
$F(000) = 600$
$D_x = 2.148$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2870 reflections
$\theta = 2.8–40.2°$
$\mu = 3.25$ mm^{-1}

T = 98 K
Prism, colourless

0.40 × 0.13 × 0.07 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.504, T_{max} = 1.000

5074 measured reflections
3775 independent reflections
3550 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°, θ_{min} = 2.7°
$h = -7 \rightarrow 7$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.09
3775 reflections
271 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 2.2885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −1.20 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
I1	0.02819 (5)	0.31600 (3)	0.57773 (2)	0.02562 (13)
I2	0.78603 (5)	−0.24672 (3)	0.69360 (2)	0.02055 (12)
F1	0.0119 (4)	0.0318 (3)	0.7123 (2)	0.0253 (6)
F2	0.2992 (5)	−0.1842 (3)	0.7543 (2)	0.0243 (6)
F3	0.7961 (5)	0.0349 (3)	0.5483 (2)	0.0237 (6)
F4	0.5096 (5)	0.2523 (3)	0.5082 (2)	0.0235 (6)
C1	0.2526 (8)	0.1487 (5)	0.6091 (3)	0.0187 (10)
C2	0.2048 (7)	0.0342 (5)	0.6718 (3)	0.0183 (9)
C3	0.3548 (8)	−0.0770 (5)	0.6931 (3)	0.0185 (9)
C4	0.5573 (8)	−0.0806 (5)	0.6541 (3)	0.0184 (9)
C5	0.6036 (7)	0.0330 (4)	0.5907 (3)	0.0168 (9)
C6	0.4545 (8)	0.1452 (5)	0.5692 (3)	0.0168 (9)
N1	0.4973 (6)	0.6357 (4)	0.3011 (3)	0.0207 (8)
N2	0.8530 (6)	0.4641 (4)	0.2683 (3)	0.0193 (8)

N3	0.7532 (6)	0.8733 (4)	0.1407 (3)	0.0208 (8)
N4	0.8477 (6)	0.6513 (4)	0.0459 (3)	0.0191 (8)
C7	0.6336 (8)	0.6725 (4)	0.2310 (3)	0.0181 (9)
C8	0.5401 (8)	0.5140 (5)	0.3545 (3)	0.0214 (10)
H8	0.4440	0.4842	0.4036	0.026*
C9	0.7207 (8)	0.4295 (4)	0.3405 (3)	0.0215 (10)
H9	0.7514	0.3457	0.3828	0.026*
C10	0.8064 (7)	0.5845 (4)	0.2107 (3)	0.0178 (9)
C11	0.5864 (8)	0.8134 (5)	0.1779 (3)	0.0205 (10)
C12	0.7097 (8)	1.0002 (5)	0.0970 (3)	0.0213 (10)
H12	0.8255	1.0442	0.0709	0.026*
C13	0.5087 (8)	1.0721 (5)	0.0870 (3)	0.0223 (10)
H13	0.4873	1.1624	0.0550	0.027*
C14	0.3393 (8)	1.0090 (5)	0.1249 (3)	0.0226 (10)
H14	0.1985	1.0552	0.1192	0.027*
C15	0.3776 (8)	0.8781 (5)	0.1710 (3)	0.0205 (10)
H15	0.2638	0.8327	0.1977	0.025*
C16	0.9470 (8)	0.6132 (4)	0.1261 (3)	0.0189 (9)
C17	0.9704 (9)	0.6689 (5)	−0.0306 (4)	0.0244 (10)
H17	0.9038	0.6948	−0.0884	0.029*
C18	1.1934 (8)	0.6509 (5)	−0.0298 (4)	0.0241 (10)
H18	1.2751	0.6654	−0.0857	0.029*
C19	1.2907 (8)	0.6117 (5)	0.0544 (4)	0.0242 (10)
H19	1.4409	0.5979	0.0573	0.029*
C20	1.1658 (7)	0.5928 (4)	0.1341 (3)	0.0191 (10)
H20	1.2281	0.5665	0.1929	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0227 (2)	0.0220 (2)	0.0325 (2)	0.00505 (13)	−0.00955 (14)	−0.01061 (15)
I2	0.02250 (19)	0.01648 (18)	0.02206 (19)	0.00093 (12)	−0.00667 (13)	−0.00489 (13)
F1	0.0179 (14)	0.0322 (16)	0.0267 (16)	−0.0065 (12)	0.0029 (12)	−0.0084 (13)
F2	0.0296 (15)	0.0220 (14)	0.0202 (15)	−0.0091 (12)	−0.0007 (12)	−0.0006 (12)
F3	0.0172 (13)	0.0283 (16)	0.0228 (15)	−0.0035 (12)	0.0027 (11)	−0.0031 (12)
F4	0.0250 (15)	0.0171 (14)	0.0234 (15)	−0.0021 (11)	−0.0037 (12)	0.0032 (11)
C1	0.017 (2)	0.018 (2)	0.021 (2)	0.0012 (18)	−0.0094 (18)	−0.0060 (19)
C2	0.018 (2)	0.021 (2)	0.018 (2)	−0.0044 (18)	0.0010 (18)	−0.0076 (18)
C3	0.025 (2)	0.016 (2)	0.015 (2)	−0.0054 (18)	−0.0046 (18)	−0.0036 (17)
C4	0.023 (2)	0.016 (2)	0.016 (2)	−0.0024 (18)	−0.0045 (18)	−0.0042 (18)
C5	0.017 (2)	0.016 (2)	0.015 (2)	0.0020 (17)	−0.0042 (17)	−0.0019 (17)
C6	0.022 (2)	0.015 (2)	0.012 (2)	−0.0050 (18)	−0.0021 (18)	−0.0007 (17)
N1	0.0182 (19)	0.0185 (19)	0.024 (2)	−0.0023 (15)	−0.0028 (16)	−0.0035 (16)
N2	0.0173 (19)	0.0190 (19)	0.021 (2)	−0.0005 (15)	−0.0022 (16)	−0.0060 (16)
N3	0.022 (2)	0.020 (2)	0.022 (2)	−0.0056 (16)	−0.0040 (16)	−0.0063 (16)
N4	0.024 (2)	0.0169 (19)	0.017 (2)	−0.0011 (15)	−0.0036 (16)	−0.0062 (15)
C7	0.022 (2)	0.016 (2)	0.016 (2)	−0.0019 (18)	−0.0047 (18)	−0.0044 (18)
C8	0.023 (2)	0.021 (2)	0.019 (2)	−0.0053 (19)	−0.0006 (19)	−0.0020 (18)

C9	0.030 (3)	0.012 (2)	0.022 (2)	−0.0043 (19)	−0.004 (2)	−0.0030 (18)
C10	0.022 (2)	0.015 (2)	0.018 (2)	−0.0013 (17)	−0.0074 (18)	−0.0069 (17)
C11	0.026 (2)	0.016 (2)	0.020 (2)	−0.0035 (18)	0.0012 (19)	−0.0052 (18)
C12	0.027 (2)	0.020 (2)	0.019 (2)	−0.0094 (19)	0.0001 (19)	−0.0038 (18)
C13	0.033 (3)	0.014 (2)	0.020 (2)	−0.0060 (19)	−0.006 (2)	−0.0026 (18)
C14	0.025 (2)	0.018 (2)	0.022 (2)	0.0032 (19)	−0.003 (2)	−0.0050 (19)
C15	0.022 (2)	0.020 (2)	0.020 (2)	−0.0082 (19)	−0.0005 (19)	−0.0024 (19)
C16	0.024 (2)	0.0089 (19)	0.023 (2)	−0.0007 (17)	−0.0031 (19)	−0.0027 (17)
C17	0.037 (3)	0.014 (2)	0.019 (2)	0.000 (2)	−0.006 (2)	−0.0005 (18)
C18	0.031 (3)	0.017 (2)	0.023 (3)	−0.0058 (19)	0.007 (2)	−0.0056 (19)
C19	0.021 (2)	0.023 (2)	0.029 (3)	−0.0014 (19)	−0.001 (2)	−0.009 (2)
C20	0.016 (2)	0.014 (2)	0.023 (2)	−0.0018 (17)	−0.0075 (18)	0.0032 (18)

Geometric parameters (Å, º)

I1—C1	2.068 (5)	C7—C11	1.497 (6)
I2—C4	2.085 (5)	C8—C9	1.385 (7)
F1—C2	1.339 (5)	C8—H8	0.9500
F2—C3	1.348 (5)	C9—H9	0.9500
F3—C5	1.348 (5)	C10—C16	1.500 (7)
F4—C6	1.346 (5)	C11—C15	1.395 (7)
C1—C6	1.385 (7)	C12—C13	1.380 (7)
C1—C2	1.398 (7)	C12—H12	0.9500
C2—C3	1.378 (7)	C13—C14	1.382 (7)
C3—C4	1.383 (7)	C13—H13	0.9500
C4—C5	1.392 (7)	C14—C15	1.377 (7)
C5—C6	1.382 (6)	C14—H14	0.9500
N1—C8	1.331 (6)	C15—H15	0.9500
N1—C7	1.340 (6)	C16—C20	1.389 (6)
N2—C9	1.340 (7)	C17—C18	1.408 (7)
N2—C10	1.345 (6)	C17—H17	0.9500
N3—C12	1.333 (6)	C18—C19	1.383 (7)
N3—C11	1.349 (6)	C18—H18	0.9500
N4—C16	1.338 (6)	C19—C20	1.383 (7)
N4—C17	1.337 (7)	C19—H19	0.9500
C7—C10	1.402 (7)	C20—H20	0.9500
C6—C1—C2	117.4 (4)	N2—C10—C16	115.6 (4)
C6—C1—I1	121.8 (4)	C7—C10—C16	124.4 (4)
C2—C1—I1	120.8 (4)	N3—C11—C15	122.8 (4)
F1—C2—C3	119.2 (4)	N3—C11—C7	117.1 (4)
F1—C2—C1	120.0 (4)	C15—C11—C7	120.1 (4)
C3—C2—C1	120.8 (4)	N3—C12—C13	124.7 (4)
F2—C3—C2	117.9 (4)	N3—C12—H12	117.6
F2—C3—C4	120.1 (4)	C13—C12—H12	117.6
C2—C3—C4	122.0 (4)	C14—C13—C12	118.1 (4)
C3—C4—C5	117.1 (4)	C14—C13—H13	121.0
C3—C4—I2	121.1 (4)	C12—C13—H13	121.0

C5—C4—I2	121.7 (4)	C13—C14—C15	119.0 (5)
F3—C5—C6	118.6 (4)	C13—C14—H14	120.5
F3—C5—C4	120.1 (4)	C15—C14—H14	120.5
C6—C5—C4	121.3 (4)	C14—C15—C11	118.9 (4)
F4—C6—C5	118.5 (4)	C14—C15—H15	120.5
F4—C6—C1	120.2 (4)	C11—C15—H15	120.5
C5—C6—C1	121.4 (4)	N4—C16—C20	124.3 (5)
C8—N1—C7	117.1 (4)	N4—C16—C10	115.5 (4)
C9—N2—C10	117.8 (4)	C20—C16—C10	120.0 (4)
C12—N3—C11	116.5 (4)	N4—C17—C18	123.3 (5)
C16—N4—C17	116.7 (4)	N4—C17—H17	118.4
N1—C7—C10	121.6 (4)	C18—C17—H17	118.4
N1—C7—C11	114.6 (4)	C19—C18—C17	118.4 (5)
C10—C7—C11	123.7 (4)	C19—C18—H18	120.8
N1—C8—C9	121.9 (4)	C17—C18—H18	120.8
N1—C8—H8	119.0	C18—C19—C20	118.9 (5)
C9—C8—H8	119.0	C18—C19—H19	120.5
N2—C9—C8	121.1 (4)	C20—C19—H19	120.5
N2—C9—H9	119.5	C16—C20—C19	118.3 (5)
C8—C9—H9	119.5	C16—C20—H20	120.8
N2—C10—C7	120.0 (4)	C19—C20—H20	120.8

C6—C1—C2—F1	−179.7 (4)	C9—N2—C10—C16	−174.1 (4)
I1—C1—C2—F1	0.1 (6)	N1—C7—C10—N2	−7.7 (7)
C6—C1—C2—C3	0.6 (7)	C11—C7—C10—N2	171.8 (4)
I1—C1—C2—C3	−179.6 (4)	N1—C7—C10—C16	171.1 (4)
F1—C2—C3—F2	0.1 (7)	C11—C7—C10—C16	−9.4 (7)
C1—C2—C3—F2	179.8 (4)	C12—N3—C11—C15	0.7 (7)
F1—C2—C3—C4	−179.6 (4)	C12—N3—C11—C7	−177.3 (4)
C1—C2—C3—C4	0.1 (7)	N1—C7—C11—N3	148.1 (4)
F2—C3—C4—C5	179.3 (4)	C10—C7—C11—N3	−31.5 (7)
C2—C3—C4—C5	−1.0 (7)	N1—C7—C11—C15	−29.9 (7)
F2—C3—C4—I2	−3.4 (6)	C10—C7—C11—C15	150.5 (5)
C2—C3—C4—I2	176.3 (4)	C11—N3—C12—C13	−0.5 (7)
C3—C4—C5—F3	−178.1 (4)	N3—C12—C13—C14	0.0 (8)
I2—C4—C5—F3	4.6 (6)	C12—C13—C14—C15	0.3 (7)
C3—C4—C5—C6	1.2 (7)	C13—C14—C15—C11	−0.1 (7)
I2—C4—C5—C6	−176.1 (3)	N3—C11—C15—C14	−0.4 (8)
F3—C5—C6—F4	−1.4 (6)	C7—C11—C15—C14	177.5 (5)
C4—C5—C6—F4	179.2 (4)	C17—N4—C16—C20	0.8 (7)
F3—C5—C6—C1	178.8 (4)	C17—N4—C16—C10	−175.5 (4)
C4—C5—C6—C1	−0.6 (7)	N2—C10—C16—N4	124.0 (4)
C2—C1—C6—F4	179.9 (4)	C7—C10—C16—N4	−54.8 (6)
I1—C1—C6—F4	0.0 (6)	N2—C10—C16—C20	−52.5 (6)
C2—C1—C6—C5	−0.3 (7)	C7—C10—C16—C20	128.7 (5)
I1—C1—C6—C5	179.9 (4)	C16—N4—C17—C18	−0.8 (7)
C8—N1—C7—C10	4.1 (7)	N4—C17—C18—C19	0.8 (7)
C8—N1—C7—C11	−175.5 (4)	C17—C18—C19—C20	−0.6 (7)

C7—N1—C8—C9	2.0 (7)	N4—C16—C20—C19	−0.6 (7)
C10—N2—C9—C8	1.1 (7)	C10—C16—C20—C19	175.5 (4)
N1—C8—C9—N2	−4.8 (8)	C18—C19—C20—C16	0.5 (7)
C9—N2—C10—C7	4.8 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···F4	0.95	2.54	3.145 (6)	121
C9—H9···F4	0.95	2.46	3.100 (6)	125
C18—H18···F2^{i}	0.95	2.52	3.341 (7)	144

Symmetry code: (i) $x+1, y+1, z-1$.