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3-Amino-1*H*-pyrazol-2-ium trifluoroacetate

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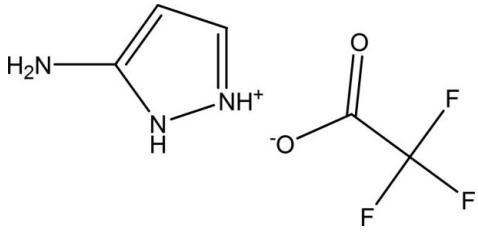
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 9.0.

The asymmetric unit of the title salt, $C_3H_6N_3^+\cdot C_2F_3O_2^-$, contains two independent 3-aminopyrazolium cations and two independent trifluoroacetate anions. The F atoms of both anions were refined as disordered over two sets of sites, with common occupancy ratios of 0.639 (12):0.361 (12). In the crystal, the cations and anions are linked *via* N—H···O hydrogen bonds, forming chains along [100] and [010].

Related literature

For biological properties of pyrazole derivatives, see: Hall *et al.* (2008); Isloor *et al.* (2009); Patel *et al.* (2010); Samshuddin *et al.* (2010). For the chemistry of aminopyrazoles, see: Giuseppe *et al.* (1991). For the medicinal activity of pyrazoles, see: Vinogradov *et al.* (1994). For related structures, see: Dobson & Gerkin (1998); Foces-Foces *et al.* (1996); Hemamalini & Fun (2010); Thanigaimani *et al.* (2012). For hydrogen-bond graph-set motifs, see: Bernstein *et al.* (1995). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_3H_6N_3^+\cdot C_2F_3O_2^-$
M_r = 197.13
Monoclinic, $P2_1/n$
a = 10.9292 (8) Å
b = 10.9332 (6) Å
c = 13.7002 (13) Å
β = 107.939 (9)°
V = 1557.5 (2) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 173 K
0.16 × 0.14 × 0.06 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.662, T_{max} = 1.000
9227 measured reflections
3031 independent reflections
2343 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.05
3031 reflections
338 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1AA···O1A^{i}	0.85 (3)	2.28 (3)	2.936 (3)	134 (2)
N1A—H1AB···O2A^{ii}	0.91 (3)	1.99 (3)	2.884 (3)	169 (3)
N2A—H2AA···O1A^{ii}	0.94 (3)	1.85 (3)	2.778 (2)	171 (3)
N3A—H3AA···O2A	0.93 (3)	1.78 (3)	2.705 (2)	172 (3)
N1B—H1BA···O2B^{iii}	0.84 (3)	2.18 (3)	2.962 (2)	153 (2)
N1B—H1BB···O2B^{iv}	0.90 (3)	2.03 (3)	2.929 (3)	173 (2)
N2B—H2BA···O1B^{iv}	0.95 (3)	1.81 (3)	2.756 (2)	174 (2)
N3B—H3BA···O1B^{v}	0.91 (3)	1.82 (3)	2.728 (2)	171 (2)

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5637).

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supplementary materials

Acta Cryst. (2013). E**69**, o1425–o1426 [doi:10.1107/S1600536813022204]

3-Amino-1*H*-pyrazol-2-ium trifluoroacetate

T. S. Yamuna, Jerry P. Jasinski, Derek R. Scadova, H. S. Yathirajan and Manpreet Kaur

1. Comment

Pyrazoles are an important class of heterocyclic compounds and many pyrazole derivatives are reported to have a broad spectrum of biological properties, e.g. antibacterial and anti-inflammatory activities (Patel *et al.*, 2010), anticancer (Hall *et al.*, 2008), antimicrobial (Samshuddin *et al.*, 2010), anti-inflammatory, antidepressant, anticonvulsant and anti-HIV properties (Isloor *et al.*, 2009). The chemistry of aminopyrazoles has been extensively investigated in the past (Giuseppe *et al.*, 1991). The considerable biological and medicinal activities of pyrazoles (Vinogradov *et al.*, 1994) for which aminopyrazoles are preferred precursors, have stimulated our investigations.

The crystal structures of some related compounds, viz., 3-aminopyrazole-4-carboxylic acid (Dobson & Gerkin, 1998), 4-(3,5-dimethylpyrazol-1-yl)benzoic acid trifluoroacetate (Foces-Foces *et al.*, 1996), 2-amino-5-methylpyridinium trifluoroacetate (Thanigaimani *et al.*, 2012) and 2-amino-5-chloropyridinium trifluoroacetate (Hemamalini & Fun, 2010) have been reported. In view of the importance of the title compound this paper reports its crystal structure.

The asymmetric unit of the title compound consists of two crystallographically independent 3-aminopyrazolium cations (A and B) and two trifluoroacetate anions (A and B) (Fig. 1). Each 3-aminopyrazolium cation is planar, with a maximum deviation of 0.0006 (2) Å for atom N2A in cation A and 0.0005 (2) Å for atom N2B in cation B. In the cations, atoms N3A and N3B are protonated. The F atoms of both anions are disordered over two sets of positions, with occupancy ratios of 0.639 (12):0.361 (12). Bond lengths and are normal (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), the A/B type 3-aminopyrazolium cations interact with the carboxylate groups of the A/B type trifluoroacetate anions through N—H···O hydrogen bonds, forming $R_2^2(8)$, $R_2^4(8)$, $R_2^4(10)$, $R_4^4(16)$ and $R_4^4(18)$ (Bernstein *et al.*, 1995) ring motifs.

2. Experimental

A mixture of commercially available 3-aminopyrazole and trifluoroacetic acid (1:3 v/v) were stirred for 15 minutes at room temperature. X-ray quality crystals were formed on slow evaporation. (m.p.: 463-468 K).

3. Refinement

All H atoms were located in a difference Fourier map and refined independently with isotropic displacement parameters [N—H = 0.84 (3)–0.95 (3) Å and C—H = 0.89 (3)–0.96 (3)Å].

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

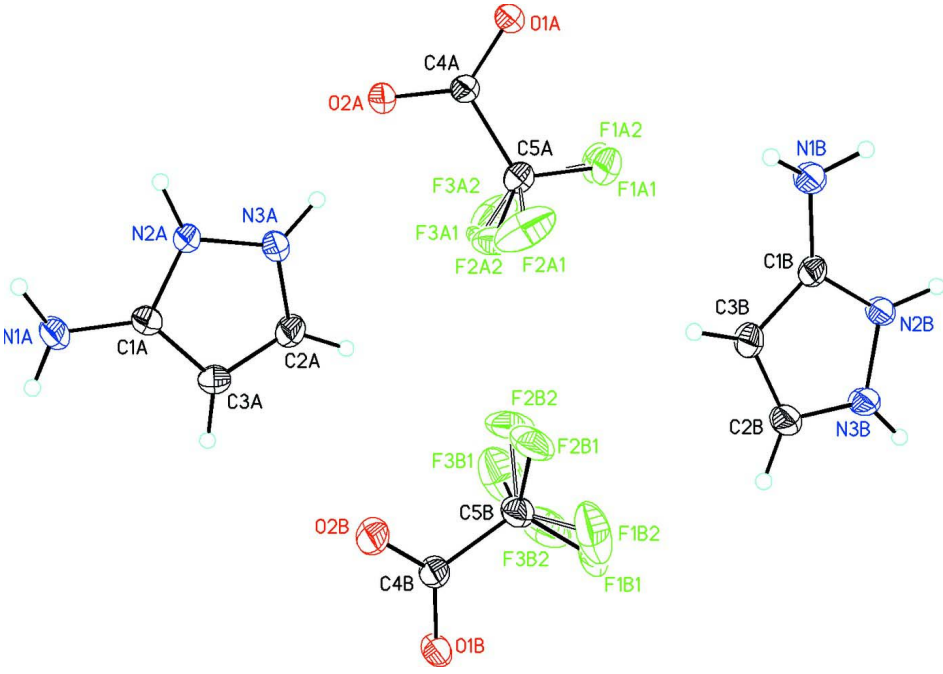

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. All disorder components are shown.

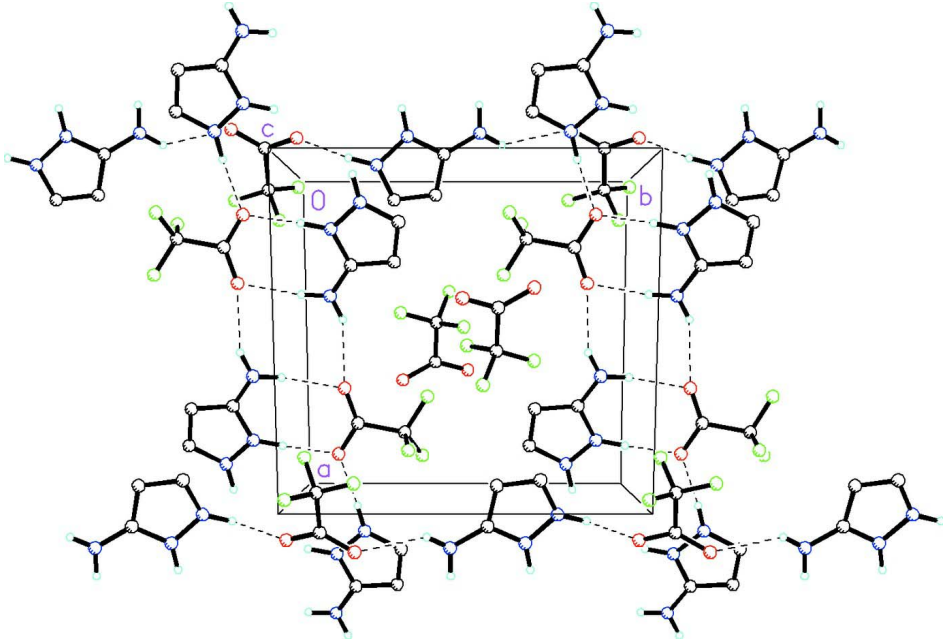

Figure 2

The crystal packing of the title compound, showing the hydrogen bonds (dashed lines) forming chains along [100] and [010]. H atoms not involved in hydrogen bonding and the minor component of disorder have been removed for clarity.

3-Amino-1*H*-pyrazol-2-ium trifluoroacetate

Crystal data

$C_3H_6N_3^+ \cdot C_2F_3O_2^-$
$M_r = 197.13$
Monoclinic, $P2_1/n$
$a = 10.9292$ (8) Å
$b = 10.9332$ (6) Å
$c = 13.7002$ (13) Å
$\beta = 107.939$ (9)°
$V = 1557.5$ (2) Å^3
$Z = 8$
$F(000) = 800$
$D_x = 1.681$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 2544 reflections
$\theta = 3.4$–72.4°
$\mu = 1.58$ mm^{-1}
$T = 173$ K
Irregular, colourless
0.16 × 0.14 × 0.06 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
$T_{min} = 0.662$, $T_{max} = 1.000$
9227 measured reflections
3031 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 72.5°$, $\theta_{min} = 4.6°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 9$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.136$
$S = 1.05$
3031 reflections
338 parameters
0 restraints
Primary atom site location: inferred from neighbouring sites
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.4559P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1A	0.56299 (19)	0.93721 (18)	0.25897 (17)	0.0384 (5)	
C2A	0.4240 (2)	0.7896 (2)	0.25222 (19)	0.0453 (5)	
H2A	0.351 (2)	0.741 (2)	0.2498 (18)	0.050 (7)*	
C3A	0.4396 (2)	0.9121 (2)	0.26406 (18)	0.0428 (5)	
H3A	0.379 (2)	0.968 (2)	0.2737 (18)	0.050 (7)*	
N1A	0.6272 (2)	1.04305 (18)	0.2644 (2)	0.0588 (6)	
H1AA	0.593 (3)	1.108 (3)	0.278 (2)	0.057 (8)*	
H1AB	0.713 (3)	1.041 (3)	0.272 (2)	0.064 (8)*	
N2A	0.61502 (17)	0.83064 (15)	0.24439 (15)	0.0396 (4)	

H2AA	0.697 (3)	0.815 (3)	0.240 (2)	0.062 (8)*	
N3A	0.52875 (17)	0.73971 (17)	0.23916 (16)	0.0440 (5)	
H3AA	0.549 (3)	0.657 (3)	0.236 (2)	0.067 (8)*	
C1B	0.28710 (18)	0.17323 (18)	0.48905 (16)	0.0351 (4)	
C2B	0.1618 (2)	0.3114 (2)	0.5268 (2)	0.0451 (5)	
H2B	0.122 (2)	0.382 (2)	0.5441 (19)	0.050 (7)*	
C3B	0.2771 (2)	0.2975 (2)	0.50783 (18)	0.0410 (5)	
H3B	0.336 (3)	0.354 (3)	0.508 (2)	0.061 (8)*	
N1B	0.37852 (18)	0.11030 (18)	0.46300 (18)	0.0472 (5)	
H1BA	0.450 (3)	0.147 (2)	0.476 (2)	0.053 (7)*	
H1BB	0.375 (3)	0.029 (3)	0.472 (2)	0.060 (8)*	
N2B	0.18060 (15)	0.11865 (16)	0.49623 (14)	0.0372 (4)	
H2BA	0.164 (2)	0.034 (3)	0.4985 (19)	0.058 (8)*	
N3B	0.10420 (17)	0.20371 (16)	0.52047 (16)	0.0431 (4)	
H3BA	0.024 (3)	0.184 (2)	0.5222 (19)	0.051 (7)*	
C4A	0.58112 (19)	0.40965 (18)	0.26078 (18)	0.0409 (5)	
C5A	0.4574 (2)	0.4142 (2)	0.29303 (18)	0.0422 (5)	
F1A1	0.4274 (7)	0.3086 (7)	0.3249 (5)	0.0619 (13)	0.639 (12)
F1A2	0.3945 (12)	0.3073 (14)	0.2818 (12)	0.075 (3)	0.361 (12)
F2A1	0.3589 (8)	0.4515 (8)	0.2173 (6)	0.0681 (17)	0.639 (12)
F2A2	0.3687 (14)	0.4932 (10)	0.2363 (13)	0.067 (3)	0.361 (12)
F3A1	0.4720 (7)	0.4955 (5)	0.3687 (6)	0.0651 (13)	0.639 (12)
F3A2	0.4800 (14)	0.4446 (15)	0.3885 (10)	0.089 (4)	0.361 (12)
O1A	0.63921 (15)	0.31128 (13)	0.27322 (15)	0.0526 (5)	
O2A	0.60816 (16)	0.50747 (14)	0.22685 (17)	0.0622 (5)	
C4B	0.23375 (19)	0.8115 (2)	0.48329 (18)	0.0413 (5)	
C5B	0.2075 (2)	0.6750 (2)	0.45833 (19)	0.0447 (5)	
F1B1	0.1329 (4)	0.6255 (3)	0.5045 (6)	0.077 (2)	0.639 (12)
F1B2	0.2028 (16)	0.6103 (8)	0.5367 (6)	0.101 (4)	0.361 (12)
F2B1	0.3162 (3)	0.6097 (3)	0.4866 (5)	0.0669 (13)	0.639 (12)
F2B2	0.2821 (9)	0.6190 (6)	0.4167 (12)	0.089 (4)	0.361 (12)
F3B1	0.1581 (7)	0.6629 (3)	0.3597 (3)	0.090 (2)	0.639 (12)
F3B2	0.0855 (7)	0.6537 (6)	0.3935 (8)	0.079 (3)	0.361 (12)
O1B	0.13834 (14)	0.86991 (13)	0.49109 (15)	0.0530 (5)	
O2B	0.34134 (14)	0.84860 (15)	0.48973 (15)	0.0538 (5)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0374 (10)	0.0299 (10)	0.0508 (12)	0.0050 (8)	0.0177 (9)	0.0021 (8)
C2A	0.0330 (11)	0.0431 (13)	0.0629 (15)	−0.0022 (9)	0.0194 (10)	0.0043 (10)
C3A	0.0351 (10)	0.0382 (12)	0.0595 (14)	0.0072 (9)	0.0208 (10)	0.0022 (10)
N1A	0.0434 (11)	0.0275 (10)	0.113 (2)	0.0008 (8)	0.0358 (12)	−0.0044 (10)
N2A	0.0340 (9)	0.0284 (9)	0.0624 (12)	0.0006 (7)	0.0238 (8)	0.0023 (8)
N3A	0.0385 (9)	0.0281 (9)	0.0701 (13)	−0.0011 (7)	0.0239 (9)	0.0017 (8)
C1B	0.0265 (9)	0.0353 (11)	0.0453 (11)	−0.0029 (7)	0.0138 (8)	0.0041 (8)
C2B	0.0464 (12)	0.0299 (11)	0.0663 (15)	−0.0029 (9)	0.0280 (11)	−0.0050 (10)
C3B	0.0344 (10)	0.0341 (11)	0.0570 (13)	−0.0096 (8)	0.0178 (9)	−0.0010 (9)
N1B	0.0302 (9)	0.0350 (10)	0.0823 (15)	−0.0018 (8)	0.0259 (9)	0.0024 (9)
N2B	0.0288 (8)	0.0279 (9)	0.0588 (11)	−0.0013 (6)	0.0192 (7)	−0.0009 (7)

N3B	0.0345 (9)	0.0330 (9)	0.0709 (13)	−0.0024 (7)	0.0298 (9)	−0.0039 (8)
C4A	0.0354 (10)	0.0301 (11)	0.0639 (14)	−0.0021 (8)	0.0252 (10)	−0.0036 (9)
C5A	0.0363 (11)	0.0397 (12)	0.0549 (13)	−0.0014 (9)	0.0201 (10)	0.0010 (9)
F1A1	0.053 (3)	0.0486 (17)	0.099 (4)	−0.004 (2)	0.045 (3)	0.015 (3)
F1A2	0.046 (5)	0.054 (3)	0.135 (10)	−0.010 (4)	0.044 (5)	0.013 (7)
F2A1	0.0376 (17)	0.094 (5)	0.071 (2)	0.011 (3)	0.0149 (16)	0.019 (3)
F2A2	0.038 (4)	0.058 (5)	0.113 (8)	0.009 (4)	0.035 (5)	0.018 (4)
F3A1	0.061 (2)	0.067 (3)	0.079 (4)	−0.001 (2)	0.039 (2)	−0.027 (2)
F3A2	0.070 (4)	0.137 (11)	0.069 (5)	−0.006 (7)	0.034 (3)	−0.015 (7)
O1A	0.0452 (9)	0.0277 (8)	0.0968 (13)	0.0022 (6)	0.0394 (9)	0.0030 (7)
O2A	0.0526 (10)	0.0302 (8)	0.1222 (16)	0.0029 (7)	0.0538 (11)	0.0110 (9)
C4B	0.0309 (10)	0.0341 (11)	0.0634 (14)	0.0007 (8)	0.0211 (10)	0.0020 (9)
C5B	0.0379 (11)	0.0350 (12)	0.0636 (15)	0.0034 (9)	0.0193 (10)	−0.0015 (10)
F1B1	0.071 (2)	0.0309 (14)	0.151 (6)	−0.0066 (15)	0.068 (3)	0.005 (2)
F1B2	0.174 (11)	0.053 (4)	0.069 (4)	−0.026 (6)	0.025 (6)	0.011 (3)
F2B1	0.0527 (15)	0.0417 (14)	0.107 (3)	0.0162 (11)	0.0249 (19)	−0.0071 (17)
F2B2	0.072 (6)	0.059 (3)	0.163 (11)	−0.002 (3)	0.076 (7)	−0.038 (5)
F3B1	0.113 (5)	0.0658 (19)	0.069 (2)	−0.017 (2)	−0.003 (2)	−0.0142 (14)
F3B2	0.050 (3)	0.060 (3)	0.108 (6)	0.002 (2)	−0.003 (3)	−0.033 (3)
O1B	0.0343 (8)	0.0290 (8)	0.1059 (14)	−0.0020 (6)	0.0366 (8)	−0.0059 (8)
O2B	0.0310 (8)	0.0434 (9)	0.0937 (13)	−0.0013 (6)	0.0290 (8)	0.0035 (8)

Geometric parameters (Å, º)

C1A—C3A	1.399 (3)	N2B—H2BA	0.95 (3)
C1A—N1A	1.344 (3)	N2B—N3B	1.358 (2)
C1A—N2A	1.338 (3)	N3B—H3BA	0.91 (3)
C2A—H2A	0.96 (3)	C4A—C5A	1.547 (3)
C2A—C3A	1.354 (3)	C4A—O1A	1.234 (2)
C2A—N3A	1.329 (3)	C4A—O2A	1.238 (3)
C3A—H3A	0.94 (3)	C5A—F1A1	1.312 (8)
N1A—H1AA	0.85 (3)	C5A—F1A2	1.341 (14)
N1A—H1AB	0.91 (3)	C5A—F2A1	1.309 (8)
N2A—H2AA	0.94 (3)	C5A—F2A2	1.351 (15)
N2A—N3A	1.357 (2)	C5A—F3A1	1.337 (7)
N3A—H3AA	0.93 (3)	C5A—F3A2	1.298 (14)
C1B—C3B	1.393 (3)	C4B—C5B	1.538 (3)
C1B—N1B	1.349 (3)	C4B—O1B	1.255 (2)
C1B—N2B	1.338 (2)	C4B—O2B	1.221 (2)
C2B—H2B	0.95 (3)	C5B—F1B1	1.295 (5)
C2B—C3B	1.372 (3)	C5B—F1B2	1.299 (8)
C2B—N3B	1.325 (3)	C5B—F2B1	1.337 (4)
C3B—H3B	0.89 (3)	C5B—F2B2	1.284 (6)
N1B—H1BA	0.84 (3)	C5B—F3B1	1.298 (4)
N1B—H1BB	0.90 (3)	C5B—F3B2	1.375 (6)
N1A—C1A—C3A	131.41 (19)	C2B—N3B—N2B	108.01 (17)
N2A—C1A—C3A	107.28 (18)	C2B—N3B—H3BA	130.5 (16)
N2A—C1A—N1A	121.30 (19)	N2B—N3B—H3BA	121.1 (16)
C3A—C2A—H2A	129.0 (15)	O1A—C4A—C5A	116.52 (18)

N3A—C2A—H2A	121.0 (15)	O1A—C4A—O2A	129.27 (19)
N3A—C2A—C3A	109.9 (2)	O2A—C4A—C5A	114.21 (17)
C1A—C3A—H3A	127.7 (15)	F1A1—C5A—C4A	113.4 (4)
C2A—C3A—C1A	106.02 (19)	F1A1—C5A—F3A1	108.0 (4)
C2A—C3A—H3A	126.3 (15)	F1A2—C5A—C4A	113.7 (7)
C1A—N1A—H1AA	118.4 (19)	F1A2—C5A—F2A2	103.9 (7)
C1A—N1A—H1AB	119.1 (18)	F2A1—C5A—C4A	111.2 (4)
H1AA—N1A—H1AB	120 (3)	F2A1—C5A—F1A1	108.0 (4)
C1A—N2A—H2AA	128.8 (18)	F2A1—C5A—F3A1	106.2 (4)
C1A—N2A—N3A	109.00 (17)	F2A2—C5A—C4A	113.1 (7)
N3A—N2A—H2AA	122.2 (18)	F3A1—C5A—C4A	109.7 (3)
C2A—N3A—N2A	107.79 (18)	F3A2—C5A—C4A	112.6 (6)
C2A—N3A—H3AA	129.0 (18)	F3A2—C5A—F1A2	105.7 (7)
N2A—N3A—H3AA	122.6 (18)	F3A2—C5A—F2A2	107.3 (8)
N1B—C1B—C3B	130.75 (19)	O1B—C4B—C5B	114.19 (18)
N2B—C1B—C3B	107.58 (17)	O2B—C4B—C5B	116.60 (19)
N2B—C1B—N1B	121.60 (19)	O2B—C4B—O1B	129.2 (2)
C3B—C2B—H2B	131.0 (15)	F1B1—C5B—C4B	113.5 (3)
N3B—C2B—H2B	119.5 (15)	F1B1—C5B—F2B1	105.8 (3)
N3B—C2B—C3B	109.57 (19)	F1B1—C5B—F3B1	110.1 (3)
C1B—C3B—H3B	125.5 (18)	F1B2—C5B—C4B	113.3 (4)
C2B—C3B—C1B	105.75 (18)	F1B2—C5B—F3B2	99.4 (5)
C2B—C3B—H3B	128.7 (18)	F2B1—C5B—C4B	111.4 (2)
C1B—N1B—H1BA	114.8 (18)	F2B2—C5B—C4B	117.5 (3)
C1B—N1B—H1BB	113.5 (17)	F2B2—C5B—F1B2	107.4 (6)
H1BA—N1B—H1BB	121 (2)	F2B2—C5B—F3B2	104.7 (5)
C1B—N2B—H2BA	128.4 (16)	F3B1—C5B—C4B	108.6 (2)
C1B—N2B—N3B	109.08 (17)	F3B1—C5B—F2B1	107.2 (3)
N3B—N2B—H2BA	121.5 (16)	F3B2—C5B—C4B	112.7 (3)

C1A—N2A—N3A—C2A	−1.0 (3)	O1A—C4A—C5A—F3A2	88.7 (8)
C3A—C1A—N2A—N3A	0.6 (3)	O2A—C4A—C5A—F1A1	177.4 (4)
C3A—C2A—N3A—N2A	1.1 (3)	O2A—C4A—C5A—F1A2	149.4 (7)
N1A—C1A—C3A—C2A	178.8 (3)	O2A—C4A—C5A—F2A1	55.5 (5)
N1A—C1A—N2A—N3A	−178.3 (2)	O2A—C4A—C5A—F2A2	31.3 (7)
N2A—C1A—C3A—C2A	0.1 (3)	O2A—C4A—C5A—F3A1	−61.7 (4)
N3A—C2A—C3A—C1A	−0.7 (3)	O2A—C4A—C5A—F3A2	−90.5 (8)
C1B—N2B—N3B—C2B	1.0 (3)	O1B—C4B—C5B—F1B1	−38.2 (4)
C3B—C1B—N2B—N3B	−0.9 (2)	O1B—C4B—C5B—F1B2	−76.1 (9)
C3B—C2B—N3B—N2B	−0.6 (3)	O1B—C4B—C5B—F2B1	−157.5 (3)
N1B—C1B—C3B—C2B	177.5 (2)	O1B—C4B—C5B—F2B2	157.7 (8)
N1B—C1B—N2B—N3B	−178.2 (2)	O1B—C4B—C5B—F3B1	84.6 (5)
N2B—C1B—C3B—C2B	0.5 (3)	O1B—C4B—C5B—F3B2	35.9 (7)
N3B—C2B—C3B—C1B	0.1 (3)	O2B—C4B—C5B—F1B1	143.9 (4)
O1A—C4A—C5A—F1A1	−3.4 (4)	O2B—C4B—C5B—F1B2	106.0 (9)
O1A—C4A—C5A—F1A2	−31.4 (7)	O2B—C4B—C5B—F2B1	24.5 (4)
O1A—C4A—C5A—F2A1	−125.3 (4)	O2B—C4B—C5B—F2B2	−20.3 (9)
O1A—C4A—C5A—F2A2	−149.5 (6)	O2B—C4B—C5B—F3B1	−93.3 (5)
O1A—C4A—C5A—F3A1	117.5 (4)	O2B—C4B—C5B—F3B2	−142.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*AA*···O1*A*^{i}	0.85 (3)	2.28 (3)	2.936 (3)	134 (2)
N1*A*—H1*AB*···O2*A*^{ii}	0.91 (3)	1.99 (3)	2.884 (3)	169 (3)
N2*A*—H2*AA*···O1*A*^{ii}	0.94 (3)	1.85 (3)	2.778 (2)	171 (3)
N3*A*—H3*AA*···O2*A*	0.93 (3)	1.78 (3)	2.705 (2)	172 (3)
N1*B*—H1*BA*···O2*B*^{iii}	0.84 (3)	2.18 (3)	2.962 (2)	153 (2)
N1*B*—H1*BB*···O2*B*^{iv}	0.90 (3)	2.03 (3)	2.929 (3)	173 (2)
N2*B*—H2*BA*···O1*B*^{iv}	0.95 (3)	1.81 (3)	2.756 (2)	174 (2)
N3*B*—H3*BA*···O1*B*^{v}	0.91 (3)	1.82 (3)	2.728 (2)	171 (2)

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, *y*−1, *z*; (v) −*x*, −*y*+1, −*z*+1.