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Crystal structure and hydrogen-bonding patterns in 5-fluorocytosinium picrate

Marimuthu Mohana,[a] Packianathan Thomas Muthiah[a]* and Colin D. McMillen[b]

[a]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India, and [b]Department of Chemistry, Clemson University, 379 H.L. Hunter Laboratories, Clemson, SC 29634, USA. *Correspondence e-mail: tommtrichy@yahoo.co.in

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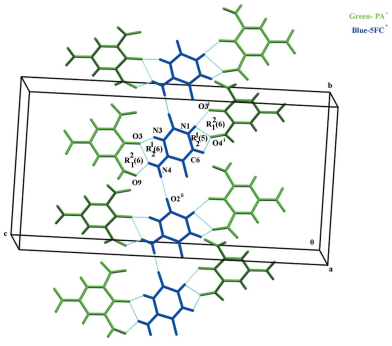
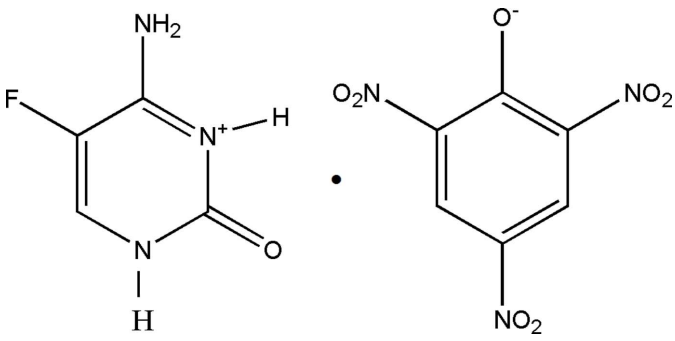
In the crystal structure of the title compound, 5-fluorocytosinium picrate, $C_4H_5FN_3O^+\cdot C_6H_2N_3O_7^-$, one N heteroatom of the 5-fluorocytosine (5FC) ring is protonated. The 5FC ring forms a dihedral angle of 19.97 (11)° with the ring of the picrate (PA^-) anion. In the crystal, the $5FC^+$ cation interacts with the PA^- anion through three-centre N—H···O hydrogen bonds, forming two conjoined rings having $R_2^1(6)$ and $R_1^2(6)$ motifs, and is extended by N—H···O hydrogen bonds and C—H···O interactions into a two-dimensional sheet structure lying parallel to (001). Also present in the crystal structure are weak C—F···π interactions.

1. Chemical context

Crystal engineering is defined as the rational design of crystalline solids through control of intermolecular interactions (hydrogen bonding, hydrophobic forces, van der Waals forces, π–π interactions and electrostatic forces). New solid forms of pharmaceuticals are designed using the crystal engineering approach. These engineered solids have technological and legal importance. Among the intermolecular interactions, hydrogen bonding is the master key for molecular recognition in biological systems because of its strength and directionality (Almarsson & Zaworoko, 2004; Desiraju, 1995). It plays a dominant role in molecular aggregates (Samuel, 1997; Tutughamiarso & Egert, 2012) and three-dimensional structure, stability and function of biomacromolecules (Gould, 1986). In particular, pyrimidine derivatives are used in the treatment of antiviral, antifungal, antitumor and cardiovascular diseases. 5-fluorocytosine (5FC) is a synthetic antimycotic compound, first synthesized in 1957 and widely used as an antitumor agent it is also active against fungal infection (Heidelberger *et al.*, 1957; Portalone & Colapietro, 2007; Vermes *et al.*, 2000). It becomes active by deamination of 5FC into 5-fluorouracil by the enzyme cytosine deaminase (CD) and inhibits RNA and DNA synthesis (Morschhäuser, 2003). Picric acid forms charge-transfer complexes with many organic compounds. It functions not only as an acceptor to form
π-stacking complexes with aromatic biomolecules, but also as an acidic ligand to form salts with polar biomolecules through specific electrostatic hydrogen-bonding interactions (In *et al.*, 1997). The present work is focused on the understanding of supramolecular hydrogen-bonding patterns exhibited by the interaction of 5FC and picric acid, giving the (1:1) title salt, $C_4H_5FN_3O^+\cdot C_6H_2N_3O_7^-$ whose structure and hydrogen-bonding patterns are reported on herein.





2. Structural commentary

The asymmetric unit contains one 5-fluorocytosinium cation ($5FC^+$) and one picrate anion (PA^-) (Fig. 1). The 5-fluorocytosine cation is protonated at the N3 atom, as is evident from the widening of the corresponding internal angle from 120.8 (5)° to 125.37 (17)° compared to neutral 5FC (Louis *et al.*, 1982). The dihedral angle between the planes of the rigs in the cation and anion is 19.97 (11)°. In the picrate (PA^-) anion, the nitro groups lie variously out of the parent benzene ring, with torsion angles C9—C8—N5—O4, C9—C10—N6—O7 and C11—C12—N7—O9 of 166.2 (2), −171.7 (2) and 147.2 (2)°, respectively.

3. Supramolecular features

In this crystal structure, the N4-amino group and protonated N3 atom of the $5FC^+$ cation interact with atoms O3 and O9 of the picrate anion through three-centre N—H···O hydrogen bonds, forming two fused-ring motifs with graph-sets $R_1^2(6)$ and $R_2^1(6)$ (Fig. 1). One of the N4-amino hydrogen atoms of the $5FC^+$ cation acts as a three-centre donor and the O3 atom of the PA^- anion acts as a three-centre acceptor. This type of interaction has also been reported in the crystal structures of 2-amino-4,6-dimethylpyrimidinium picrate (Subashini *et al.*, 2006) and 2-amino-4,6- dimethoxypyrimidinium picrate, pyrimethaminium picrate dimethyl sulfoxide (Thanigaimani *et al.*, 2009). Similarly, the other hetero nitrogen atom (N1) of the cation and both the phenolate O3^i and a nitro O4^i atom of a PA^- anion form an $R_1^2(6)$ ring motif through N—H···O hydrogen bonds with a second C—H···O4^i interaction, closing an $R_2^1(5)$ ring (Table 1). A similar type of interaction has also been observed in the crystal structure of cytosinium hydrogen chloroanilate monohydrate (Gotoh *et al.*, 2006).

Further, the symmetry-related O2^{ii} atom and the amino group of the $5FC^+$ cation are connected through an N—H···O hydrogen bond, forming a two-dimensional supramolecular network lying parallel to (001) (Fig. 2). Also present in the crystal structure is a weak C5—F5···π interaction (Fig. 3) between $5FC^+$ cations [C5···Cg^{iv} = 3.4002 (19) Å; C—F···Cg = 88.34 (12)°, where Cg is the centroid of the N1–C6 ring; symmetry code: (iv) $-x$, $-y$, $-z$ + 1]. A similar angle [90.5 (2)°] has been reported for a C—F···Cg interaction in an acridinium trifluoromethane sulfonate compound (Sikorski *et al.*, 2005).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^i	0.88	1.92	2.794 (3)	175
N1—H1···O4^i	0.88	2.56	3.021 (3)	114
N3—H3···O3	0.88	2.22	2.915 (2)	136
N4—H4*A*···O3	0.88	2.10	2.828 (2)	139
N4—H4*A*···O9	0.88	2.18	2.782 (3)	125
N4—H4*B*···O2^{ii}	0.88	1.96	2.832 (3)	171
C6—H6···O4^i	0.95	2.51	3.003 (3)	113

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

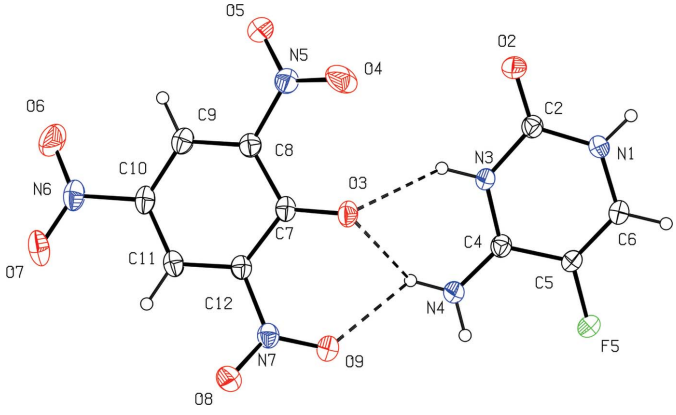


Figure 1
The naming scheme for the $5FC^+$ cation and the PA^- anion in the title compound, showing 30% probability level displacement ellipsoids. Dashed lines represent hydrogen bonds.

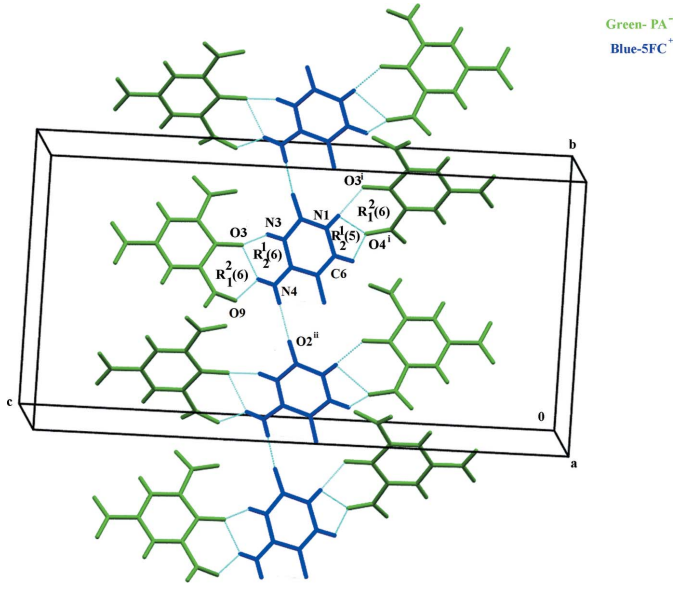


Figure 2
A view of the supramolecular network formed *via* N—H···O and C—H···O interactions. Dashed lines represent hydrogen bonds. For symmetry codes, see Table 1.

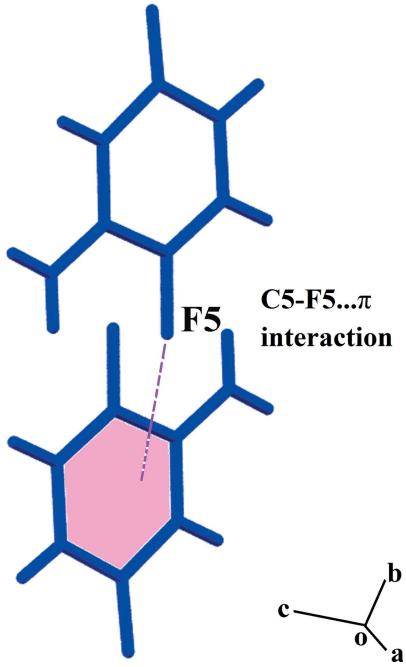


Figure 3
A view of the C5—F5···π interaction between 5FC$^+$ cations.

4. Database survey

The crystal structures of 5-fluorocytosine monohydrates (Louis *et al.*, 1982; Portalone & Colapietro, 2006; Portalone & Colapietro, 2007; Portalone, 2011), polymorphs (Hulme & Tocher, 2006; Tutughamiarso & Egert, 2012), salts (Perumalla *et al.*, 2013) and co-crystals (Tutughamiarso *et al.*, 2012; da Silva *et al.*, 2014) have been reported in the literature. From our laboratory, 5-fluorocytosinium salicylate (Prabakaran *et al.*, 2001), 5-fluorocytosinium 3-hydroxypicolinate (Karthikeyan *et al.*, 2014) and 5-fluorocytosine melamine (Mohana *et al.*, 2016) have been reported. Various salts and co-crystals of picric acid have also been reported in the literature (Subashini *et al.*, 2006; Thanigaimani *et al.*, 2009; Nagata *et al.*, 1995; Smith *et al.*, 2004; Gotoh *et al.*, 2004).

5. Synthesis and crystallization

A hot aqueous solution of 5-fluorocytosine (32 mg) and picric acid (57 mg) were mixed in a 1:1 molar ratio. The resulting solution was warmed to 353 K wrong symmetry description - inversion centre in central benzene ring over a water bath for half an hour and kept for slow evaporation. After a week, colourless prismatic crystals were obtained.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were positioned geometrically (C—H = 0.95 Å and N—H = 0.88 Å) and were refined using a riding model with U_{iso}(H) = 1.2U_{eq}(parent atom).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_5FN_3O^+·C_6H_2N_3O_7^-$
M_r	358.22
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	200
a, *b*, *c* (Å)	7.7463 (15), 13.235 (3), 25.642 (5)
V (Å^3)	2628.9 (9)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.17
Crystal size (mm)	0.65 × 0.58 × 0.20
Data collection	
Diffractometer	Rigaku AFC-8S
Absorption correction	Multi-scan multi-scan
T_{min}, T_{max}	0.899, 0.967
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21815, 2779, 2367
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.633
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.058, 0.174, 1.09
No. of reflections	2779
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.36

Computer programs: *CrystalClear* (Rigaku/MSC, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008), *POVRay* (Cason, 2004) and *publCIF* (Westrip, 2010).

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Acta Cryst. (2017). E**73**, 361-364 [https://doi.org/10.1107/S205698901700216X]

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Computing details

Data collection: *CrystalClear* (Rigaku/MSC, 2008); cell refinement: *CrystalClear* (Rigaku/MSC, 2008); data reduction: *CrystalClear* (Rigaku/MSC, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008) and *POVRay* (Cason, 2004); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

5-Fluorocytosinium picrate

Crystal data

$C_4H_5FN_3O^+·C_6H_2N_3O_7^-$
M_r = 358.22
Orthorhombic, *Pbca*
a = 7.7463 (15) Å
b = 13.235 (3) Å
c = 25.642 (5) Å
V = 2628.9 (9) Å^3
Z = 8
F(000) = 1456
D_x = 1.810 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2779 reflections
θ = 3.1–26.7°
μ = 0.17 mm^{-1}
T = 200 K
Prism, colorless
0.65 × 0.58 × 0.20 mm

Data collection

Rigaku AFC-8S diffractometer
Radiation source: fine focus sealed tube
Detector resolution: 14.6199 pixels mm^{-1}
ω scans
Absorption correction: multi-scan multi-scan
T_{min} = 0.899, T_{max} = 0.967
21815 measured reflections
2779 independent reflections
2367 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 26.7°, θ_{min} = 3.1°
h = −9→7
k = −16→16
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.174
S = 1.09
2779 reflections
226 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1025P)^2 + 1.2366P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.4311 (2)	0.65661 (11)	0.61738 (6)	0.0381 (4)
O9	0.5493 (2)	0.46460 (13)	0.62650 (7)	0.0440 (4)
O7	0.5646 (3)	0.58196 (18)	0.85486 (7)	0.0566 (5)
O8	0.7432 (2)	0.45799 (14)	0.68664 (7)	0.0469 (4)
C7	0.4418 (3)	0.65628 (15)	0.66650 (8)	0.0317 (5)
N7	0.6116 (2)	0.49512 (14)	0.66734 (7)	0.0353 (4)
C12	0.5282 (3)	0.57726 (16)	0.69555 (8)	0.0317 (4)
C8	0.3714 (3)	0.73340 (16)	0.70030 (8)	0.0338 (5)
C10	0.4631 (3)	0.65060 (18)	0.77790 (8)	0.0365 (5)
O4	0.2970 (3)	0.83845 (18)	0.63172 (8)	0.0664 (7)
N5	0.2811 (3)	0.81933 (15)	0.67800 (8)	0.0390 (4)
O5	0.1900 (3)	0.87035 (16)	0.70710 (7)	0.0595 (6)
C11	0.5410 (3)	0.57451 (16)	0.74889 (8)	0.0344 (5)
H11	0.601989	0.521474	0.765720	0.041*
O6	0.3831 (4)	0.70675 (18)	0.85946 (8)	0.0733 (7)
N6	0.4708 (3)	0.64684 (16)	0.83447 (8)	0.0448 (5)
C9	0.3783 (3)	0.72956 (17)	0.75414 (9)	0.0366 (5)
H9	0.325057	0.780799	0.774507	0.044*
F5	0.2136 (2)	0.44284 (10)	0.45073 (6)	0.0484 (4)
O2	0.0618 (2)	0.81443 (11)	0.51702 (7)	0.0412 (4)
N3	0.1841 (2)	0.66094 (13)	0.53164 (6)	0.0320 (4)
H3	0.209477	0.679151	0.563747	0.038*
N1	0.0672 (3)	0.69947 (14)	0.45092 (7)	0.0371 (4)
H1	0.019456	0.742373	0.429023	0.044*
N4	0.3114 (3)	0.50588 (14)	0.54809 (7)	0.0383 (4)
H4A	0.338817	0.526201	0.579703	0.046*
H4B	0.339680	0.444694	0.537710	0.046*
C2	0.1011 (3)	0.73142 (15)	0.50045 (8)	0.0325 (5)
C4	0.2293 (3)	0.56620 (15)	0.51674 (8)	0.0316 (4)
C5	0.1785 (3)	0.53785 (16)	0.46564 (8)	0.0348 (5)
C6	0.1035 (3)	0.60450 (18)	0.43367 (9)	0.0392 (5)
H6	0.075454	0.585605	0.398941	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0529 (10)	0.0359 (8)	0.0256 (7)	−0.0065 (7)	−0.0044 (6)	0.0023 (6)
O9	0.0528 (10)	0.0445 (9)	0.0347 (8)	0.0036 (7)	−0.0071 (7)	−0.0055 (7)
O7	0.0523 (11)	0.0861 (15)	0.0315 (9)	−0.0037 (10)	−0.0075 (8)	0.0120 (9)

O8	0.0448 (9)	0.0477 (10)	0.0483 (10)	0.0065 (7)	−0.0101 (8)	0.0000 (8)
C7	0.0347 (10)	0.0337 (10)	0.0268 (10)	−0.0097 (8)	−0.0011 (8)	0.0030 (7)
N7	0.0386 (10)	0.0369 (9)	0.0305 (9)	−0.0042 (7)	−0.0001 (7)	0.0035 (7)
C12	0.0335 (10)	0.0331 (10)	0.0286 (10)	−0.0057 (8)	−0.0010 (8)	0.0025 (8)
C8	0.0373 (11)	0.0315 (10)	0.0327 (10)	−0.0057 (8)	−0.0022 (8)	0.0014 (8)
C10	0.0408 (12)	0.0434 (12)	0.0252 (10)	−0.0119 (9)	−0.0015 (8)	0.0014 (8)
O4	0.0806 (15)	0.0708 (14)	0.0478 (11)	0.0296 (11)	0.0199 (10)	0.0262 (10)
N5	0.0424 (10)	0.0379 (10)	0.0368 (10)	−0.0034 (8)	0.0003 (8)	0.0009 (8)
O5	0.0814 (15)	0.0547 (12)	0.0424 (10)	0.0228 (10)	−0.0041 (9)	−0.0079 (8)
C11	0.0357 (11)	0.0380 (10)	0.0296 (10)	−0.0076 (8)	−0.0047 (8)	0.0058 (8)
O6	0.122 (2)	0.0654 (13)	0.0320 (9)	0.0087 (13)	0.0120 (11)	−0.0020 (9)
N6	0.0538 (12)	0.0518 (12)	0.0287 (10)	−0.0135 (10)	−0.0011 (9)	0.0027 (8)
C9	0.0396 (12)	0.0386 (11)	0.0317 (11)	−0.0097 (9)	0.0015 (8)	−0.0019 (8)
F5	0.0673 (10)	0.0373 (7)	0.0404 (8)	0.0123 (6)	−0.0140 (7)	−0.0128 (6)
O2	0.0538 (10)	0.0292 (8)	0.0406 (9)	0.0029 (7)	−0.0023 (7)	−0.0004 (6)
N3	0.0404 (10)	0.0302 (9)	0.0252 (8)	0.0019 (7)	−0.0033 (7)	−0.0028 (6)
N1	0.0491 (11)	0.0347 (9)	0.0274 (9)	0.0077 (8)	−0.0028 (8)	0.0032 (7)
N4	0.0514 (11)	0.0310 (9)	0.0324 (9)	0.0053 (8)	−0.0094 (8)	−0.0031 (7)
C2	0.0380 (11)	0.0308 (11)	0.0288 (10)	−0.0023 (8)	0.0005 (8)	0.0012 (8)
C4	0.0360 (10)	0.0303 (10)	0.0285 (10)	−0.0039 (8)	−0.0006 (8)	0.0000 (8)
C5	0.0439 (11)	0.0312 (10)	0.0294 (10)	0.0031 (8)	−0.0032 (9)	−0.0057 (8)
C6	0.0473 (12)	0.0418 (12)	0.0284 (10)	0.0055 (10)	−0.0053 (9)	−0.0049 (8)

Geometric parameters (Å, º)

O3—C7	1.262 (3)	O6—N6	1.225 (3)
O9—N7	1.222 (3)	C9—H9	0.9500
O7—N6	1.240 (3)	F5—C5	1.342 (2)
O8—N7	1.235 (3)	O2—C2	1.217 (3)
C7—C8	1.446 (3)	N3—C4	1.357 (3)
C7—C12	1.448 (3)	N3—C2	1.387 (3)
N7—C12	1.457 (3)	N3—H3	0.8800
C12—C11	1.372 (3)	N1—C6	1.362 (3)
C8—C9	1.383 (3)	N1—C2	1.364 (3)
C8—N5	1.452 (3)	N1—H1	0.8800
C10—C9	1.377 (3)	N4—C4	1.299 (3)
C10—C11	1.389 (3)	N4—H4A	0.8800
C10—N6	1.453 (3)	N4—H4B	0.8800
O4—N5	1.219 (3)	C4—C5	1.419 (3)
N5—O5	1.229 (3)	C5—C6	1.337 (3)
C11—H11	0.9500	C6—H6	0.9500
O3—C7—C8	124.81 (19)	C10—C9—C8	119.2 (2)
O3—C7—C12	123.1 (2)	C10—C9—H9	120.4
C8—C7—C12	112.08 (18)	C8—C9—H9	120.4
O9—N7—O8	122.5 (2)	C4—N3—C2	125.37 (17)
O9—N7—C12	119.83 (18)	C4—N3—H3	117.3
O8—N7—C12	117.63 (18)	C2—N3—H3	117.3

C11—C12—C7	124.4 (2)	C6—N1—C2	123.29 (18)
C11—C12—N7	116.32 (18)	C6—N1—H1	118.4
C7—C12—N7	119.24 (18)	C2—N1—H1	118.4
C9—C8—C7	123.9 (2)	C4—N4—H4A	120.0
C9—C8—N5	116.14 (19)	C4—N4—H4B	120.0
C7—C8—N5	119.89 (18)	H4A—N4—H4B	120.0
C9—C10—C11	121.4 (2)	O2—C2—N1	123.8 (2)
C9—C10—N6	119.2 (2)	O2—C2—N3	121.46 (19)
C11—C10—N6	119.5 (2)	N1—C2—N3	114.70 (18)
O4—N5—O5	122.3 (2)	N4—C4—N3	121.33 (19)
O4—N5—C8	119.8 (2)	N4—C4—C5	123.0 (2)
O5—N5—C8	117.87 (19)	N3—C4—C5	115.65 (19)
C12—C11—C10	118.9 (2)	C6—C5—F5	122.10 (19)
C12—C11—H11	120.6	C6—C5—C4	120.8 (2)
C10—C11—H11	120.6	F5—C5—C4	117.05 (19)
O6—N6—O7	123.5 (2)	C5—C6—N1	120.0 (2)
O6—N6—C10	118.5 (2)	C5—C6—H6	120.0
O7—N6—C10	117.9 (2)	N1—C6—H6	120.0
O4—N5—C8—C7	−16.2 (3)	O3—C7—C8—C9	177.2 (2)
O4—N5—C8—C9	166.2 (2)	C12—C7—C8—N5	179.5 (2)
O5—N5—C8—C7	163.6 (2)	C12—C7—C8—C9	−3.0 (3)
O5—N5—C8—C9	−14.0 (3)	O3—C7—C12—N7	1.8 (3)
O6—N6—C10—C9	9.2 (4)	O3—C7—C12—C11	−179.6 (2)
O6—N6—C10—C11	−170.7 (2)	C8—C7—C12—N7	−178.00 (19)
O7—N6—C10—C9	−171.7 (2)	N5—C8—C9—C10	−179.5 (2)
O7—N6—C10—C11	8.4 (3)	C7—C8—C9—C10	3.0 (4)
O8—N7—C12—C7	147.0 (2)	C8—C9—C10—N6	179.8 (2)
O8—N7—C12—C11	−31.8 (3)	C8—C9—C10—C11	−0.3 (4)
O9—N7—C12—C7	−34.0 (3)	N6—C10—C11—C12	178.0 (2)
O9—N7—C12—C11	147.2 (2)	C9—C10—C11—C12	−1.9 (3)
C2—N1—C6—C5	−1.1 (4)	C10—C11—C12—N7	−179.6 (2)
C6—N1—C2—O2	−176.4 (2)	C10—C11—C12—C7	1.7 (4)
C6—N1—C2—N3	3.1 (3)	N3—C4—C5—F5	−176.70 (18)
C2—N3—C4—C5	−3.0 (3)	N3—C4—C5—C6	5.1 (3)
C4—N3—C2—O2	178.6 (2)	N4—C4—C5—F5	2.2 (3)
C4—N3—C2—N1	−0.9 (3)	N4—C4—C5—C6	−175.9 (2)
C2—N3—C4—N4	178.0 (2)	F5—C5—C6—N1	178.7 (2)
O3—C7—C8—N5	−0.2 (3)	C4—C5—C6—N1	−3.3 (4)
C8—C7—C12—C11	0.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.88	1.92	2.794 (3)	175
N1—H1···O4^{i}	0.88	2.56	3.021 (3)	114
N3—H3···O3	0.88	2.22	2.915 (2)	136
N4—H4*A*···O3	0.88	2.10	2.828 (2)	139

N4—H4*A*···O9	0.88	2.18	2.782 (3)	125
N4—H4*B*···O2^{ii}	0.88	1.96	2.832 (3)	171
C6—H6···O4^{i}	0.95	2.51	3.003 (3)	113

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