

Synthesis and crystal structure of 2-[(2,3,5,6-tetrafluoropyridin-4-yl)amino]ethyl methacrylate

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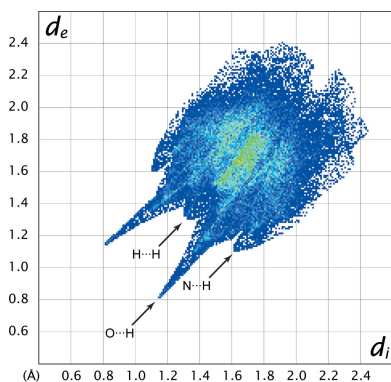
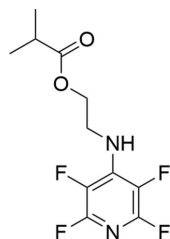
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Keywords: crystal structure; perfluoropyridine; C—H...F interaction.**CCDC reference:** 2263932**Supporting information:** this article has supporting information at journals.iucr.org/e

In the title compound, $C_{11}H_{10}F_4N_2O_2$, the conformation about the N—C—C—O bond is *gauche* [torsion angle = $61.84(13)^\circ$]. In the crystal, N—H...O hydrogen bonds link the molecules into [010] chains, which are cross-linked by C—H...F and C—H... π contacts. Hirshfeld surface analysis was conducted to aid in the visualization of these various influences on the packing. This analysis showed that the largest contribution to the surface contacts arises from F...H/H...F interactions (35.6%), followed by O...H/H...O (17.8%) and H...H (12.7%).

1. Chemical context

Perfluoropyridine (C_5NF_5 ; PFPy) is an ideal candidate to use in the preparation of complex fluorinated compounds and materials as PFPy is reactive towards nucleophilic addition (Sandford, 2012). Furthermore, our group and others have demonstrated that this addition can be regio-selectively controlled, with stoichiometric addition to the 4-(*para*-) position being exclusive with a broad range of nucleophiles (Brittain & Cobb, 2019; Peloquin *et al.*, 2020; Seyb & Kerres, 2013). Sequential addition can also be accomplished at the 3,5-(*meta*-) positions (Corley *et al.*, 2019; Houck *et al.*, 2021). As part of our ongoing work in this area, the synthesis and single-crystal structure of the title compound, $C_{11}H_{10}F_4N_2O_2$, is reported herein.



2. Structural commentary

The title compound (Fig. 1) crystallizes in the monoclinic space group $P2_1/n$ with one molecule in the asymmetric unit. The N2—C6 bond is rotated by only $15.81(8)^\circ$ from the C1—C5/N1 ring plane, presumably to encourage conjugation of the nitrogen atom lone pair with the aromatic ring π system, which is reflected in the C3—N2 bond length of $1.3522(16)$ Å; the C3—N2—C6—C7 torsion angle is $-81.68(16)^\circ$. The amine nitrogen atom (N2) and ester oxygen atom (O1) are *gauche* to one another, with N2—C6—C7—O1 = $61.84(13)^\circ$. The C10



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

Cg11 is the centroid of the C1–C5/N1 ring.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N2–HN2...O2 ⁱ	0.811 (18)	2.119 (17)	2.8296 (15)	146.3 (15)
C6–H6B...F3	0.99	2.23	2.9004 (15)	124
C7–H7B...F3 ⁱⁱ	0.99	2.57	3.5368 (15)	167
C7–H7B...F4 ⁱⁱ	0.99	2.63	3.3646 (16)	131
C7–H7A...Cg1 ⁱⁱⁱ	0.99	2.89	3.6047 (15)	130

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

methyl group is oriented in such a fashion as to enable a weak C–H... π interaction with the aromatic ring of an adjacent molecule (Table 1).

3. Supramolecular features

The main directional interactions in the crystal structure of the title compound are of the type C–H...F, N–H...O and C–H... π (Table 1). The N–H...O hydrogen bonds link the molecules into [010] chains, with adjacent molecules related by

a 2_1 screw axis. Weak hydrogen-bonding interactions are observed between one hydrogen atom bound to each carbon atom of the two-carbon (C6/C7) linker unit between the amine nitrogen atom and the ester, and F3 as acceptor. One of these interactions is intramolecular (C6–H6A...F3) with the other being intermolecular (C7–H7A...F3). A hydrogen-bonding interaction occurs between the secondary amine and the carbonyl oxygen atom (N2–H1N2...O2). Finally, a weak C–H... π interaction is observed between H7B and the pyridine ring π system.

Hirshfeld surface analysis was used to investigate the presence of hydrogen bonds and intermolecular interactions in the crystal structure. The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were generated by *CrystalExplorer17.5* (Turner *et al.*, 2017), using standard surface resolution with the three-dimensional d_{norm} surfaces plotted over a fixed color scale of -0.025 (red) to 1.38 (blue) a.u.; the pale-red spots symbolize short contacts and negative d_{norm} values on the corresponding surface plots shown in Fig. 2, associated with their relative contributions to the Hirshfeld surface.

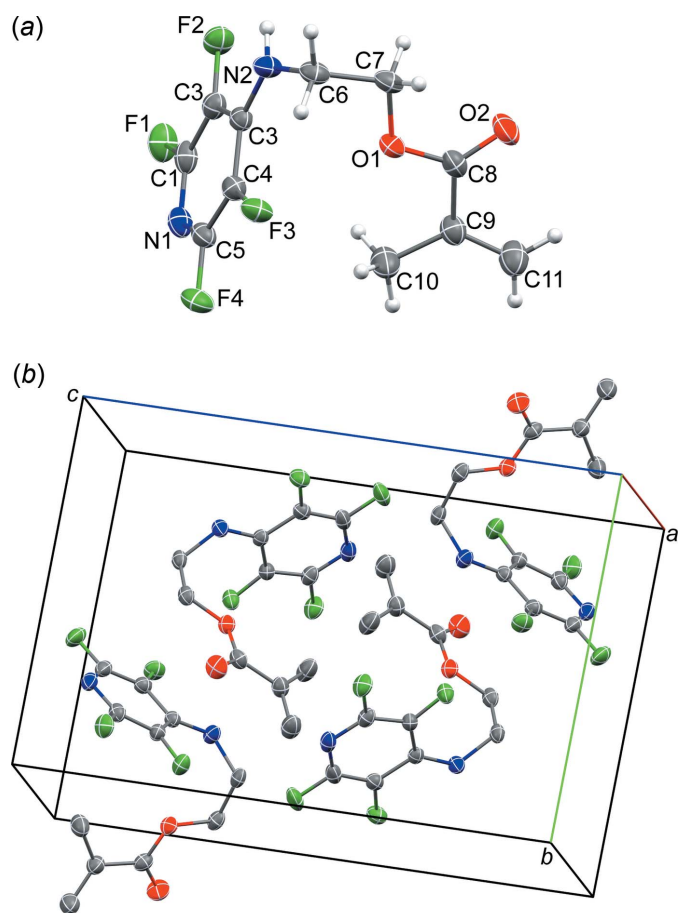


Figure 1
The molecular structure of the title compound (a) and the unit-cell packing (b). Displacement ellipsoids are shown at the 50% probability level.

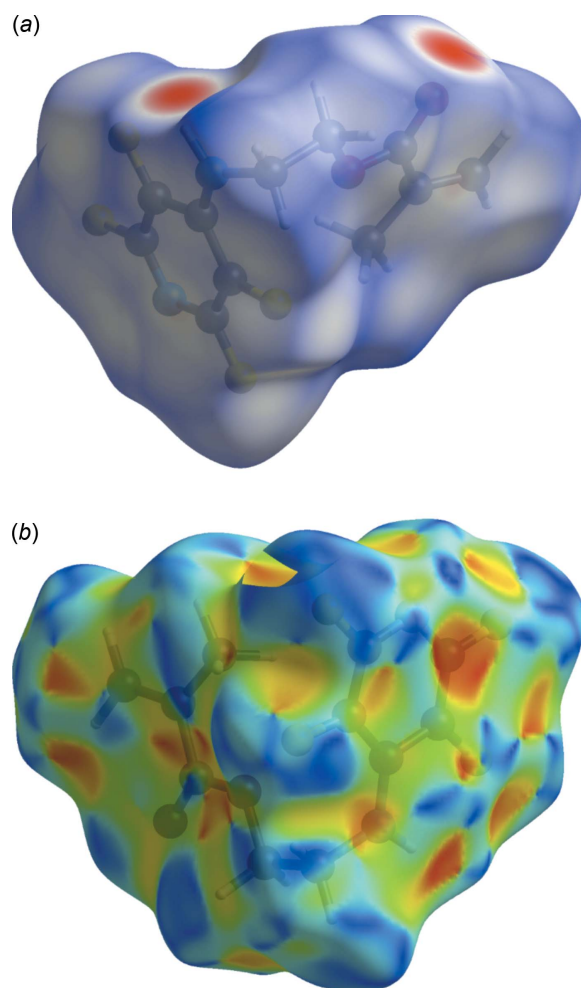


Figure 2
Map of d_{norm} (a) and shape index (b) onto the Hirshfeld surface for the title compound.

Table 2

Percentage contribution of inter-atomic contacts to the Hirshfeld surface of the title compound.

Contact	Percentage contribution
F...H/H...F	35.6
H...H	17.8
C...H/H...C	12.7
N...H/H...N	8.7
O...H/H...O	8.7
F...F	6.3
O...C/C...O	2.5
F...O/O...F	2.4
F...N/N...F	1.8
C...F/F...C	1.7
C...C	1.4
N...C/C...N	0.3

The largest contribution to the overall crystal packing is from F...H/H...F interactions (35.6%) (Table 2). However, the spike in the fingerprint plot (Fig. 3) associated with this contact is masked by that of the O...H/H...O contacts, which appears in the plot at $0.80 \text{ \AA} < (d_i + d_e) < 1.15 \text{ \AA}$. The H...H and C...H/H...C contacts have the second and third largest contributions, at 17.8 and 12.7%, respectively. Smaller spikes on the shoulder of the fingerprint plot, appearing at $1.15 \text{ \AA} < (d_i + d_e) < 1.160 \text{ \AA}$, correspond to the N...H/H...N contacts.

4. Database survey

A search of the November 2019 release of the Cambridge Structure Database (Groom *et al.*, 2016), with updates through November 2012, was performed using the program *ConQuest*

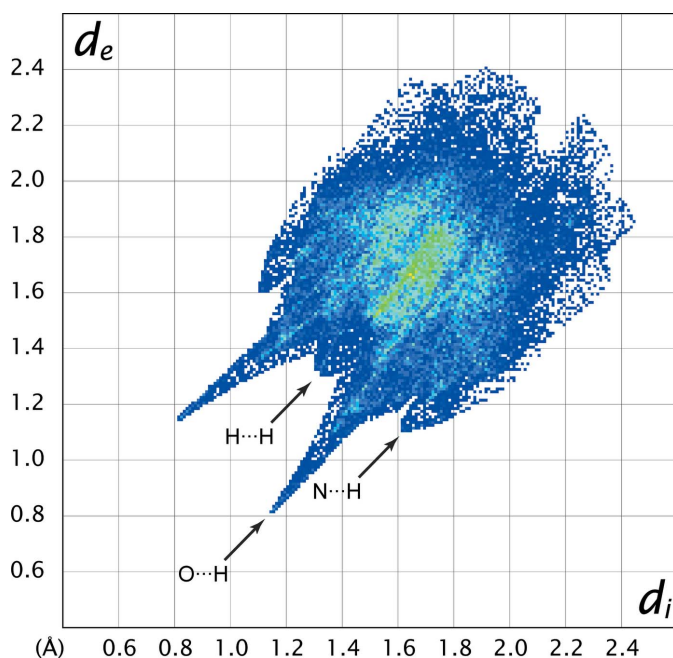


Figure 3
The overall two-dimensional fingerprint plot for the title compound.

(Bruno *et al.*, 2002). The search was limited to 2,3,5,6-tetrafluoropyridine-based compounds with a secondary amine nitrogen atom bound to the ring in the 4-position. This search resulted in 19 hits: the C—C—N—C torsion angles indicate planarity, presumably due to conjugation of the nitrogen lone pair into the pyridine ring π system, in the majority of cases. In cases of non-planarity, this is typically due to steric factors of the substituent on the nitrogen atom or conjugation of that nitrogen lone pair into the π system of the substituent. For example, in CSD refcode NIXMEN (Ranjbar-Karimi *et al.*, 2008), the bulk of a phenyl ring attached to the nitrogen atom substituent discourages planarity, resulting in a torsion angle of 37.4° . In TAPRAD (Yamaguchi *et al.*, 1992), the conjugation of the nitrogen lone pair is into a urea substituent, *vice* the pyridine ring, with a torsion angle of 38.7° .

5. Synthesis and crystallization

2-[(Perfluoropyridin-4-yl)amino]ethan-1-ol was synthesized using a known method and used without further purification (Peloquin, *et al.*, 2020). Methacryloyl chloride was purchased from Sigma and distilled under reduced pressure prior to use.

A 500 ml round-bottom flask equipped with an addition funnel was charged with 2-[(perfluoropyridin-4-yl)amino]ethan-1-ol (13.4 g, 62.3 mmol), trimethylamine (10.7 ml, 77.2 mmol) and diethyl ether (300 ml). The solution was stirred under nitrogen at 273–278 K for 15 minutes. Next, a solution of methacryloyl chloride (7.50 ml, 76.8 mmol) in ether (10 ml) was added dropwise to the round-bottom flask using an addition funnel. The solution was allowed to gradually warm to room temperature and was stirred for 96 h under nitrogen. Precipitated salts were removed by vacuum filtration and the filtrate was concentrated under reduced pressure. Crystals of the title compound in the form of colorless needles were obtained by recrystallization from a solution in warm ($\sim 328 \text{ K}$) hexanes (9.0 g, 50.7%): m.p. 335–336 K; ^1H NMR (500 MHz, CDCl_3): δ 6.01 (s, vinyl, 1H), 5.61 (s, vinyl, 1H), 4.90 (bs, $-\text{NHCH}_2\text{CH}_2\text{O}-$, 1H), 4.38 (t, $-\text{NHCH}_2\text{CH}_2\text{O}-$, 2H, $^3J = 5.0 \text{ Hz}$), 3.86 (q, $-\text{NHCH}_2\text{CH}_2\text{O}-$, 2H, $^3J = 5.3 \text{ Hz}$), 1.93 (s, $\text{CH}_2=\text{C}(\text{CH}_3)-$, 3H); ^{19}F NMR (471 MHz, CDCl_3): δ -93.6 (bs, 2F), -163.4 (bs, 2F); ^{13}C NMR (125 MHz, CDCl_3): δ 167.8 (C=O), 135.8 ($\text{CH}_2=\text{C}(\text{CH}_3)-$), 126.4 [$\text{CH}_2=\text{C}(\text{CH}_3)-$], 63.7 ($-\text{OCH}_2\text{CH}_2\text{NH}-$), 44.1 ($-\text{OCH}_2\text{CH}_2\text{NH}-$), 18.3 [$\text{CH}_2=\text{C}(\text{CH}_3)-$].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. N-bound H atoms were refined freely. C-bound H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$.

Funding information

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Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₁ H ₁₀ F ₄ N ₂ O ₂
<i>M</i> _r	278.21
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	106
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.8588 (1), 10.7797 (2), 15.7707 (2)
β (°)	91.251 (1)
<i>V</i> (Å ³)	1165.74 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.15
Crystal size (mm)	0.44 × 0.18 × 0.17
Data collection	
Diffractometer	XtaLAB Synergy, Single source at offset/far, HyPix3000
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Rigaku OD, 2019)
<i>T</i> _{min} , <i>T</i> _{max}	0.705, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	33062, 2583, 2211
<i>R</i> _{int}	0.035
(sin θ/λ) _{max} (Å ⁻¹)	0.647
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.035, 0.090, 1.06
No. of reflections	2583
No. of parameters	177
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.28, -0.21

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020) and *OLEX2* (Dolomanov *et al.*, 2009).

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Synthesis and crystal structure of 2-[(2,3,5,6-tetrafluoropyridin-4-yl)amino]ethyl methacrylate

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Computing details

Data collection: *APEX3* v2017.3-0 (Bruker, 2017); cell refinement: *SAINT* V8.38A (Bruker, 2017); data reduction: *SAINT* V8.38A (Bruker, 2017); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *Olex2* 1.5 (Dolomanov *et al.*, 2009).

2-[(2,3,5,6-Tetrafluoropyridin-4-yl)amino]ethyl 2-methylprop-2-enoate

Crystal data

$C_{11}H_{10}F_4N_2O_2$

$M_r = 278.21$

Monoclinic, $P2_1/n$

$a = 6.8588$ (1) Å

$b = 10.7797$ (2) Å

$c = 15.7707$ (2) Å

$\beta = 91.251$ (1)°

$V = 1165.74$ (3) Å³

$Z = 4$

$F(000) = 568$

$D_x = 1.585$ Mg m⁻³

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

Cell parameters from 19836 reflections

$\theta = 2.3$ – 27.2 °

$\mu = 0.15$ mm⁻¹

$T = 106$ K

Needle, colourless

$0.44 \times 0.18 \times 0.17$ mm

Data collection

XtaLAB Synergy, Single source at offset/far,

HyPix3000

diffractometer

Radiation source: micro-focus sealed X-ray tube

φ and ω scans

Absorption correction: gaussian

(CrysAlis PRO; Rigaku OD, 2019)

$T_{\min} = 0.705$, $T_{\max} = 1.000$

33062 measured reflections

2583 independent reflections

2211 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 27.4$ °, $\theta_{\min} = 2.3$ °

$h = -8 \rightarrow 8$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.090$

$S = 1.06$

2583 reflections

177 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.4834P]$

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

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.28$ e Å⁻³

$\Delta\rho_{\min} = -0.21$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.76605 (14)	0.04660 (8)	0.49959 (5)	0.0400 (2)
F2	0.49913 (12)	0.06997 (8)	0.37165 (5)	0.0334 (2)
F3	0.92779 (11)	0.36294 (8)	0.24890 (5)	0.0301 (2)
F4	1.17024 (11)	0.32149 (9)	0.37827 (5)	0.0364 (2)
O1	0.53522 (13)	0.47979 (9)	0.28749 (6)	0.0261 (2)
O2	0.30721 (15)	0.62510 (10)	0.30633 (7)	0.0391 (3)
N1	0.96939 (17)	0.18455 (11)	0.43992 (7)	0.0296 (3)
N2	0.56174 (17)	0.22514 (11)	0.23936 (7)	0.0267 (3)
C1	0.8023 (2)	0.12386 (13)	0.43516 (8)	0.0293 (3)
C2	0.66735 (19)	0.13523 (12)	0.37096 (8)	0.0258 (3)
C3	0.69653 (18)	0.21724 (12)	0.30299 (8)	0.0228 (3)
C4	0.87510 (19)	0.28051 (12)	0.30859 (8)	0.0241 (3)
C5	0.99991 (19)	0.25973 (13)	0.37622 (8)	0.0274 (3)
C6	0.53726 (19)	0.32687 (13)	0.17900 (8)	0.0266 (3)
H6A	0.468848	0.295683	0.127349	0.032*
H6B	0.667341	0.356903	0.162348	0.032*
C7	0.42353 (19)	0.43344 (13)	0.21475 (8)	0.0272 (3)
H7A	0.406113	0.499531	0.171663	0.033*
H7B	0.293237	0.405086	0.232375	0.033*
C8	0.45919 (19)	0.57648 (13)	0.32828 (9)	0.0276 (3)
C9	0.5847 (2)	0.61826 (14)	0.40162 (9)	0.0306 (3)
C10	0.7559 (2)	0.54178 (16)	0.42728 (10)	0.0417 (4)
H10A	0.843816	0.534069	0.379396	0.063*
H10B	0.711927	0.459166	0.444381	0.063*
H10C	0.825125	0.581580	0.475012	0.063*
C11	0.5387 (3)	0.72537 (16)	0.43920 (10)	0.0430 (4)
H11A	0.617410	0.756041	0.484859	0.052*
H11B	0.427248	0.770700	0.420212	0.052*
HN2	0.467 (3)	0.1814 (16)	0.2450 (10)	0.032 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0534 (6)	0.0383 (5)	0.0284 (4)	0.0099 (4)	0.0041 (4)	0.0129 (4)
F2	0.0342 (5)	0.0303 (4)	0.0360 (5)	-0.0056 (3)	0.0052 (3)	0.0048 (3)
F3	0.0244 (4)	0.0381 (5)	0.0277 (4)	-0.0070 (3)	-0.0027 (3)	0.0070 (3)
F4	0.0247 (4)	0.0491 (5)	0.0351 (5)	-0.0030 (4)	-0.0091 (3)	-0.0017 (4)
O1	0.0213 (5)	0.0304 (5)	0.0264 (5)	0.0017 (4)	-0.0040 (4)	0.0011 (4)
O2	0.0270 (5)	0.0447 (6)	0.0453 (6)	0.0115 (5)	-0.0054 (4)	0.0008 (5)

N1	0.0328 (6)	0.0332 (6)	0.0228 (6)	0.0102 (5)	-0.0038 (5)	-0.0007 (5)
N2	0.0236 (6)	0.0292 (6)	0.0270 (6)	-0.0065 (5)	-0.0051 (4)	0.0039 (5)
C1	0.0382 (8)	0.0281 (7)	0.0216 (6)	0.0111 (6)	0.0035 (5)	0.0028 (5)
C2	0.0276 (7)	0.0241 (6)	0.0260 (6)	0.0012 (5)	0.0038 (5)	-0.0004 (5)
C3	0.0229 (6)	0.0238 (6)	0.0217 (6)	0.0024 (5)	-0.0001 (5)	-0.0018 (5)
C4	0.0242 (6)	0.0263 (6)	0.0217 (6)	0.0012 (5)	0.0001 (5)	0.0008 (5)
C5	0.0228 (6)	0.0329 (7)	0.0265 (7)	0.0043 (5)	-0.0034 (5)	-0.0047 (6)
C6	0.0243 (6)	0.0342 (7)	0.0211 (6)	-0.0043 (5)	-0.0051 (5)	0.0044 (5)
C7	0.0203 (6)	0.0345 (7)	0.0266 (7)	-0.0031 (5)	-0.0062 (5)	0.0062 (6)
C8	0.0227 (6)	0.0309 (7)	0.0295 (7)	0.0034 (5)	0.0021 (5)	0.0065 (6)
C9	0.0310 (7)	0.0341 (7)	0.0269 (7)	0.0055 (6)	0.0005 (5)	0.0016 (6)
C10	0.0419 (9)	0.0459 (9)	0.0369 (8)	0.0100 (7)	-0.0106 (7)	-0.0114 (7)
C11	0.0490 (10)	0.0442 (9)	0.0356 (8)	0.0130 (7)	-0.0057 (7)	-0.0044 (7)

Geometric parameters (Å, °)

F1—C1	1.3413 (16)	C4—C5	1.3714 (18)
F2—C2	1.3516 (15)	C6—H6A	0.9900
F3—C4	1.3495 (15)	C6—H6B	0.9900
F4—C5	1.3444 (16)	C6—C7	1.505 (2)
O1—C7	1.4540 (15)	C7—H7A	0.9900
O1—C8	1.3367 (17)	C7—H7B	0.9900
O2—C8	1.2105 (16)	C8—C9	1.4961 (19)
N1—C1	1.3201 (19)	C9—C10	1.484 (2)
N1—C5	1.3111 (18)	C9—C11	1.339 (2)
N2—C3	1.3522 (16)	C10—H10A	0.9800
N2—C6	1.4594 (17)	C10—H10B	0.9800
N2—HN2	0.811 (18)	C10—H10C	0.9800
C1—C2	1.3625 (19)	C11—H11A	0.9500
C2—C3	1.4072 (18)	C11—H11B	0.9500
C3—C4	1.4030 (18)		
C8—O1—C7	116.31 (10)	C7—C6—H6A	109.1
C5—N1—C1	114.56 (11)	C7—C6—H6B	109.1
C3—N2—C6	126.76 (11)	O1—C7—C6	106.82 (10)
C3—N2—HN2	114.8 (11)	O1—C7—H7A	110.4
C6—N2—HN2	115.4 (12)	O1—C7—H7B	110.4
F1—C1—C2	118.98 (13)	C6—C7—H7A	110.4
N1—C1—F1	116.09 (12)	C6—C7—H7B	110.4
N1—C1—C2	124.93 (13)	H7A—C7—H7B	108.6
F2—C2—C1	120.90 (12)	O1—C8—C9	112.50 (11)
F2—C2—C3	117.95 (11)	O2—C8—O1	122.86 (13)
C1—C2—C3	121.13 (12)	O2—C8—C9	124.62 (13)
N2—C3—C2	119.91 (12)	C10—C9—C8	118.83 (13)
N2—C3—C4	126.72 (12)	C11—C9—C8	117.68 (13)
C4—C3—C2	113.32 (11)	C11—C9—C10	123.46 (14)
F3—C4—C3	121.52 (11)	C9—C10—H10A	109.5
F3—C4—C5	118.55 (12)	C9—C10—H10B	109.5

C5—C4—C3	119.92 (12)	C9—C10—H10C	109.5
F4—C5—C4	117.72 (12)	H10A—C10—H10B	109.5
N1—C5—F4	116.16 (11)	H10A—C10—H10C	109.5
N1—C5—C4	126.12 (13)	H10B—C10—H10C	109.5
N2—C6—H6A	109.1	C9—C11—H11A	120.0
N2—C6—H6B	109.1	C9—C11—H11B	120.0
N2—C6—C7	112.48 (11)	H11A—C11—H11B	120.0
H6A—C6—H6B	107.8		
F1—C1—C2—F2	-0.02 (19)	C1—N1—C5—C4	1.0 (2)
F1—C1—C2—C3	178.48 (11)	C1—C2—C3—N2	178.87 (12)
F2—C2—C3—N2	-2.59 (18)	C1—C2—C3—C4	1.25 (18)
F2—C2—C3—C4	179.79 (11)	C2—C3—C4—F3	179.97 (11)
F3—C4—C5—F4	-1.19 (18)	C2—C3—C4—C5	-0.49 (18)
F3—C4—C5—N1	178.86 (12)	C3—N2—C6—C7	-81.68 (16)
O1—C8—C9—C10	-8.07 (19)	C3—C4—C5—F4	179.25 (11)
O1—C8—C9—C11	170.13 (13)	C3—C4—C5—N1	-0.7 (2)
O2—C8—C9—C10	173.30 (15)	C5—N1—C1—F1	-179.66 (11)
O2—C8—C9—C11	-8.5 (2)	C5—N1—C1—C2	-0.2 (2)
N1—C1—C2—F2	-179.47 (12)	C6—N2—C3—C2	160.42 (13)
N1—C1—C2—C3	-1.0 (2)	C6—N2—C3—C4	-22.3 (2)
N2—C3—C4—F3	2.5 (2)	C7—O1—C8—O2	-0.88 (19)
N2—C3—C4—C5	-177.92 (13)	C7—O1—C8—C9	-179.54 (11)
N2—C6—C7—O1	61.78 (13)	C8—O1—C7—C6	179.42 (11)
C1—N1—C5—F4	-178.91 (11)		

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

Cg11 is the centroid of the C1—C5/N1 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—HN2 \cdots O2 ⁱ	0.811 (18)	2.119 (17)	2.8296 (15)	146.3 (15)
C6—H6B \cdots F3	0.99	2.23	2.9004 (15)	124
C7—H7B \cdots F3 ⁱⁱ	0.99	2.57	3.5368 (15)	167
C7—H7B \cdots F4 ⁱⁱ	0.99	2.63	3.3646 (16)	131
C7—H7A \cdots Cg1 ⁱⁱⁱ	0.99	2.89	3.6047 (15)	130

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