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(*E*)-3-(4-Fluorophenyl)-1-[1-(4-fluorophenyl)-5-methyl-1*H*-1,2,3-triazol-4-yl]prop-2-en-1-one

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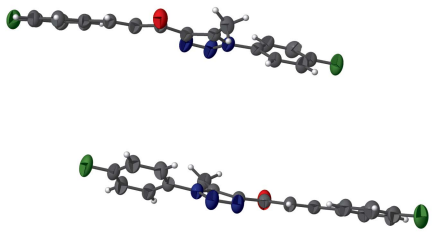
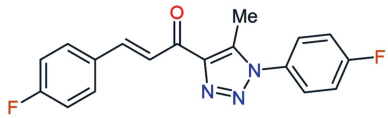
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{18}H_{13}F_2N_3O$, comprises two molecules with similar conformations. In the crystal, weak C—H···F interactions form chains of molecules and the chains are stacked to form layers parallel to (101).

3D view



Chemical scheme



Structure description

The asymmetric unit comprises two molecules of $C_{18}H_{13}F_2N_3O$ (Fig. 1) with similar conformations (r.m.s. overlay fit = 0.180 Å). In the C1 molecule, the dihedral angles between the triazole ring and the adjacent and remote fluorobenzene rings are 39.63 (11) and 17.88 (11)°, respectively. Equivalent values for the C19 molecule are 34.67 (10) and 16.55 (11)°, respectively.

In the crystal, very weak C—H···F interactions link the molecules into chains (Table 1, Fig. 2) and the chains are stacked to form layers parallel to (101) (Fig. 3). Weak aromatic π–π stacking is also observed [shortest centroid–centroid separation = 3.7332 (12) Å].

Synthesis and crystallization

1-[1-(4-Fluorophenyl)-5-methyl-1*H*-1,2,3-triazol-4-yl]ethanone, 4-fluorobenzaldehyde and sodium hydroxide (10%) were mixed in ethanol at 20–25°C for 4 h. Yellow plates (m.p. 167–168°C) were obtained following recrystallization from dimethylformamide solution of the solid obtained after work-up.

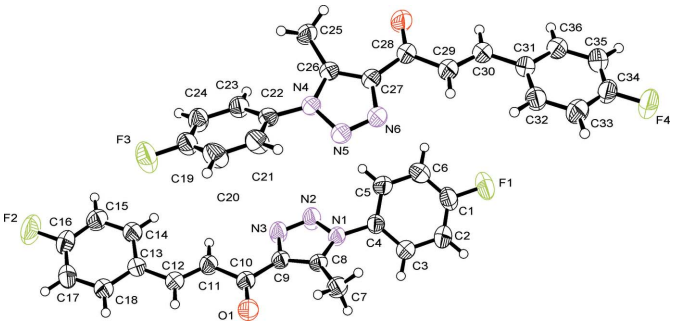


Figure 1
An *ORTEP* representation of the two unique molecules showing 50% probability ellipsoids.

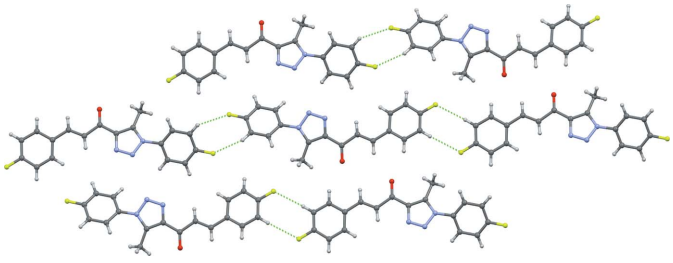


Figure 2
Intermolecular C—H···F interactions forming chains.

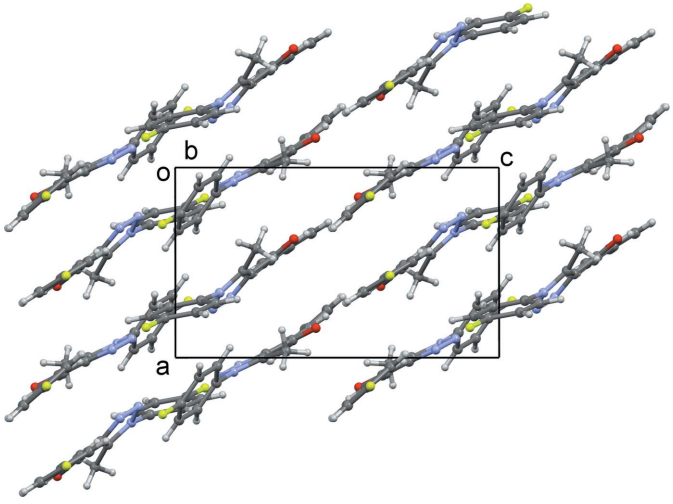


Figure 3
Crystal packing showing layers parallel to (101).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24···F1^{i}	0.93	2.73	3.418 (2)	132
C35—H35···F2^{ii}	0.93	2.70	3.608 (2)	164
C2—H2···F3^{iii}	0.93	2.65	3.395 (2)	137
C17—H17···F4^{iv}	0.93	2.62	3.546 (2)	178

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{13}F_2N_3O$
M_r	325.31
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.1891 (4), 14.1804 (6), 14.5050 (6)
α, β, γ (°)	68.075 (4), 84.220 (4), 74.627 (4)
V (Å^3)	1506.65 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.33 × 0.21 × 0.10
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.503, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26379, 7530, 4890
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.700
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.141, 1.05
No. of reflections	7530
No. of parameters	435
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.21

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Funding information

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full crystallographic data

IUCrData (2018). **3**, x171841 [https://doi.org/10.1107/S2414314617018417]

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(*E*)-3-(4-Fluorophenyl)-1-[1-(4-fluorophenyl)-5-methyl-1*H*-1,2,3-triazol-4-yl]prop-2-en-1-one

Crystal data

$C_{18}H_{13}F_2N_3O$
M_r = 325.31
Triclinic, $P\overline{1}$
a = 8.1891 (4) Å
b = 14.1804 (6) Å
c = 14.5050 (6) Å
α = 68.075 (4)°
β = 84.220 (4)°
γ = 74.627 (4)°
V = 1506.65 (13) Å^3
Z = 4
$F(000)$ = 672
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6895 reflections
θ = 4.2–27.7°
μ = 0.11 mm^{-1}
T = 296 K
Plate, yellow
0.33 × 0.21 × 0.10 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.503, T_{max} = 1.000
26379 measured reflections
7530 independent reflections
4890 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 29.8°, θ_{min} = 3.0°
h = −11→11
k = −19→19
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.141
S = 1.05
7530 reflections
435 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.4741P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Experimental. Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

Refinement. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C), and were allowed to spin about the C—C bond. Aromatic C—H distances were set to 0.93 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2075 (3)	0.01266 (16)	0.03379 (16)	0.0604 (5)
C2	0.2384 (3)	0.05994 (16)	−0.06481 (16)	0.0667 (6)
H2	0.2281	0.1319	−0.0926	0.080*
C3	0.2854 (3)	−0.00171 (14)	−0.12258 (14)	0.0574 (5)
H3	0.3067	0.0286	−0.1901	0.069*
C4	0.3003 (2)	−0.10814 (13)	−0.07944 (13)	0.0451 (4)
C5	0.2665 (3)	−0.15357 (15)	0.02006 (14)	0.0589 (5)
H5	0.2756	−0.2254	0.0484	0.071*
C6	0.2191 (3)	−0.09221 (17)	0.07755 (15)	0.0645 (6)
H6	0.1956	−0.1218	0.1448	0.077*
C7	0.5744 (2)	−0.10855 (15)	−0.24935 (15)	0.0554 (5)
H7A	0.5199	−0.0457	−0.3017	0.083*
H7B	0.6744	−0.1441	−0.2748	0.083*
H7C	0.6049	−0.0907	−0.1968	0.083*
C8	0.4564 (2)	−0.17840 (12)	−0.21012 (12)	0.0407 (4)
C9	0.4406 (2)	−0.26215 (13)	−0.23169 (13)	0.0434 (4)
C10	0.5329 (2)	−0.30726 (13)	−0.30344 (13)	0.0459 (4)
C11	0.5127 (2)	−0.41066 (14)	−0.29353 (14)	0.0484 (4)
H11	0.4446	−0.4428	−0.2426	0.058*
C12	0.5872 (2)	−0.45986 (13)	−0.35404 (13)	0.0466 (4)
H12	0.6513	−0.4247	−0.4056	0.056*
C13	0.5791 (2)	−0.56363 (13)	−0.34807 (13)	0.0452 (4)
C14	0.4970 (3)	−0.62760 (15)	−0.27110 (14)	0.0562 (5)
H14	0.4438	−0.6037	−0.2214	0.067*
C15	0.4930 (3)	−0.72559 (16)	−0.26704 (16)	0.0636 (5)
H15	0.4386	−0.7682	−0.2152	0.076*
C16	0.5715 (3)	−0.75854 (15)	−0.34159 (17)	0.0614 (5)
C17	0.6531 (3)	−0.69911 (16)	−0.41866 (16)	0.0638 (5)
H17	0.7049	−0.7236	−0.4682	0.077*
C18	0.6566 (3)	−0.60140 (15)	−0.42123 (14)	0.0549 (5)
H18	0.7123	−0.5599	−0.4733	0.066*
C19	1.2425 (2)	−0.66173 (15)	0.01546 (14)	0.0517 (4)
C20	1.3283 (3)	−0.59030 (17)	0.01026 (15)	0.0616 (5)

H20	1.4229	−0.5834	−0.0306	0.074*
C21	1.2736 (3)	−0.52812 (16)	0.06637 (14)	0.0586 (5)
H21	1.3317	−0.4792	0.0641	0.070*
C22	1.1323 (2)	−0.53858 (13)	0.12588 (12)	0.0414 (4)
C23	1.0451 (2)	−0.61035 (13)	0.12862 (13)	0.0470 (4)
H23	0.9485	−0.6164	0.1678	0.056*
C24	1.1016 (2)	−0.67331 (15)	0.07298 (14)	0.0534 (5)
H24	1.0446	−0.7226	0.0747	0.064*
C25	0.9663 (3)	−0.58167 (13)	0.34081 (14)	0.0547 (5)
H25A	0.8549	−0.5847	0.3290	0.082*
H25B	0.9730	−0.5846	0.4076	0.082*
H25C	1.0483	−0.6400	0.3318	0.082*
C26	1.0016 (2)	−0.48221 (13)	0.26976 (12)	0.0413 (4)
C27	0.9802 (2)	−0.38655 (13)	0.27927 (13)	0.0463 (4)
C28	0.9078 (2)	−0.35116 (13)	0.36098 (13)	0.0478 (4)
C29	0.9169 (3)	−0.24485 (14)	0.34965 (14)	0.0526 (4)
H29	0.9774	−0.2092	0.2962	0.063*
C30	0.8435 (2)	−0.19792 (14)	0.41170 (13)	0.0494 (4)
H30	0.7826	−0.2348	0.4641	0.059*
C31	0.8486 (2)	−0.09345 (13)	0.40616 (13)	0.0468 (4)
C32	0.9495 (3)	−0.03399 (15)	0.33795 (15)	0.0558 (5)
H32	1.0171	−0.0611	0.2938	0.067*
C33	0.9505 (3)	0.06391 (16)	0.33501 (16)	0.0609 (5)
H33	1.0179	0.1031	0.2895	0.073*
C34	0.8501 (3)	0.10242 (14)	0.40055 (16)	0.0572 (5)
C35	0.7489 (3)	0.04812 (15)	0.46811 (16)	0.0614 (5)
H35	0.6812	0.0765	0.5114	0.074*
C36	0.7492 (3)	−0.05020 (14)	0.47070 (14)	0.0556 (5)
H36	0.6811	−0.0884	0.5168	0.067*
N1	0.34173 (18)	−0.17422 (11)	−0.13693 (11)	0.0452 (3)
N2	0.2574 (2)	−0.25153 (13)	−0.11516 (13)	0.0586 (4)
N3	0.3186 (2)	−0.30441 (12)	−0.17205 (12)	0.0549 (4)
N4	1.07488 (19)	−0.46919 (11)	0.17951 (10)	0.0453 (3)
N5	1.0991 (2)	−0.36974 (12)	0.13550 (11)	0.0628 (5)
N6	1.0419 (2)	−0.32099 (12)	0.19610 (12)	0.0606 (4)
O1	0.62385 (19)	−0.26083 (11)	−0.36626 (10)	0.0658 (4)
O2	0.84447 (19)	−0.40717 (10)	0.43345 (10)	0.0636 (4)
F1	0.1592 (2)	0.07284 (11)	0.09065 (10)	0.0896 (4)
F2	0.5683 (2)	−0.85579 (10)	−0.33684 (12)	0.0940 (5)
F3	1.29847 (17)	−0.72282 (11)	−0.04006 (10)	0.0808 (4)
F4	0.85150 (19)	0.19891 (9)	0.39781 (11)	0.0828 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0705 (13)	0.0620 (12)	0.0615 (12)	−0.0169 (10)	0.0053 (10)	−0.0377 (11)
C2	0.0948 (16)	0.0473 (11)	0.0667 (13)	−0.0239 (11)	0.0071 (12)	−0.0275 (10)
C3	0.0817 (14)	0.0459 (10)	0.0473 (10)	−0.0225 (10)	0.0058 (10)	−0.0167 (9)

C4	0.0502 (10)	0.0429 (9)	0.0470 (10)	−0.0160 (7)	0.0068 (8)	−0.0202 (8)
C5	0.0767 (14)	0.0467 (10)	0.0513 (11)	−0.0178 (9)	0.0158 (10)	−0.0177 (9)
C6	0.0807 (15)	0.0627 (13)	0.0494 (11)	−0.0168 (11)	0.0130 (10)	−0.0232 (10)
C7	0.0626 (12)	0.0536 (11)	0.0584 (11)	−0.0315 (9)	0.0137 (9)	−0.0214 (9)
C8	0.0446 (9)	0.0378 (8)	0.0396 (8)	−0.0150 (7)	0.0058 (7)	−0.0119 (7)
C9	0.0486 (10)	0.0383 (9)	0.0441 (9)	−0.0165 (7)	0.0061 (7)	−0.0135 (7)
C10	0.0508 (10)	0.0415 (9)	0.0459 (9)	−0.0147 (8)	0.0056 (8)	−0.0154 (8)
C11	0.0548 (10)	0.0448 (10)	0.0503 (10)	−0.0186 (8)	0.0080 (8)	−0.0201 (8)
C12	0.0534 (10)	0.0427 (9)	0.0441 (9)	−0.0136 (8)	0.0024 (8)	−0.0154 (8)
C13	0.0494 (10)	0.0434 (9)	0.0434 (9)	−0.0112 (7)	0.0010 (8)	−0.0167 (8)
C14	0.0694 (13)	0.0512 (11)	0.0520 (11)	−0.0205 (9)	0.0122 (9)	−0.0222 (9)
C15	0.0754 (14)	0.0521 (11)	0.0656 (13)	−0.0279 (10)	0.0132 (11)	−0.0191 (10)
C16	0.0702 (13)	0.0431 (10)	0.0762 (14)	−0.0150 (9)	−0.0031 (11)	−0.0260 (10)
C17	0.0777 (14)	0.0532 (11)	0.0676 (13)	−0.0141 (10)	0.0098 (11)	−0.0339 (11)
C18	0.0654 (12)	0.0490 (10)	0.0509 (10)	−0.0154 (9)	0.0099 (9)	−0.0205 (9)
C19	0.0542 (11)	0.0545 (11)	0.0509 (10)	−0.0130 (9)	0.0063 (9)	−0.0260 (9)
C20	0.0556 (11)	0.0835 (15)	0.0582 (12)	−0.0335 (11)	0.0210 (9)	−0.0338 (11)
C21	0.0649 (12)	0.0717 (13)	0.0562 (11)	−0.0410 (10)	0.0155 (10)	−0.0293 (10)
C22	0.0491 (9)	0.0405 (9)	0.0368 (8)	−0.0168 (7)	0.0013 (7)	−0.0127 (7)
C23	0.0494 (10)	0.0464 (10)	0.0497 (10)	−0.0193 (8)	0.0099 (8)	−0.0197 (8)
C24	0.0593 (11)	0.0508 (10)	0.0608 (11)	−0.0248 (9)	0.0106 (9)	−0.0272 (9)
C25	0.0724 (13)	0.0399 (9)	0.0494 (10)	−0.0208 (9)	0.0156 (9)	−0.0126 (8)
C26	0.0470 (9)	0.0380 (9)	0.0384 (8)	−0.0143 (7)	0.0024 (7)	−0.0112 (7)
C27	0.0602 (11)	0.0378 (9)	0.0424 (9)	−0.0185 (8)	0.0013 (8)	−0.0121 (7)
C28	0.0579 (11)	0.0399 (9)	0.0460 (10)	−0.0137 (8)	0.0012 (8)	−0.0151 (8)
C29	0.0681 (12)	0.0442 (10)	0.0484 (10)	−0.0203 (9)	0.0048 (9)	−0.0167 (8)
C30	0.0587 (11)	0.0440 (10)	0.0459 (10)	−0.0146 (8)	0.0020 (8)	−0.0159 (8)
C31	0.0558 (10)	0.0409 (9)	0.0444 (9)	−0.0111 (8)	−0.0017 (8)	−0.0163 (8)
C32	0.0642 (12)	0.0547 (11)	0.0561 (11)	−0.0203 (9)	0.0095 (9)	−0.0271 (9)
C33	0.0696 (13)	0.0536 (11)	0.0655 (13)	−0.0276 (10)	0.0049 (10)	−0.0211 (10)
C34	0.0723 (13)	0.0405 (10)	0.0627 (12)	−0.0126 (9)	−0.0131 (10)	−0.0205 (9)
C35	0.0789 (14)	0.0496 (11)	0.0587 (12)	−0.0101 (10)	0.0024 (10)	−0.0275 (10)
C36	0.0706 (13)	0.0474 (10)	0.0488 (10)	−0.0163 (9)	0.0077 (9)	−0.0184 (9)
N1	0.0529 (8)	0.0399 (7)	0.0481 (8)	−0.0206 (6)	0.0114 (7)	−0.0185 (7)
N2	0.0677 (10)	0.0558 (9)	0.0683 (10)	−0.0358 (8)	0.0276 (8)	−0.0333 (9)
N3	0.0636 (10)	0.0495 (9)	0.0645 (10)	−0.0296 (7)	0.0232 (8)	−0.0301 (8)
N4	0.0620 (9)	0.0388 (7)	0.0398 (7)	−0.0238 (7)	0.0061 (7)	−0.0132 (6)
N5	0.1073 (14)	0.0463 (9)	0.0442 (9)	−0.0409 (9)	0.0165 (9)	−0.0161 (7)
N6	0.0997 (13)	0.0444 (9)	0.0451 (9)	−0.0340 (9)	0.0108 (9)	−0.0162 (7)
O1	0.0836 (10)	0.0560 (8)	0.0648 (9)	−0.0332 (7)	0.0338 (8)	−0.0273 (7)
O2	0.0879 (10)	0.0489 (8)	0.0548 (8)	−0.0250 (7)	0.0209 (7)	−0.0193 (7)
F1	0.1226 (12)	0.0847 (9)	0.0852 (9)	−0.0274 (8)	0.0181 (8)	−0.0605 (8)
F2	0.1197 (12)	0.0538 (7)	0.1244 (12)	−0.0332 (8)	0.0155 (9)	−0.0458 (8)
F3	0.0878 (9)	0.0880 (9)	0.0915 (9)	−0.0308 (7)	0.0328 (7)	−0.0623 (8)
F4	0.1129 (11)	0.0499 (7)	0.0981 (10)	−0.0264 (7)	−0.0075 (8)	−0.0345 (7)

Geometric parameters (Å, º)

C1—F1	1.359 (2)	C19—C24	1.363 (3)
C1—C6	1.362 (3)	C20—C21	1.376 (3)
C1—C2	1.364 (3)	C20—H20	0.9300
C2—C3	1.385 (3)	C21—C22	1.378 (2)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.377 (2)	C22—C23	1.377 (2)
C3—H3	0.9300	C22—N4	1.431 (2)
C4—C5	1.376 (3)	C23—C24	1.381 (2)
C4—N1	1.430 (2)	C23—H23	0.9300
C5—C6	1.379 (3)	C24—H24	0.9300
C5—H5	0.9300	C25—C26	1.485 (2)
C6—H6	0.9300	C25—H25A	0.9600
C7—C8	1.488 (2)	C25—H25B	0.9600
C7—H7A	0.9600	C25—H25C	0.9600
C7—H7B	0.9600	C26—N4	1.352 (2)
C7—H7C	0.9600	C26—C27	1.378 (2)
C8—N1	1.353 (2)	C27—N6	1.365 (2)
C8—C9	1.375 (2)	C27—C28	1.467 (2)
C9—N3	1.365 (2)	C28—O2	1.220 (2)
C9—C10	1.465 (2)	C28—C29	1.476 (2)
C10—O1	1.222 (2)	C29—C30	1.319 (2)
C10—C11	1.471 (2)	C29—H29	0.9300
C11—C12	1.324 (2)	C30—C31	1.465 (2)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.460 (2)	C31—C36	1.388 (2)
C12—H12	0.9300	C31—C32	1.398 (3)
C13—C18	1.387 (2)	C32—C33	1.375 (3)
C13—C14	1.392 (2)	C32—H32	0.9300
C14—C15	1.378 (3)	C33—C34	1.367 (3)
C14—H14	0.9300	C33—H33	0.9300
C15—C16	1.371 (3)	C34—F4	1.357 (2)
C15—H15	0.9300	C34—C35	1.361 (3)
C16—C17	1.360 (3)	C35—C36	1.380 (3)
C16—F2	1.362 (2)	C35—H35	0.9300
C17—C18	1.380 (3)	C36—H36	0.9300
C17—H17	0.9300	N1—N2	1.3701 (19)
C18—H18	0.9300	N2—N3	1.294 (2)
C19—C20	1.355 (3)	N4—N5	1.3735 (19)
C19—F3	1.358 (2)	N5—N6	1.292 (2)
F1—C1—C6	118.35 (19)	C21—C20—H20	120.5
F1—C1—C2	118.77 (19)	C20—C21—C22	119.83 (17)
C6—C1—C2	122.86 (18)	C20—C21—H21	120.1
C1—C2—C3	118.45 (19)	C22—C21—H21	120.1
C1—C2—H2	120.8	C23—C22—C21	120.20 (16)
C3—C2—H2	120.8	C23—C22—N4	121.59 (15)

C4—C3—C2	119.59 (18)	C21—C22—N4	118.11 (15)
C4—C3—H3	120.2	C22—C23—C24	119.75 (16)
C2—C3—H3	120.2	C22—C23—H23	120.1
C5—C4—C3	120.70 (17)	C24—C23—H23	120.1
C5—C4—N1	117.69 (15)	C19—C24—C23	118.68 (17)
C3—C4—N1	121.52 (16)	C19—C24—H24	120.7
C4—C5—C6	119.75 (18)	C23—C24—H24	120.7
C4—C5—H5	120.1	C26—C25—H25A	109.5
C6—C5—H5	120.1	C26—C25—H25B	109.5
C1—C6—C5	118.65 (19)	H25A—C25—H25B	109.5
C1—C6—H6	120.7	C26—C25—H25C	109.5
C5—C6—H6	120.7	H25A—C25—H25C	109.5
C8—C7—H7A	109.5	H25B—C25—H25C	109.5
C8—C7—H7B	109.5	N4—C26—C27	103.98 (14)
H7A—C7—H7B	109.5	N4—C26—C25	125.31 (15)
C8—C7—H7C	109.5	C27—C26—C25	130.60 (16)
H7A—C7—H7C	109.5	N6—C27—C26	108.92 (15)
H7B—C7—H7C	109.5	N6—C27—C28	120.75 (15)
N1—C8—C9	103.99 (14)	C26—C27—C28	130.32 (15)
N1—C8—C7	124.74 (15)	O2—C28—C27	121.35 (15)
C9—C8—C7	131.19 (15)	O2—C28—C29	122.77 (17)
N3—C9—C8	109.02 (15)	C27—C28—C29	115.88 (15)
N3—C9—C10	120.88 (15)	C30—C29—C28	123.18 (17)
C8—C9—C10	130.09 (15)	C30—C29—H29	118.4
O1—C10—C9	120.54 (15)	C28—C29—H29	118.4
O1—C10—C11	122.96 (16)	C29—C30—C31	126.38 (17)
C9—C10—C11	116.48 (15)	C29—C30—H30	116.8
C12—C11—C10	122.81 (16)	C31—C30—H30	116.8
C12—C11—H11	118.6	C36—C31—C32	117.71 (16)
C10—C11—H11	118.6	C36—C31—C30	119.36 (16)
C11—C12—C13	126.70 (17)	C32—C31—C30	122.93 (16)
C11—C12—H12	116.7	C33—C32—C31	121.17 (18)
C13—C12—H12	116.7	C33—C32—H32	119.4
C18—C13—C14	117.89 (16)	C31—C32—H32	119.4
C18—C13—C12	119.41 (16)	C34—C33—C32	118.52 (19)
C14—C13—C12	122.69 (16)	C34—C33—H33	120.7
C15—C14—C13	121.32 (18)	C32—C33—H33	120.7
C15—C14—H14	119.3	F4—C34—C35	118.76 (19)
C13—C14—H14	119.3	F4—C34—C33	118.50 (19)
C16—C15—C14	118.13 (19)	C35—C34—C33	122.74 (17)
C16—C15—H15	120.9	C34—C35—C36	118.30 (19)
C14—C15—H15	120.9	C34—C35—H35	120.8
C17—C16—F2	119.13 (19)	C36—C35—H35	120.8
C17—C16—C15	122.97 (18)	C35—C36—C31	121.56 (18)
F2—C16—C15	117.90 (19)	C35—C36—H36	119.2
C16—C17—C18	118.12 (19)	C31—C36—H36	119.2
C16—C17—H17	120.9	C8—N1—N2	110.51 (13)
C18—C17—H17	120.9	C8—N1—C4	132.05 (14)

C17—C18—C13	121.57 (18)	N2—N1—C4	117.40 (13)
C17—C18—H18	119.2	N3—N2—N1	107.40 (13)
C13—C18—H18	119.2	N2—N3—C9	109.07 (14)
C20—C19—F3	118.33 (16)	C26—N4—N5	110.53 (14)
C20—C19—C24	122.52 (17)	C26—N4—C22	132.38 (14)
F3—C19—C24	119.15 (17)	N5—N4—C22	117.07 (13)
C19—C20—C21	119.01 (17)	N6—N5—N4	107.30 (13)
C19—C20—H20	120.5	N5—N6—C27	109.27 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24···F1^{i}	0.93	2.73	3.418 (2)	132
C35—H35···F2^{ii}	0.93	2.70	3.608 (2)	164
C2—H2···F3^{iii}	0.93	2.65	3.395 (2)	137
C17—H17···F4^{iv}	0.93	2.62	3.546 (2)	178

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