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1-[3-(2-Benzyloxy-6-hydroxy-4-methylphenyl)-5-[3,5-bis(trifluoromethyl)phenyl]-4,5-dihydro-1*H*-pyrazol-1-yl]propane-1-one

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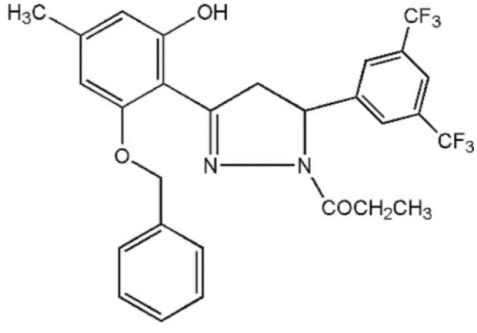
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.070; wR factor = 0.246; data-to-parameter ratio = 12.8.

In the title compound, $C_{28}H_{24}F_6N_2O_3$, the mean plane of the central pyrazoline ring forms dihedral angles of 2.08 (9) and 69.02 (16)° with the 2-benzyloxy-6-hydroxy-4-methylphenyl and 3,5-bis(trifluoromethyl)phenyl rings, respectively. The dihedral angle between the mean planes of the pyrazoline and 3,5-bis(trifluoromethyl)phenyl rings is 68.97 (9)°. An intramolecular O—H···N hydrogen bond is observed, which forms an S(6) graph-set motif. In the crystal, pairs of weak C—H···F halogen interactions link the molecules into inversion dimers while molecular chains along [100] are formed by C—H···O contacts.

Related literature

For pharmacalogical and anticancer properties of pyrazoline derivatives, see: Smith *et al.* (2001). For graph-set motifs, see: Bernstein *et al.*, (1995). For related structures, see: Patel *et al.* (2007, 2012).



Experimental

Crystal data

$C_{28}H_{24}F_6N_2O_3$
M_r = 550.49
Monoclinic, $P2_1/n$
a = 4.8822 (2) Å
b = 23.4752 (9) Å
c = 22.4311 (9) Å
β = 91.494 (2)°
V = 2569.97 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 273 K
0.54 × 0.34 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.951, T_{max} = 0.988
19610 measured reflections
4514 independent reflections
2491 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.246
S = 1.00
4514 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O16—H16···N2	0.82	1.84	2.568 (3)	147
C31—H31···O9^{i}	0.93	2.67	3.490 (4)	148
C21—H21···F37^{ii}	0.93	2.72	3.488 (6)	140
C29—H29···F33^{iii}	0.93	2.64	3.490 (5)	152

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2162).

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supporting information

Acta Cryst. (2013). E**69**, o840 [doi:10.1107/S160053681301180X]

1-[3-(2-Benzyloxy-6-hydroxy-4-methylphenyl)-5-[3,5-bis(trifluoromethyl)-phenyl]-4,5-dihydro-1*H*-pyrazol-1-yl]propane-1-one

U. H. Patel, S. A. Gandhi, V. M. Barot and N. V. S. Varma

S1. Comment

Pyrazoline derivatives, prominent nitrogen containing heterocyclic compounds, play an important role in medicinal chemistry. These derivatives are found to possess antidepressant, antioxidant, anti- inflammatory (Smith *et al.*, 2001), anticonvulsant, antimicrobial, antiviral, monoamine oxidase (MAO-A and MAO-B) inhibitor, and anticancer activity. Our on-going research is focused on the synthesis and crystal structures of related pyrazoline derivatives of these types of heterocyclic compounds (Patel *et al.* 2007, Patel *et al.* 2012). We report here the synthesis and crystal structure of the title compound, $C_{28}H_{24}N_2O_3F_6$, (I).

In (I), propionaldehyde, 3-benzyloxy-5-methyl-phenol and 1,3-bis-trifluro methyl benzene are bonded to N1, C3 and C5 of the pyrazoline ring, respectively. The dihedral angles between the mean planes of the pyrazoline ring and the 3-benzyl-oxy-5-methyl-phenol (C10—C15) and 1,3-bis-trifluro methyl benzene rings (C26—C31) are 2.03 (15)° and 69.02 (16)° respectively. An intra-molecular O16—H16···N2 hydrogen bond (Fig.1) forms an S1,1(6) graph set motif configuration (Bernstein *et al.*, 1995). The mean plane of the propionaldehyde group (C6—C8/O9) is inclined by 12.56 (13)° to the meam plane of the pyrazoline ring. Weak C—H···F Halogen intermolecular interactions are observed that form inversion dimers (Fig. 2).

S2. Experimental

1-[2-benzyloxy-6-hydroxy-4-methyl phenyl]-3-(3, 5-bis (trifluoromethyl) phenyl)prop-2-en-1-one (5 g m, 0.01 mole), hydrazine hydrate (0.70 g m, 0.014 mole) and butanoic acid (20 ml) were heated to 115–120 °C for 4 h. The resulting solution was concentrated and allowed to cool and then poured into ice. The resulting solid was filtered, washed with water, dried and rystallized from methanol as pale yellow needles.

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with C—H lengths of 0.93Å, 0.98Å (CH) or 0.96Å (CH_3) and O—H lengths of 0.82Å. The isotropic displacement parameters for these atoms were set to 1.19 to 1.20 (CH, CH_2), 1.50 (CH_3) or 1.49 (OH) times U_{eq} of the parent atom.

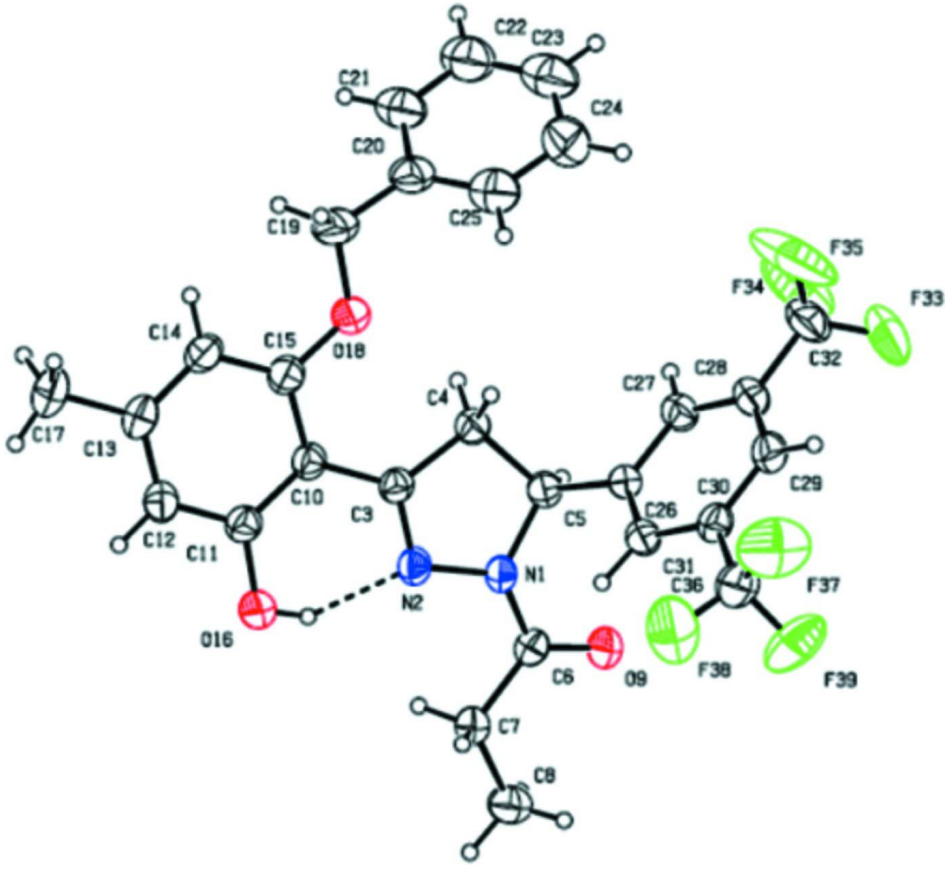

Figure 1

Molecular structure of the title compound,showing the atom labeling scheme with 50% probability displacement ellipsoids. The dashed line represents an O—H···N intramolecular hydrogen bond which forms an S1,1(6) graph set motif.

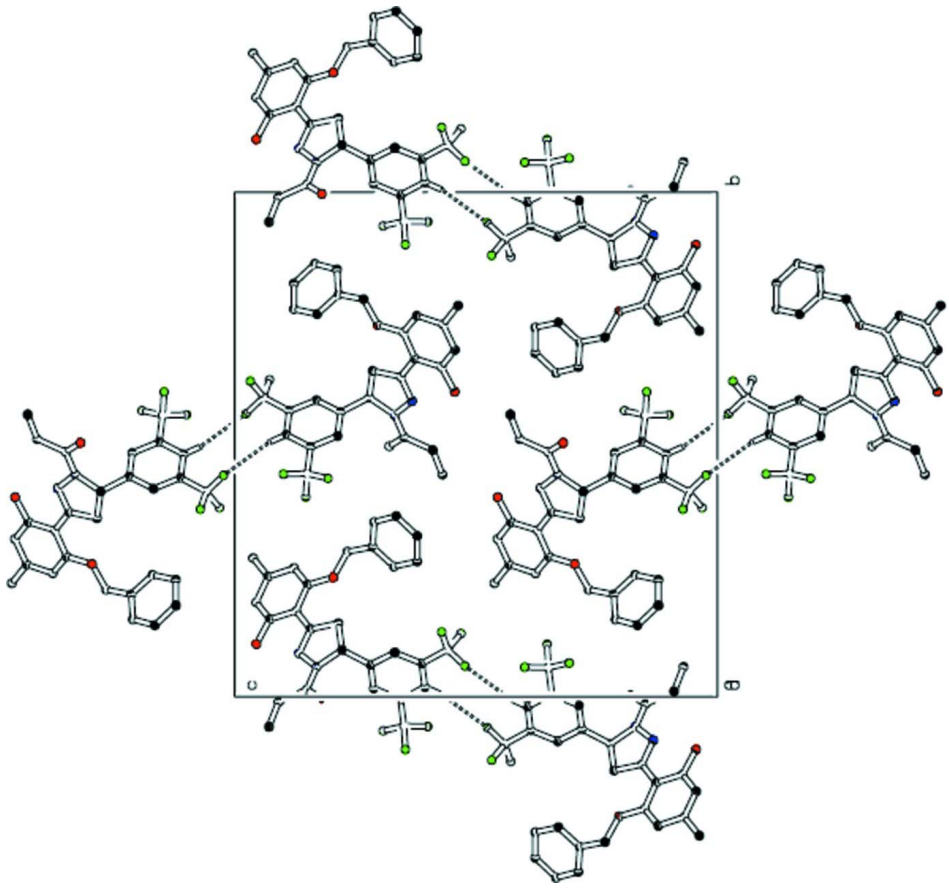

Figure 2

Molecular packing diagram the title compound. Dashed lines indicate weak C—H···F halogen intermolecular interactions which are displayed as inversion dimers. H atoms not involved with these weak intermolecular interactions have been deleted for clarity.

1-[3-(2-Benzyloxy-6-hydroxy-4-methylphenyl)-5-[3,5-bis(trifluoromethyl)phenyl]-4,5-dihydro-1*H*-pyrazol-1-yl]propane-1-one

Crystal data

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Hall symbol: -P 2yn
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c = 22.4311 (9) Å
β = 91.494 (2)°
V = 2569.97 (18) Å^3
Z = 4
$F(000)$ = 1136
D_x = 1.423 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 2.9–27.7°
μ = 0.12 mm^{-1}
T = 273 K
Needle, white
0.54 × 0.34 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
CCD scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.951, T_{max} = 0.988

19610 measured reflections
4514 independent reflections
2491 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
$h = -5 \rightarrow 5$
$k = -27 \rightarrow 27$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.246$
$S = 1.00$
4514 reflections
352 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
$w = 1/[\sigma^2(F_o^2) + (0.1524P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Special details

Experimental. IR (cm^{-1}): 2929 (C—H str. (*asym*) alkyl), 1458 (C—H def (*asym*)alkyl), 1387(C—H def (*sym*) alkyl), 3072 (C—H str.arom.), 1593. (C=Cstr. arom.), 1128 (C—H i.p.def arom.), 847 (C—H o.o.p.def.arom.), 1272 (C—O—C (*sym*) ether), 1066 (C—O—C (*asym*) ether), 3380($OH_{str.}$ phenol). 1659 (N—CO¬ CH_2CH_3), 1379 (N-$COCH_2CH_3$ def., pyrazoline), 1588 (C=N str., pyrazoline), 2863 (C—H ring (str.), pyrazoline), 682 (C—H def. of CH_2, pyrazoline), 1197 (C—N str., pyrazoline), 1117 (C—F str.).
1H NMR ($CDCl_3$) δp.p.m.: 0.96 (trip, 3H, J=7.3 &7.2 Hz), 1.70 (Qur, 2H),2.31(s,3*H*), 3.36 (dd, 1H, J=15.3 & 3.5 Hz), 3.83 (dd, 1H, J=11.7 & 7.2 Hz), 5.02 (s, 2H), 5.32 (trip, 1H, J= 3.1 & 8.08 Hz), 6.33 (S, 1H), 6.52 (S,1H), 7.16–7.23(m, 8H), 11.24 (s, 1H).
^{13}C NMR ($CDCl_3$) δp.p.m.: 21.98(C-1, CH_3), 70.91 (C-2,CH_2 C6 H5), 159.37(C-3,Pyrazoline), 46.49 (C-4,Pyrazoline), 57.92 (C-5, Pyrazoline), 170.03(C-6,CO CH_2 CH_3), 36.15 (C-7,CO CH_2 CH_3), 13.83 (C-8, CO CH_2 CH_3), 124.44(C-9, CF_3), 124.44 (C-10, CF_3).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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}
N1	0.1214 (5)	0.55900 (10)	0.66924 (11)	0.0539 (7)
N2	0.3088 (5)	0.58603 (11)	0.63303 (10)	0.0543 (7)
C3	0.3815 (6)	0.63423 (12)	0.65664 (13)	0.0496 (8)
C4	0.2432 (7)	0.64580 (13)	0.71404 (14)	0.0579 (8)
H4A	0.135	0.6804	0.7115	0.069*
H4B	0.3757	0.6492	0.7468	0.069*
C5	0.0589 (6)	0.59313 (13)	0.72178 (13)	0.0515 (8)
H5	−0.1338	0.6048	0.7195	0.062*
C6	−0.0355 (7)	0.51471 (13)	0.64937 (14)	0.0543 (8)
C7	0.0403 (7)	0.48937 (15)	0.59035 (15)	0.0658 (9)
H7A	0.2281	0.476	0.5933	0.079*

H7B	0.0315	0.519	0.5602	0.079*
C8	−0.1418 (8)	0.44063 (16)	0.57049 (18)	0.0830 (12)
H8A	−0.0827	0.4265	0.5327	0.124*
H8B	−0.3277	0.4537	0.5665	0.124*
H8C	−0.1307	0.4106	0.5995	0.124*
O9	−0.2171 (5)	0.49645 (10)	0.68000 (10)	0.0699 (7)
C10	0.5820 (6)	0.67000 (13)	0.62685 (13)	0.0532 (8)
C11	0.6938 (7)	0.65374 (13)	0.57238 (14)	0.0571 (8)
C12	0.8825 (7)	0.68729 (15)	0.54402 (15)	0.0654 (9)
H12	0.9499	0.6755	0.5076	0.079*
C13	0.9730 (7)	0.73805 (15)	0.56867 (17)	0.0640 (9)
C14	0.8683 (7)	0.75504 (14)	0.62281 (16)	0.0657 (10)
H14	0.9278	0.7889	0.6402	0.079*
C15	0.6766 (7)	0.72210 (14)	0.65103 (15)	0.0605 (9)
O16	0.6203 (5)	0.60455 (10)	0.54461 (10)	0.0770 (8)
H16	0.5078	0.5877	0.5646	0.115*
C17	1.1739 (8)	0.77503 (17)	0.53729 (18)	0.0844 (12)
H17A	1.2123	0.8083	0.5609	0.127*
H17B	1.0976	0.7863	0.4992	0.127*
H17C	1.3404	0.7542	0.5317	0.127*
O18	0.5648 (6)	0.73696 (10)	0.70381 (11)	0.0824 (8)
C19	0.6523 (9)	0.78764 (16)	0.73329 (19)	0.0842 (12)
H19A	0.6385	0.8197	0.7061	0.101*
H19B	0.842	0.7839	0.7467	0.101*
C20	0.4748 (8)	0.79714 (18)	0.78508 (18)	0.0758 (11)
C21	0.3242 (9)	0.8464 (2)	0.7888 (2)	0.0907 (13)
H21	0.3401	0.8733	0.7586	0.109*
C22	0.1532 (11)	0.8579 (3)	0.8341 (3)	0.1063 (15)
H22	0.0572	0.8921	0.8352	0.128*
C23	0.1262 (10)	0.8189 (3)	0.8770 (3)	0.1106 (17)
H23	0.0065	0.8262	0.9077	0.133*
C24	0.2689 (13)	0.7684 (3)	0.8775 (2)	0.1151 (17)
H24	0.2502	0.742	0.908	0.138*
C25	0.4458 (10)	0.7582 (2)	0.8295 (2)	0.0996 (14)
H25	0.5438	0.7242	0.8283	0.12*
C26	0.1172 (6)	0.56381 (12)	0.78105 (13)	0.0485 (8)
C27	0.0104 (7)	0.58758 (14)	0.83107 (14)	0.0611 (9)
H27	−0.1031	0.6192	0.827	0.073*
C28	0.0657 (8)	0.56612 (15)	0.88733 (15)	0.0690 (10)
C29	0.2329 (8)	0.51930 (16)	0.89386 (15)	0.0690 (10)
H29	0.2723	0.5044	0.9315	0.083*
C30	0.3422 (7)	0.49453 (13)	0.84349 (15)	0.0603 (9)
C31	0.2878 (6)	0.51677 (13)	0.78742 (14)	0.0546 (8)
H31	0.365	0.5003	0.7541	0.065*
C32	−0.0504 (12)	0.5936 (2)	0.94053 (18)	0.0946 (14)
C36	0.5136 (10)	0.44223 (17)	0.8505 (2)	0.0807 (12)
F37	0.3614 (6)	0.39586 (11)	0.85326 (17)	0.1375 (12)
F38	0.6768 (7)	0.43269 (13)	0.80719 (16)	0.1480 (14)

F39	0.6615 (8)	0.44101 (13)	0.89967 (16)	0.1546 (14)
F33	−0.1600 (12)	0.56096 (17)	0.97657 (17)	0.219 (3)
F34	0.1149 (8)	0.6254 (3)	0.9680 (2)	0.235 (3)
F35	−0.2551 (10)	0.6284 (2)	0.92844 (15)	0.190 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0651 (17)	0.0526 (16)	0.0442 (15)	−0.0098 (13)	0.0082 (12)	0.0046 (12)
N2	0.0614 (16)	0.0565 (17)	0.0448 (15)	−0.0068 (13)	0.0004 (12)	0.0073 (12)
C3	0.0554 (18)	0.0452 (18)	0.0480 (18)	0.0006 (14)	−0.0038 (14)	0.0049 (14)
C4	0.071 (2)	0.0496 (18)	0.054 (2)	0.0050 (15)	0.0087 (16)	0.0039 (15)
C5	0.0540 (18)	0.0507 (18)	0.0499 (18)	0.0048 (14)	0.0050 (14)	0.0034 (14)
C6	0.0599 (19)	0.0476 (18)	0.055 (2)	−0.0019 (15)	0.0010 (16)	0.0059 (15)
C7	0.074 (2)	0.064 (2)	0.059 (2)	−0.0114 (17)	0.0156 (17)	−0.0002 (16)
C8	0.091 (3)	0.076 (3)	0.083 (3)	−0.017 (2)	0.015 (2)	−0.023 (2)
O9	0.0737 (15)	0.0703 (16)	0.0666 (16)	−0.0161 (12)	0.0206 (12)	0.0007 (12)
C10	0.0591 (19)	0.0504 (18)	0.0498 (19)	−0.0019 (15)	0.0004 (15)	0.0066 (14)
C11	0.067 (2)	0.0492 (18)	0.055 (2)	−0.0003 (16)	−0.0012 (16)	0.0047 (16)
C12	0.073 (2)	0.065 (2)	0.059 (2)	−0.0020 (18)	0.0139 (17)	0.0091 (17)
C13	0.062 (2)	0.059 (2)	0.071 (2)	−0.0037 (17)	0.0012 (17)	0.0181 (18)
C14	0.080 (2)	0.0501 (19)	0.067 (2)	−0.0122 (17)	0.0000 (19)	0.0046 (16)
C15	0.066 (2)	0.059 (2)	0.056 (2)	−0.0091 (16)	−0.0026 (16)	0.0033 (16)
O16	0.0990 (19)	0.0673 (16)	0.0659 (16)	−0.0194 (13)	0.0254 (13)	−0.0101 (12)
C17	0.084 (3)	0.077 (3)	0.093 (3)	−0.017 (2)	0.012 (2)	0.022 (2)
O18	0.108 (2)	0.0729 (17)	0.0669 (17)	−0.0386 (14)	0.0217 (14)	−0.0174 (13)
C19	0.094 (3)	0.067 (2)	0.092 (3)	−0.022 (2)	0.011 (2)	−0.020 (2)
C20	0.082 (3)	0.070 (3)	0.075 (3)	−0.015 (2)	−0.001 (2)	−0.019 (2)
C21	0.095 (3)	0.089 (3)	0.089 (3)	−0.005 (3)	0.003 (2)	−0.026 (2)
C22	0.112 (4)	0.104 (4)	0.103 (4)	−0.005 (3)	0.006 (3)	−0.019 (3)
C23	0.100 (4)	0.123 (5)	0.109 (4)	−0.007 (3)	0.007 (3)	−0.048 (4)
C24	0.147 (5)	0.117 (4)	0.081 (4)	−0.023 (4)	0.004 (3)	−0.006 (3)
C25	0.112 (4)	0.094 (3)	0.093 (4)	−0.004 (3)	0.000 (3)	−0.011 (3)
C26	0.0526 (18)	0.0464 (17)	0.0467 (18)	−0.0022 (13)	0.0056 (14)	0.0002 (13)
C27	0.072 (2)	0.0548 (19)	0.057 (2)	0.0073 (16)	0.0118 (17)	0.0005 (16)
C28	0.095 (3)	0.063 (2)	0.050 (2)	0.003 (2)	0.0152 (18)	−0.0002 (17)
C29	0.090 (3)	0.069 (2)	0.048 (2)	−0.011 (2)	0.0017 (18)	0.0079 (17)
C30	0.071 (2)	0.0503 (19)	0.060 (2)	−0.0009 (16)	0.0009 (17)	0.0112 (16)
C31	0.0609 (19)	0.0533 (19)	0.0497 (19)	0.0025 (15)	0.0049 (15)	0.0012 (15)
C32	0.141 (4)	0.098 (3)	0.046 (2)	0.014 (3)	0.010 (3)	−0.008 (2)
C36	0.099 (3)	0.065 (3)	0.078 (3)	0.011 (2)	−0.009 (3)	0.018 (2)
F37	0.136 (2)	0.0594 (16)	0.216 (3)	0.0071 (15)	−0.006 (2)	0.0306 (18)
F38	0.167 (3)	0.128 (2)	0.152 (3)	0.088 (2)	0.065 (2)	0.053 (2)
F39	0.187 (3)	0.125 (2)	0.148 (3)	0.057 (2)	−0.078 (2)	0.0105 (19)
F33	0.400 (7)	0.148 (3)	0.119 (3)	0.008 (4)	0.160 (4)	−0.001 (2)
F34	0.156 (3)	0.362 (7)	0.188 (4)	−0.068 (4)	0.061 (3)	−0.206 (5)
F35	0.242 (4)	0.229 (4)	0.102 (2)	0.119 (4)	0.033 (3)	−0.038 (2)

Geometric parameters (Å, º)

N1—C6	1.360 (4)	C17—H17C	0.96
N1—N2	1.392 (3)	O18—C19	1.421 (4)
N1—C5	1.464 (4)	C19—C20	1.484 (5)
N2—C3	1.295 (4)	C19—H19A	0.97
C3—C10	1.464 (4)	C19—H19B	0.97
C3—C4	1.495 (4)	C20—C25	1.362 (6)
C4—C5	1.541 (4)	C20—C21	1.374 (6)
C4—H4A	0.97	C21—C22	1.359 (6)
C4—H4B	0.97	C21—H21	0.93
C5—C26	1.517 (4)	C22—C23	1.338 (7)
C5—H5	0.98	C22—H22	0.93
C6—O9	1.214 (4)	C23—C24	1.376 (8)
C6—C7	1.506 (5)	C23—H23	0.93
C7—C8	1.509 (5)	C24—C25	1.418 (7)
C7—H7A	0.97	C24—H24	0.93
C7—H7B	0.97	C25—H25	0.93
C8—H8A	0.96	C26—C27	1.368 (4)
C8—H8B	0.96	C26—C31	1.388 (4)
C8—H8C	0.96	C27—C28	1.379 (5)
C10—C11	1.404 (4)	C27—H27	0.93
C10—C15	1.411 (4)	C28—C29	1.374 (5)
C11—O16	1.356 (4)	C28—C32	1.482 (5)
C11—C12	1.380 (5)	C29—C30	1.390 (5)
C12—C13	1.381 (5)	C29—H29	0.93
C12—H12	0.93	C30—C31	1.381 (4)
C13—C14	1.389 (5)	C30—C36	1.492 (5)
C13—C17	1.499 (5)	C31—H31	0.93
C14—C15	1.380 (5)	C32—F33	1.244 (6)
C14—H14	0.93	C32—F34	1.251 (6)
C15—O18	1.362 (4)	C32—F35	1.315 (6)
O16—H16	0.82	C36—F38	1.291 (5)
C17—H17A	0.96	C36—F39	1.303 (5)
C17—H17B	0.96	C36—F37	1.320 (5)
C6—N1—N2	122.0 (3)	H17A—C17—H17C	109.5
C6—N1—C5	123.7 (3)	H17B—C17—H17C	109.5
N2—N1—C5	112.0 (2)	C15—O18—C19	119.7 (3)
C3—N2—N1	109.7 (2)	O18—C19—C20	108.4 (3)
N2—C3—C10	119.6 (3)	O18—C19—H19A	110
N2—C3—C4	112.7 (3)	C20—C19—H19A	110
C10—C3—C4	127.7 (3)	O18—C19—H19B	110
C3—C4—C5	103.3 (2)	C20—C19—H19B	110
C3—C4—H4A	111.1	H19A—C19—H19B	108.4
C5—C4—H4A	111.1	C25—C20—C21	117.1 (4)
C3—C4—H4B	111.1	C25—C20—C19	123.0 (4)
C5—C4—H4B	111.1	C21—C20—C19	119.9 (4)

H4A—C4—H4B	109.1	C22—C21—C20	123.5 (5)
N1—C5—C26	114.8 (2)	C22—C21—H21	118.2
N1—C5—C4	102.3 (2)	C20—C21—H21	118.2
C26—C5—C4	111.5 (2)	C23—C22—C21	118.5 (5)
N1—C5—H5	109.3	C23—C22—H22	120.8
C26—C5—H5	109.3	C21—C22—H22	120.8
C4—C5—H5	109.3	C22—C23—C24	122.4 (5)
O9—C6—N1	119.9 (3)	C22—C23—H23	118.8
O9—C6—C7	123.9 (3)	C24—C23—H23	118.8
N1—C6—C7	116.2 (3)	C23—C24—C25	117.3 (5)
C6—C7—C8	113.8 (3)	C23—C24—H24	121.4
C6—C7—H7A	108.8	C25—C24—H24	121.4
C8—C7—H7A	108.8	C20—C25—C24	121.2 (5)
C6—C7—H7B	108.8	C20—C25—H25	119.4
C8—C7—H7B	108.8	C24—C25—H25	119.4
H7A—C7—H7B	107.7	C27—C26—C31	118.7 (3)
C7—C8—H8A	109.5	C27—C26—C5	117.8 (3)
C7—C8—H8B	109.5	C31—C26—C5	123.3 (3)
H8A—C8—H8B	109.5	C26—C27—C28	122.1 (3)
C7—C8—H8C	109.5	C26—C27—H27	118.9
H8A—C8—H8C	109.5	C28—C27—H27	118.9
H8B—C8—H8C	109.5	C29—C28—C27	119.4 (3)
C11—C10—C15	116.1 (3)	C29—C28—C32	120.0 (3)
C11—C10—C3	121.4 (3)	C27—C28—C32	120.6 (4)
C15—C10—C3	122.5 (3)	C28—C29—C30	119.2 (3)
O16—C11—C12	116.5 (3)	C28—C29—H29	120.4
O16—C11—C10	121.8 (3)	C30—C29—H29	120.4
C12—C11—C10	121.7 (3)	C31—C30—C29	120.9 (3)
C11—C12—C13	121.2 (3)	C31—C30—C36	120.1 (3)
C11—C12—H12	119.4	C29—C30—C36	119.0 (3)
C13—C12—H12	119.4	C30—C31—C26	119.7 (3)
C12—C13—C14	118.5 (3)	C30—C31—H31	120.2
C12—C13—C17	121.2 (4)	C26—C31—H31	120.2
C14—C13—C17	120.3 (3)	F33—C32—F34	109.3 (5)
C15—C14—C13	120.6 (3)	F33—C32—F35	100.3 (5)
C15—C14—H14	119.7	F34—C32—F35	101.9 (5)
C13—C14—H14	119.7	F33—C32—C28	115.8 (4)
O18—C15—C14	123.2 (3)	F34—C32—C28	113.7 (5)
O18—C15—C10	114.9 (3)	F35—C32—C28	114.2 (4)
C14—C15—C10	121.9 (3)	F38—C36—F39	107.1 (4)
C11—O16—H16	109.5	F38—C36—F37	104.6 (4)
C13—C17—H17A	109.5	F39—C36—F37	104.0 (3)
C13—C17—H17B	109.5	F38—C36—C30	114.8 (3)
H17A—C17—H17B	109.5	F39—C36—C30	113.8 (4)
C13—C17—H17C	109.5	F37—C36—C30	111.6 (4)

N1—C6—C7—C8	−179.7 (3)	C15—O18—C19—C20	173.2 (3)
C14—C15—O18—C19	−2.2 (5)	O18—C19—C20—C21	−120.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O16—H16···N2	0.82	1.84	2.568 (3)	147
C31—H31···O9^{i}	0.93	2.67	3.490 (4)	148
C21—H21···F37^{ii}	0.93	2.72	3.488 (6)	140
C29—H29···F33^{iii}	0.93	2.64	3.490 (5)	152

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