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1-(2′-Ethoxy-4′-fluoro-[1,1′-biphenyl]-4-yl)-4-phenyl-1*H*-1,2,3-triazole

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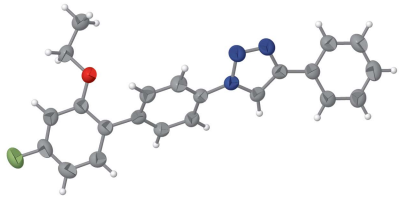
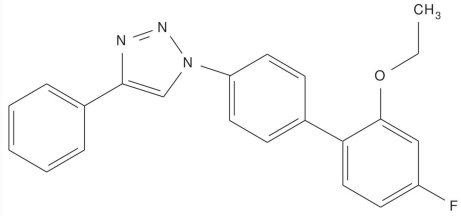
In the title compound, $C_{22}H_{18}FN_3O$, the triazole ring is planar. The plane of the triazole ring makes dihedral angles of 19.31 (10), 20.52 (10) and 39.82 (9)° with the planes of the benzene rings, indicating the overall nonplanarity of the molecule. No classical hydrogen bonds were observed in the structure.

3D view



Chemical scheme



Structure description

Nitrogen-containing heterocyclic compounds, such as 1,2,3-triazoles, have a wide-ranging biological spectrum, including anticancer activity (Duan *et al.*, 2013), antitubercular activity (Somu *et al.*, 2006), anti-HIV activity, antibacterial activity, antiallergic activity and selective β_3-adrenergic receptor agonism (Brockunier *et al.*, 2000). They also have a wide range of other applications, such as dyes, corrosion inhibition, photostabilizers, photographic materials, and in the field of agrochemicals. Owing to their wide range of biological and technical interest and as a part of our ongoing research on triazoles (Ashwini *et al.*, 2016), the title compound was synthesized from the 1,3-dipolar cyclo-addition of an azide an and alkyne in the presence of a copper(I) catalyst to form a 1,4-disubstituted triazoles, contributing to the popularization of 'click' chemistry as a highly effective method for the functionalization of triazoles.

In the title compound (Fig. 1), the triazole ring is planar, with atom N1 deviating by 0.004 (1) Å from the mean plane. The plane of the triazole ring makes dihedral angles of 19.31 (10), 20.52 (10) and 39.82 (9)°, respectively, with the planes of the C3–C8, C9–C14 and C15–C20 benzene rings, indicating the non-planarity of the molecule as a whole. The ethoxy group lies in the plane of the fluorophenyl ring and is in an antiperiplanar

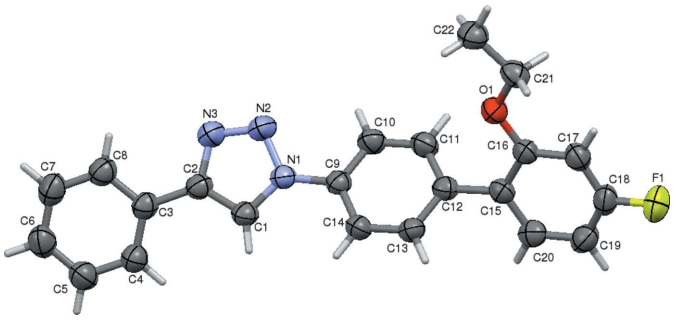


Figure 1
A view of the title molecule, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

conformation, as indicated by the torsion angle of −175.08 (16)°. No classical hydrogen bonds were observed in the structure.

Synthesis and crystallization

1-(4-Bromophenyl)-4-phenyl-1,2,3-triazole (1 mmol), 2-ethoxy-4-fluorobenzenboronic acid (1.2 mmol) and K_2CO_3 (3 mmol) were added to a mixture of ethanol, water and 1,4-dioxane in the ratio of 1:1:5 and taken into a pressure tube. The reaction mixture was stirred for 15 min in the presence of nitrogen gas to create inert atmosphere. Then Dikis, *i.e.* $[PdCl_2(PPh_3)_2]$, was added as a catalyst (0.1 mmol) to the reaction mass. The reaction mass was heated between 393 to 403 K for 30 min in a sealed tube and the progress of the reaction was monitored by thin-layer chromatography. The resultant mixture was filtered through a Celite bed and the filtrate concentrated under reduced pressure to remove the ethanol using a roto-evaporator. The reaction mass was extracted with ethyl acetate followed by a brine wash and dried over anhydrous sodium sulfate. The organic layer was evaporated under reduced pressure to get a crude product which was purified by column chromatography using 60:120 silica gel and EtOAc–hexane as a eluent to get the desired triazole as a white solid. Single crystals suitable for X-ray diffraction studies were obtained by the slow evaporation method by using ethanol as the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}FN_3O$
M_r	359.39
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	24.392 (3), 5.9336 (8), 12.3651 (16)
β (°)	100.828 (8)
V (Å^3)	1757.8 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.75
Crystal size (mm)	0.30 × 0.27 × 0.26
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.805, 0.828
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12946, 2882, 2093
R_{int}	0.062
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.140, 1.04
No. of reflections	2882
No. of parameters	246
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161712 [https://doi.org/10.1107/S2414314616017120]

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Crystal data

$C_{22}H_{18}FN_3O$
M_r = 359.39
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 24.392 (3) Å
b = 5.9336 (8) Å
c = 12.3651 (16) Å
β = 100.828 (8)°
V = 1757.8 (4) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.358 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2093 reflections
θ = 7.2–64.5°
μ = 0.75 mm^{-1}
T = 296 K
Rectangle, white
0.30 × 0.27 × 0.26 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Rotating Anode
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.805, T_{max} = 0.828
12946 measured reflections
2882 independent reflections
2093 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 64.5°, θ_{min} = 7.2°
h = −28→24
k = −6→6
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.140
S = 1.04
2882 reflections
246 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
$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 0.0093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), FC*=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.0014 (4)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of F^2 > 2sigma(F^2) is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.05300 (5)	0.8669 (2)	−0.28028 (9)	0.0837 (5)
O1	0.11703 (5)	0.4164 (2)	0.03622 (10)	0.0574 (5)
N1	0.31578 (6)	0.5776 (2)	0.40783 (12)	0.0492 (5)
N2	0.32422 (7)	0.3614 (3)	0.44199 (15)	0.0703 (7)
N3	0.35374 (8)	0.3674 (3)	0.54193 (15)	0.0696 (7)
C1	0.33979 (7)	0.7201 (3)	0.48777 (14)	0.0498 (7)
C2	0.36432 (7)	0.5852 (3)	0.57278 (15)	0.0487 (7)
C3	0.39749 (7)	0.6463 (3)	0.68042 (15)	0.0491 (7)
C4	0.42250 (8)	0.8577 (3)	0.69861 (16)	0.0575 (7)
C5	0.45458 (9)	0.9110 (4)	0.79905 (17)	0.0654 (8)
C6	0.46224 (9)	0.7563 (4)	0.88317 (17)	0.0699 (9)
C7	0.43748 (9)	0.5467 (4)	0.86671 (16)	0.0668 (8)
C8	0.40571 (8)	0.4912 (4)	0.76674 (15)	0.0574 (7)
C9	0.28234 (7)	0.6239 (3)	0.30256 (15)	0.0460 (6)
C10	0.27337 (8)	0.4560 (3)	0.22393 (16)	0.0543 (7)
C11	0.23700 (8)	0.4932 (3)	0.12618 (15)	0.0538 (7)
C12	0.20939 (7)	0.6977 (3)	0.10390 (14)	0.0460 (6)
C13	0.22149 (8)	0.8679 (3)	0.18198 (15)	0.0514 (7)
C14	0.25738 (8)	0.8324 (3)	0.28107 (16)	0.0519 (7)
C15	0.16868 (7)	0.7360 (3)	−0.00005 (14)	0.0467 (7)
C16	0.12240 (8)	0.5936 (3)	−0.03169 (14)	0.0477 (7)
C17	0.08372 (8)	0.6410 (3)	−0.12668 (15)	0.0551 (7)
C18	0.09231 (9)	0.8241 (4)	−0.18843 (15)	0.0583 (7)
C19	0.13686 (9)	0.9642 (4)	−0.16214 (16)	0.0619 (8)
C20	0.17441 (8)	0.9187 (3)	−0.06678 (15)	0.0545 (7)
C21	0.06654 (8)	0.2878 (3)	0.01397 (16)	0.0559 (7)
C22	0.06763 (9)	0.1172 (4)	0.10339 (17)	0.0650 (8)
H1	0.33970	0.87680	0.48550	0.0600*
H4	0.41740	0.96370	0.64220	0.0690*
H5	0.47120	1.05240	0.81010	0.0780*
H6	0.48400	0.79250	0.95100	0.0840*
H7	0.44240	0.44250	0.92390	0.0800*
H8	0.38950	0.34910	0.75630	0.0690*
H10	0.29180	0.31860	0.23690	0.0650*
H11	0.23080	0.37900	0.07380	0.0650*
H13	0.20510	1.00880	0.16720	0.0620*
H14	0.26470	0.94760	0.33280	0.0620*
H17	0.05250	0.54980	−0.14780	0.0660*
H19	0.14180	1.08580	−0.20670	0.0740*

H20	0.20480	1.01430	−0.04640	0.0650*
H21A	0.06330	0.21250	−0.05660	0.0670*
H21B	0.03460	0.38660	0.01090	0.0670*
H22A	0.10050	0.02550	0.10880	0.0980*
H22B	0.03500	0.02350	0.08660	0.0980*
H22C	0.06810	0.19290	0.17210	0.0980*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0920 (10)	0.0886 (10)	0.0600 (8)	0.0091 (7)	−0.0124 (7)	0.0138 (6)
O1	0.0568 (9)	0.0542 (9)	0.0559 (8)	−0.0108 (6)	−0.0027 (6)	0.0035 (6)
N1	0.0496 (9)	0.0376 (9)	0.0565 (9)	−0.0019 (7)	−0.0003 (7)	0.0027 (7)
N2	0.0877 (13)	0.0413 (11)	0.0711 (12)	0.0010 (9)	−0.0126 (10)	0.0049 (8)
N3	0.0853 (13)	0.0454 (12)	0.0675 (11)	0.0005 (9)	−0.0126 (10)	0.0052 (8)
C1	0.0464 (11)	0.0408 (12)	0.0590 (11)	−0.0039 (8)	0.0018 (9)	0.0015 (9)
C2	0.0451 (11)	0.0430 (12)	0.0566 (11)	0.0010 (8)	0.0058 (9)	0.0049 (9)
C3	0.0433 (11)	0.0487 (12)	0.0536 (11)	0.0057 (9)	0.0046 (9)	0.0036 (9)
C4	0.0575 (12)	0.0529 (14)	0.0580 (12)	0.0006 (9)	0.0004 (10)	0.0045 (9)
C5	0.0657 (14)	0.0556 (14)	0.0690 (14)	0.0025 (10)	−0.0023 (11)	−0.0058 (11)
C6	0.0723 (15)	0.0705 (17)	0.0603 (13)	0.0116 (12)	−0.0045 (11)	−0.0079 (11)
C7	0.0704 (14)	0.0714 (17)	0.0561 (12)	0.0140 (12)	0.0052 (11)	0.0100 (11)
C8	0.0569 (13)	0.0531 (13)	0.0606 (12)	0.0046 (9)	0.0067 (10)	0.0064 (10)
C9	0.0425 (10)	0.0415 (11)	0.0516 (10)	−0.0029 (8)	0.0026 (8)	0.0026 (8)
C10	0.0547 (12)	0.0430 (12)	0.0627 (12)	0.0061 (9)	0.0043 (10)	−0.0028 (9)
C11	0.0561 (12)	0.0451 (12)	0.0579 (11)	−0.0005 (9)	0.0050 (10)	−0.0087 (9)
C12	0.0470 (11)	0.0407 (11)	0.0501 (10)	−0.0034 (8)	0.0088 (8)	−0.0010 (8)
C13	0.0567 (12)	0.0373 (11)	0.0572 (11)	0.0011 (8)	0.0028 (9)	0.0025 (8)
C14	0.0557 (12)	0.0418 (12)	0.0541 (11)	−0.0035 (9)	−0.0002 (9)	−0.0041 (9)
C15	0.0522 (12)	0.0433 (12)	0.0445 (10)	0.0011 (8)	0.0088 (8)	−0.0045 (8)
C16	0.0554 (12)	0.0430 (12)	0.0432 (10)	0.0023 (9)	0.0056 (9)	−0.0031 (8)
C17	0.0572 (12)	0.0554 (13)	0.0497 (11)	0.0016 (10)	0.0026 (9)	−0.0073 (9)
C18	0.0662 (14)	0.0624 (14)	0.0425 (10)	0.0133 (11)	0.0003 (10)	0.0013 (9)
C19	0.0777 (15)	0.0546 (14)	0.0539 (12)	0.0080 (11)	0.0140 (11)	0.0102 (10)
C20	0.0584 (13)	0.0490 (13)	0.0572 (11)	−0.0002 (9)	0.0134 (10)	−0.0005 (9)
C21	0.0475 (12)	0.0567 (13)	0.0612 (12)	−0.0070 (9)	0.0042 (9)	−0.0070 (10)
C22	0.0634 (13)	0.0575 (15)	0.0721 (14)	−0.0083 (10)	0.0074 (11)	0.0008 (10)

Geometric parameters (Å, º)

F1—C18	1.366 (2)	C15—C20	1.385 (3)
O1—C16	1.367 (2)	C16—C17	1.390 (3)
O1—C21	1.431 (2)	C17—C18	1.367 (3)
N1—N2	1.354 (2)	C18—C19	1.358 (3)
N1—C1	1.348 (2)	C19—C20	1.377 (3)
N1—C9	1.427 (2)	C21—C22	1.496 (3)
N2—N3	1.309 (3)	C1—H1	0.9300
N3—C2	1.358 (3)	C4—H4	0.9300

C1—C2	1.367 (3)	C5—H5	0.9300
C2—C3	1.467 (3)	C6—H6	0.9300
C3—C4	1.395 (3)	C7—H7	0.9300
C3—C8	1.395 (3)	C8—H8	0.9300
C4—C5	1.375 (3)	C10—H10	0.9300
C5—C6	1.374 (3)	C11—H11	0.9300
C6—C7	1.381 (3)	C13—H13	0.9300
C7—C8	1.370 (3)	C14—H14	0.9300
C9—C10	1.381 (3)	C17—H17	0.9300
C9—C14	1.382 (3)	C19—H19	0.9300
C10—C11	1.376 (3)	C20—H20	0.9300
C11—C12	1.390 (3)	C21—H21A	0.9700
C12—C13	1.390 (3)	C21—H21B	0.9700
C12—C15	1.487 (2)	C22—H22A	0.9600
C13—C14	1.382 (3)	C22—H22B	0.9600
C15—C16	1.406 (3)	C22—H22C	0.9600

C16—O1—C21	118.06 (14)	C15—C20—C19	122.56 (18)
N2—N1—C1	110.23 (15)	O1—C21—C22	108.89 (16)
N2—N1—C9	119.62 (14)	N1—C1—H1	127.00
C1—N1—C9	130.03 (14)	C2—C1—H1	127.00
N1—N2—N3	107.05 (16)	C3—C4—H4	120.00
N2—N3—C2	109.44 (17)	C5—C4—H4	120.00
N1—C1—C2	105.29 (15)	C4—C5—H5	120.00
N3—C2—C1	107.98 (16)	C6—C5—H5	120.00
N3—C2—C3	122.21 (17)	C5—C6—H6	120.00
C1—C2—C3	129.81 (17)	C7—C6—H6	120.00
C2—C3—C4	121.23 (16)	C6—C7—H7	120.00
C2—C3—C8	120.43 (17)	C8—C7—H7	120.00
C4—C3—C8	118.32 (17)	C3—C8—H8	120.00
C3—C4—C5	120.68 (18)	C7—C8—H8	120.00
C4—C5—C6	120.3 (2)	C9—C10—H10	120.00
C5—C6—C7	119.8 (2)	C11—C10—H10	120.00
C6—C7—C8	120.5 (2)	C10—C11—H11	119.00
C3—C8—C7	120.5 (2)	C12—C11—H11	119.00
N1—C9—C10	119.43 (16)	C12—C13—H13	119.00
N1—C9—C14	120.22 (16)	C14—C13—H13	119.00
C10—C9—C14	120.31 (17)	C9—C14—H14	120.00
C9—C10—C11	119.58 (17)	C13—C14—H14	120.00
C10—C11—C12	121.50 (17)	C16—C17—H17	121.00
C11—C12—C13	117.70 (16)	C18—C17—H17	121.00
C11—C12—C15	121.66 (16)	C18—C19—H19	121.00
C13—C12—C15	120.64 (16)	C20—C19—H19	121.00
C12—C13—C14	121.45 (17)	C15—C20—H20	119.00
C9—C14—C13	119.32 (17)	C19—C20—H20	119.00
C12—C15—C16	121.32 (16)	O1—C21—H21A	110.00
C12—C15—C20	120.59 (16)	O1—C21—H21B	110.00
C16—C15—C20	118.05 (16)	C22—C21—H21A	110.00

O1—C16—C15	117.13 (15)	C22—C21—H21B	110.00
O1—C16—C17	123.12 (17)	H21A—C21—H21B	108.00
C15—C16—C17	119.72 (16)	C21—C22—H22A	109.00
C16—C17—C18	118.82 (18)	C21—C22—H22B	109.00
F1—C18—C17	117.08 (19)	C21—C22—H22C	109.00
F1—C18—C19	119.37 (19)	H22A—C22—H22B	109.00
C17—C18—C19	123.55 (19)	H22A—C22—H22C	109.00
C18—C19—C20	117.3 (2)	H22B—C22—H22C	110.00

C21—O1—C16—C15	171.58 (16)	N1—C9—C10—C11	173.95 (17)
C21—O1—C16—C17	−6.3 (2)	C14—C9—C10—C11	−3.5 (3)
C16—O1—C21—C22	−175.08 (16)	N1—C9—C14—C13	−174.70 (17)
C1—N1—N2—N3	−0.7 (2)	C10—C9—C14—C13	2.8 (3)
C9—N1—N2—N3	−177.13 (16)	C9—C10—C11—C12	0.8 (3)
N2—N1—C1—C2	0.9 (2)	C10—C11—C12—C13	2.7 (3)
C9—N1—C1—C2	176.86 (17)	C10—C11—C12—C15	−177.98 (17)
N2—N1—C9—C10	−19.9 (2)	C11—C12—C13—C14	−3.4 (3)
N2—N1—C9—C14	157.63 (17)	C15—C12—C13—C14	177.19 (17)
C1—N1—C9—C10	164.46 (18)	C11—C12—C15—C16	55.8 (2)
C1—N1—C9—C14	−18.1 (3)	C11—C12—C15—C20	−126.4 (2)
N1—N2—N3—C2	0.2 (2)	C13—C12—C15—C16	−124.8 (2)
N2—N3—C2—C1	0.4 (2)	C13—C12—C15—C20	53.0 (2)
N2—N3—C2—C3	−178.95 (17)	C12—C13—C14—C9	0.8 (3)
N1—C1—C2—N3	−0.8 (2)	C12—C15—C16—O1	−1.1 (3)
N1—C1—C2—C3	178.51 (18)	C12—C15—C16—C17	176.85 (17)
N3—C2—C3—C4	159.79 (19)	C20—C15—C16—O1	−178.96 (16)
N3—C2—C3—C8	−18.8 (3)	C20—C15—C16—C17	−1.0 (3)
C1—C2—C3—C4	−19.4 (3)	C12—C15—C20—C19	−178.16 (18)
C1—C2—C3—C8	162.00 (19)	C16—C15—C20—C19	−0.3 (3)
C2—C3—C4—C5	−178.43 (18)	O1—C16—C17—C18	179.02 (18)
C8—C3—C4—C5	0.2 (3)	C15—C16—C17—C18	1.2 (3)
C2—C3—C8—C7	178.86 (18)	C16—C17—C18—F1	−179.11 (17)
C4—C3—C8—C7	0.2 (3)	C16—C17—C18—C19	−0.1 (3)
C3—C4—C5—C6	−0.3 (3)	F1—C18—C19—C20	177.84 (18)
C4—C5—C6—C7	−0.2 (3)	C17—C18—C19—C20	−1.2 (3)
C5—C6—C7—C8	0.6 (3)	C18—C19—C20—C15	1.4 (3)
C6—C7—C8—C3	−0.6 (3)		