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Bis[2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl] benzene-2,4-dicarboxylate

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Key indicators

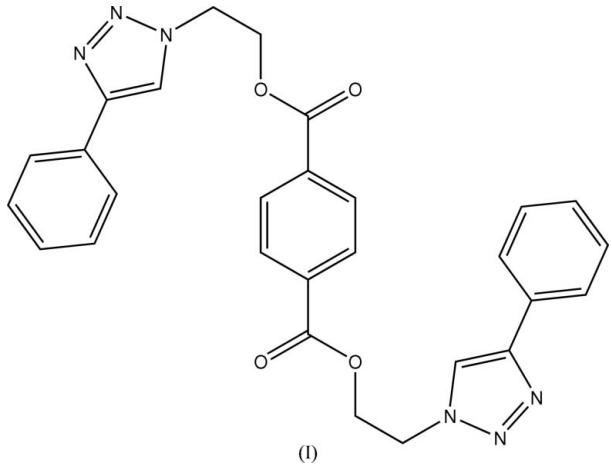
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.071
wR factor = 0.137
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{28}H_{24}N_6O_4$, crystallizes with one half-molecule in the asymmetric unit, the other half being generated by a center of inversion. In the crystal structure, molecules are linked into ribbons along the *a* axis by weak C—H···N hydrogen bonds.

Comment

1,2,3-Triazoles are important target molecules due to their importance as potent pharmacophores. Many 1,2,3-triazoles have been found to be potent antimicrobial (Chen *et al.*, 2000) and anti-inflammatory agents (Banu & Dinakar, 1999). The title triazole, (I), was synthesized *via* [3 + 2]-cycloaddition between azide and acetylene compounds. This reaction generally results in the corresponding 1,4-disubstituted 1,2,3-triazoles in high yields.



(I)

The title compound, (I), has a crystallographically imposed center of symmetry. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angles between the triazole ring and its attached benzene ring is 21.4 (2)°, and that between the triazole ring and the central benzene ring is 56.9 (2)°, while the two benzene rings make an angle of 43.0 (2)° with each other. In the crystal structure, molecules are linked into a ribbon along the *a* axis (Fig. 2) by C8—H8*A*···N1 hydrogen bonds (Table 2).

Experimental

To a solution of bis(2-azidoethyl)terephthalate (1 g, 3.3 mmol) in toluene (10 ml), were added successively phenylacetylene (1.6 ml, 16.5 mmol), CuI (0.66 g, 3.3 mmol) and diisopropyl ether (5 ml). The mixture was stirred at 323 K for 20 h. After concentration, the resulting solid was recrystallized from dimethylformamide (DMF),

yielding the title compound, (I). A solution of (I) in DMF was allowed to stand at 323 K for 2 d and colourless needle-shaped crystals suitable for X-ray crystallographic analysis were grown by slow evaporation.

Crystal data

$C_{28}H_{24}N_6O_4$
M_r = 508.53
Monoclinic, $P2_1/c$
a = 5.538 (3) Å
b = 30.783 (17) Å
c = 7.930 (5) Å
β = 107.617 (11)°
V = 1288.6 (12) Å^3
Z = 2
D_x = 1.311 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 535 reflections
θ = 2.6–18.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Needle, colourless
0.43 × 0.08 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.962, T_{max} = 0.996
7423 measured reflections
2535 independent reflections
1226 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 26.0°
$h = -5 \rightarrow 6$
$k = -38 \rightarrow 32$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.137
S = 1.03
2535 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C11	1.335 (4)	N3—C9	1.464 (4)
O1—C10	1.446 (3)	C9—C10	1.498 (4)
O2—C11	1.208 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···N1^{i}	0.93	2.49	3.363 (5)	156

Symmetry code: (i) $x+1, y, z$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2 U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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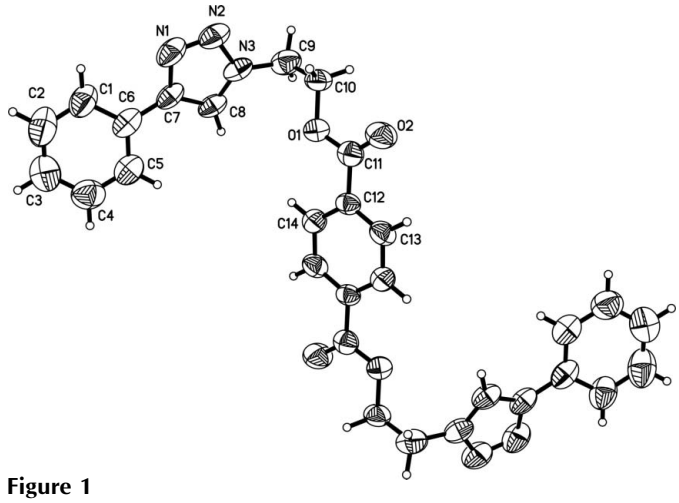

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $2-x, 1-y, 2-z$.

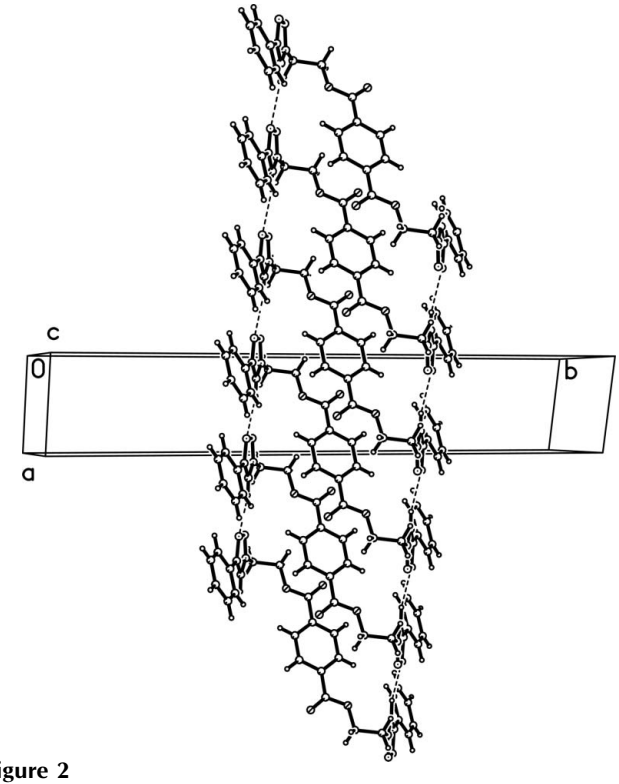

Figure 2
A view down the c axis, showing the ribbon along the a axis. Hydrogen bonds are indicated by dashed lines.

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