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(*E*)-1-(Naphthalen-1-yl)-3-(1-phenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one

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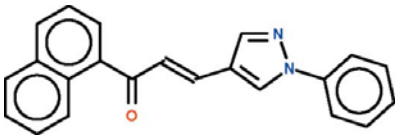
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.140; data-to-parameter ratio = 16.9.

In the title molecule, $C_{22}H_{16}N_2O$, the phenyl ring is twisted slightly with respect to the plane of the central pyrazole ring [dihedral angle = 14.8 (2)°]; the central ring is connected to the naphthyl ring through a —CH=CH—C(=O)— fragment, whose C=C double bond has an *E* configuration. The pyrazole ring and naphthalene ring system are twisted by 46.3 (1)°. Weak intermolecular C—H···O hydrogen bonds link the molecules, forming supramolecular chains running along the *a* axis. The crystal studied was a non-merohedral twin with a component ratio of 0.544 (2):0.456 (2).

Related literature

For related structures; see: Diánez & López-Castro (1990); Jones *et al.* (1984). For the synthesis, see: Finar (1961); Finar & Lord (1959); Jones *et al.* (1984).



Experimental

Crystal data

$C_{22}H_{16}N_2O$ M_r = 324.37
Monoclinic, $P2_1/n$
a = 5.8457 (6) Å
b = 10.322 (2) Å
c = 26.626 (2) Å
β = 92.322 (9)°
V = 1605.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.25 × 0.10 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.980, T_{max} = 0.992
3824 measured reflections
3825 independent reflections
2494 reflections with $I > 2\sigma(I)$
R_{int} = 0.105

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.140
S = 0.96
3825 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1^{i}	0.95	2.46	3.397 (4)	167

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); 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: XU5313).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Diánez, M. J. & López-Castro, A. (1990). *Acta Cryst.* C**46**, 1718–1720.
Finar, I. L. (1961). *J. Chem. Soc.* pp. 674–679.
Finar, I. L. & Lord, G. H. (1959). *J. Chem. Soc.* pp. 1819–1823.
Jones, R. A., Gonzalez, B. A., Arques, J. S., Pardo, J. Q. & King, T. J. (1984). *J. Chem. Soc. Perkin Trans. 1*, pp. 1423–1425.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.