Crystal structure of 2-(1-benzyl-3-phenyl-1H-pyrazol-5-yl)-5-(4-nitrobenzylthio)-1,3,4-oxadiazole, C_{25}H_{19}N_{5}O_{3}S

Abstract
C_{25}H_{19}N_{5}O_{3}S, monoclinic, P2_{1}/c (no. 14), \( a = 16.715(2) \text{ Å} \), \( b = 11.2677(15) \text{ Å} \), \( c = 12.6490(17) \text{ Å} \), \( \beta = 110.818(2)^\circ \), \( V = 2226.7(5) \text{ Å}^3 \), \( Z = 4 \), \( R_{gt}(F) = 0.0424 \), \( wR_{ref}(F^2) = 0.1037 \), \( T = 296 \text{ K} \).

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material
5-(1-Benzyl-3-phenyl-1H-pyrazol-5-yl)-1,3,4-oxadiazole-2-thiol (1.67 g, 5.0 mmol) and 4-nitrobenzyl chloride (0.86 g, 5.0 mmol) were mixed in acetonitrile (25 mL), \( \text{K}_2\text{CO}_3 \) (0.69 g, 5.0 mmol) was added and the mixture was stirred under reflux for 3 hours. The solution was concentrated by vacuum evaporation and the residue was poured onto crushed ice. The precipitate was collected by filtration, washed with water and cold ethanol to afford the title compound as white solid in 78.7% yield [1]. Crystals were obtained by slow evaporation of a solution in acetonitrile at room temperature.

Experimental details
All H atoms were placed in idealized positions and treated as riding on their parent atoms, with \( d(\text{C—H}) = 0.97 \text{ Å} \) (methylene), \( U_{iso}(\text{H}) = 1.5U_{eq}(\text{C}) \) and \( d(\text{C—H}) = 0.93 \text{ Å} \) (aromatic), \( U_{iso}(\text{H}) = 1.2U_{eq}(\text{C}) \).

Discussion
In recent years, 1,3,4-oxadiazoles have received much attention due to their application in fluorescence dyes [2] and some pharmacological properties, such as enzyme inhibition, anti-convulsant, anti-inflammatory and anti-tumour activities [3–6]. Pyrazole are as well known for their important biological and pharmaceutical activities [7]. The rational combination of 1,3,4-oxadiazole and pyrazole should provide excellent fluorescence properties and biological activities [8]. In continuation of our development of compounds containing...
The core of the title compound consists of one pyrazolyl and one 1,3,4-oxadiazolyl moiety. The pyrazolyl ring (N1/N2/C9/C8/C7) and 1,3,4-oxadiazolyl ring (N3/N4/C11/C10) are almost coplanar with an angle of 4.2° between them. The angle between the planes of the phenyl (C1/C2/C3/C4/C5/C6) and the pyrazolyl plane (N1/N2/C9/C8/C7) is 76°. The planes of the benzyl (C13/C14/C15/C16/C17) and the pyrazolyl moiety (N1/N2/C9/C8/C7) are twisted by an angle of 72.4°. Bond lengths and angles are within the ranges [1].

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### References


