

Single-crystal X-ray structure determinations were performed at room temperature on a Stoe IPS II diffractometer using monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å). A multiscan absorption correction was applied. The data reduction, including an empirical absorption correction using spherical harmonics, implemented in LANA. The crystal structures were solved by direct methods using the online version of WinGX [1] and then refined by full-matrix least-squares (SHELXL2014) on F<sup>2</sup> [2,3]. The nonhydrogen atoms were refined anisotropically. All of the hydrogen atoms were positioned geometrically in idealized positions and refined with the riding model approximation, with Uiso(H) = 1.2 or 1.5 Ueq(C). The molecular graphics the program MERCURY from the CSD package was used [4].

For the reported compound, the crystals are small resulting in very weak diffraction data and poor resolution. The structure was solved by direct methods. The data used for the refinement are up to a resolution of 2-theta = 37.7 degrees as the intensity of the data dropped rapidly after this point. The flack parameter ( $x = -0.901$ ) was refined by full-matrix least squares (i.e., using the TWIN/BASF commands in the SHELXL.ins file) [5]. Hydrogen atoms were included in calculated positions.

Due to poor diffraction of the crystal, some alerts show in the CheckCif file such as low value of sine (theta\_max) of 0.5554, low resolution of 23.25 degree, diffraction fraction of full theta is low (0.952) and low bond precision on some C-C bonds. The final R1 and wR2 values are acceptable.

## References

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