**STRUCTURE REPORT**

**Crystallographer:** F. Engelhardt

**ID code:** IDCODE Date: DATE

**Sample by:** USER

**Compound:**

**Formula sum:** SUM

**Formula moieties:** MOI

PICTURE

**Figure 1**. Molecular structure of the title compound in the crystalline state. Thermal ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

**Crystallographic Data and Details on Structure Refinement**

formula sum SUM

formula weight WEIGHT

crystal size (mm) SIZE mm

crystal system CRYSSYSTEM

space group SPGRP

unit cell parameters

a (Å) CELLA

b (Å) CELLB

c (Å) CELLC

α (deg) ALPHA

β (deg) BETA

γ (deg) GAMMA

unit cell volume V (Å3) VOLUME

molecules per cell z ZERR

crystallographic density μ calcd (g cm-3) DENSITY

absorption coefficient µ (mm-1) MU

diffractometer STOE IPDS 2T

radiation (λ [Å]) graphite-monochromated Mo-Kα (0.71073)

temperature (°C) -173.15

scan type ω scan (increment 1.5°, exposure 1 min)

completeness of dataset COMPLETENESS%

θ range of data collection (deg) THETAMIN to THETAMAX

reflections collected COLLRFL

independent reflections UNIQUE

independent reflections with I>2σ(I) UNIQUE2S

structure solution method dual-space structure solution (SHELXT)

refinement method full-matrix least-squares on F2 (SHELXL 2016/4)

absorption correction method ABSCORR

range of transmission factors TMAX and TMIN

data / parameters / restraints DATA / PARAM / RESTR

goodness of fit (GooF) [all data] GOOF

final R values

R1 [all data, I ≥ 2σ (I)] R1ALL, R12SIG

wR2 [all data, I ≥ 2σ (I)]] WR2ALL, WR2SIG

largest difference peak and hole HIGHPEAK and DEEPHOLE eÅ-3

Refinement special details:

SPECIAL