**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.

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| --- | --- |
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**Crystallographic Data and Details on Structure Refinement**

formulasum 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

** (deg) ALPHA

** (deg) BETA

*γ*(deg) GAMMA

unit cell volume *V* (Å3) VOLUME

molecules per cell *z* ZERR

crystallographic density **calcd (g cm-3) DENSITY

absorption coefficient *µ* (mm-1) MU

diffractometer STOE IPDS 2T

radiation (**[Å]) graphite-monochromated Mo-K (0.71073)

temperature (°C) -173.15

scan type ** scan (increment 1.5°, exposure 1 min)

completeness of dataset COMPLETENESS%

** range of data collection (deg) THETAMIN to THETAMAX

reflections collected COLLRFL

independent reflections UNIQUE

independent reflections with *I*>2**(*I*) UNIQUE2S

structure solution method dual-space structure solution (SHELXT)

refinement method full-matrix least-squares on *F*2 (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

*R*1 [all data, *I* ≥ 2** (*I*)] R1ALL, R12SIG

*wR*2 [all data, *I* ≥ 2** (*I*)]] WR2ALL, WR2SIG

largest difference peak and hole HIGHPEAK and DEEPHOLE eÅ-3

Refinement special details: