checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lms12209b2_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: lms12209b2_0m

Bond precision: C-C = 0.0039 A Wavelength=1.54178

Cell: a=7.0846(7) b=12.2015(12) c=23.936(2)
alpha=90 beta=98.375(4) gamma=90
Temperature: 267 K

	Calculated	Reported
Volume	2047.0(3)	2047.1(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	C19 H16 F N O4 S [+ solvent]	C19 H16 F N O4 S
Sum formula	C19 H16 F N O4 S [+ solvent]	C19 H16 F N O4 S
Mr	373.39	373.39
Dx,g cm-3	1.212	1.212
Z	4	4
Mu (mm-1)	1.676	1.676
F000	776.0	776.0
F000'	779.82	
h,k,lmax	8,15,29	8,15,29
Nref	4053	4016
Tmin,Tmax	0.980,0.983	0.537,0.753
Tmin'	0.967	

Correction method= # Reported T Limits: Tmin=0.537 Tmax=0.753
AbsCorr = NONE

Data completeness= 0.991 Theta(max)= 72.419

R(reflections)= 0.0550(3585)

wR2(reflections)= 0.1768(4016)

S = 1.095 Npar= 235

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.828 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 22 Report

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Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 183 A**3
PLAT767_ALERT_4_G INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 15 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock lms12209b2_0m - ellipsoid plot