checkCIF/PLATON report

Structure factors have been supplied for datablock(s) g23053

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: g23053

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Bond precision:    C-C = 0.0019 A            Wavelength=1.54178

Cell:            a=3.9311(3)        b=6.7913(5)        c=31.150(2)
                 alpha=93.740(3)   beta=91.628(3)    gamma=93.783(3)
Temperature:     100 K

                  Calculated                   Reported
Volume            827.59(10)                   827.61(11)
Space group       P -1                         P -1
Hall group        -P 1                         -P 1
Moiety formula    C42 H16 F10 O4 S2            ?
Sum formula       C42 H16 F10 O4 S2            C42 H16 F10 O4 S2
Mr                838.67                       838.67
Dx,g cm-3         1.683                        1.683
Z                 1                            1
Mu (mm-1)         2.407                        2.407
F000              422.0                        422.0
F000'             424.31
h,k,lmax          4,8,39                       4,8,39
Nref              3504                         3472
Tmin,Tmax         0.589,0.965                  0.163,0.282
Tmin'             0.452

Correction method= # Reported T Limits: Tmin=0.163 Tmax=0.282
AbsCorr = MULTI-SCAN

Data completeness= 0.991          Theta(max)= 77.493

R(reflections)= 0.0321( 3327)                    wR2(reflections)=
                                                 0.0858( 3472)
S = 1.031                 Npar= 281
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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 G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   14 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms   13 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   6 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records   2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   19 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records   1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used   0.0200 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0400 Report
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd   1)   21% Note
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond C7   – C8   .   1.43 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   306 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
             0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   30 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   1 Note
            -4 0 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ....   3.696 Note
            Predicted wR2: Based on SigI**2 2.32 or SHELX Weight 8.32
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   21 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
   0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  27 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  14 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 15/07/2024; check.def file version of 15/07/2024

Datablock g23053 - ellipsoid plot