checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JF3162FFMI

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: JF3162FFMI

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Bond precision:    C-C = 0.0032 A              Wavelength=0.71073

Cell:              a=9.9964(9)     b=7.9885(7)              c=27.840(3)
                   alpha=90        beta=97.4283(14)         gamma=90
Temperature:       90 K

                   Calculated                  Reported
Volume             2204.5(4)                   2204.5(3)
Space group        P 21/c                      P 21/c
Hall group         -P 2ybc                     -P 2ybc
Moiety formula     2(C20.50 H16 Cl2 N7.50 O4   2(C20.50 H16 Cl2 N7.50 O4
                   S)                          S)
Sum formula        C41 H32 Cl4 N15 O8 S2       C41 H32 Cl4 N15 O8 S2
Mr                 1068.74                     1068.74
Dx,g cm-3          1.610                       1.610
Z                  2                           2
Mu (mm-1)          0.437                       0.437
F000               1094.0                      1094.0
F000'              1096.07
h,k,lmax           12,10,36                    12,10,36
Nref               5064                        5054
Tmin,Tmax          0.883,0.980                 0.831,0.932
Tmin'              0.883

Correction method= # Reported T Limits: Tmin=0.831 Tmax=0.932
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 27.505


R(reflections)= 0.0416( 3417)                      wR2(reflections)=
                                                   0.0943( 5054)
S = 1.025                   Npar= 380
```

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

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PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records        1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N21        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21        Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        3% Note
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl1      ..O18       .      3.16 Ang.
                                      1+x,3/2-y,-1/2+z  =      4_675 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H10B     ..O11       .      2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H20      ..CL3       .      2.87 Ang.
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL    2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        10 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         6 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
  12 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   8 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 06/07/2023; check.def file version of 30/06/2023

NOMOVE FORCED

Prob = 50
Temp = 90

-23 Y

- (60723)

PLATON-Aug 11 6:09:37 2023

Z -149 JF3162FFMI   P 21/c   R = 0.04   RES= O-124 X