checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 3-130-1

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Bond precision:   C-C = 0.0127 A          Wavelength=1.54184

Cell:              a=9.8460(1)      b=15.3637(2)      c=17.0733(3)
                   alpha=90         beta=90           gamma=90
Temperature:       293 K

                 Calculated                Reported
Volume           2582.70(6)                2582.70(6)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C21 H31 F I N3 Pd         C21 H31 F I N3 Pd
Sum formula      C21 H31 F I N3 Pd         C21 H31 F I N3 Pd
Mr               577.79                    577.79
Dx,g cm-3        1.486                     1.486
Z                4                         4
Mu (mm-1)        15.306                    15.306
F000             1144.0                    1144.0
F000'            1146.09
h,k,lmax         12,19,21                  11,19,21
Nref             5280[ 2984]               5108
Tmin,Tmax        0.199,0.294               0.432,1.000
Tmin'            0.094

Correction method= # Reported T Limits: Tmin=0.432 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.97        Theta(max)= 74.234

R(reflections)= 0.0553( 4724)                wR2(reflections)=
                                             0.1557( 5108)
S = 1.035                 Npar= 181
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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 C

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C1       -C6       .       1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01275 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C14      - C16      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C15      - C16      .       1.43 Ang.
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         10 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.51 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          9 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0001 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0005 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0070 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0090 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0006 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0006 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0006 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0006 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0001 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0001 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I1       --Pd1      .        9.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --C7       .        8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --C17      .        6.0 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .       1.82 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        241 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.4 Low
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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
   7 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
  15 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 06/01/2024; check.def file version of 05/01/2024

Datablock 3-130-1 - ellipsoid plot