checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kr186_01_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: kr186_01_0m

```
Bond precision:    = 0.0000 A                    Wavelength=0.71073

Cell:              a=6.9383(6)       b=5.5231(5)      c=13.0772(14)
                   alpha=90          beta=90          gamma=90
Temperature:       172 K

                   Calculated                Reported
Volume             501.13(8)                 501.13(8)
Space group        C m m a                   C m m e
Hall group         -C 2b 2                   -C 2b 2
Moiety formula     C0.75 H0.75 I0.25 N0.50   C3 H3 I N2
Sum formula        C0.75 H0.75 I0.25 N0.50   C3 H3 I N2
Mr                 48.49                     193.97
Dx,g cm-3          2.571                     2.571
Z                  16                        4
Mu (mm-1)          6.230                     6.230
F000               352.0                     352.0
F000'              350.22
h,k,lmax           10,8,19                   10,8,19
Nref               512                       483
Tmin,Tmax                                    0.502,0.746
Tmin'

Correction method= # Reported T Limits: Tmin=0.502 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.943            Theta(max)= 31.903

                                            wR2(reflections)=
R(reflections)= 0.0302( 426)                0.0682( 483)

S = 1.198                Npar= 55
```

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...   Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...   Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...   Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....   8.78 Note
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4   Please Check

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   4 Check
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records   1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records   1 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   0.0010 Report
PLAT300_ALERT_4_G Atom Site Occupancy of I1   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1   Constrained at   0.125 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A   Constrained at   0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2   Constrained at   0.125 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3   Constrained at   0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 1)   2.25 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #   10 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers   1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   39 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   29 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   1 Note

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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  17 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 10/05/2023; check.def file version of 10/05/2023