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: shoji04

```
Bond precision:   C-C = 0.0157 A              Wavelength=0.71075

Cell:            a=11.1593(16)     b=9.9827(16)         c=30.073(4)
                 alpha=90          beta=95.774(3)       gamma=90
Temperature:     296 K

                 Calculated                  Reported
Volume           3333.1(8)                   3333.1(9)
Space group      C c                         C 1 c 1
Hall group       C -2yc                      C -2yc
Moiety formula   C22 H19 N O                 C22 H19 N O
Sum formula      C22 H19 N O                 C22 H19 N O
Mr               313.38                      313.40
Dx,g cm-3        1.249                       1.249
Z                8                           8
Mu (mm-1)        0.076                       0.076
F000             1328.0                      1328.0
F000'            1328.52
h,k,lmax         14,12,38                    14,12,38
Nref             7574[ 3790]                 6901
Tmin,Tmax        0.973,0.985                 0.985,0.985
Tmin'            0.970

Correction method= # Reported T Limits: Tmin=0.985 Tmax=0.985
AbsCorr = NONE

Data completeness= 1.82/0.91      Theta(max)= 27.395

R(reflections)= 0.0937( 3167)     wR2(reflections)= 0.3157( 6901)

S = 1.288                  Npar= 433
```

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 B**
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.01568 Ang.

🟡 **Alert level C**
ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
            However values have been given for Tmin and Tmax. Remove
            these if an absorption correction has not been applied.
   From the CIF: _exptl_absorpt_correction_T_min   0.985
   From the CIF: _exptl_absorpt_correction_T_max   0.985
RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
            Weighted R factor given   0.316
STRVA01_ALERT_2_C   Chirality of atom sites is inverted?
            From the CIF: _refine_ls_abs_structure_Flack   2.600
            From the CIF: _refine_ls_abs_structure_Flack_su   1.000
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..   46 %
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.32 Report
PLAT085_ALERT_2_C SHELXL default weighting scheme is not optimized   Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C3   -- C42   ..   0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C4   -- C7   ..   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C18   -- C33   ..   0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20   -- C38   ..   0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28   -- C37   ..   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6   -- C29   ..   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30   -- C48   ..   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31   -- C43   ..   0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C39   -- C44   ..   0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C38 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C47 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C31 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1 Note
            C22 H19 N O
PLAT907_ALERT_2_C Flack x > 0.5, Structure needs to be Inverted? .   2.60 Check

---

⚪ **Alert level G**
CHEMS02_ALERT_1_G Please check that you have entered the correct
            _publ_requested_category classification of your compound;
            FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
            FO or CO or EO for organic.
            From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
            From the CIF: _chemical_formula_sum:C22 H19 N1 O1
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF   Please Do !
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .   1.000 Report
PLAT792_ALERT_1_G The Model has Chirality at C4   (Polar SPGR)   S Verify
PLAT792_ALERT_1_G The Model has Chirality at C6   (Polar SPGR)   S Verify
PLAT792_ALERT_1_G The Model has Chirality at C7   (Polar SPGR)   R Verify
PLAT792_ALERT_1_G The Model has Chirality at C14   (Polar SPGR)   R Verify
PLAT792_ALERT_1_G The Model has Chirality at C22   (Polar SPGR)   R Verify
PLAT792_ALERT_1_G The Model has Chirality at C23   (Polar SPGR)   S Verify
PLAT792_ALERT_1_G The Model has Chirality at C24   (Polar SPGR)   S Verify
PLAT792_ALERT_1_G The Model has Chirality at C25   (Polar SPGR)   R Verify
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI ..... Please Check

---

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
  20 **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

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
11 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 08/07/2016; check.def file version of 05/07/2016

NOMOVE FORCED

Prob = 50
Temp = 296

71 Y

PLATON-Jul 21 11:18:13 2016 - (70316)

Z 158   shoji04   C 1 c 1   R = 0.09   RES=   0 -175 X