checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kv690

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: kv690

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Bond precision:   C-C = 0.0021 A              Wavelength=0.71073

Cell:          a=11.3880(4)        b=11.8845(4)        c=15.3829(5)
               alpha=75.0794(12)  beta=75.9749(13)  gamma=84.3937(13)
Temperature: 150 K

                 Calculated                Reported
Volume           1950.38(12)               1950.38(12)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C38 H39 Mn2 N4 O6, F6 P   C76 H78 Mn4 N8 O12, 2(F6
                                           P)
Sum formula      C38 H39 F6 Mn2 N4 O6 P    C76 H78 F12 Mn4 N8 O12 P2
Mr               902.58                    1805.16
Dx,g cm-3        1.537                     1.537
Z                2                         1
Mu (mm-1)        0.768                     0.768
F000             924.0                     924.0
F000'            926.03
h,k,lmax         15,16,21                  15,16,21
Nref             11122                     10872
Tmin,Tmax        0.871,0.977               0.644,0.746
Tmin'            0.794

Correction method= # Reported T Limits: Tmin=0.644 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.978          Theta(max)= 29.742

R(reflections)= 0.0319( 9134)      wR2(reflections)= 0.0828( 10872)

S = 1.022                  Npar= 520
```

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

```
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       3.6 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        P1 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        39 Ang3
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        42 Report
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⚪ Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT012_ALERT_1_G No     _shelx_res_checksum found in CIF ........  Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   2.00 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)        4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      205 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       22 Note
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 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 27/03/2017; check.def file version of 24/03/2017