checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C2c_a

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: C2c_a

```
Bond precision:  C-C = 0.0075 A          Wavelength=0.71073

Cell:              a=17.84(6)     b=9.32(3)          c=22.76(8)
                   alpha=90       beta=99.67(6)      gamma=90
Temperature:       100 K

                 Calculated                Reported
Volume           3731(22)                  3730(21)
Space group      C 2/c                     C 2/c
Hall group       -C 2yc                    -C 2yc
Moiety formula   C49 H30 F6 O3 S           ?
Sum formula      C49 H30 F6 O3 S           C49 H30 F6 O3 S
Mr               812.79                    812.79
Dx,g cm-3        1.447                     1.447
Z                4                         4
Mu (mm-1)        0.163                     0.163
F000             1672.0                    1672.0
F000'            1673.50
h,k,lmax         21,11,27                  21,11,27
Nref             3352                      3352
Tmin,Tmax        0.978,0.983               0.516,0.746
Tmin'            0.918

Correction method= # Reported T Limits: Tmin=0.516 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.198

R(reflections)= 0.0781( 2664)     wR2(reflections)= 0.2019( 3352)

S = 1.209                 Npar= 343
```

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

```
PLAT149_ALERT_3_B s.u. on the   beta    Angle is Too Large .......       0.06 Degree
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
```

Alert level C

```
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................       9.77 Note
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.060 Ang.
PLAT148_ALERT_3_C s.u. on the      b    - Axis is (Too) Large ....     0.0300 Ang.
PLAT148_ALERT_3_C s.u. on the      c    - Axis is (Too) Large ....      0.080 Ang.
PLAT215_ALERT_3_C Disordered F4        has ADP max/min Ratio .....        3.6 Note
PLAT215_ALERT_3_C Disordered F5        has ADP max/min Ratio .....        3.7 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00748 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.349 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.852 Check
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          3 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      18.17 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O1       --C2       .        6.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of S1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C27        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         29% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F5       ..C15            2.77 Ang.
                                                x,-1+y,z  =      1_545 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         18 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         54% Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

```
  37 ALERT level G = General information/check it is not something unexpected

   1 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
  14 ALERT type 3 Indicator that the structure quality may be low
  26 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT149_C2c_a
;
PROBLEM: s.u. on the   beta    Angle is Too Large .......       0.06 Degree
RESPONSE: ...
;
_vrf_PLAT934_C2c_a
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
RESPONSE: ...
;
_vrf_PLAT088_C2c_a
;
PROBLEM: Poor Data / Parameter Ratio ....................       9.77 Note
RESPONSE: ...
;
_vrf_PLAT148_C2c_a
;
PROBLEM: s.u. on the      a    - Axis is (Too) Large ....      0.060 Ang.
RESPONSE: ...
;
_vrf_PLAT215_C2c_a
;
PROBLEM: Disordered F4        has ADP max/min Ratio .....        3.6 Note
RESPONSE: ...
;
_vrf_PLAT340_C2c_a
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............    0.00748 Ang.
RESPONSE: ...
;
_vrf_PLAT906_C2c_a
;
PROBLEM: Large K Value in the Analysis of Variance ......     12.349 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 18/09/2020; check.def file version of 20/08/2020

Datablock C2c_a - ellipsoid plot

