checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2222a

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: 2222a

```
Bond precision:  C-C = 0.0031 A          Wavelength=1.34138

Cell:           a=26.9960(11)    b=20.4249(9)      c=17.8631(7)
                alpha=90         beta=93.411(2)    gamma=90
Temperature:    193 K

                Calculated                Reported
Volume          9832.1(7)                 9832.1(7)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C57 H36 [+ solvent]       C57 H36
Sum formula     C57 H36 [+ solvent]       C57 H36
Mr              720.86                    720.86
Dx,g cm-3       0.974                     0.974
Z               8                         8
Mu (mm-1)       0.267                     0.269
F000            3024.0                    3024.0
F000'           3029.87
h,k,lmax        32,24,21                  32,24,21
Nref            18067                     18003
Tmin,Tmax                                 0.213,0.301
Tmin'

Correction method= # Reported T Limits: Tmin=0.213 Tmax=0.301
AbsCorr = NONE

Data completeness= 0.996          Theta(max)= 53.994

R(reflections)= 0.0522( 11040)    wR2(reflections)= 0.1500( 18003)

S = 0.958                 Npar= 1027
```

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

```
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
```

Alert level C

```
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
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C02X     --C033     .        5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C02K     --C02Z     .        7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C034     --C036     .        6.3 s.u.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -1.456 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        186 Note
PLAT793_ALERT_4_G Model has Chirality at C008        (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C00E        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C00L        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C010        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C016        (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C01P        (Centro SPGR)          R Verify
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
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         57 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value     0.0137 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
```

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

   5 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
   5 ALERT type 3 Indicator that the structure quality may be low
  10 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_PLAT053_2222a
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT054_2222a
;
PROBLEM: Medium  Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
```

```
;
_vrf_PLAT055_2222a
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT230_2222a
;
PROBLEM: Hirshfeld Test Diff for    C02X     --C033     .        5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT905_2222a
;
PROBLEM: Negative K value in the Analysis of Variance ...     -1.456 Report
RESPONSE: ...
;
_vrf_PLAT911_2222a
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
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 16/07/2020; check.def file version of 12/07/2020

Datablock 2222a - ellipsoid plot