checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wky

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: wky

```
Bond precision:   C-C = 0.0020 A          Wavelength=1.54178

Cell:             a=10.3413(4)     b=17.8703(7)         c=20.9013(9)
                  alpha=90         beta=100.077(2)      gamma=90
Temperature:      150 K

                 Calculated                Reported
Volume           3803.0(3)                 3803.0(3)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C42 H48 O10               C21 H24 O5
Sum formula      C42 H48 O10               C21 H24 O5
Mr               712.80                    356.40
Dx,g cm-3        1.245                     1.245
Z                4                         8
Mu (mm-1)        0.720                     0.720
F000             1520.0                    1520.0
F000'            1524.84
h,k,lmax                                   12,22,26
Nref                                       3873
Tmin,Tmax        0.866,0.866               0.010,0.087
Tmin'            0.866

Correction method= # Reported T Limits: Tmin=0.010 Tmax=0.087
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 74.776

R(reflections)= 0.0664( 3615)                wR2(reflections)=
                                             0.1673( 3873)
S = 1.060                  Npar= 236
```

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
             Calc: C42 H48 O10
             Rep.: C21 H24 O5
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         54 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.378 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         13 Report
                2  0  0,  -1  1  2,  -7  5  2,  -1  3  3,  -4  0  4,  -2  0  4,
                4  0  4,  -1  1  4,   4  8  4,  -1  1  5,  -4  0  6,   8  0  6,
               -6  0 22,
```

Alert level G

```
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         51 Note
             O001    O002    O003    O004    O005    C006    C007    H007
             C008    H00A    H00B    C009    C00A    H00C    C00B    H00D
             C00C    C00D    H00E    H00F    C00E    C00F    C00G    H00G
             C00H    H00H    C00I    H00I    C00J    H00J    C00K    C00L
             H00L    C00M    H00K    H00M    C00N    H00N    H00O    C00O
             H00P    H00Q    C00P    H00R    H00S    C00Q    H00T    H00U
             C00R    H00V    H00W
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         21 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
              -1  3  3,  -1  1  4,  -1  1  5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          5 Check
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
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 29/11/2023; check.def file version of 14/09/2023

Datablock wky - ellipsoid plot