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 = 0.0031 A          Wavelength=0.71073

Cell:             a=10.0159(2)     b=21.1579(6)         c=15.1788(4)
                  alpha=90         beta=102.956(1)      gamma=90
Temperature:      170 K
```

	Calculated	Reported
Volume	3134.74(14)	3134.73(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C38 H40 O8	C38 H40 O8
Sum formula	C38 H40 O8	C38 H40 O8
Mr	624.70	624.70
Dx,g cm-3	1.324	1.324
Z	4	4
Mu (mm-1)	0.092	0.092
F000	1328.0	1328.0
F000'	1328.69	
h,k,lmax		13,27,19
Nref		7180
Tmin,Tmax	0.982,0.982	0.702,0.746
Tmin'	0.982	

```
Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.746
AbsCorr = ?

Data completeness=                  Theta(max)= 27.496

R(reflections)= 0.0643( 5781)                    wR2(reflections)=
                                                 0.1445( 7180)
S = 1.089                  Npar= 415
```

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

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT410_ALERT_2_C Short Intra H...H Contact  H00P     ..H01K     .       1.93 Ang.
                                                      x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H00A     ..H00Z     .       1.99 Ang.
                                                      x,y,z  =      1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      7.341 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
                2  0  2,  -9  6  5,
```

Alert level G

```
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         86 Note
              O001    O002    O003    O004    O005    O006    O007    O008
              C009    C00A    C00B    H00B    C00C    H00C    C00D    C00E
              C00F    C00G    C00H    H00H    C00I    H00I    C00J    H00J
              C00K    C00L    C00M    C00N    H00N    C00O    H00O    C00P
              H00P    C00Q    H00Q    C00R    H00R    C00S    C00T    H00T
              C00U    H00U    C00V    H00V    C00W    H00A    H00D    C00X
              H00X    C00Y    H00Y    C00Z    H00Z    C010    H01A    H01B
              C011    H01C    H01D    C012    H01E    H01F    C013    H01G
              H01H    C014    H01I    H01J    C015    H01K    H01L    C016
              H01M    H01N    C017    H01O    H01P    C018    H01Q    H01R
              C019    H01S    H01T    C01A    H01U    H01V
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
```

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
4 **ALERT level G** = General information/check it is not something unexpected

1 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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 14/11/2023; check.def file version of 14/09/2023

Datablock wky - ellipsoid plot