checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 211213lt_auto

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: 211213lt_auto

```
Bond precision:    C-C = 0.0025 A            Wavelength=1.54184

Cell:              a=21.1226(2)      b=21.1226(2)      c=10.9251(1)
                   alpha=90          beta=90           gamma=120
Temperature:       100 K

                   Calculated                Reported
Volume             4221.35(9)                4221.34(9)
Space group        P 61                      P 61
Hall group         P 61                      P 61
Moiety formula     C35 H28 O [+ solvent]     C35 H28 O
Sum formula        C35 H28 O [+ solvent]     C35 H28 O
Mr                 464.57                    464.57
Dx,g cm-3          1.097                     1.096
Z                  6                         6
Mu (mm-1)          0.493                     0.493
F000               1476.0                    1476.0
F000'              1479.92
h,k,lmax           26,26,13                  25,25,13
Nref               5643[ 2978]               4767
Tmin,Tmax          0.977,0.980               0.875,1.000
Tmin'              0.893

Correction method= # Reported T Limits: Tmin=0.875 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.60/0.84      Theta(max)= 73.094
```

R(reflections)= 0.0272(4625)   wR2(reflections)= 0.0745(4767)

S = 1.070   Npar= 328

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
```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         70 %
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● Alert level G
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PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .     0.300 Report
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............   0.00010 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O10            107.2 Degree
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........         ! Info
PLAT791_ALERT_4_G Model has Chirality at C3          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C4          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C7          (Sohnke SpGr)          S Verify
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         58 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         6 Info
```

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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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   7 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 13/07/2021; check.def file version of 13/07/2021