checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-La

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: 3-La

```
Bond precision:   C-C = 0.0044 A           Wavelength=1.54178

Cell:           a=12.3417(3)       b=15.7328(3)      c=18.9830(4)
                alpha=86.423(1)    beta=81.658(1)    gamma=68.732(1)
Temperature:    120 K

                Calculated                  Reported
Volume          3398.35(13)                 3398.35(13)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
Moiety formula  C56 H89 La O4 P4, 2(C7 H8)  C56 H89 La O4 P4, 2(C7 H8)
Sum formula     C70 H105 La O4 P4           C70 H105 La O4 P4
Mr              1273.33                     1273.32
Dx,g cm-3       1.244                       1.244
Z               2                           2
Mu (mm-1)       6.085                       6.085
F000            1348.0                      1348.0
F000'           1350.50
h,k,lmax        15,19,23                    15,19,23
Nref            13544                       13416
Tmin,Tmax       0.405,0.515                 0.409,0.754
Tmin'           0.257

Correction method= # Reported T Limits: Tmin=0.409 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.991            Theta(max)= 72.750

R(reflections)= 0.0350( 13076)                wR2(reflections)=
                                              0.0865( 13416)
S = 1.034                  Npar= 738
```

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

```
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.79Ang From La1            3.05 eA-3
```

Author Response: The residual density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (La)

Alert level C

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         63 Report
                   5  2  0,   6  2  0,   5  6  0,  -5 -7  1,   2 -6  1,  -4 -4  1,
                  -3 -4  1,   0  1  1,   3  3  1,   6  3  1,   7  8  1,  -5 -5  2,
                  -4 -5  2,   1  0  2,   9 10  2,  -4 -5  3,  -3 -5  3,  -4 -4  3,
                  -3 -3  3,   3  1  3,  -2 -8  4, -14 -6  4,  -3 -6  4,  -5 -5  4,
                   5  0  4,   5-13  5,  -1 -6  5,  -6 -3  6,   6 -9  7,  -9-15  9,
                  -5 -5  9,  -9-14 10, -10-13 10,   0-13 10,   1 -6 10,  -1-15 11,
                  -9-13 11,  -8-13 11, -10-12 11,  -1 -5 11,   0 -5 11,   1 -5 11,
                  -3 -1 11,   0-12 12,   1 -8 12, -10 -6 12,   0 -4 12,  -8 -9 13,
                 -10 -2 13,  -1 -1 13,   1 -1 13,   2 -1 13,   2  2 13,  -3-14 14,
                  -1-13 14,   2 -2 14,   1  0 14,  -3-11 15,   2 -5 15,   3 -1 15,
                   5 10 15,  -4-12 16,  -7  0 17,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From La1           -1.72 eA-3
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          1 Report
              H4
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.63 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C65      --C66      .        6.0 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for La1       (III)      .       3.20 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         64 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
                 -1-10 19,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.734 Note
              Predicted wR2: Based on SigI**2  3.16 or SHELX Weight  8.36
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 Info
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 22/08/2024; check.def file version of 21/08/2024

Datablock 3-La - ellipsoid plot