# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 200721a

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: 200721a

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```
Bond precision:   Y- O = 0.0069 A          Wavelength=0.71073

Cell:             a=6.8110(4)     b=9.5833(6)          c=10.5124(7)
                  alpha=90        beta=105.512(7)      gamma=90
Temperature:      293 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 661.17(8) | 661.17(8) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | Mo4 O15 Y2 | Mo4 O15 Y2 |
| Sum formula | Mo4 O15 Y2 | Mo4 O15 Y2 |
| Mr | 801.58 | 801.58 |
| Dx,g cm-3 | 4.026 | 4.026 |
| Z | 2 | 2 |
| Mu (mm-1) | 12.429 | 12.429 |
| F000 | 732.0 | 732.0 |
| F000' | 707.48 | |
| h,k,lmax | 8,11,13 | 8,11,13 |
| Nref | 1351 | 1342 |
| Tmin,Tmax | 0.556,0.780 | 0.257,1.000 |
| Tmin' | 0.532 | |

```
Correction method= # Reported T Limits: Tmin=0.257 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993           Theta(max)= 26.372

R(reflections)= 0.0531( 1217)                    wR2(reflections)=
                                                 0.1306( 1342)
S = 1.076                  Npar= 98
```

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          3 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Mo2              2.11 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Mo2              2.11 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From O7               2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.85Ang From Y1               1.79 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From Mo2              1.71 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From O4               1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Mo2              1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From O1              -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From Mo2             -2.04 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.69Ang From Mo1             -1.86 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.15Ang From Mo1             -1.86 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Mo2             -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.41Ang From Y1              -1.75 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.28Ang From Y1              -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.11Ang From Mo1             -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From Mo2             -1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.98Ang From O7              -1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From O2              -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From Mo2             -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From Mo2             -1.55 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From O8      .        1.16 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From O6      .       -1.33 eA-3
```

## Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Mo1       (VI)      .       5.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo2       (VI)      .       5.88 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y1        (III)     .       3.31 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.9 Low
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
23 **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
22 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
1 ALERT type 4 Improvement, methodology, query or suggestion
4 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.

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**PLATON version of 28/11/2022; check.def file version of 28/11/2022**

**Datablock 200721a** - ellipsoid plot