checkCIF/PLATON report

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

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: 200721b

```
Bond precision:    Y- O = 0.0071 A           Wavelength=0.71073

Cell:              a=6.8176(5)     b=9.5857(6)          c=10.5127(8)
                   alpha=90        beta=105.512(8)      gamma=90
Temperature:       323 K

                   Calculated                Reported
Volume             662.00(9)                 662.00(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          4.021                     4.021
Z                  2                         2
Mu (mm-1)          12.413                    12.413
F000               732.0                     732.0
F000'              707.48
h,k,lmax           8,11,13                   8,11,13
Nref               1353                      1349
Tmin,Tmax                                    0.129,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.129 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 26.372


R(reflections)= 0.0495( 1210)                wR2(reflections)=
                                             0.1229( 1349)
S = 0.891                  Npar= 98
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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 A
EXPT005_ALERT_1_A _exptl_crystal_description is missing
            Crystal habit description.
            The following tests will not be performed.
            CRYSR_01
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ....   Please Do !

🟠 Alert level B
PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE.   293 Degree

🟡 Alert level C
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...   Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...   Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...   Please Check
PLAT213_ALERT_2_C Atom O5   has ADP max/min Ratio .....   3.2 prolat
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   3 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02Ang From Y1   1.87 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From O4   1.56 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.16Ang From O3   1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From O5   -1.71 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From Mo1   -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From Mo1   -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From Mo1   -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From Y1   -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.36Ang From O3   -1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.62Ang From Mo2   -1.51 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From O4   .   1.04 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From O4   . -1.23 eA-3

⚪ Alert level G
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   8.09 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Mo1   (VI)   .   6.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo2   (VI)   .   5.87 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y1   (III)   .   3.31 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   3.6 Low

   2 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
  17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  11 **ALERT level G** = General information/check it is not something unexpected

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 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_EXPT005_200721b
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_PLAT699_200721b
;
PROBLEM: Missing _exptl_crystal_description Value .......    Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

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