

```
R(reflections)= 0.0324( 582)      wR2(reflections)=
S = 1.073                        0.0918( 609)
Npar= 55
```

---

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. 0.81Ang From Mo1 2.77 eA-3

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#### Alert level C

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.87Ang From Mo2 1.84 eA-3  
PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.56Ang From Mo2 -1.65 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.74Ang From O1 . 0.60 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.98Ang From O4 . 0.55 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.45Ang From O1 . 0.49 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.97Ang From O2 . 0.48 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.92Ang From O5 . 0.46 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.67Ang From O2 . 0.44 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.58Ang From O3 . 0.41 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.61Ang From O6 . -1.15 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 1.00Ang From O4 . -0.66 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.71Ang From O4 . -0.60 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.97Ang From O3 . -0.57 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.95Ang From O5 . -0.55 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.79Ang From O3 . -0.43 eA-3

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#### Alert level G

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ Please Check  
PLAT158\_ALERT\_4\_G The Input Unitcell is NOT Standard/Reduced ..... Please Check  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Mo1 (VI) . 5.97 Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Mo2 (VI) . 5.85 Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
16 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 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.

