

```
R(reflections)= 0.0933( 3641)      wR2(reflections)=
S = 1.069                        0.2713( 6678)
Npar= 247
```

---

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

DIFMN02\_ALERT\_2\_B The minimum difference density is  $< -0.1 \times Z_{MAX} \times 1.00$

\_refine\_diff\_density\_min given = -0.853

Test value = -0.800

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 1.17 eA-3

PLAT098\_ALERT\_2\_B Large Reported Min. (Negative) Residual Density -0.85 eA-3

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C00Q --C00R . 9.7 s.u.

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#### Alert level C

DIFMN03\_ALERT\_1\_C The minimum difference density is  $< -0.1 \times Z_{MAX} \times 0.75$

The relevant atom site should be identified.

DIFMX02\_ALERT\_1\_C The maximum difference density is  $> 0.1 \times Z_{MAX} \times 0.75$

The relevant atom site should be identified.

PLAT084\_ALERT\_3\_C High wR2 Value (i.e.  $> 0.25$ ) ..... 0.27 Report

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N004 --C00N . 5.5 s.u.

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 13.564 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.253 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.88Ang From O002 . -0.65 eA-3

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#### Alert level G

PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ Please Check

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.5000 Check

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 46 Note

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= 0.600 480 Note

PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 2 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 1 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

4 **ALERT level B** = A potentially serious problem, consider carefully

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

9 **ALERT level G** = General information/check it is not something unexpected

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

10 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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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.

