

```
R(reflections)= 0.0747( 2233)      wR2(reflections)=
S = 1.086                        0.2005( 2770)
Npar= 200
```

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

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00543 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 14.667 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.117 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 35 Report
5 0 0, 5 8 0, -5 8 1, 5 8 1, -4 9 1, -5 0 2,
4 10 3, -1 0 4, -4 8 4, 1 10 4, 1 10 5, -3 7 7,
-2 1 13, -2 0 14, -2 1 14, -2 1 15, 5 3 16, 5 3 17,
5 3 18, 4 6 18, -1 0 20, -1 1 20, -2 8 21, -2 2 22,
0 6 22, -2 1 23, -2 3 23, -3 0 24, -4 1 24, -3 1 24,
-4 2 24, -3 2 24, -4 3 24, -3 3 24, -4 2 25,



Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.29 Why ?
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O001 . 109.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 38 Note
O001 O002 N003 C004 C005 C006 H006 C007
H007 C009 C00A H00A C00B C00C H00C C00D
H00D C00E H00E C00F C00G H00G C00H H00B
H00F C00I H00I C00J H00H H00J C00K H00K
C00L H00L C00M H00M H00N H00O
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 140 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.71 Note
Predicted wR2: Based on SigI**2 4.25 or SHELX Weight 19.17
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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 06/01/2024; check.def file version of 05/01/2024

