

```
R(reflections)= 0.0733( 5873)      wR2(reflections)=
S = 1.025                        0.2179( 8960)
Npar= 621
```

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.127

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.127 Report

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00483 Ang.



Alert level G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF Please Check

PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 106.5 Degree

PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 . 106.7 Degree

PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 . 106.2 Degree

PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 . 106.3 Degree

PLAT434_ALERT_2_G Short Inter HL..HL Contact F1 ..F4 . 2.79 Ang.

1+x,y,z = 1_655 Check

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note

C26 H22 B F5 O2

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.6 Low

PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

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

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

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

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

7 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

1 ALERT type 4 Improvement, methodology, query or suggestion

0 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.

