

```
R(reflections)= 0.0220( 654)      wR2(reflections)=
S = 1.557                        0.0605( 657)
Npar= 30
```

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check



Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.806 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.94Ang From Sn1 1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From Sn1 -1.81 eA-3



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0 0.998 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.66 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 50% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 70.0 Degree

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **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

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

-43 Y

PLATON-Apr 27 07:54:46 2023 - (281122)

Z -147 HR514_0m

P 4/m n c R = 0.02

RES= 0-101 X

NOMOVE FORCED

Prob	=	50
Temp	=	100