

```
R(reflections)= 0.0204( 103)      wR2(reflections)=
S = 1.208                        0.0491( 108)
Npar= 11
```

---

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



PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio .....	9.82 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	V1 Check
PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on	V1 -1.48 eA-3

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### Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 )	88% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....	! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check

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

- 3 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  
2 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

