

```
R(reflections)= 0.0417( 3579)      wR2(reflections)=
S = 1.091                        0.1021( 3774)
Npar= 310
```

---

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

PLAT234_ALERT_4_C	Large Hirshfeld Difference P1	--F2	.	0.16	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			Ru1	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		P1	0.160	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		P2	0.115	Check
PLAT330_ALERT_2_C	Large Aver Phenyl C-C Dist C6	--C11	.	1.41	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....			2.546	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595		16	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....			10	Note

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#### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...			14	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			24.79	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records			4	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P1		Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P2		Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )			21%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....			72	Note
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
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still			87%	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			3	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....				Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..			50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			2	Info

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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  
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
14 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 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.

