

```
R(reflections)= 0.0311( 5678)      wR2(reflections)=
S = 1.051                        0.0772( 6074)
Npar= 330
```

---

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.

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### Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.4 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	5.9 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C4S Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00867 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	10 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.73Ang From Cs2	1.60 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.87Ang From O1S .	0.56 eA-3

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### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C10 H30 B18 Cl4 Co1 Cs1 O2  
Atom count from \_chemical\_formula\_moiety:C6 H12 Cs1 O2

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.59 Why ?
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem c/2	94 %Fit
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1' Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2' Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C2 .	1.62 Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1' - C2' .	1.62 Ang.
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H2SC ..H4 .	2.10 Ang.
	3/2-y,-1/2+x,1/4+z =	3_645 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	12 Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.18 Ratio
PLAT774_ALERT_1_G	Check X-Y Bond in CIF: Cs1 --Cs2 ..	4.44 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	44.50 Deg.
	O1S -C1S -CS1 1_555 1_555 1_555 .....	# 480 Check
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	11 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 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  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
18 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
15 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  
3 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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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.

