

```
R(reflections)= 0.0240( 1474)      wR2(reflections)=
S = 1.087                        0.0616( 1507)
Npar= 143
```

---

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

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.15	Do !
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	....	3.11	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.596	3	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.13Ang From Cel	2.31	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.03Ang From O4	-0.50	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4A	.	-0.38	eA-3

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### Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			
	not performed for this radiation type.			
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		4	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		2	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c	12/a	Note
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O6	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	14%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	.	106.1	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6	.	107.3	Degree
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		7	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cel	(III)	3.32	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		18	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		94%	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		4	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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
24 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
11 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

