

```
R(reflections)= 0.0404( 6588)      wR2(reflections)=
S = 1.043                        0.1014( 7846)
Npar= 487
```

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C29	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	U1	Check	
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.01492	Ang.	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		4	Report	
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.90Ang	From N9	1.95	eA-3	
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.12Ang	From N15	-1.65	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H5B	.	-0.53	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H19	.	-0.33	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H24A	.	-0.32	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H25A	.	-0.34	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H30	.	-0.31	eA-3	



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	12	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	13.00	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	4	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV)	3.87	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	48	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

