

```
R(reflections)= 0.0337( 1279)      wR2(reflections)=
S = 1.126                        0.0886( 1356)
Npar= 144
```

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.42 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.596	5 Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check



Alert level G

PLAT300_ALERT_4_G	Atom Site Occupancy of S1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7	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 C11	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6C	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 H11	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	81% Note	
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	31 Check	
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info	
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	4 Check	
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	90% Note	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.5 Low	
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	133.5 Degree	

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
33 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.

