

```
R(reflections)= 0.0424( 4113)      wR2(reflections)=
S = 1.000                        0.0832( 4113)
Npar= 334
```

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check
PLAT737_ALERT_1_C	D...A Calc 2.8944(15), Rep 2.894(5)		3.3 s.u.-R
	O3 -O14 1_555 1_555	#	1 Check
PLAT737_ALERT_1_C	D...A Calc 3.0026(17), Rep 3.003(5)		2.9 s.u.-R
	O9 -O14 1_555 1_555	#	4 Check
PLAT737_ALERT_1_C	D...A Calc 2.8837(17), Rep 2.884(5)		2.9 s.u.-R
	O14 -O6 1_555 1_555	#	15 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600		20 Report

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	12 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed 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 C12 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H91 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H92 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H101 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H102 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H103 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H113 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H114 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H115 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H116 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H121 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H122 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H123 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H171 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H172 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H173 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H174 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H182 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H183 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H184 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H191 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H192 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H201 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H202 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H203 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H211 Constrained at	0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H212	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H213	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H221	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H223	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H224	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H143	Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H144	Constrained at	0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)		14% Note
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data		Please Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints		18 Note
PLAT882_ALERT_1_G No Datum for _diffn_reflns_av_unetI/netI		Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		88 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked		! Info
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ...		2 Check

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 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
 42 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

