

```
R(reflections)= 0.0713( 2724)      wR2(reflections)=
S = 1.026                        0.2048( 3543)
Npar= 294
```

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 B

PLAT921_ALERT_1_B R1 in the CIF and FCF Differ by 0.0111 Check

Author Response: The supplied FCF is corresponded with the CIF produced in the same least squares refinement job, the reason for this alert is not clear.

PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by 0.0279 Check

Author Response: The supplied FCF is corresponded with the CIF produced in the same least squares refinement job, the reason for this alert is not clear.



Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00508 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 38 Report
PLAT923_ALERT_1_C S Values in the CIF and FCF Differ by 0.146 Check
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by -0.0027 Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 13 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 18 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of F1 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1A Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2A Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3A Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4 Constrained at 0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4A Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4B Constrained at 0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 80% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 . 106.3 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact F1A ..C3 . 2.93 Ang.
1/2-x,-1/2+y,1/2-z = 2_545 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 123 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 9 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 39 Note

0	ALERT level A	= Most likely a serious problem - resolve or explain
2	ALERT level B	= A potentially serious problem, consider carefully
5	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
25	ALERT level G	= General information/check it is not something unexpected
4	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
7	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
17	ALERT type 4	Improvement, methodology, query or suggestion
0	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.

