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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 B

PLAT410\_ALERT\_2\_B Short Intra H...H Contact H17 ..H26 . 1.82 Ang.  
x,y,z = 1\_555 Check

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#### Alert level C

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 5.0 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.82Ang From F12 1.71 eA-3  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.55Ang From F21 1.62 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.00Ang From N7 . 0.91 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H26 . -0.71 eA-3

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#### Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 11 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 11.86 Why ?  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 5 Report  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for F12 --C10 . 8.0 s.u.  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for F20 --C15 . 8.7 s.u.  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for F23 --C10 . 5.7 s.u.  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C4 Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C9 Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C10 Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C15 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F10 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F11 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F12 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F16 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F17 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F18 Constrained at 0.75 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F19 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F20 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F21 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F22 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F23 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F24 Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O1W Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H1WA Constrained at 0.25 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H1WB Constrained at 0.25 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 15% Note  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O1W ..C26 . 2.84 Ang.  
x,y,z = 1\_555 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2 Note  
PLAT780\_ALERT\_1\_G Coordinates do not Form a Properly Connected Set Please Do !

|                   |  |     |      |
|-------------------|--|-----|------|
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints .....         | 66  | 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  | 29  | Note |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 5   | Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity .....       | 4.9 | Low  |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 0   | Info |

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| 0  | <b>ALERT level A</b> | = Most likely a serious problem - resolve or explain         |
| 1  | <b>ALERT level B</b> | = A potentially serious problem, consider carefully          |
| 8  | <b>ALERT level C</b> | = Check. Ensure it is not caused by an omission or oversight |
| 38 | <b>ALERT level G</b> | = General information/check it is not something unexpected   |
|    |                      |  |
| 3  | ALERT type 1         | CIF construction/syntax error, inconsistent or missing data  |
| 18 | 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              |
| 18 | ALERT type 4         | Improvement, methodology, query or suggestion                |
| 2  | 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.

