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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 C**

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C1	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....	4.894	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta (Min).		8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	14	Report

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		9	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		2	Report
PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	.....	Please Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		14	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of S1A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S1	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16	Constrained at	0.2	Check
PLAT301_ALERT_3_G	Main Residue Disorder	.....(Resd 1 )	21%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....	26	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	533	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		11	Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		3	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ		2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.		3	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 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.

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**PLATON version of 06/07/2023; check.def file version of 30/06/2023**

