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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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT051_ALERT_1_C	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	2.07 %
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.62 Report
PLAT723_ALERT_1_C	Torsion Calc -83.00, Rep 75(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-LI5	3_676 1_555 1_555 1_555 #	29 Check
PLAT723_ALERT_1_C	Torsion Calc 97.00, Rep -105(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-LI5	3_676 1_555 1_555 3_676 #	30 Check
PLAT723_ALERT_1_C	Torsion Calc 43.00, Rep -158(24) Dev...	159.00 Sigma
LI4 -LI4 -LI12-LI15	3_676 1_555 1_555 1_555 #	31 Check
PLAT723_ALERT_1_C	Torsion Calc 34.00, Rep -168(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S1	3_676 1_555 1_555 1_565 #	32 Check
PLAT723_ALERT_1_C	Torsion Calc -146.00, Rep 12(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S1	3_676 1_555 1_555 3_666 #	33 Check
PLAT723_ALERT_1_C	Torsion Calc 141.00, Rep -61(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S2	3_676 1_555 1_555 3_666 #	34 Check
PLAT723_ALERT_1_C	Torsion Calc -39.00, Rep 119(19) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S2	3_676 1_555 1_555 1_565 #	35 Check
PLAT723_ALERT_1_C	Torsion Calc -55.00, Rep 103(20) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S3	3_676 1_555 1_555 1_555 #	36 Check
PLAT723_ALERT_1_C	Torsion Calc 125.00, Rep -77(20) Dev...	158.00 Sigma
LI4 -LI4 -LI12-S3	3_676 1_555 1_555 3_676 #	37 Check
PLAT723_ALERT_1_C	Torsion Calc -1.00, Rep 2(19) Dev...	3.00 Sigma
LI6 -LI5 -LI13-S6	3_666 1_555 1_555 2_655 #	111 Check
PLAT723_ALERT_1_C	Torsion Calc 1.00, Rep 4(20) Dev...	3.00 Sigma
LI7 -LI5 -LI13-S6	1_555 1_555 1_555 2_655 #	131 Check
PLAT723_ALERT_1_C	Torsion Calc 23.00, Rep 25(30) Dev...	2.00 Sigma
LI8 -LI8 -LI14-I1	3_655 1_555 1_555 1_545 #	136 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.098 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report
PLAT926_ALERT_1_C	Reported and Calculated R1 Differ by .....	-0.0014 Check
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by .....	-0.0016 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.72Ang From S4	1.70 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.50Ang From Li7	1.62 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.85Ang From S4	1.61 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.19Ang From S2	1.53 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.24Ang From I1	1.52 eA-3



### Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3 Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.68890 Ang.
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0010 Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0010 Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6 )	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7 )	100% Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 8 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 9 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 10 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 11 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 12 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 13 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 14 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 15 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 16 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 17 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 2 )	0.94	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 6 )	0.96	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 7 )	0.52	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 8 )	0.33	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 9 )	0.37	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 10 )	0.30	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 11 )	0.47	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 12 )	0.48	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 13 )	0.48	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 14 )	0.07	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 15 )	0.28	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 16 )	0.09	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 17 )	0.18	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		16	Note
	Li			
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		71	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		5	Note
PLAT984_ALERT_1_G	The I-f' = -0.7738 Deviates from the B&C-Value		-0.4882	Check
PLAT984_ALERT_1_G	The Li-f' = -0.0007 Deviates from the B&C-Value		0.0003	Check
PLAT984_ALERT_1_G	The S-f' = 0.1048 Deviates from the B&C-Value		0.1187	Check
PLAT984_ALERT_1_G	The Si-f' = 0.0672 Deviates from the B&C-Value		0.0783	Check
PLAT985_ALERT_1_G	The I-f" = 1.7195 Deviates from the B&C-Value		1.7230	Check

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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  
 24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 43 **ALERT level G** = General information/check it is not something unexpected

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

