
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

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 .	2.09 %
PLAT723_ALERT_1_C	Torsion Calc 116.00, Rep 33(12) Dev...	83.00 Sigma
	LI4 -LI4 -LI12-LI5 3_676 1_555 1_555 3_676 #	31 Check
PLAT723_ALERT_1_C	Torsion Calc -64.00, Rep -147(12) Dev...	83.00 Sigma
	LI4 -LI4 -LI12-LI5 3_676 1_555 1_555 1_555 #	32 Check
PLAT723_ALERT_1_C	Torsion Calc -122.00, Rep 156(15) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-LI15 3_676 1_555 1_555 3_676 #	33 Check
PLAT723_ALERT_1_C	Torsion Calc 58.00, Rep -24(15) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-LI15 3_676 1_555 1_555 1_555 #	34 Check
PLAT723_ALERT_1_C	Torsion Calc 52.00, Rep -31(7) Dev...	83.00 Sigma
	LI4 -LI4 -LI12-S1 3_676 1_555 1_555 1_565 #	35 Check
PLAT723_ALERT_1_C	Torsion Calc -129.00, Rep 149(7) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-S1 3_676 1_555 1_555 3_666 #	36 Check
PLAT723_ALERT_1_C	Torsion Calc -22.00, Rep -104(7) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-S2 3_676 1_555 1_555 1_565 #	37 Check
PLAT723_ALERT_1_C	Torsion Calc 158.00, Rep 76(7) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-S2 3_676 1_555 1_555 3_666 #	38 Check
PLAT723_ALERT_1_C	Torsion Calc 143.00, Rep 61(8) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-S3 3_676 1_555 1_555 3_676 #	39 Check
PLAT723_ALERT_1_C	Torsion Calc -37.00, Rep -119(8) Dev...	82.00 Sigma
	LI4 -LI4 -LI12-S3 3_676 1_555 1_555 1_555 #	40 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	-0.0017 Check



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 4)	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)	0.97 Check

PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 4)	0.98	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 6)	0.89	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 7)	0.56	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 8)	0.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 9)	0.34	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 10)	0.37	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 11)	0.30	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 12)	0.47	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 13)	0.44	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 14)	0.08	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 15)	0.22	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 16)	0.17	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 17)	0.20	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		59	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		619	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.1	Low
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

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 46 **ALERT level G** = General information/check it is not something unexpected

19 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
 5 ALERT type 3 Indicator that the structure quality may be low
 33 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

