
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

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.06 Note
PLAT332_ALERT_2_C	Large Phenyl C-C Range C00A -C14 .	0.16 Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	82 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	6 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0050 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0050 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0050 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C00A --C14 .	6.8 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C006 --C1A .	5.8 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of N0 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N003 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C0 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C008 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00D Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00E Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00F Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00H Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00I Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00J Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00K Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00L Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00M Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00N Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00Q Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00R Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00S Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00T Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00U Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00W Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00Y Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C00Z Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C010 Constrained at	0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C011 Constrained at	0.8 Check

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PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	60	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1146	Note

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

5	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
8	ALERT type 3	Indicator that the structure quality may be low
142	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.

