
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**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	O4	--C1	.	6.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	C3	--C4	.	5.2 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	O9	--C19	.	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	C19	--C20	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test Diff	for	C20	--C21	.	6.0 s.u.
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as	Compared to	Neighbors of	C16	Check

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij	Restrained non-H Atoms ...				5	Report
PLAT005_ALERT_5_G	No Embedded Refinement	Details Found	in the CIF				Please Do !
PLAT398_ALERT_2_G	Deviating	C-O-C	Angle From 120	for O4		105.7	Degree
PLAT398_ALERT_2_G	Deviating	C-O-C	Angle From 120	for O9		104.6	Degree
PLAT789_ALERT_4_G	Atoms with Negative	_atom_site_disorder_group	#			2	Check
PLAT860_ALERT_3_G	Number of Least-Squares	Restraints			40	Note
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and	Succeeded by	SHELXL/		2018	Note

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

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

