
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 B

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	40.54	Check
PLAT090_ALERT_3_B	Poor Data / Parameter Ratio (Zmax > 18)	5.96	Note
PLAT213_ALERT_2_B	Atom Oh1 has ADP max/min Ratio	4.7	oblate
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	Oh1	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	Ow	Check

Alert level C

DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.		
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.46	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.74	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	5.0	Ratio

Alert level G

FORMU01_ALERT_2_G	There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data. Atom count from _chemical_formula_sum:H20 O21 S1 Zn7.82 Atom count from the _atom_site data: O21 S1 Zn7.811		
CELLZ01_ALERT_1_G	Difference between formula and atom_site contents detected.		
CELLZ01_ALERT_1_G	WARNING: H atoms missing from atom site list. Is this intentional? From the CIF: _cell_formula_units_Z 2 From the CIF: _chemical_formula_sum H20 O21 S Zn7.82 TEST: Compare cell contents of formula and atom_site data		
	atom Z*formula cif sites diff		
	H 40.00 0.00 40.00		
	O 42.00 42.00 0.00		
	S 2.00 2.00 0.00		
	Zn 15.64 15.62 0.02		
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.5000	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder	17%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	7	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

7 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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.

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