
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

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of B01P Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.2 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report
-1 1 0, 1 1 0, 0 2 0, 0 -1 1, -3 0 1, -1 0 1,
1 0 1, 0 1 1, -1 -2 2, 1 -2 2, 1 -1 2, 0 0 2,
-1 -1 3, 1 1 3,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) F1 --B01P . 5.5 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) F00B --B01P . 7.6 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) F0 --B01P . 7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Au01 --P003 . 5.8 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 60% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 108 Note
Au01 P002 P003 P004 P005 F006 C007 H007
C008 H008 C009 C00A F00B C00C H00C C00D
H00D C00E C00F C00G C00H H00H C00I C00J
H00J C00K H00K C00L H00L C00M H00M C00N
H00N C00O H00O C00P H00P C00Q C00R H00R
C00S H00S C00T H00T C00U C00V H00V C00W
H00W C00X H00X C00Y H00Y C00Z H00Z C010
H010 C011 H011 C012 H012 C013 H013 C014
H014 C015 H015 C016 H016 C017 H017 F018
C019 H019 C01A H01A C01B H01B C01C H01C
C01D H01D C01E H01E C01F H01F C01G H01G
C01H H01H C01I H01I C01J H01J C01K H01K
C01L H01L C01M H01M C01N H01N C01O H01O
B01P F01Q F01R F0
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
0 1 0, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
-3 0 1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 4 Note
0 0 1, 0 1 0, 1 1 0, 1 1 3,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.53 Note
Predicted wR2: Based on SigI**2 1.49 or SHELX Weight 3.72
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

16 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
8 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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