
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

PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) 5.69 Note
PLAT430_ALERT_2_B Short Inter D...A Contact O1W ..O2W . 2.76 Ang.
1-x+y,y,z = 5_655 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O1W ..N1 . 2.86 Ang.
x,y,z = 1_555 Check

Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 6.270
Value of mu given = 6.150
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 0.030
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.94 %
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
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
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O2W 0.142 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From O1W . 0.53 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 16 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0 0.950 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 24.74 Why ?
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group R-3m Check
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 35% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O1W Check

PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	O2W	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O2W ..C6 .	2.81 Ang.
		x,y,z =	1_555 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		11 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2 (III) .		3.71 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		97 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		2 Note
PLAT982_ALERT_1_G	The C-f' = 0.0192 Deviates from IT-value =		0.0181 Check
PLAT982_ALERT_1_G	The Fe-f' = -1.0935 Deviates from IT-value =		-1.1336 Check
PLAT982_ALERT_1_G	The N-f' = 0.0330 Deviates from IT-value =		0.0311 Check
PLAT982_ALERT_1_G	The O-f' = 0.0517 Deviates from IT-value =		0.0492 Check
PLAT983_ALERT_1_G	The Fe-f" = 3.1934 Deviates from IT-Value =		3.1974 Check
PLAT983_ALERT_1_G	The O-f" = 0.0336 Deviates from IT-Value =		0.0322 Check

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

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 17 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

PLATON version of 20/01/2022; check.def file version of 19/01/2022

