
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**

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
yellowish

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

| | | | | | |
|-------------------|--|------------------------|---------------------------------|-------|--------|
| PLAT213_ALERT_2_C | Atom O13 | has ADP max/min Ratio | | 3.8 | prolat |
| PLAT220_ALERT_2_C | NonSolvent | Resd 1 O | Ueq(max)/Ueq(min) Range | 6.0 | Ratio |
| PLAT222_ALERT_3_C | NonSolvent | Resd 1 H | Uiso(max)/Uiso(min) Range | 9.4 | Ratio |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | Tb01 | Check |
| PLAT245_ALERT_2_C | U(iso) H1A | Smaller than U(eq) O20 | by | 0.018 | Ang**2 |
| PLAT245_ALERT_2_C | U(iso) H1B | Smaller than U(eq) O20 | by | 0.018 | Ang**2 |
| PLAT975_ALERT_2_C | Check Calcd Resid. Dens. | 0.84Ang From O20 | . | 1.18 | eA-3 |
| PLAT975_ALERT_2_C | Check Calcd Resid. Dens. | 0.97Ang From O20 | . | 0.64 | eA-3 |
| PLAT975_ALERT_2_C | Check Calcd Resid. Dens. | 1.07Ang From O13 | . | 0.42 | eA-3 |
| PLAT976_ALERT_2_C | Check Calcd Resid. Dens. | 0.44Ang From O13 | . | -0.53 | eA-3 |
| PLAT976_ALERT_2_C | Check Calcd Resid. Dens. | 0.67Ang From O13 | . | -0.53 | eA-3 |
| PLAT977_ALERT_2_C | Check Negative Difference Density on H1B | | . | -0.33 | eA-3 |

● **Alert level G**

| | | | | | |
|-------------------|--|----------------------|---|-------|--------------|
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms | | | 5 | Report |
| PLAT128_ALERT_4_G | Alternate Setting for Input Space Group | C2/c | | I2/a | Note |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Tb01 --O2 | . | 13.4 | s.u. |
| PLAT300_ALERT_4_G | Atom Site Occupancy of O19 | Constrained at | | 0.7 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of O18 | Constrained at | | 0.3 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H1C | Constrained at | | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H13C | Constrained at | | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H19A | Constrained at | | 0.7 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H18A | Constrained at | | 0.3 | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder |(Resd 1) | | 2% | Note |
| PLAT303_ALERT_2_G | Full Occupancy Atom H100 | with # Connections | | 2.00 | Check |
| PLAT416_ALERT_2_G | Short Intra D-H..H-D | H1 ..H1C | . | 0.98 | Ang. |
| | | x,y,z = | | 1_555 | Check |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact | O5 ..C2 | . | 2.96 | Ang. |
| | | 3/2-x,1/2-y,1-z = | | 7_656 | Check |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact | O9 ..C29 | . | 2.96 | Ang. |
| | | 3/2-x,-1/2+y,3/2-z = | | 4_646 | Check |
| PLAT605_ALERT_4_G | Largest Solvent Accessible VOID in the Structure | | | 179 | A**3 |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | | 1 | Note |
| PLAT767_ALERT_4_G | INS Embedded LIST 6 Instruction Should be LIST 4 | | | | Please Check |
| PLAT869_ALERT_4_G | ALERTS Related to the Use of SQUEEZE | Suppressed | | | ! Info |
| 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). | | | 2 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | | 18 | Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | | | 4.8 | Low |
| PLAT961_ALERT_5_G | Dataset Contains no Negative Intensities | | | | Please Check |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | | | 8 | Info |

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

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

14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 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
12 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.

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