

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MC22029

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: MC22029

| | | | |
|------------------------|----------------|--------------------|---------------|
| Bond precision: | C-C = 0.0016 Å | Wavelength=0.71073 | |
| Cell: | a=21.1676 (5) | b=15.6626 (4) | c=11.8892 (3) |
| | alpha=90 | beta=90 | gamma=90 |
| Temperature: | 120 K | | |
| | Calculated | Reported | |
| Volume | 3941.74 (17) | 3941.72 (17) | |
| Space group | P 21 21 21 | P 21 21 21 | |
| Hall group | P 2ac 2ab | P 2ac 2ab | |
| Moiety formula | C49 H53 Al | C49 H53 Al | |
| Sum formula | C49 H53 Al | C49 H53 Al | |
| Mr | 668.89 | 668.95 | |
| Dx, g cm ⁻³ | 1.127 | 1.127 | |
| Z | 4 | 4 | |
| Mu (mm ⁻¹) | 0.084 | 0.084 | |
| F000 | 1440.0 | 1440.9 | |
| F000' | 1440.71 | | |
| h, k, lmax | 32, 23, 18 | 32, 23, 17 | |
| Nref | 14834 [8107] | 13850 | |
| Tmin, Tmax | 0.974, 0.982 | 0.981, 0.981 | |
| Tmin' | 0.974 | | |

Correction method= # Reported T Limits: Tmin=0.981 Tmax=0.981
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.93 Theta(max)= 32.980

| | |
|---------------------------------|-------------------|
| R(reflections)= 0.0383 (11861) | wR2(reflections)= |
| S = 1.068 | 0.0564 (13850) |
| Npar= 928 | |

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

| | | |
|--|----|-------|
| PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). | 12 | Note |
| PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. | 3 | Check |



Alert level C

| | | |
|---|-----|-------|
| PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range | 5.0 | Ratio |
|---|-----|-------|



Alert level G

| | | |
|--|--------|--------|
| PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... | 50 | Report |
| PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical | ? | Check |
| PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... | Please | Check |
| PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records | 1 | Report |
| PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters | 2 | Info |
| PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 | 361 | Note |
| PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... | 2 | Check |
| PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. | 23 | Info |
| PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used | Please | Note |

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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-

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.

