

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5

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: 5

Bond precision: C-C = 0.0045 Å Wavelength=0.71073

Cell: a=13.060(6) b=19.92(1) c=21.490(11)
 alpha=65.028(6) beta=87.853(7) gamma=89.408(7)

Temperature: 296 K

	Calculated	Reported
Volume	5064(4)	5064(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C65 H47 Al3 F3 N6 O9 [+ solvent]	?
Sum formula	C65 H47 Al3 F3 N6 O9 [+ solvent]	C65 H47 Al3 F3 N6 O9
Mr	1194.03	1194.02
Dx, g cm ⁻³	0.783	0.783
Z	2	2
Mu (mm ⁻¹)	0.080	0.080
F000	1234.0	1234.0
F000'	1234.96	
h,k,lmax	15,23,25	15,23,25
Nref	17579	17212
Tmin,Tmax	0.967,0.984	0.964,0.982
Tmin'	0.967	

Correction method= # Reported T Limits: Tmin=0.964 Tmax=0.982
AbsCorr = MULTI-SCAN

Data completeness= 0.979 Theta(max)= 24.858

R(reflections)= 0.0556(9858) wR2(reflections)= 0.1635(17212)

S = 1.014 Npar= 778

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**

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 6 Check

 **Alert level C**

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.979 Why?
PLAT230_ALERT_2_C Hirshfeld Test Diff for O9 --C65 . 7.0 s.u.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00452 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -15.024 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.274 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.591 361 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.98A From O8 0.42 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01A From O9 0.41 eA-3

 **Alert level G**

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

