

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compoundAIL33

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: compoundAIL33

Bond precision:	C-C = 0.0060 A	Wavelength=0.78224	
Cell:	a=34.0652(3)	b=34.0652(3)	c=18.1656(2)
	alpha=90	beta=90	gamma=120
Temperature:	83 K		
	Calculated	Reported	
Volume	18255.9(4)	18255.9(4)	
Space group	R -3	R -3 :h	
Hall group	-R 3	-R 3	
Moiety formula	6(C57 H30 Al N3 O3), C0.90 H1.80 Cl1.80, 6(C2 H3 N)	6(C57 H30 Al N3 O3), C0.90 H1.80 Cl1.80, 6(C2 H3 N)	
Sum formula	C354.90 H199.80 Al6 Cl1.80 N24 O18	C354.90 H199.80 Al6 Cl1.80 N24 O18	
Mr	5313.68	5313.67	
Dx, g cm ⁻³	1.450	1.450	
Z	3	3	
Mu (mm ⁻¹)	0.161	0.161	
F000	8249.4	8249.0	
F000'	8255.94		
h,k,lmax	40,40,21	40,40,21	
Nref	7002	6965	
Tmin,Tmax	0.997,0.998	0.977,1.034	
Tmin'	0.997		

Correction method= # Reported T Limits: Tmin=0.977 Tmax=1.034
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.499

R(reflections)= 0.0791(5595) wR2(reflections)= 0.2317(6965)

S = 1.124 Npar= 613

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	1 Check
	C73	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C72 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N4	0.165 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.006 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.979 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	6 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.590	31 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	5 Note

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3 Note
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	30.22 Why ?
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.78224 Ang.
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Al01 --O2 .	5.5 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1 Constrained at	0.3 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C73 Constrained at	0.9 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H73 Constrained at	0.3 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	4.50 Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C009 -C018 .	1.44 Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C013 -C017 .	1.44 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	58 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Al01 (III) .	3.07 Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	60% Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	19 Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	21 Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info
PLAT984_ALERT_1_G	The C-f' = -0.0020 Deviates from the B&C-Value	0.0041 Check
PLAT984_ALERT_1_G	The Al-f' = 0.0674 Deviates from the B&C-Value	0.0767 Check
PLAT984_ALERT_1_G	The Cl-f' = 0.1427 Deviates from the B&C-Value	0.1721 Check
PLAT984_ALERT_1_G	The N-f' = -0.0031 Deviates from the B&C-Value	0.0078 Check
PLAT984_ALERT_1_G	The O-f' = -0.0041 Deviates from the B&C-Value	0.0135 Check

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
11 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.

