

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound1

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: Compound1

Bond precision: C-C = 0.0021 A Wavelength=0.71073

Cell: a=24.0888(13) b=11.7687(6) c=20.4327(11)
 alpha=90 beta=111.559(1) gamma=90

Temperature: 103 K

	Calculated	Reported
Volume	5387.3(5)	5387.3(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C44 H82 Al2 Ho2 N2	C44 H82 Al2 Ho2 N2
Sum formula	C44 H82 Al2 Ho2 N2	C44 H82 Al2 Ho2 N2
Mr	1022.94	1022.93
Dx,g cm-3	1.261	1.261
Z	4	4
Mu (mm-1)	2.974	2.974
F000	2080.0	2080.0
F000'	2079.21	
h,k,lmax	33,16,28	33,16,28
Nref	7904	7898
Tmin,Tmax	0.248,0.679	0.080,0.624
Tmin'	0.092	

Correction method= # Reported T Limits: Tmin=0.080 Tmax=0.624
AbsCorr = NUMERICAL

Data completeness= 0.999 Theta(max)= 30.057

R(reflections)= 0.0172(7569) wR2(reflections)= 0.0466(7898)

S = 1.042 Npar= 239

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**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.22	Report
PLAT731_ALERT_1_C	Bond Calc 3.2486(6), Rep 3.24874(15)	4	su-Rat
	HO1 -HO1 1.555 7.556	6	Check
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	1	Note

● **Alert level G**

PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.79	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	7.63	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ho1 -- C2 ..	5.4	su
PLAT303_ALERT_2_G	Full Occupancy H-Atom H1C with # Connections	2.00	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2	Check
PLAT605_ALERT_4_G	Structure Contains Solvent Accessible VOIDS of .	173	A**3
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed		! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...	1	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	6	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 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*, 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 21/06/2015; check.def file version of 21/06/2015

