

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision:    C-C = 0.0034 Å                      Wavelength=0.71073

Cell:                      a=10.135(9)              b=18.687(14)              c=19.155(15)  
                            alpha=90              beta=104.73(2)              gamma=90

Temperature:            100 K

	Calculated	Reported
Volume	3509(5)	3509(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30.84 H54.52 Al B2 N4, 0.159(C H3)	C31 H55 Al B2 N4
Sum formula	C31 H55 Al B2 N4	C31 H55 Al B2 N4
Mr	532.39	532.39
Dx, g cm <sup>-3</sup>	1.008	1.008
Z	4	4
Mu (mm <sup>-1</sup> )	0.081	0.081
F000	1168.0	1168.0
F000'	1168.54	
h,k,lmax	12,22,23	12,22,23
Nref	6621	6558
Tmin,Tmax	0.976,0.986	0.662,0.735
Tmin'	0.975	

Correction method= # Reported T Limits: Tmin=0.662 Tmax=0.735  
AbsCorr = MULTI-SCAN

Data completeness= 0.990                      Theta(max)= 25.620

R(reflections)= 0.0574( 4722)              wR2(reflections)= 0.1319( 6558)

S = 1.059                      Npar= 443

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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

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.132

PLAT220_ALERT_2_C	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT222_ALERT_3_C	Non-Solv.	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.5	Ratio
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible	VOIDS of	.			34	Ang**3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....				9.459	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.					0	Info



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...					9	Report
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12 .....					0.132	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ						Please Check
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records					1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records					3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records					3	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	All	--N3	.		7.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	All	--N4	.		6.4	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1	)			15%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2	)				100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	Resd 1				92.36	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	Resd 2				0.64	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact B1	..C28B				2.55	Ang.
		x,y,z =				1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....					7	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....					48	Note
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					63	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...					1	Note

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

2 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  
7 ALERT type 3 Indicator that the structure quality may be low  
8 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 03/05/2019; check.def file version of 29/04/2019**

Datablock I - ellipsoid plot

