

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TPP\_Al\_phsalMe2

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: TPP\_Al\_phsalMe2

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Bond precision:    C-C = 0.0053 Å                      Wavelength=0.71073

Cell:                a=13.324(13)                b=13.763(13)                c=14.190(14)  
                      alpha=91.243(14)        beta=104.039(13)        gamma=101.050(12)  
Temperature:        273 K

	Calculated	Reported
Volume	2471(4)	2471(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H26 Al N2 O4, C24 H20 P, 2(C2 H3 N)	?
Sum formula	C58 H52 Al N4 O4 P	C58 H52 Al N4 O4 P
Mr	926.99	926.98
Dx, g cm <sup>-3</sup>	1.246	1.246
Z	2	2
Mu (mm <sup>-1</sup> )	0.125	0.125
F000	976.0	976.0
F000'	976.69	
h, k, lmax	15, 16, 16	15, 16, 16
Nref	8725	8574
Tmin, Tmax	0.990, 0.991	0.890, 0.990
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.890 Tmax=0.990  
AbsCorr = MULTI-SCAN

Data completeness= 0.983                      Theta(max)= 25.030

R(reflections)= 0.0581( 5628)	wR2(reflections)= 0.1771( 8574)
S = 1.017	Npar= 947

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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.

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#### Alert level C

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	9.05	Note
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C56	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C58	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N3	0.132	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00527	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	4.604	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	146	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H5'A .	-0.31	eA-3

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	72	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	104	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	36	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	273	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	273	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) All --O4' .	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) All --N1' .	6.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	97%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C16' -C21' .	1.42	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C7 -C12	0.48	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C16 -C21	0.54	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C22 -C27	0.56	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C7' -C12'	0.49	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C16' -C21'	0.54	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C22' -C27'	0.57	Ang.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C15	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	3	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5' --C6'	1.70	Ang.
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1458	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	36%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	5	Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

28 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

15 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  
8 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

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**PLATON version of 20/01/2022; check.def file version of 19/01/2022**

