

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: DAP

Bond precision: C-C = 0.0192 Å Wavelength=0.41390

Cell: a=15.88000(5) b=15.99245(4) c=24.15056(8)
 alpha=90 beta=90 gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	6133.28(3)	6133.28(3)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	Al5 O28 P7, 2(C3 H6 N2.57), O1.15	?
Sum formula	C6 H12 Al5 N5.14 O29.15 P7 ?	
Mr	974.23	0.00
Dx,g cm-3	2.110	0.000
Z	8	8
Mu (mm-1)	0.161	0.000
F000	3898.0	0.0
F000'	3899.81	
h,k,lmax	13,13,20	
Nref	1899	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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 A

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
 Label identifying the atom site 1.
GEOM003_ALERT_1_A _geom_bond_distance is missing

Distance between atom sites 1 and 2.
 GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
 Label identifying the atom site 2.
 GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
 Label identifying the atom site 3.

PLAT043_ALERT_1_A	Check Reported Molecular Weight	0.00
PLAT047_ALERT_1_A	SumFormula Not Given	?
PLAT075_ALERT_1_A	Occupancy 1. greater than 1.0 for	OW1
PLAT075_ALERT_1_A	Occupancy 1. greater than 1.0 for	N11
PLAT075_ALERT_1_A	Occupancy 1. greater than 1.0 for	N15
PLAT075_ALERT_1_A	Occupancy 1. greater than 1.0 for	N21
PLAT075_ALERT_1_A	Occupancy 1. greater than 1.0 for	N25



Alert level B

PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds	0.0192 Ang
-------------------	---------------------------------------	------------



Alert level C

REFI015_ALERT_1_A _refine_ls_shift/su_max is missing
 Maximum shift/s.u. ratio after final refinement cycle.
 The following tests will not be performed
 SHFSU_01

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT142_ALERT_4_C	su on b - Axis Small or Missing	0.00004 Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing	0.00008 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C12 - H1 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C12 - H2 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C13 - H3 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C13 - H4 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C14 - H5 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C14 - H6 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C22 - H8 ...	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C23 - H9 ...	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C23 - H10 ...	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C24 - H11 ...	1.13 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C24 - H12 ...	1.11 Ang.
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C12 - C13 ...	1.66 Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1

A15 O28 P7



Alert level G

PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	2
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	OW1
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1
PLAT793_ALERT_4_G	The Model has Chirality at P1 (Verify)	S
PLAT793_ALERT_4_G	The Model has Chirality at P2 (Verify)	S
PLAT793_ALERT_4_G	The Model has Chirality at P3 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at P4 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at P6 (Verify)	S
PLAT793_ALERT_4_G	The Model has Chirality at P7 (Verify)	R
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al1 (III)	2.83
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al2 (III)	2.88
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al3 (III)	2.74
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al4 (III)	3.16
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al5 (III)	2.92
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Al6 (III)	3.08
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	42
PLAT950_ALERT_5_G	Reported and Calculated Hmax Values Differ by ..	13
PLAT951_ALERT_5_G	Reported and Calculated Kmax Values Differ by ..	13

PLAT952_ALERT_5_G	Reported and Calculated Lmax Values Differ by ..	20
PLAT984_ALERT_1_G	The Al-f' = 0.032 Deviates from the B&C-Value	0.020
PLAT984_ALERT_1_G	The O-f' = 0.003 Deviates from the B&C-Value	0.002
PLAT984_ALERT_1_G	The P-f' = 0.055 Deviates from the B&C-Value	0.035
PLAT985_ALERT_1_G	The Al-f" = 0.031 Deviates from the B&C-Value	0.017
PLAT985_ALERT_1_G	The O-f" = 0.004 Deviates from the B&C-Value	0.002
PLAT985_ALERT_1_G	The P-f" = 0.058 Deviates from the B&C-Value	0.031

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

19 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 ALERT type 2 Indicator that the structure model may be wrong or deficient
 13 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 10 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*, 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.

