

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TPP_Al_Me4azp2_01

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_Me4azp2_01

Bond precision: C-C = 0.0060 A Wavelength=0.71073

Cell: a=21.806 (4) b=21.822 (4) c=20.800 (4)
 alpha=90 beta=101.314 (3) gamma=90

Temperature: 90 K

	Calculated	Reported
Volume	9705 (3)	9705 (3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
	C32 H32 Al N4 O4, C30 H26	
Moiety formula	Al N4 O4, 2(C24 H20 P), 3(O), 2(C H3)	?
Sum formula	C112 H104 Al2 N8 O11 P2	C56 H55 Al N4 O5.50 P
Mr	1853.93	929.99
Dx, g cm ⁻³	1.269	1.273
Z	4	8
Mu (mm ⁻¹)	0.130	0.130
F000	3904.0	3928.0
F000'	3906.84	
h, k, lmax	25, 25, 24	25, 25, 24
Nref	8570	8549
Tmin, Tmax	0.985, 0.994	0.910, 0.990
Tmin'	0.981	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 25.030

R(reflections)= 0.0698(5440)

wR2(reflections)=
0.2098(8549)

S = 1.062

Npar= 987

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 B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 05 Check

Author Response: The oxygen atom is a water molecule.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) 06 Check

Author Response: The oxygen atom is a water molecule.

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by ..	6.05 Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio		8.66 Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.01 Report
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2	--C7	0.17 Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	05	0.153 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	06	0.174 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		9.129 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	21 Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.85Ang From O6	. -0.50 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.69Ang From O6	. -0.48 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.66Ang From O6	. -0.47 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang From O6	. -0.42 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.82Ang From O6	. -0.41 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C56 H55 Al1 N4 O5.5 P1
Atom count from the _atom_site data: C56 H52 Al1 N4 O5.5 P1

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C56 H55 Al1 N4 O5.5 P1
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	448.00	448.00	0.00

H	440.00	416.00	24.00
Al	8.00	8.00	0.00
N	32.00	32.00	0.00
O	44.00	44.00	0.00
P	8.00	8.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	81	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	107	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	25.49	Why ?
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	28	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C28 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C28' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C29 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C29' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C30 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C30' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21' Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27'	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H29	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H29'	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32F	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		98%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		97%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)		0.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)		2.06	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 7)		1.94	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		6	Note
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4 --C8		1.76	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5 --C6		1.82	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9 --C14		1.80	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4' --C8'		1.77	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5' --C6'		1.82	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9' --C14'		1.79	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	0			
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		1606	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		33%	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully

16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
107 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
22 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
87 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

