

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TPP_Al_azpCl2_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_azpCl2_01

Bond precision:	C-C = 0.0070 A	Wavelength=0.71073	
Cell:	a=13.424 (2) alpha=90	b=16.380 (3) beta=90	c=41.151 (7) gamma=90
Temperature:	90 K		
	Calculated	Reported	
Volume	9049 (3)	9048 (3)	
Space group	P n a 21	P n a 21	
Hall group	P 2c -2n	P 2c -2n	
Moiety formula	C24 H12 Al Cl4 N4 O4, C24 H20 P [+ solvent]	?	
Sum formula	C48 H32 Al Cl4 N4 O4 P [+ solvent]	C48 H32 Al Cl4 N4 O4 P	
Mr	928.53	928.52	
Dx, g cm ⁻³	1.363	1.363	
Z	8	8	
Mu (mm ⁻¹)	0.365	0.365	
F000	3808.0	3808.0	
F000'	3815.34		
h, k, lmax	17, 21, 53	17, 21, 53	
Nref	20762 [10526]	19535	
Tmin, Tmax	0.978, 0.996	0.860, 1.000	
Tmin'	0.864		

Correction method= # Reported T Limits: Tmin=0.860 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.86/0.94

Theta (max)= 27.480

R(reflections)= 0.0460 (14707)

wR2(reflections)=
0.0961 (19535)

S = 1.008

Npar= 1118

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.440
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.050
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00701 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 325 A**3
PLAT767_ALERT_4_G INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT794_ALERT_5_G Tentative Bond Valency for Al1 (III) . 3.13 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2 (III) . 3.10 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
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). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info
PLAT992_ALERT_5_G Repd & Actual `_reflns_number_gt` Values Differ by 3 Check

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

2 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
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
3 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

