checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Al_Buazp_293K

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: Al_Buazp_293K

Bond precision: C-C = 0.0046 A   Wavelength=0.71073

Cell: a=13.374(7)   b=14.095(8)   c=16.593(9)
               alpha=96.179(8)   beta=106.731(7)   gamma=103.041(7)
Temperature: 293 K

	Calculated	Reported
Volume	2868(3)	2868(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H48 Al N4 O4, C24 H20 P	?
Sum formula	C64 H68 Al N4 O4 P	C64 H68 Al N4 O4 P
Mr	1015.17	1015.17
Dx,g cm-3	1.176	1.176
Z	2	2
Mu (mm-1)	0.113	0.113
F000	1080.0	1080.0
F000'	1080.72	
h,k,lmax	15,16,19	15,16,19
Nref	10147	10014
Tmin,Tmax	0.956,0.989	0.940,0.990
Tmin'	0.956	

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.987   Theta(max)= 25.030

R(reflections)= 0.0562(7356)   wR2(reflections)= 0.1648(10014)

S = 1.044   Npar= 1125

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 B**
PLAT334_ALERT_2_B Small Aver. Benzene C-C Dist C21   -C26   1.33 Ang.

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🟡 **Alert level C**
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....   8.90 Note
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_C Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT213_ALERT_2_C Atom C11'   has ADP max/min Ratio .....   3.7 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.1 Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00458 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.595   129 Report
PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by   12 Check

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⚪ **Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   96 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   122 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records   6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   15 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N4   --C32   .   11.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C33   --C35   .   6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C37   --C39   .   7.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --O1   .   5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --O3   .   9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --O4   .   5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --N3   .   5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --O3'   .   9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --O4'   .   10.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Al1   --N3'   .   13.5 s.u.
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   98% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C27   -C32   .   1.45 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C27'   -C32'   .   1.48 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C21   -C26   0.44 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C27   -C32   0.44 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C21'   -C26'   0.49 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C27'   -C32'   0.48 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O1'   ..C63   .   2.98 Ang.
                                             1+x,y,z =   1_655 Check
PLAT721_ALERT_1_G Bond   Calc   0.97000, Rep   0.96000 Dev...   0.01 Ang.
          C20'   -H20F   1_555 1_555 ....   # 114 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C31'   --C32'   1.72 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 ....   1878 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   47% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   1.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   12 Info

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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  24 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT334_Al_Buazp_293K
;
PROBLEM: Small Aver. Benzene C-C Dist C21      -C26          1.33 Ang.
RESPONSE: ...
;
# end Validation Reply Form
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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.

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

Datablock Al_Buazp_293K - ellipsoid plot