

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1-La

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: 1-La

Bond precision: C-C = 0.0139 A

Wavelength=1.54178

Cell: a=13.3143(11) b=15.3515(16) c=26.489(3)
 alpha=104.015(9) beta=94.387(6) gamma=110.588(6)
Temperature: 120 K

	Calculated	Reported
Volume	4839.0(9)	4839.0(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C84 H132 La2 O6 P6, 1.5(C6 H14)	C84 H132 La2 O6 P6, 1.5(C6 H14)
Sum formula	C93 H153 La2 O6 P6	C93 H153 La2 O6 P6
Mr	1830.80	1830.78
Dx, g cm ⁻³	1.257	1.257
Z	2	2
Mu (mm ⁻¹)	8.025	8.025
F000	1926.0	1926.0
F000'	1928.11	
h,k,lmax	16,19,32	16,18,32
Nref	19355	19092
Tmin,Tmax	0.500,0.628	0.477,0.754
Tmin'	0.230	

Correction method= # Reported T Limits: Tmin=0.477 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.986

Theta(max)= 73.000

R(reflections)= 0.0650(13088)

wR2(reflections)=
0.1647(19092)

S = 1.018

Npar= 1003

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.140

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C86 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C89 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C90 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C85 0.106 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C88 0.111 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01386 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C92 - C93 . 1.38 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 105 Report

8 1 2, 6 3 2, 7 3 2, 4-15 3, -9 1 3, 6 3 3,
6 4 3, 9-17 4, 5-15 4, -10 -1 4, -9 1 4, -13 4 4,
5 5 4, -10 -5 5, 8-14 6, 3 -8 6, 2 -7 6, 3 -7 6,
12-15 7, 2 -8 7, 3 -8 7, 3 6 7, 2 -8 8, 3 -8 8,
4 -8 8, 4 -6 8, 8-17 9, 6-15 9, 2 -9 9, 3 -9 9,
4 -9 9, 1 -8 9, 0 -7 9, 3 -7 9, -8 5 9, 0 7 9,
5-15 10, 1 -9 10, 2 -9 10, 3 -9 10, 4 -9 10, 1 -8 10,
2 -8 10, 0 -7 10, -8 4 10, 1 8 10, 13-14 11, 2 -9 11,
0 -8 11, 1 -8 11, 0 -7 11, -6 6 11, 3-17 12, -2-13 12,
0 -8 12, 1 -8 12, 0 -5 13, 0 -4 13, 6 5 13, -1 7 14,
2 5 19, 5-16 21, 6-16 21, 4-15 22, 5-15 22, 6-15 22,
7-15 22, 9 -3 22, 3-15 23, 4-15 23, 5-15 23, 6-15 23,
4-14 23, 5-14 23, 2-15 24, 3-15 24, 4-15 24, 3-14 24,
4-14 24, 5-14 24, 6-14 24, 1 -7 24, 1 -1 24, -5 1 24,
2-14 25, 3-14 25, 4-14 25, 5-14 25, 4-13 25, -2 -7 25,
-3 -6 25, 1 -4 25, 0 -3 25, -3 1 25, -2 1 25, 3-13 26,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From La1 1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02Ang From La2 1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From La2 1.62 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From La1 1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.64Ang From La1 -2.14 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From La2 -2.13 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From La1 -2.04 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From La2 -1.60 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.88Ang From O4 . 0.96 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 6 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.140 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 28.59 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) La2 --O4 . 5.3 s.u.
PLAT344_ALERT_2_G Unusual sp3 Angle Range in Solvent/Ion for C92 Check
PLAT774_ALERT_1_G Check X-Y Bond in CIF: La1 --La2 .. 4.05 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C6 H14 2 Note
PLAT794_ALERT_5_G Tentative Bond Valency for La1 (III) . 2.98 Info

PLAT794_ALERT_5_G	Tentative Bond Valency for La2 (III) .	2.95	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	39	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
	0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	149	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	1.604	Note
	Predicted wR2: Based on SigI**2 10.27 or SHELX Weight 16.18		
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
0 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 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
8 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 22/08/2024; check.def file version of 21/08/2024

Datablock 1-La - ellipsoid plot

