checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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: 4

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Bond precision:   C-C = 0.0300 A          Wavelength=1.54178

Cell:             a=17.482(5)     b=22.364(6)          c=23.567(6)
                  alpha=90        beta=102.640(6)      gamma=90
Temperature:      120 K

                 Calculated                Reported
Volume           8991(4)                   8991(4)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C84 H131 K3 La O6 P6      C84 H131 K3 La O6 P6
Sum formula      C84 H131 K3 La O6 P6      C84 H131 K3 La O6 P6
Mr               1678.93                   1678.91
Dx,g cm-3        1.240                     1.240
Z                4                         4
Mu (mm-1)        6.284                     6.284
F000             3548.0                    3548.0
F000'            3561.52
h,k,lmax         18,23,24                  17,18,23
Nref             10417                     8184
Tmin,Tmax        0.391,0.504               0.378,0.750
Tmin'            0.247

Correction method= # Reported T Limits: Tmin=0.378 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.786           Theta(max)= 52.874

R(reflections)= 0.1144( 5118)                    wR2(reflections)=
                                                 0.2479( 8184)
S = 1.126                  Npar= 936
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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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5171

Author Response: The data was largely incomplete due to poor diffraction and resolution

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.786 Why?

Author Response: The data was largely incomplete due to poor diffraction and resolution

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Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03 Ang.

Author Response: The data was largely incomplete due to poor diffraction and resolution

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.517 1624 Report

16	0	0,	15	1	0,	16	1	0,	17	1	0,	17	2	0,	13	3	0,
14	4	0,	13	6	0,	13	8	0,	12	9	0,	12	10	0,	15	12	0,
3	14	0,	14	14	0,	0	16	0,	2	16	0,	6	17	0,	7	17	0,
8	17	0,	9	17	0,	10	17	0,	11	17	0,	0	18	0,	1	18	0,
2	18	0,	4	18	0,	5	18	0,	6	18	0,	7	18	0,	8	18	0,
9	18	0,	10	18	0,	11	18	0,	-17	0	1,	-15	0	1,	-1	0	1,
15	0	1,	17	0	1,	-17	1	1,	-16	1	1,	-15	1	1,	15	1	1,
16	1	1,	17	1	1,	-17	2	1,	13	2	1,	17	2	1,	-14	3	1,
-14	4	1,	-14	5	1,	-13	7	1,	13	7	1,	-13	8	1,	-16	10	1,
-12	10	1,	12	10	1,	11	11	1,	11	12	1,	10	13	1,	-6	14	1,
-5	14	1,	-4	14	1,	-3	14	1,	-2	15	1,	-6	16	1,	5	16	1,
-12	17	1,	-11	17	1,	-10	17	1,	-9	17	1,	-8	17	1,	-7	17	1,
-3	17	1,	0	17	1,	5	17	1,	7	17	1,	8	17	1,	9	17	1,
10	17	1,	11	17	1,	-11	18	1,	-10	18	1,	-9	18	1,	-8	18	1,
-7	18	1,	-6	18	1,	-3	18	1,	-2	18	1,	-1	18	1,	0	18	1,
1	18	1,	2	18	1,	3	18	1,	5	18	1,	6	18	1,	7	18	1,

Author Response: The data was largely incomplete due to poor diffraction and resolution

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Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.137 Report
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 8.74 Note

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         K3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C39 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .........        C68 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     11.991 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.880 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       La1       1.06 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H55B      .      -0.32 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          96 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     290.92 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C68 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C67      - C68      .       1.56 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: K2       --K3        ..       4.03 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      43.40 Deg.
              O5   -C57  -K2      1_555   1_555   1_555 ......     #  476 Check
PLAT794_ALERT_5_G Tentative Bond Valency for La1       (III)     .       2.93 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1622 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         16 Note
               -9  1 18,  -8  3 17,  -8  7 15,  -8  8 14,  -7  0 19,  -7  1 19,
               -7  2 19,  -7  5 18,  -7  6 15,  -6  2 19,  -5  0 19,  -5  2 18,
               -4  1 19,  -4  1 20,  -4 10 17,  -3  1 20,
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           5 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ           5 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.237 Note
              Predicted wR2: Based on SigI**2  5.85 or SHELX Weight 22.01
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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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 22/08/2024; check.def file version of 21/08/2024

Datablock 4 - ellipsoid plot