checkCIF/PLATON report

Structure factors have been supplied for datablock(s) latflfac3

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: latflfac3

Bond precision: C-C = 0.0078 A   Wavelength=1.54184

Cell: a=8.2940(3)   b=27.8547(9)   c=19.0060(8)
               alpha=90   beta=101.943(4)   gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	4295.9(3)	4295.9(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C36 H17 F24 La O9	C36 H17 F24 La O9
Sum formula	C36 H17 F24 La O9	C36 H17 F24 La O9
Mr	1188.41	1188.41
Dx,g cm-3	1.837	1.837
Z	4	4
Mu (mm-1)	9.147	9.147
F000	2312.0	2312.0
F000'	2317.86	
h,k,lmax	10,34,23	10,33,23
Nref	8729	8469
Tmin,Tmax	0.401,0.774	0.660,1.000
Tmin'	0.002	

Correction method= # Reported T Limits: Tmin=0.660 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.970   Theta(max)= 74.038

R(reflections)= 0.0442(7377)   wR2(reflections)= 0.1293(8469)

S = 1.025   Npar= 661

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

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PLAT213_ALERT_2_C Atom F56              has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom F54B             has ADP max/min Ratio .....      3.2 prolat
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F69    -- C68     ..      5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C64    -- C66     ..      6.2 s.u.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......   2.688 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        6 Report
PLAT975_ALERT_2_C Check Calcd Residual Density  0.81A From        O3    0.59 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Note
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       4 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....    0.69 mm
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records       1 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C17 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C35 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C53 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..       4 % Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact F33     .. F33     ..    2.78 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters       1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      18 Note
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     237 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        2 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 27/03/2017; check.def file version of 24/03/2017