checkCIF/PLATON report

Structure factors have been supplied for datablock(s) marc004a

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: marc004a

Bond precision: C-C = 0.0015 A   Wavelength=1.54178

Cell: a=19.9030(8)   b=11.3141(5)   c=22.0976(9)
                 alpha=90   beta=90.020(2)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4976.0(4)	4976.0(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C28 H18 O5, C7 H8	C28 H18 O5, C7 H8
Sum formula	C35 H26 O5	C35 H26 O5
Mr	526.56	526.56
Dx,g cm-3	1.406	1.406
Z	8	8
Mu (mm-1)	0.753	0.753
F000	2208.0	2208.0
F000'	2214.78	
h,k,lmax	24,14,27	24,14,27
Nref	5158	5111
Tmin,Tmax	0.863,0.873	0.707,0.754
Tmin'	0.863	

Correction method= # Reported T Limits: Tmin=0.707 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.991   Theta(max)= 75.481

R(reflections)= 0.0356(4759)   wR2(reflections)= 0.0994(5111)

S = 1.040   Npar= 445

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
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   10 Report

Alert level G
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   7 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2)   13.44 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3)   1.56 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   30 Note
PLAT793_ALERT_4_G Model has Chirality at C1   (Centro SPGR)   R Verify
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   37 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...   3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   25 Info

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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
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   0 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
   3 ALERT type 3 Indicator that the structure quality may be low
   8 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.