checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TRY_a

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: TRY_a

```
Bond precision:   C-C = 0.0109 A          Wavelength=0.71073

Cell:              a=8.702(3)     b=20.224(7)          c=11.877(4)
                   alpha=90       beta=98.716(9)       gamma=90
Temperature:       296 K
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	Calculated	Reported
Volume	2066.1(12)	2066.2(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H30 O4	C24 H30 O4
Sum formula	C24 H30 O4	C24 H30 O4
Mr	382.48	382.50
Dx,g cm-3	1.230	1.230
Z	4	4
Mu (mm-1)	0.082	0.082
F000	824.0	824.0
F000'	824.39	
h,k,lmax	8,19,11	8,19,11
Nref	1911	1903
Tmin,Tmax	0.971,0.976	0.971,0.976
Tmin'	0.952	

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Correction method= # Reported T Limits: Tmin=0.971 Tmax=0.976
AbsCorr = MULTI-SCAN

Data completeness= 0.996           Theta(max)= 19.924

R(reflections)= 0.1078( 1729)                    wR2(reflections)=
                                                 0.2744( 1903)
S = 1.006                 Npar= 230
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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

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THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.4795
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Alert level B

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PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       1.05 eA-3
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C23      --C24      .       10.3 s.u.
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01088 Ang.
PLAT416_ALERT_2_B Short Intra D-H..H-D       H2       ..H3       .       1.07 Ang.
                                                    x,y,z  =      1_555 Check
PLAT921_ALERT_1_B R1  in the CIF and FCF Differ by ..............    -0.0131 Check
PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by ..............    -0.0291 Check
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Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =     -0.623
           Test value =     -0.600
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
SHFSU01_ALERT_2_C  The absolute value of parameter shift to su ratio > 0.05
           Absolute value of the parameter shift to su ratio given   0.069
           Additional refinement cycles may be required.
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ...      2.600 Sigma
PLAT080_ALERT_2_C Maximum Shift/Error ...........................       0.07 Why ?
PLAT082_ALERT_2_C High R1 Value .................................       0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.27 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................       8.27 Note
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density     -0.62 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C18      --C24      .        6.8 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C19      --C24      .       1.36 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range     C19       -C24      .       0.16 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C9       - C18      .       1.42 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....      7.194 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.479         8 Report
PLAT923_ALERT_1_C S    Values in the CIF and FCF Differ by .......     -0.118 Check
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PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      10.52 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H20       .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22       .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23       .      -0.32 eA-3
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      13.53 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
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        65% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  29 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 18/05/2022; check.def file version of 17/05/2022

Datablock TRY_a - ellipsoid plot