checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rrc1_abs

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: rrc1_abs

Bond precision: C-C = 0.0038 A   Wavelength=1.54184

Cell: a=12.3108(1)   b=17.9164(1)   c=18.8197(1)
               alpha=109.473(1)   beta=101.931(1)   gamma=102.210(1)
Temperature: 100 K

	Calculated	Reported
Volume	3647.78(6)	3647.77(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C74.62 H89.43 N10 O15, 0.191(C2 H3), 3(H2 O)	C75 H90 N10 O15, 3(H2 O)
Sum formula	C75 H96 N10 O18	C75 H96 N10 O18
Mr	1425.62	1425.61
Dx,g cm-3	1.298	1.298
Z	2	2
Mu (mm-1)	0.768	0.768
F000	1520.0	1520.0
F000'	1524.85	
h,k,lmax	15,22,23	15,22,23
Nref	15447	15316
Tmin,Tmax	0.894,0.956	0.564,1.000
Tmin'	0.858	

Correction method= # Reported T Limits: Tmin=0.564 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.992   Theta(max)= 77.143

R(reflections)= 0.0746(13641)   wR2(reflections)= 0.2298(15316)

S = 1.047   Npar= 1077

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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DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =      -0.774
           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.
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      0.79 eA-3
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density     -0.77 eA-3
PLAT213_ALERT_2_C Atom C58           has ADP max/min Ratio .....      3.2 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1   C   Ueq(max)/Ueq(min) Range      5.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range      4.9 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45       --C46       .      5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C53       --C59       .      7.0 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C53 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H7        ..H50C      .      1.98 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H8        ..H59C      .      1.95 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H10       ..H74C      .      1.99 Ang.
                                             x,y,z  =      1_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2        --H2        .      Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.479 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        14 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .       1 Check
PLAT922_ALERT_1_C wR2 in the CIF and FCF Differ by ...............      0.0021 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      26 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      31 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............      16 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ    Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.14 Report
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes    are Equal ..(Note)    0.0001 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       9 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records       8 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records       1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       5 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records       3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records       6 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )     14% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )    100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )  189.05 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )    0.95 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O13A      .      99.9 Degree
PLAT411_ALERT_2_G Short Inter H...H Contact  H46B      ..H48B      .      1.81 Ang.
                                             x,y,z  =      1_555 Check
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PLAT411_ALERT_2_G Short Inter H...H Contact     H55A     ..H47C     .        2.03 Ang.
                                                2-x,1-y,2-z  =      2_767 Check
PLAT411_ALERT_2_G Short Inter H...H Contact     H55A     ..H47D     .        1.92 Ang.
                                                2-x,1-y,2-z  =      2_767 Check
PLAT411_ALERT_2_G Short Inter H...H Contact     H55B     ..H47D     .        1.75 Ang.
                                                2-x,1-y,2-z  =      2_767 Check
PLAT411_ALERT_2_G Short Inter H...H Contact     H56      ..H47D     .        2.06 Ang.
                                                2-x,1-y,2-z  =      2_767 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X          H9       ..H62B     .        2.00 Ang.
                                                x,y,z  =           1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     O9       ..C48B     .        2.34 Ang.
                                                x,y,z  =           1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C30      ..C72A     .        3.00 Ang.
                                                1-x,2-y,1-z  =      2_676 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C33      ..C72A     .        3.12 Ang.
                                                1-x,2-y,1-z  =      2_676 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C34      ..C72A     .        2.81 Ang.
                                                1-x,2-y,1-z  =      2_676 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C35      ..C72A     .        2.77 Ang.
                                                1-x,2-y,1-z  =      2_676 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C46      ..C48B     .        2.74 Ang.
                                                x,y,z  =           1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact     C55      ..C47A     .        2.78 Ang.
                                                2-x,1-y,2-z  =      2_767 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C48B     --C47A          1.77 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       40 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        2 Note
                 C2 H3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       488 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       117 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         8 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         3 Check
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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
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  40 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  32 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 20/01/2022; check.def file version of 19/01/2022