checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp15v3_293k_auto_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: exp15v3_293k_auto_a

Bond precision: C-C = 0.0049 A   Wavelength=1.54184

Cell: a=6.6111(6)   b=8.1247(5)   c=10.0546(4)
               alpha=89.986(4)   beta=85.856(5)   gamma=82.196(7)
Temperature: 293 K

	Calculated	Reported
Volume	533.64(6)	533.64(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C8 H9 N O2, C2 H3 N	C8 H9 N O2, C2 H3 N
Sum formula	C10 H12 N2 O2	C10 H12 N2 O2
Mr	192.22	192.22
Dx,g cm-3	1.196	1.196
Z	2	2
Mu (mm-1)	0.697	0.697
F000	204.0	204.0
F000'	204.64	
h,k,lmax	7,9,11	7,9,11
Nref	1889	1862
Tmin,Tmax	0.778,0.858	0.126,1.000
Tmin'	0.706	

Correction method= # Reported T Limits: Tmin=0.126 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.986   Theta(max)= 66.736

R(reflections)= 0.1015(1333)   wR2(reflections)=
                                                      0.2545(1862)

S = 1.040   Npar= 175

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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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
            Rint given   0.142
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ........     0.142 Report
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C10 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)      2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N2     0.111 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00487 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    96.197 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     3.431 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    28.638 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     3.011 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     4.442 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.504 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     4.296 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.596        27 Report
             -7  2  0,  -7  3  0,  -7  1  1,  -7  2  1,   7 -3  2,  -7  0  2,
             -7  1  2,  -6  1  2,  -7  2  2,   7 -2  3,  -7  0  3,   7  0  3,
             -7  1  3,  -6  1  3,  -6  2  3,  -6  3  3,  -6  4  3,  -7 -1  4,
             -7  0  4,  -6  2  4,  -6  3  4,   7  1  5,  -6  2  5,  -6  3  5,
              7  2  6,  -5 -2  7,   6  4  7,
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⚪ **Alert level G**

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      19 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)     293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)     293 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      40 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     33% Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........   6.204 Note
            Predicted wR2: Based on SigI**2  4.10 or SHELX Weight 24.47
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       0 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
  14 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  13 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.

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