

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) barb_mel_2

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: barb_mel_2

Bond precision: C-C = 0.0040 Å Wavelength=1.54184

Cell: a=5.0575(4) b=12.1663(9) c=15.7377(11)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	968.36(12)	968.36(12)
Space group	C c c 2	C c c 2
Hall group	C 2 -2c	C 2 -2c
Moiety formula	C4 H3 N2 O3, C3 H7 N6	C3 H7 N6, C4 H3 N2 O3
Sum formula	C7 H10 N8 O3	C7 H10 N8 O3
Mr	254.23	254.23
Dx,g cm-3	1.744	1.744
Z	4	4
Mu (mm-1)	1.211	1.211
F000	528.0	528.0
F000'	529.89	
h,k,lmax	6,14,19	6,14,19
Nref	920[480]	843
Tmin,Tmax	0.957,0.988	0.632,1.000
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.632 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.76/0.92 Theta(max)= 69.937

R(reflections)= 0.0303(801) wR2(reflections)= 0.0834(843)

S = 1.104 Npar= 105

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 B

PLAT089_ALERT_3_B Poor Data / Parameter Ratio (Zmax < 18) 4.55 Note

Author Response: Diffraction data were collected with enough redundancy, but the model contains H atoms, which were localized from difference Fourier maps and refined with individual isotropic displacement parameters without any restraints. And since all refinement parameters, including high bond precision, are quite low, and the structural model is reliable, we believe that this alert is not crucial.



Alert level C

PLAT245_ALERT_2_C U(iso) H4 Smaller than U(eq) N4 by 0.011 Ang**2
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
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
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 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.

