

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB2

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: MAB2

Bond precision: C-C = 0.0028 A

Wavelength=0.71075

Cell: a=9.4616(4) b=9.4780(3) c=19.8856(8)
 alpha=86.483(3) beta=81.244(3) gamma=75.624(3)
Temperature: 100 K

| | Calculated | Reported |
|------------------------|--------------------------------------|--------------------------------------|
| Volume | 1706.79(12) | 1706.79(12) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C16 H28 N4, 2(B5 H4 O10), 3(H2 O) | C16 H28 N4, 2(B5 H4 O10), 3(H2 O) |
| Sum formula | C16 H42 B10 N4 O23 | C16 H42 B10 N4 O23 |
| Mr | 766.64 | 766.63 |
| Dx, g cm ⁻³ | 1.492 | 1.492 |
| Z | 2 | 2 |
| Mu (mm ⁻¹) | 0.129 | 0.129 |
| F000 | 800.0 | 800.0 |
| F000' | 800.54 | |
| h, k, lmax | 12, 12, 25 | 12, 12, 25 |
| Nref | 7833 | 7820 |
| Tmin, Tmax | 0.985, 0.999 | 0.609, 1.000 |
| Tmin' | 0.965 | |

Correction method= # Reported T Limits: Tmin=0.609 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max) = 27.484

R(reflections)= 0.0457(5988)

wR2(reflections)=
0.1431(7820)

S = 0.970

Npar= 537

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**

PLAT420_ALERT_2_B D-H Bond Without Acceptor O23 --H23A . Please Check

 **Alert level C**

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.753 Check

 **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 16 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 5 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 10 Report
H21A H21B H22A H22B H22C H22D H23A H23B H23C H23D
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0025 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0025 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O22A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22D Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O23A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23D Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 8) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 5) 1.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 6) 1.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 7) 1.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 8) 1.50 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X H12 ..H23A . 2.10 Ang.
x,1+y,z = 1_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O10 ..C14 . 2.98 Ang.
x,y,z = 1_555 Check
PLAT726_ALERT_2_G H...A Calc 1.94000, Rep 1.93000 Dev... 0.01 Ang.
H21B -O22 1_555 1_555 # 12 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 21 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.9 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.52 Note
Predicted wR2: Based on SigI**2 3.17 or SHELX Weight 15.28
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
24 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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 *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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