checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB6

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: MAB6

Bond precision: = 0.0000 A Wavelength=1.54178

Cell: a=9.3096(6) b=9.3175(3) c=9.3733(6)
alpha=76.598(5) beta=85.611(5) gamma=79.947(4)
Temperature: 100 K

	Calculated	Reported
Volume	778.22(8)	778.22(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	0.5(B10 H8 O20), B5 H4 O10, 2(C7 H14 N3)	B5 H4 O10, C7 H14 N3
Sum formula	C14 H36 B10 N6 O20	C7 H18 B5 N3 O10
Mr	716.59	358.29
Dx,g cm-3	1.529	1.529
Z	1	2
Mu (mm-1)	1.133	1.133
F000	372.0	372.0
F000'	373.44	
h,k,lmax	11,11,11	11,11,11
Nref	2858	2836
Tmin,Tmax	0.861,0.978	0.803,1.000
Tmin'	0.788	

Correction method= # Reported T Limits: Tmin=0.803 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 68.221

R(reflections)= 0.0561(2429) wR2(reflections)= 0.1747(2836)

S = 1.076 Npar= 459

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

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PLAT088_ALERT_3_B Poor Data / Parameter Ratio ....................       6.18 Note
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Alert level C

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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.001 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         19 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H2A       .      -0.31 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         20 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         50 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         12 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         27 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
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PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0600 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0300 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of O3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O12 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O13 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O14 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O15 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O16 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O17 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O19 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B12 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B13 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B14 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B15 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )      9.50 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      1234 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.7 Low
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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
  4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
133 **ALERT level G** = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 33 ALERT type 3 Indicator that the structure quality may be low
 97 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 *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 28/11/2022; check.def file version of 28/11/2022

Datablock MAB6 - ellipsoid plot