

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: O- B = 0.0043 A Wavelength=0.71075

Cell: a=8.3998(5) b=9.1406(7) c=18.2066(13)
 alpha=78.439(6) beta=86.810(5) gamma=88.118(6)
Temperature: 100 K

	Calculated	Reported
Volume	1367.07(17)	1367.07(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(B5 H4 O10), C10 H26 N2	2(B5 H4 O10), 2(C5 H13 N)
Sum formula	C10 H34 B10 N2 O20	C10 H34 B10 N2 O20
Mr	610.49	610.49
Dx,g cm-3	1.483	1.483
Z	2	2
Mu (mm-1)	0.130	0.130
F000	636.0	636.0
F000'	636.45	
h,k,lmax	10,11,23	10,11,23
Nref	6265	6146
Tmin,Tmax	0.994,0.999	0.727,1.000
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.727 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.981 Theta(max)= 27.486

R(reflections)= 0.0748(2997) wR2(reflections)= 0.1850(6146)

S = 1.005 Npar= 561

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

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49%	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7	Note
PLAT430_ALERT_2_C	Short Inter D...A Contact O2 ..015 .	2.87	Ang.
	x,y,z =	1_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	14.957	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.420	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	77	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	30	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	18	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	13	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	4	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	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
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
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	20.03	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4	17.97	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 5	16.47	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 6	5.05	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O12 ..C41	2.96	Ang.
	-1+x,y,z =	1_455	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	38	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	388	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	41	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **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
15 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 *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.

