

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: d832

Bond precision:	C-C = 0.0074 Å	Wavelength=0.71073
Cell:	a=15.6350(14)	b=18.2157(18) c=28.691(3)
	alpha=90	beta=91.787(3) gamma=90
Temperature:	291 K	
	Calculated	Reported
Volume	8167.3(14)	8167.3(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C60 H42 Br8 Cu3 N8 Na O16, C6 H2 N3 O7 [+ solvent]	C60 H42 Br8 Cu3 N8 Na O16, C6 H2 N3 O7
Sum formula	C66 H44 Br8 Cu3 N11 Na O23 [+ solvent]	C66 H44 Br8 Cu3 N11 Na O23
Mr	2211.96	2212.01
Dx, g cm ⁻³	1.799	1.799
Z	4	4
Mu (mm ⁻¹)	4.771	4.771
F000	4316.0	4316.0
F000'	4312.94	
h,k,lmax	20,23,37	20,23,37
Nref	18872	18150
Tmin,Tmax	0.331,0.385	
Tmin'	0.306	

Correction method= Not given

Data completeness= 0.962 Theta(max)= 27.552

R(reflections)= 0.0568(12034) wR2(reflections)= 0.1310(18150)

S = 1.032 Npar= 1009

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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low	0.975	Why?
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given		Please Do !
PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.16	Do !
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		N9 Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00739	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H10 ..H13	1.98	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H16 ..H21	1.93	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H40 ..H43	1.95	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact	Br2 ..O7	3.19	Ang.

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	11	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.10	Why ?
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C11 -C20	1.42	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C61 -C66	0.15	Ang.
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	111.5	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O7	111.5	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O13	112.7	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O21 ..C39	3.01	Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note

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

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

