

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FR10

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: FR10

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=9.4765(3) b=9.2067(3) c=24.1253(7)
 alpha=90 beta=92.1209(7) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2103.43(11)	2103.42(11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H18 Br N O6	C23 H18 Br N O6
Sum formula	C23 H18 Br N O6	C23 H18 Br N O6
Mr	484.28	484.29
Dx,g cm-3	1.529	1.529
Z	4	4
Mu (mm-1)	1.995	1.995
F000	984.0	984.0
F000'	983.33	
h,k,lmax	13,13,35	13,13,35
Nref	7002	7000
Tmin,Tmax	0.768,0.878	0.061,0.103
Tmin'	0.572	

Correction method= # Reported T Limits: Tmin=0.061 Tmax=0.103
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 31.510

R(reflections)= 0.0400(5348) wR2(reflections)= 0.1023(7000)

S = 1.046 Npar= 293

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.

PLAT971 ALERT 2 C Check Calcd Resid. Dens. 0.80A From Br1 1.59 eA-3

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O6	107.0	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O5 ..C1	2.99	Ang.
	3/2-x,-1/2+y,1/2-z =	2_645	Check
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	5	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	17	Info

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

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

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.

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock FR10 - ellipsoid plot

