

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: I

Bond precision:	C-C = 0.0040 A	Wavelength=0.71075
Cell:	a=13.9090(18) b=15.0426(17) c=14.801(2)	alpha=90 beta=107.5390(17) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	2952.8(6)	2952.9(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H40 B4 Cl2 Er2 N24 O4, 2(C H2 Cl2)	C42 H40 B4 Cl2 Er2 N24 O4, 2(C H2 Cl2)
Sum formula	C44 H44 B4 Cl6 Er2 N24 O4	C44 H44 B4 Cl6 Er2 N24 O4
Mr	1563.49	1563.47
Dx, g cm ⁻³	1.758	1.758
Z	2	2
Mu (mm ⁻¹)	3.158	3.153
F000	1532.0	1532.0
F000'	1533.10	
h,k,lmax	18,19,19	18,19,19
Nref	6768	6746
Tmin,Tmax	0.538,0.532	0.464,0.532
Tmin'	0.527	

Correction method= # Reported T Limits: Tmin=0.464 Tmax=0.532
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.483

R(reflections)= 0.0262(6432) wR2(reflections)= 0.0553(6746)

S = 1.133 Npar= 379

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ...	2.48	Report
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C12	0.078	Check
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C1 - C2	1.53	Ang.



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.13	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1 -C3_a	1.44	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C H2 C12	2	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI		Please Do !

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

Datablock I - ellipsoid plot

