

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: Er

Bond precision:	C-C = 0.0099 A	Wavelength=0.71073
Cell:	a=18.7290 (5)	b=14.8702 (4) c=11.1918 (4)
	alpha=90	beta=90 gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	3116.96 (16)	3116.95 (16)
Space group	C m c 21	C m c 21
Hall group	C 2c -2	C 2c -2
Moiety formula	C23 H19 Cl2 Er N5 O4, C6 H16 N	C23 H19 Cl2 Er N5 O4, C6 H16 N
Sum formula	C29 H35 Cl2 Er N6 O4	C29 H35 Cl2 Er N6 O4
Mr	769.79	769.79
Dx, g cm-3	1.640	1.640
Z	4	4
Mu (mm-1)	2.908	2.908
F000	1540.0	1540.0
F000'	1540.63	
h, k, lmax	25, 20, 15	25, 20, 15
Nref	4312 [2264]	3427
Tmin, Tmax	0.712, 0.748	0.959, 1.000
Tmin'	0.479	
Correction method= # Reported T Limits:	Tmin=0.959 Tmax=1.000	
AbsCorr = MULTI-SCAN		
Data completeness=	1.51/0.79	Theta(max)= 29.065
R(reflections)=	0.0331 (3085)	wR2(reflections)= 0.0551 (3427)
S =	0.960	Npar= 212

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 A**

PLAT214_ALERT_2_A Atom C2C (Anion/Solvent) ADP max/min Ratio 6.5 prolat
PLAT410_ALERT_2_A Short Intra H...H Contact H2C1 ..H2C1 . 1.59 Ang.
-2-x,y,z = 4_355 Check

 **Alert level B**

PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C1C - C2C . 1.32 Ang.

 **Alert level C**

PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 6.6 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 9.5 Ratio
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C2C Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N1C Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00992 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C23 H19 C12 Er N5 O4

 **Alert level G**

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C3C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3C1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3C2 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 29% Note
PLAT344_ALERT_2_G Unusual sp3 Angle Range in Solvent/Ion for C2C Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C15 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H3C1 ..H2C2 . 1.83 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H3C2 ..H2C2 . 1.77 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 11 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 7 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C6 H16 N
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.3 Low

2 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

18 **ALERT level G** = General information/check it is not something unexpected

0 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
2 ALERT type 3 Indicator that the structure quality may be low
17 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 13/07/2021; check.def file version of 13/07/2021

