checkCIF/PLATON report

Structure factors have been supplied for datablock(s) er

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 = 0.0069 A Wavelength=0.71073

Cell: a=11.5236(10) b=20.3299(17) c=25.596(2)
alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	5996.5(9)	5996.5(9)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C46 H39 Er N10 O4, 4(C H Cl3), H2 O	C46 H39 Er N10 O4, 4(C H Cl3), H2 O
Sum formula	C50 H45 Cl12 Er N10 O5	C50 H45 Cl12 Er N10 O5
Mr	1458.62	1458.62
Dx,g cm-3	1.616	1.616
Z	4	4
Mu (mm-1)	1.988	1.988
F000	2908.0	2908.0
F000’	2914.83	
h,k,lmax	15,27,34	15,27,34
Nref	15957[8724]	15895
Tmin,Tmax	0.438,0.646	0.584,0.746
Tmin’	0.405	

Correction method= # Reported T Limits: Tmin=0.584 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.82/1.00 Theta(max)= 28.999

R(reflections)= 0.0288(15325) wR2(reflections)= 0.0721(15895)

S = 1.176 Npar= 744

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

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PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        3.5 Ratio
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of        C3S Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of        C1S Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.8 Note
PLAT414_ALERT_2_C Short Intra D-H..H-X       H5A      ..H17C            1.98 Ang.
                                                    x,y,z  =      1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.43A   From Cl1X           1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.37A   From Cl1X          -1.77 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.90A   From N4             0.43 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         17 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.010 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          6 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        75% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        50% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        50% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          7 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         14 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 ...          2 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...          2 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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
   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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   9 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

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 22/12/2019; check.def file version of 13/12/2019

Datablock er - ellipsoid plot