

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mx118_21_auto

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: mx118_21_auto

Bond precision:	C-C = 0.0121 Å	Wavelength=0.71073	
Cell:	a=14.2457(2)	b=14.2457(2)	c=21.5746(5)
	alpha=90	beta=90	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	4378.35(16)	4378.35(16)	
Space group	P -4 n 2	P -4 n 2	
Hall group	P -4 -2n	P -4 -2n	
Moiety formula	C20 H12 Er Na O12	C20 H12 Er Na O12	
Sum formula	C20 H12 Er Na O12	C20 H12 Er Na O12	
Mr	634.55	634.55	
Dx, g cm ⁻³	1.925	1.925	
Z	8	8	
Mu (mm ⁻¹)	3.918	3.918	
F000	2456.0	2456.0	
F000'	2455.58		
h, k, lmax	21, 21, 32	19, 19, 30	
Nref	7721 [4142]	6598	
Tmin, Tmax	0.391, 0.375	0.320, 1.000	
Tmin'	0.361		

Correction method= # Reported T Limits: Tmin=0.320 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.59/0.85 Theta(max)= 32.158

R(reflections)= 0.0377(5639)	wR2(reflections)= 0.0934(6598)
S = 1.047	Npar= 308

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

PLAT213_ALERT_2_C	Atom C4	has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom C14	has ADP max/min Ratio	3.7	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 O	Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	06	Check
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	09	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.01206	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .		39	Ang**3
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		8	Note
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.73A	From C6	1.55	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.17A	From Er2	1.51	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.66A	From Er2	-1.77	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.72A	From Er1	-1.70	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.68A	From Er2	-1.60	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Er2	1.21	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Er1	1.14	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.03A	From O11	0.92	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.76A	From O2	0.84	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H20		-0.39	eA-3

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	108.1	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6	106.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O9	109.4	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O12	107.4	Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for Er1 (III)	3.01	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Er2 (III)	3.07	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	314	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ	2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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

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

20 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

25 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
3 ALERT type 4 Improvement, methodology, query or suggestion
6 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

