

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2023ncs0627_1a

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: 2023ncs0627_1a

Bond precision: C-C = 0.0019 Å Wavelength=0.71073

Cell: a=12.0715(1) b=13.3070(1) c=16.3072(1)
 alpha=94.525(1) beta=94.532(1) gamma=115.175(1)
Temperature: 100 K

	Calculated	Reported
Volume	2344.83(4)	2344.83(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H42 Er N3 O11 P2, 2(C30 H21 O P)	C60 H42 Er N3 O11 P2, 2(C30 H21 O P)
Sum formula	C120 H84 Er N3 O13 P4	C120 H84 Er N3 O13 P4
Mr	2067.04	2067.04
Dx, g cm ⁻³	1.464	1.464
Z	1	1
Mu (mm ⁻¹)	1.034	1.034
F000	1057.0	1057.0
F000'	1057.56	
h, k, lmax	17, 19, 23	17, 19, 23
Nref	14303	14302
Tmin, Tmax	0.771, 0.902	0.783, 0.927
Tmin'	0.704	

Correction method= # Reported T Limits: Tmin=0.783 Tmax=0.927
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 30.507

R(reflections)= 0.0250(13199)

wR2(reflections)=
0.0675(14302)

S = 1.046

Npar= 694

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.

