

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

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 34 Ang**3

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT300_ALERT_4_G	Atom Site Occupancy of Er1 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O11 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O12 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O13 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O21 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O22 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O23 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O31 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O32 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O33 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N10 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N20 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N30 Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	17% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact O13 ..C54 .	2.93 Ang.
	-1+x,y,z =	1_455 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3 ..C3 .	3.09 Ang.
	2-x,2-y,-z =	2_775 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	14.59 Deg.
	ER1 -O1 -ER1 2_665 1_555 1_555 #	73 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	12 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C30 H21 O P	
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1 Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Densitv.	17 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
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
23 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
0 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.

