

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xln23

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: xln23

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Bond precision:	C-C = 0.0094 Å	Wavelength=1.54178
Cell:	a=19.4879(3)      b=14.7720(2)      c=21.4793(3)	
	alpha=90      beta=90.3530(14)      gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	6183.24(15)	6183.22(16)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C51 Er F51 O8 P2, C H2 Cl2	C51 Er F51 O8 P2, C H2 Cl2
Sum formula	C52 H2 Cl2 Er F51 O8 P2	C52 H2 Cl2 Er F51 O8 P2
Mr	2023.64	2023.64
Dx,g cm-3	2.174	2.174
Z	4	4
Mu (mm-1)	5.786	5.786
F000	3876.0	3876.0
F000'	3863.42	
h,k,lmax	23,17,25	23,17,25
Nref	11316[ 5662]	9617
Tmin,Tmax	0.118,0.099	0.423,1.000
Tmin'	0.005	

Correction method= # Reported T Limits: Tmin=0.423 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.85      Theta(max)= 68.230

R(reflections)= 0.0323( 9617)      wR2(reflections)= 0.0832( 9617)

S = 1.053      Npar= 1073

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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.

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### 🟡 Alert level B

PLAT090_ALERT_3_B	Poor Data / Parameter Ratio (Zmax > 18) .....	5.24	Note
PLAT213_ALERT_2_B	Atom F45B has ADP max/min Ratio .....	5.0	prolat
PLAT213_ALERT_2_B	Atom F48 has ADP max/min Ratio .....	4.1	prolat
PLAT213_ALERT_2_B	Atom F50 has ADP max/min Ratio .....	4.5	prolat
PLAT213_ALERT_2_B	Atom C18 has ADP max/min Ratio .....	4.6	prolat
PLAT434_ALERT_2_B	Short Inter HL..HL Contact F12 .. F46A ..	2.38	Ang.
PLAT987_ALERT_1_B	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check

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### 🟡 Alert level C

PLAT213_ALERT_2_C	Atom F8 has ADP max/min Ratio .....	3.7	oblate
PLAT213_ALERT_2_C	Atom F18 has ADP max/min Ratio .....	3.1	oblate
PLAT213_ALERT_2_C	Atom F22 has ADP max/min Ratio .....	3.3	prolat
PLAT213_ALERT_2_C	Atom F23 has ADP max/min Ratio .....	3.1	prolat
PLAT213_ALERT_2_C	Atom F28 has ADP max/min Ratio .....	3.3	oblate
PLAT213_ALERT_2_C	Atom F34 has ADP max/min Ratio .....	3.4	prolat
PLAT213_ALERT_2_C	Atom F37 has ADP max/min Ratio .....	3.5	prolat
PLAT213_ALERT_2_C	Atom F38 has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C	Atom F46B has ADP max/min Ratio .....	3.3	prolat
PLAT213_ALERT_2_C	Atom F51 has ADP max/min Ratio .....	3.8	prolat
PLAT213_ALERT_2_C	Atom F45A has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C	Atom F47A has ADP max/min Ratio .....	3.6	prolat
PLAT213_ALERT_2_C	Atom C10 has ADP max/min Ratio .....	3.3	prolat
PLAT213_ALERT_2_C	Atom C21 has ADP max/min Ratio .....	3.5	oblate
PLAT213_ALERT_2_C	Atom C40 has ADP max/min Ratio .....	3.3	oblate
PLAT213_ALERT_2_C	Atom C43 has ADP max/min Ratio .....	3.8	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	4.9	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent F Ueq(max)/Ueq(min) Range	5.7	Ratio
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for .....	C47	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0094	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C51 Er F51 O8 P2	1	Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	43	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much smaller I(calc) .	4	Check

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### 🟡 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	22	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....	0.80	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	28.98	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
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
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for .....	C46	Check
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for .....	C51	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	Percentage = 3	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F18 .. C17 ..	2.90	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F33 .. C27 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F34 .. C36 ..	2.94	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F44 .. C3 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F44 .. C2 ..	2.93	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C12 .. F46B ..	3.11	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F4 .. F22 ..	2.77	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F19 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F12 .. F42 ..	2.78	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 .. F23 ..	2.73	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 .. F39 ..	2.82	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F17 .. F47A ..	2.73	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F22 .. F33 ..	2.83	Ang.

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F24	.. F37	..	2.77 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F29	.. F46A	..	2.81 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F29	.. F32	..	2.82 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F29	.. F47B	..	2.83 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F30	.. F34	..	2.78 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F32	.. F47A	..	2.72 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F38	.. F47B	..	2.66 Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#		2 Note
	C H2 Cl2			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....			149 Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..			! Info
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....			Please Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
7 **ALERT level B** = A potentially serious problem, consider carefully  
23 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
34 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
49 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
7 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*, 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.

