

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) olsn163

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: olsn163

Bond precision:	C-C = 0.0093 A	Wavelength=0.71073
Cell:	a=11.8578(2)	b=22.9499(4) c=11.9125(2)
	alpha=90	beta=104.640(2) gamma=90
Temperature:	102 K	
	Calculated	Reported
Volume	3136.56(10)	3136.56(10)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C51 Eu F51 O8 P2, C H2 Cl2	C51 Eu F51 O8 P2, C H2 Cl2
Sum formula	C52 H2 Cl2 Eu F51 O8 P2	C52 H2 Cl2 Eu F51 O8 P2
Mr	2008.35	2008.34
Dx,g cm-3	2.126	2.126
Z	2	2
Mu (mm-1)	1.343	1.343
F000	1928.0	1928.0
F000'	1930.75	
h,k,lmax	15,29,15	15,29,15
Nref	13881[7118]	11452
Tmin,Tmax	0.530,0.715	0.839,1.000
Tmin'	0.506	

Correction method= # Reported T Limits: Tmin=0.839 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.61/0.83 Theta(max)= 27.100

R(reflections)= 0.0335(10913) wR2(reflections)= 0.0838(11452)

S = 1.110 Npar= 1045

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 B

PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Th(Min) ...	12	Report
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	8	Check

Alert level C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	6.80	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0093	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	32	Ang3
PLAT915_ALERT_3_C	Low Friedel Pair Coverage	64	%
PLAT973_ALERT_2_C	Check Calcd Positive Residual Density on Eul	1.39	eA-3
PLAT975_ALERT_2_C	Check Calcd Residual Density 0.68A From 08	0.49	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density 0.93A From 07	-0.52	eA-3

Alert level G

PLAT033_ALERT_4_G	Flack x Value Deviates > 2*sigma from Zero	-0.024	Note
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for	C37	Check
PLAT242_ALERT_2_G	Low Ueq as Compared to Neighbors for	C41	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F13 .. C23 ..	2.92	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F23 .. C11 ..	2.90	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 .. F27 ..	2.69	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 .. F40 ..	2.84	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6 .. F48 ..	2.63	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 .. F30 ..	2.72	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F15 .. F23 ..	2.73	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F16 .. F43 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F18 .. F37 ..	2.76	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F18 .. F24 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F29 .. F49 ..	2.81	Ang.

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
7 **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
17 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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*, 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.

