

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DP_PDP067_ErRe3_270K

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: DP_PDP067_ErRe3_270K

Bond precision:	C-C = 0.0215 A	Wavelength=0.71073	
Cell:	a=41.6196(10)	b=41.6196(10)	c=7.6943(3)
	alpha=90	beta=90	gamma=120
Temperature:	270 K		
	Calculated	Reported	
Volume	11542.4(7)	11542.4(7)	
Space group	R -3	R -3	
Hall group	-R 3	-R 3	
Moiety formula	3(C30 H30 Er Re3), C	?	
Sum formula	C91 H90 Er3 Re9	C91 H90 Er3 Re9	
Mr	3361.31	3361.20	
Dx,g cm-3	2.901	2.901	
Z	6	6	
Mu (mm-1)	17.367	17.367	
F000	9090.0	9090.0	
F000'	9041.21		
h, k, lmax	50, 50, 9	50, 50, 9	
Nref	4729	4720	
Tmin, Tmax	0.540, 0.707	0.400, 0.720	
Tmin'	0.123		

Correction method= # Reported T Limits: Tmin=0.400 Tmax=0.720
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.400

R(reflections)= 0.0410(3894) wR2(reflections)= 0.0793(4720)

S = 1.128 Npar= 310

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

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds	0.0215 Ang.
PLAT972_ALERT_2_B	Check Calcd Resid. Dens. 2.36A From C31	-2.72 eA-3

🟡 Alert level C

PLAT213_ALERT_2_C	Atom C9	has ADP max/min Ratio	3.4 prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference C26	--C30	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C29	--C30	0.18 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C8	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Re3	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.565	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.92A	From C31	-1.64 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H6		-0.50 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H7		-0.37 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H8		-0.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H15		-0.38 eA-3

🟢 Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	497.29	Why ?
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 2)	0.33 Check
PLAT344_ALERT_2_G	Unusual sp?	Angle Range in Solvent/Ion for	C31 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31	..C31	2.98 Ang.
		$4/3-x, 2/3-y, 2/3-z =$	16_655 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0 Info

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

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

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **ALERT level G** = General information/check it is not something unexpected

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

15 **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

4 **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* 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.

