

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ppr4

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: ppr4

Bond precision:	C-C = 0.0033 A	Wavelength=0.71073	
Cell:	a=10.8259 (6)	b=14.9846 (7)	c=16.4034 (8)
	alpha=90	beta=95.786 (2)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2647.4 (2)	2647.4 (2)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C16 H22 Eu N9 O9, C2 H3 N	C16 H22 Eu N9 O9, C2 H3 N	
Sum formula	C18 H25 Eu N10 O9	C18 H25 Eu N10 O9	
Mr	677.45	677.44	
Dx, g cm ⁻³	1.700	1.700	
Z	4	4	
Mu (mm ⁻¹)	2.434	2.434	
F000	1352.0	1352.0	
F000'	1351.91		
h, k, lmax	15, 21, 23	15, 21, 23	
Nref	8116	8022	
Tmin, Tmax	0.784, 0.823	0.615, 0.746	
Tmin'	0.784		

Correction method= # Reported T Limits: Tmin=0.615 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 30.524

R(reflections)= 0.0276 (6803)	wR2(reflections)= 0.0581 (8022)
S = 1.072	Npar= 350

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 C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O4	--N8	.	5.7 s.u.
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of		C17 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			11 Report



Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Eu1	--O1	.	5.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Eu1	--O2	.	5.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Eu1	--O4	.	7.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Eu1	--O8	.	5.7 s.u.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			83 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File				26 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			4.6 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				4 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
2 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.

